



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 10:09 pm GMT

PDB ID : 6ZMI
EMDB ID : EMD-11292
Title : SARS-CoV-2 Nsp1 bound to the human LYAR-80S ribosome complex
Authors : Thoms, M.; Buschauer, R.; Ameismeier, M.; Denk, T.; Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2020-07-02
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

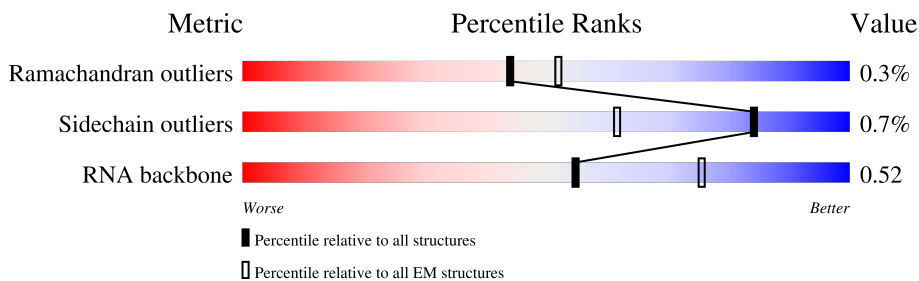
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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





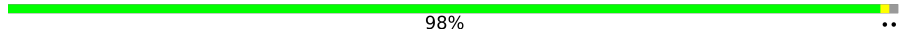
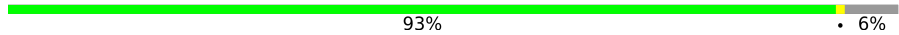
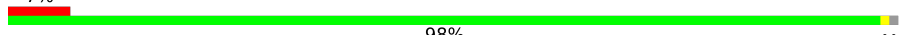
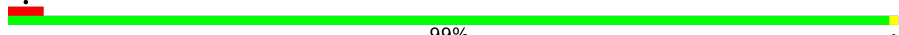

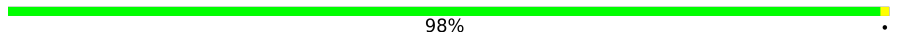
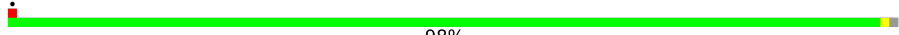

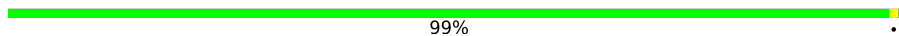








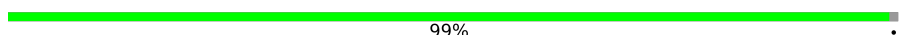





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L5	5066	
2	L7	121	
3	L8	157	
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	

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Mol	Chain	Length	Quality of chain
9	LF	248	 90% 9%
10	LG	266	 89% 9%
11	LH	192	 98% ..
12	LI	214	 93% 6%
13	LJ	178	 98% ..
14	LL	211	 99% .
15	LM	215	 63% .. 35%
16	LN	204	 98% .
17	LO	203	 98% ..
18	LP	184	 82% . 17%
19	LQ	188	 99% ..
20	LR	196	 94% . 5%
21	LS	176	 99% .
22	LT	160	 96% ..
23	LU	128	 78% . 21%
24	LV	140	 93% . 6%
25	LW	157	 78% . 21%
26	LX	156	 77% 23%
27	LY	145	 92% . 8%
28	LZ	136	 99% .
29	La	148	 99% ..
30	Lb	159	 69% 31%
31	Lc	115	 85% 15%
32	Ld	125	 84% . 14%
33	Le	135	 94% . 5%

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Mol	Chain	Length	Quality of chain
34	Lf	110	95% 5%
35	Lg	117	5% 96%
36	Lh	123	98%
37	Li	105	96%
38	Lj	97	87% 11%
39	Lk	70	99%
40	Ll	51	96%
41	Lm	128	41% 59%
42	Ln	25	96%
43	Lo	106	99%
44	Lp	92	99%
45	Lr	137	91% 9%
46	Ls	317	52% 60% 38%
47	Lt	165	82% 80% 15%
48	Lz	217	87% 98%
49	S2	1869	67% 24% 7%
50	SA	295	75% 25%
51	SB	264	81% 19%
52	SD	243	6% 92% 7%
53	SE	263	99%
54	SF	204	89% 10%
55	SH	194	12% 92%
56	SI	208	98%
57	SK	165	59% 41%
58	SL	158	7% 96%

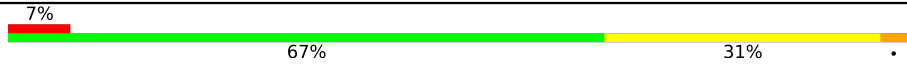


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Mol	Chain	Length	Quality of chain
59	SP	145	6% 88% 11%
60	SQ	146	97%
61	SR	135	5% 97%
62	SS	152	95% 5%
63	ST	145	97%
64	SU	119	8% 87% 13%
65	SV	83	98%
66	SX	143	93% 5%
67	Sa	115	88% 11%
68	Sc	69	90% 7%
69	Sd	56	96%
70	Sg	317	11% 98%
71	SC	293	75% 24%
72	SG	249	8% 94% 5%
73	SJ	194	93% 5%
74	SM	132	55% 89% 8%
75	SN	151	99%
76	SO	151	5% 91% 7%
77	SW	130	98%
78	SY	133	6% 96%
79	SZ	125	57% 40%
80	Sb	84	98%
81	Se	59	15% 98%
82	Sf	156	17% 42% 57%
83	CA	394	86% 89% 10%

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Mol	Chain	Length	Quality of chain
84	CC	75	
85	CE	379	
86	i	180	

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 225122 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L5	3773	80138	35655	14589	26122	3772	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L7	120	2561	1141	456	844	120	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LB	402	3238	2060	608	556	14	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LC	368	2927	1840	583	489	15	0	0

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LD	293	2382	1507	434	427	14	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6.

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

- Molecule 9 is a protein called 60S ribosomal protein L7.

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

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LG	241	1927	1228	371	324	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LH	190	1518	956	284	272	6	0	0

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LI	202	1634	1037	314	269	14	0	0

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LJ	176	1410	888	263	253	6	0	0

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

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

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called 60S ribosomal protein L17.

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

- Molecule 19 is a protein called 60S ribosomal protein L18.

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

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	LS	175	1453	925	283	235	10	0	0

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LU	101	825	529	144	150	2	0	0

- Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LV	131	979	618	184	172	5	0	0

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LW	124	1015	634	207	170	4	0	0

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LX	120	985	630	185	169	1	0	0

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Lb	109	876	546	189	137	4	0	0

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Lc	98	764	485	135	138	6	0	0

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

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

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Li	102	832	521	177	129	5	0	0

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Lm	52	429	266	90	67	6	0	0

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ls	196	Total	C	N	O	S	0	0
			1496	952	259	276	9		

- Molecule 47 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lt	141	Total	C	N	O	S	0	0
			1046	652	191	199	4		

- Molecule 48 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 49 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	S2	1740	36899	16459	6598	12103	1739	0	0

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

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

- Molecule 51 is a protein called 40S ribosomal protein S3a.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	SD	227	1765	1125	317	315	8	0	0

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

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

- Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	SF	184	1461	914	276	264	7	0	0

- Molecule 55 is a protein called 40S ribosomal protein S7.

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

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	SI	206	1686	1058	332	291	5	0	0

- Molecule 57 is a protein called 40S ribosomal protein S10.

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

- Molecule 58 is a protein called 40S ribosomal protein S11.

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

- Molecule 59 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	SP	129	1061	672	202	180	7	0	0

- Molecule 60 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	SQ	144	1142	726	216	197	3	0	0

- Molecule 61 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	SR	135	1090	685	202	198	5	0	0

- Molecule 62 is a protein called 40S ribosomal protein S18.

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

- Molecule 63 is a protein called 40S ribosomal protein S19.

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

- Molecule 64 is a protein called 40S ribosomal protein S20.

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

- Molecule 65 is a protein called 40S ribosomal protein S21.

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

- Molecule 66 is a protein called 40S ribosomal protein S23.

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

- Molecule 67 is a protein called 40S ribosomal protein S26.

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

- Molecule 68 is a protein called 40S ribosomal protein S28.

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

- Molecule 69 is a protein called 40S ribosomal protein S29.

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

- Molecule 70 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 71 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	SC	222	1725	1115	298	302	10	0	0

- Molecule 72 is a protein called 40S ribosomal protein S6.

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

- Molecule 73 is a protein called 40S ribosomal protein S9.

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

- Molecule 74 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	SM	122	940	590	164	177	9	0	0

- Molecule 75 is a protein called 40S ribosomal protein S13.

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

- Molecule 76 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	SO	140	1049	642	204	197	6	0	0

- Molecule 77 is a protein called 40S ribosomal protein S15a.

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

- Molecule 78 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 79 is a protein called 40S ribosomal protein S25.

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

- Molecule 80 is a protein called 40S ribosomal protein S27.

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

- Molecule 81 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Se	58	Total	C	N	O	S	0	0
			443	271	98	73	1		

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 83 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	CA	354	Total	C	N	O	S	4	0
			2764	1744	475	528	17		

- Molecule 84 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
84	CC	75	1589	710	279	525	75	0	0

- Molecule 85 is a protein called Cell growth-regulating nucleolar protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
85	CE	72	603	395	105	103	0	0

- Molecule 86 is a protein called Non-structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	i	33	263	160	47	55	1	0	0

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	L5	212	Total	Mg	0
			212	212	
87	L7	3	Total	Mg	0
			3	3	
87	L8	4	Total	Mg	0
			4	4	
87	LA	1	Total	Mg	0
			1	1	
87	LI	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	
87	LV	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	Lg	1	Total	Mg	0
			1	1	
87	Lj	1	Total	Mg	0
			1	1	
87	S2	30	Total	Mg	0
			30	30	

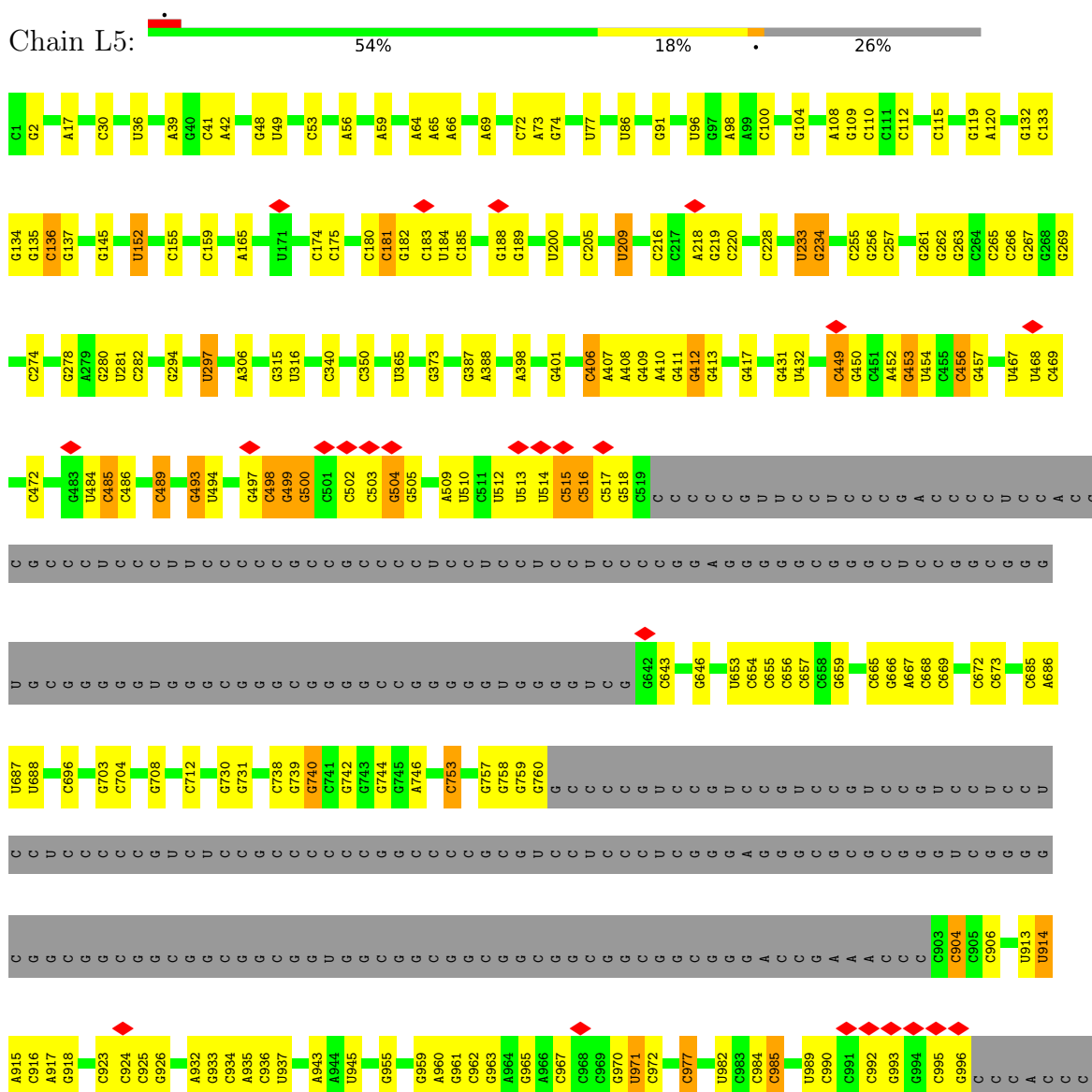
- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

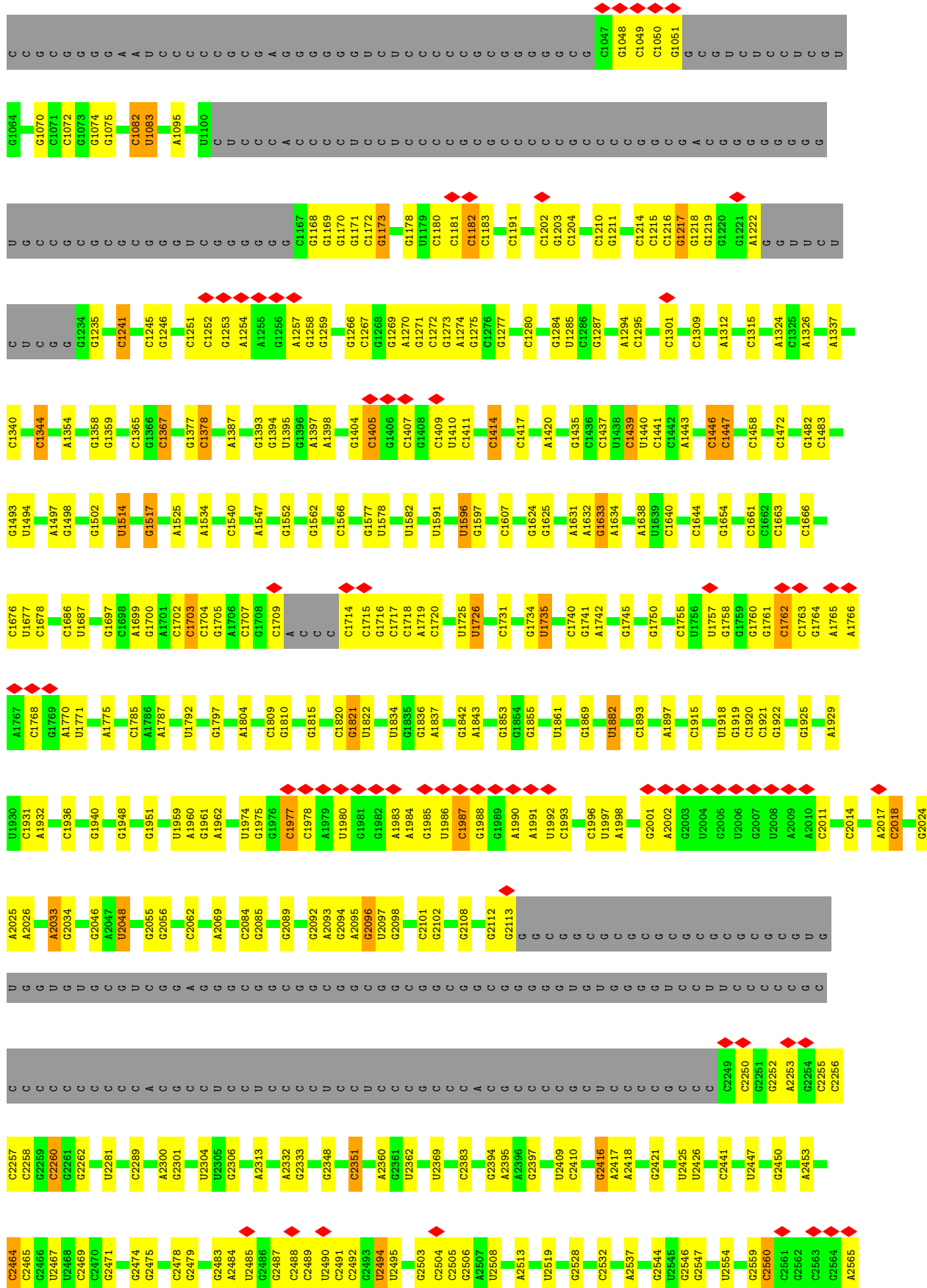
Mol	Chain	Residues	Atoms		AltConf
88	Lg	1	Total 1	Zn 1	0
88	Lj	1	Total 1	Zn 1	0
88	Lm	1	Total 1	Zn 1	0
88	Lo	1	Total 1	Zn 1	0
88	Lp	1	Total 1	Zn 1	0
88	Sa	1	Total 1	Zn 1	0
88	Sd	1	Total 1	Zn 1	0
88	Sf	1	Total 1	Zn 1	0

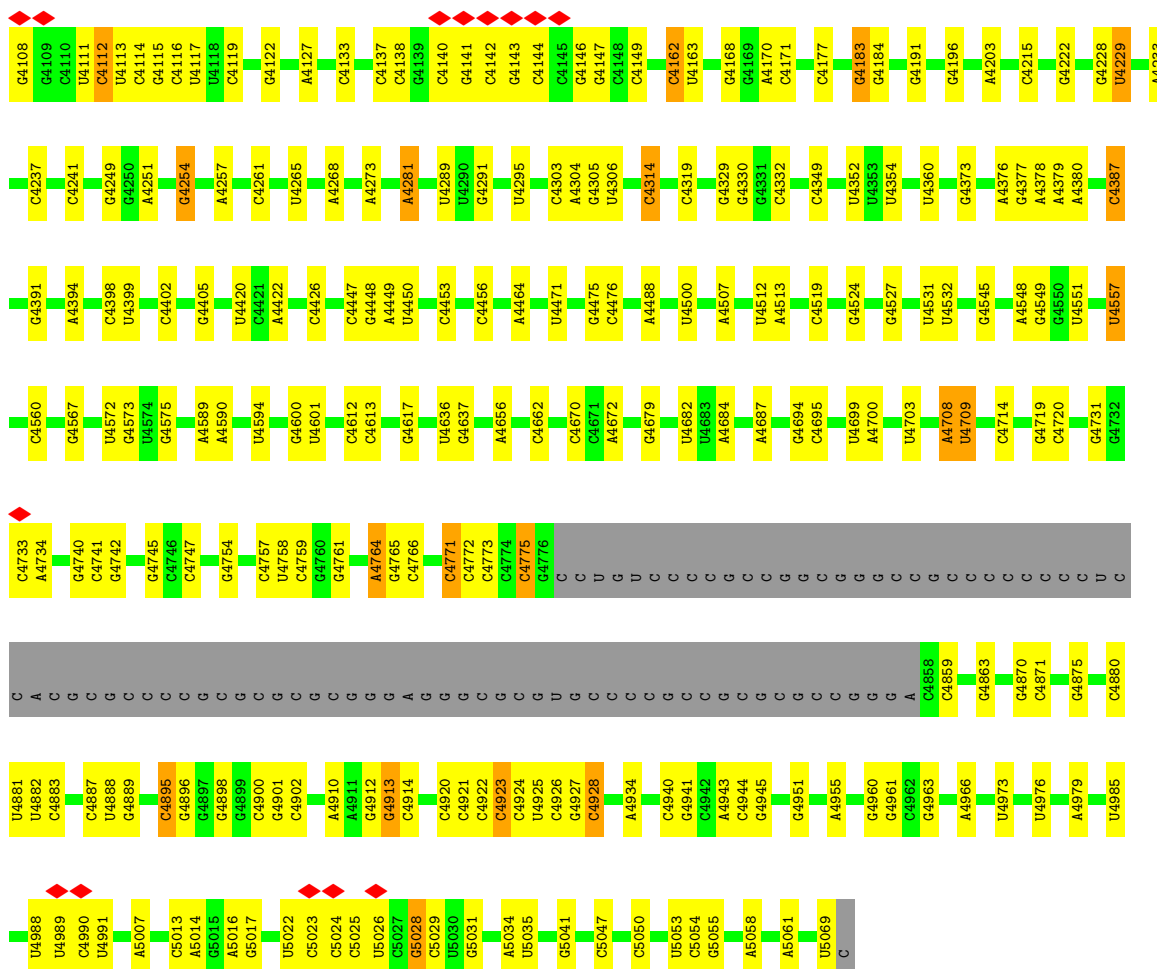
3 Residue-property plots [i](#)

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

• Molecule 1: 28S ribosomal RNA



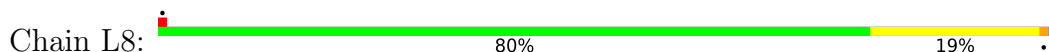




• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA



• Molecule 4: 60S ribosomal protein L8

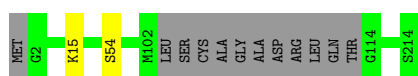




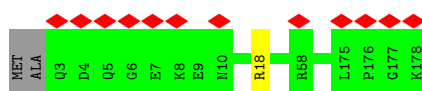
• Molecule 11: 60S ribosomal protein L9



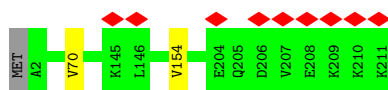
• Molecule 12: 60S ribosomal protein L10-like



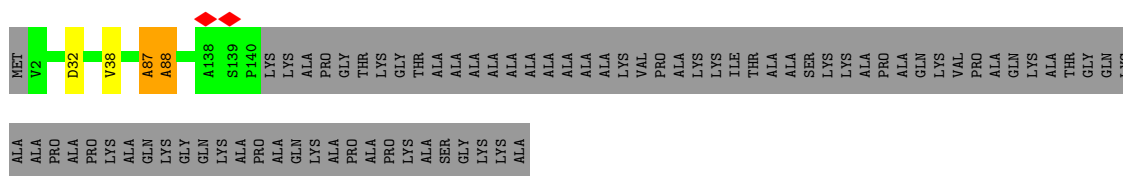
• Molecule 13: 60S ribosomal protein L11



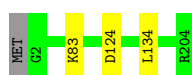
• Molecule 14: 60S ribosomal protein L13



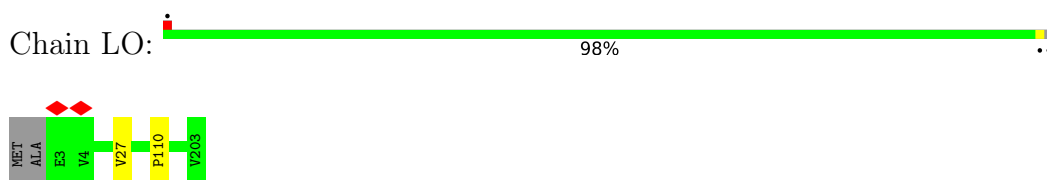
• Molecule 15: 60S ribosomal protein L14



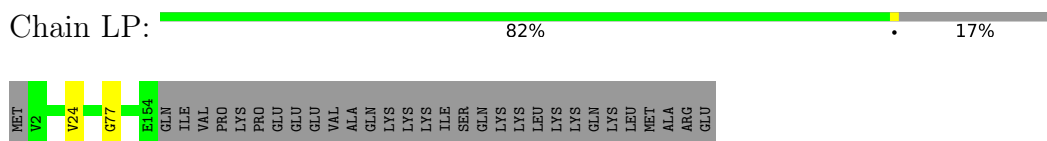
• Molecule 16: 60S ribosomal protein L15



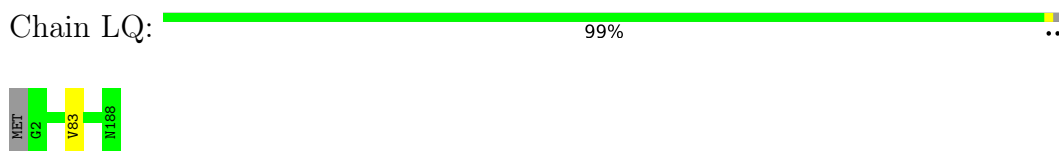
- Molecule 17: 60S ribosomal protein L13a



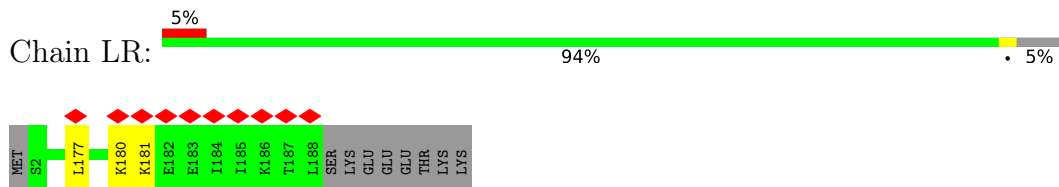
- Molecule 18: 60S ribosomal protein L17



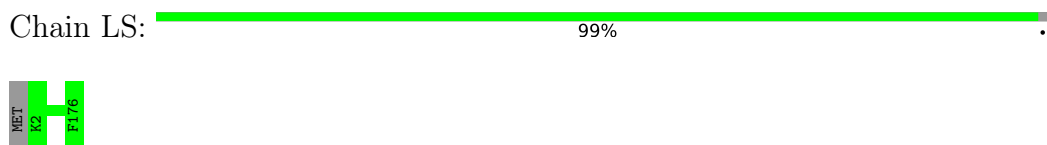
- Molecule 19: 60S ribosomal protein L18



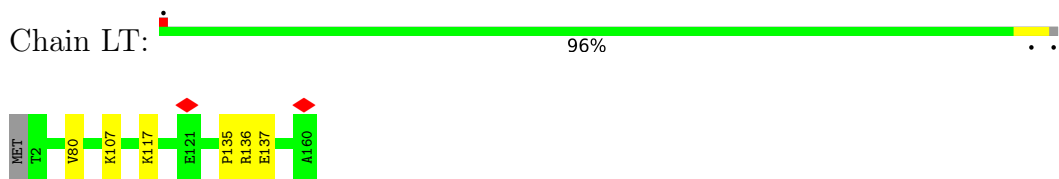
- Molecule 20: 60S ribosomal protein L19



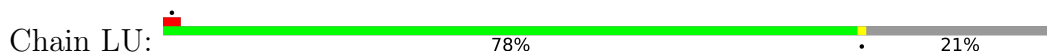
- Molecule 21: 60S ribosomal protein L18a

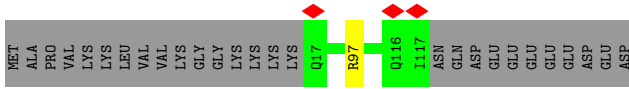


- Molecule 22: 60S ribosomal protein L21

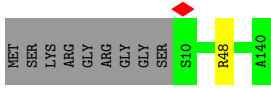


- Molecule 23: 60S ribosomal protein L22

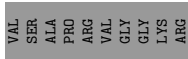
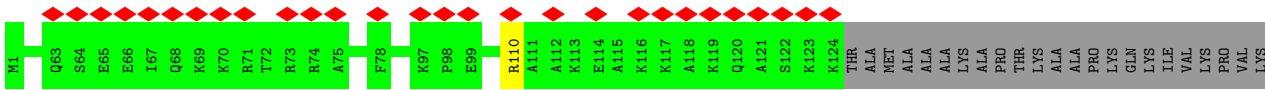
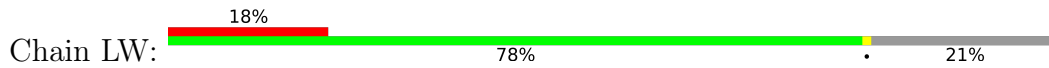




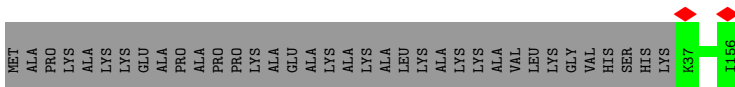
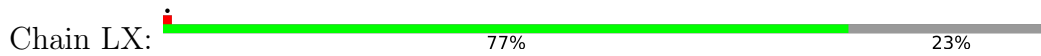
• Molecule 24: 60S ribosomal protein L23



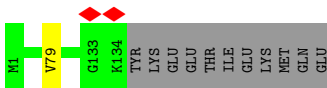
• Molecule 25: 60S ribosomal protein L24



• Molecule 26: 60S ribosomal protein L23a



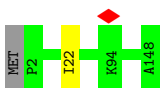
• Molecule 27: 60S ribosomal protein L26



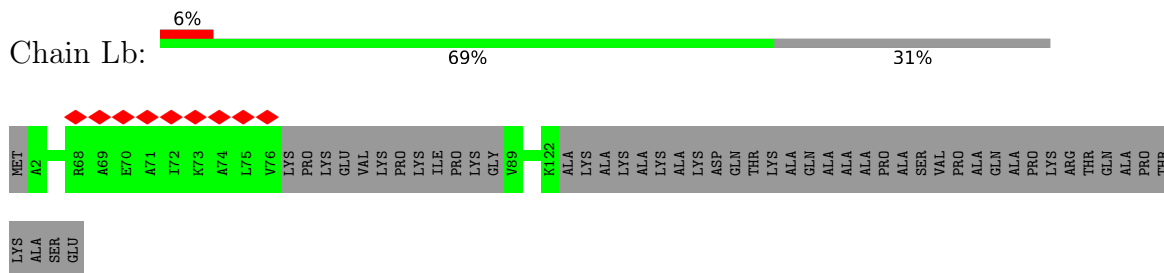
• Molecule 28: 60S ribosomal protein L27



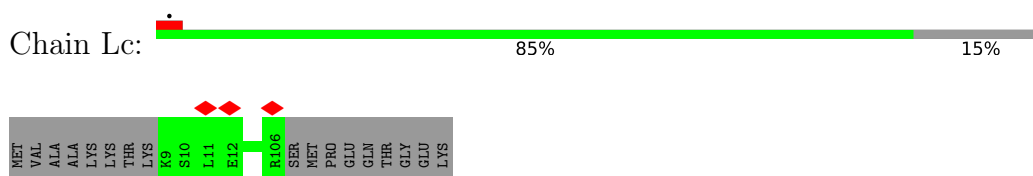
• Molecule 29: 60S ribosomal protein L27a



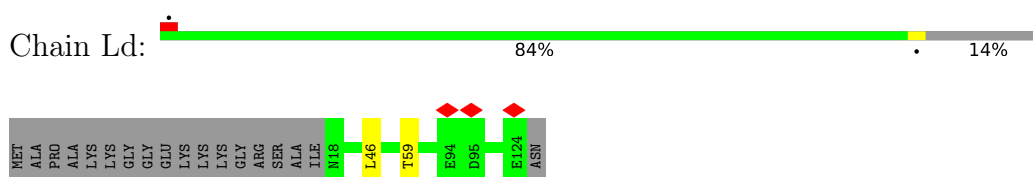
• Molecule 30: 60S ribosomal protein L29



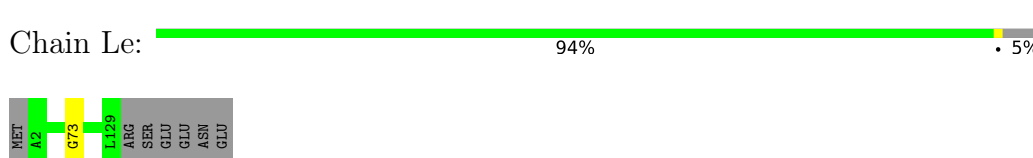
• Molecule 31: 60S ribosomal protein L30



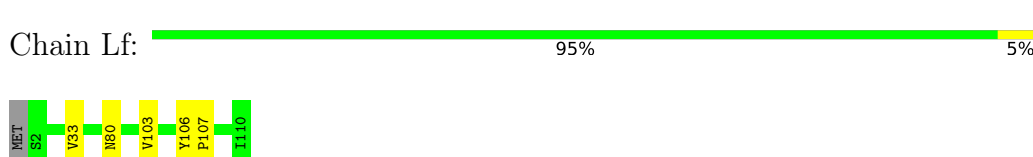
• Molecule 32: 60S ribosomal protein L31



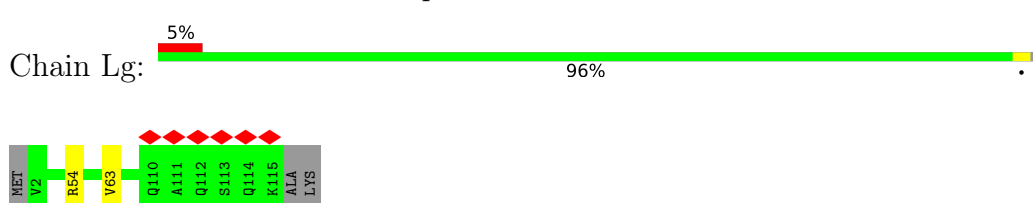
• Molecule 33: 60S ribosomal protein L32



• Molecule 34: 60S ribosomal protein L35a

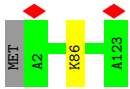


• Molecule 35: 60S ribosomal protein L34

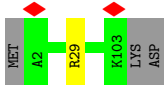


• Molecule 36: 60S ribosomal protein L35

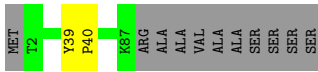
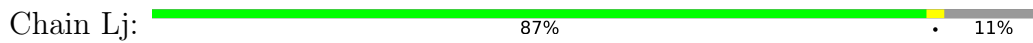




- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37



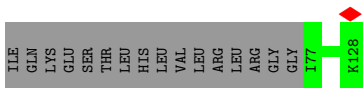
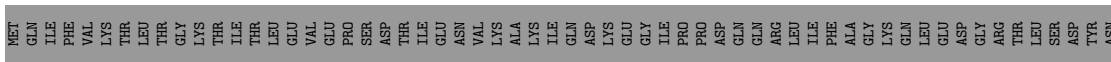
- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39



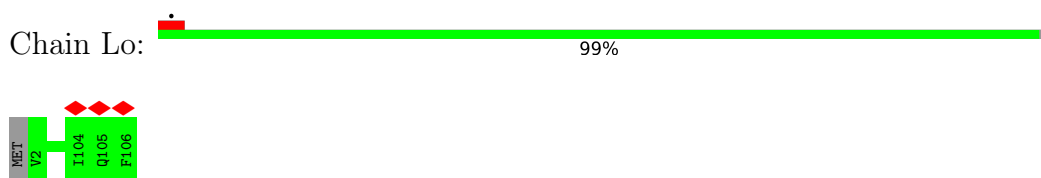
- Molecule 41: Ubiquitin-60S ribosomal protein L40



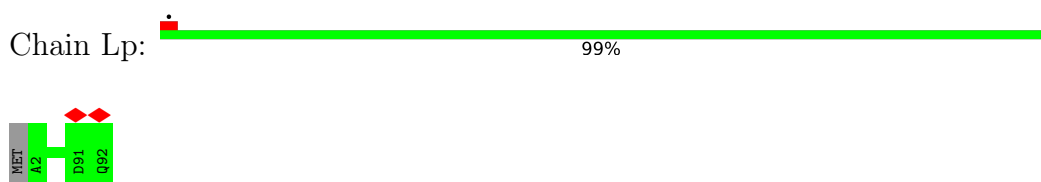
- Molecule 42: 60S ribosomal protein L41



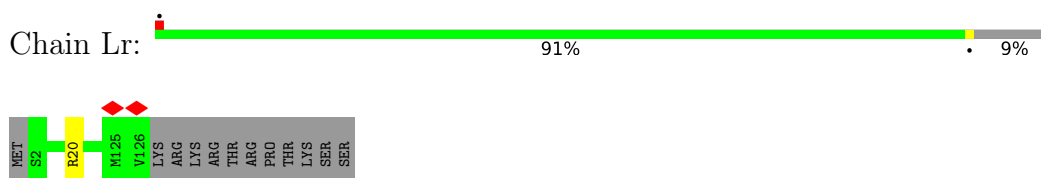
- Molecule 43: 60S ribosomal protein L36a



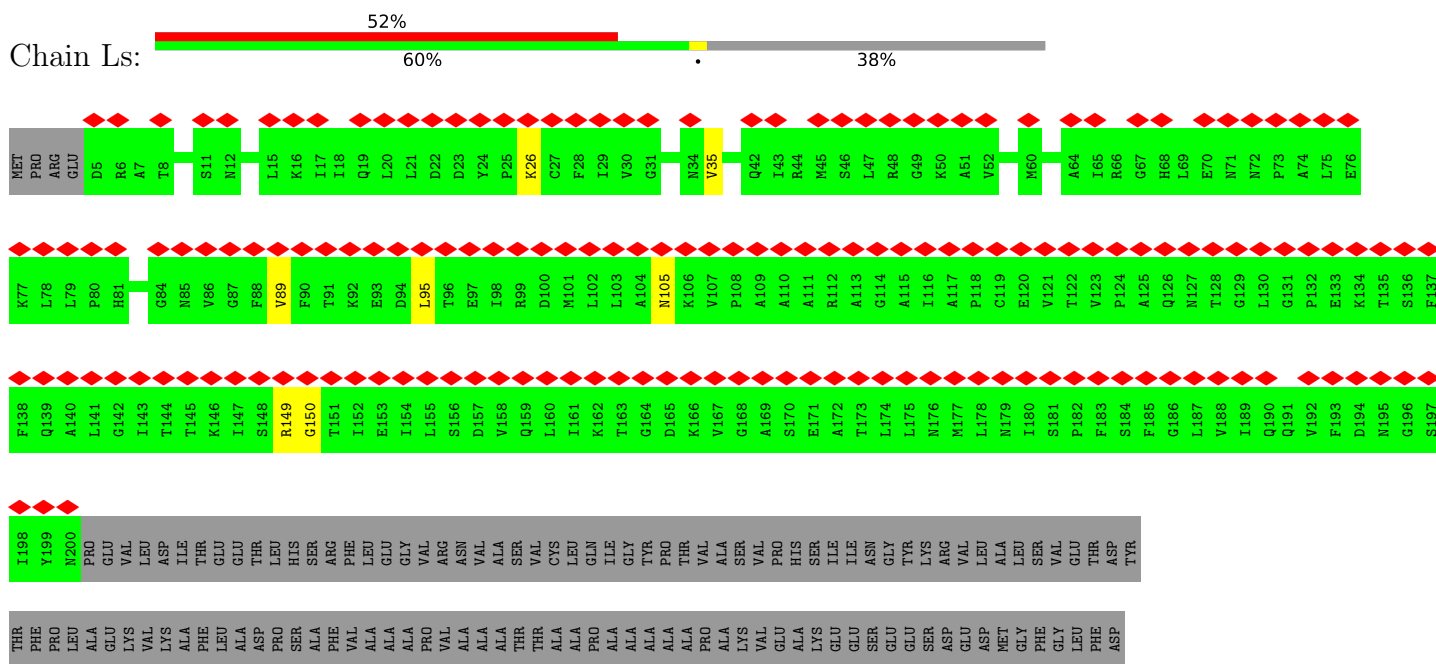
- Molecule 44: 60S ribosomal protein L37a



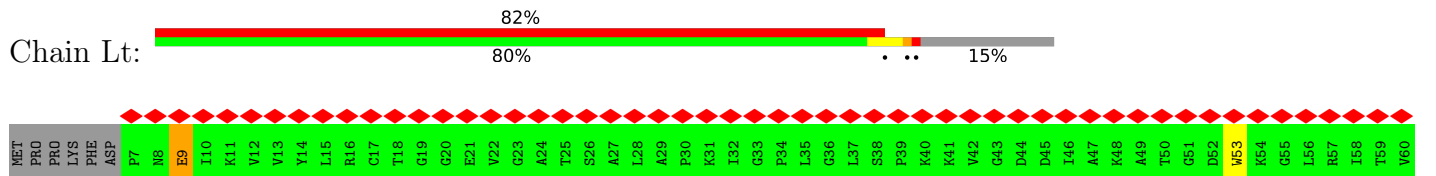
- Molecule 45: 60S ribosomal protein L28

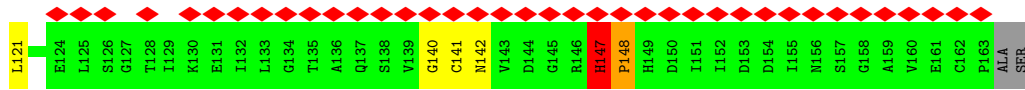


- Molecule 46: 60S acidic ribosomal protein P0

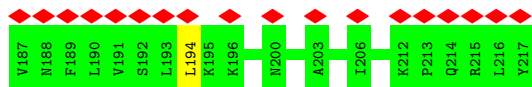
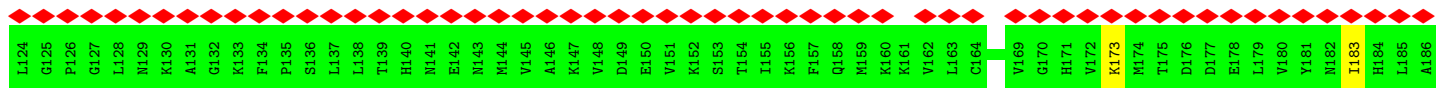
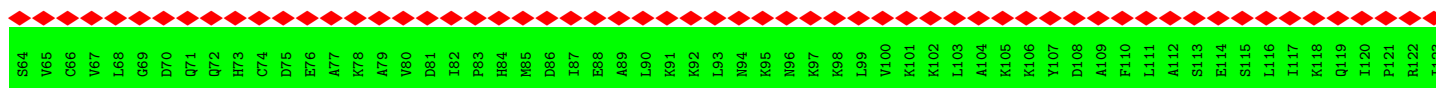
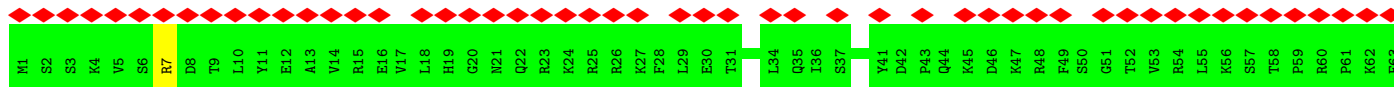
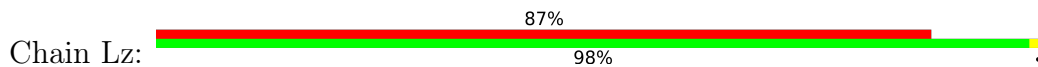


- Molecule 47: 60S ribosomal protein L12

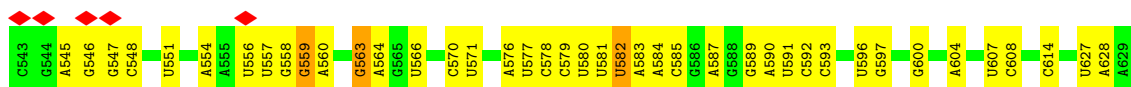


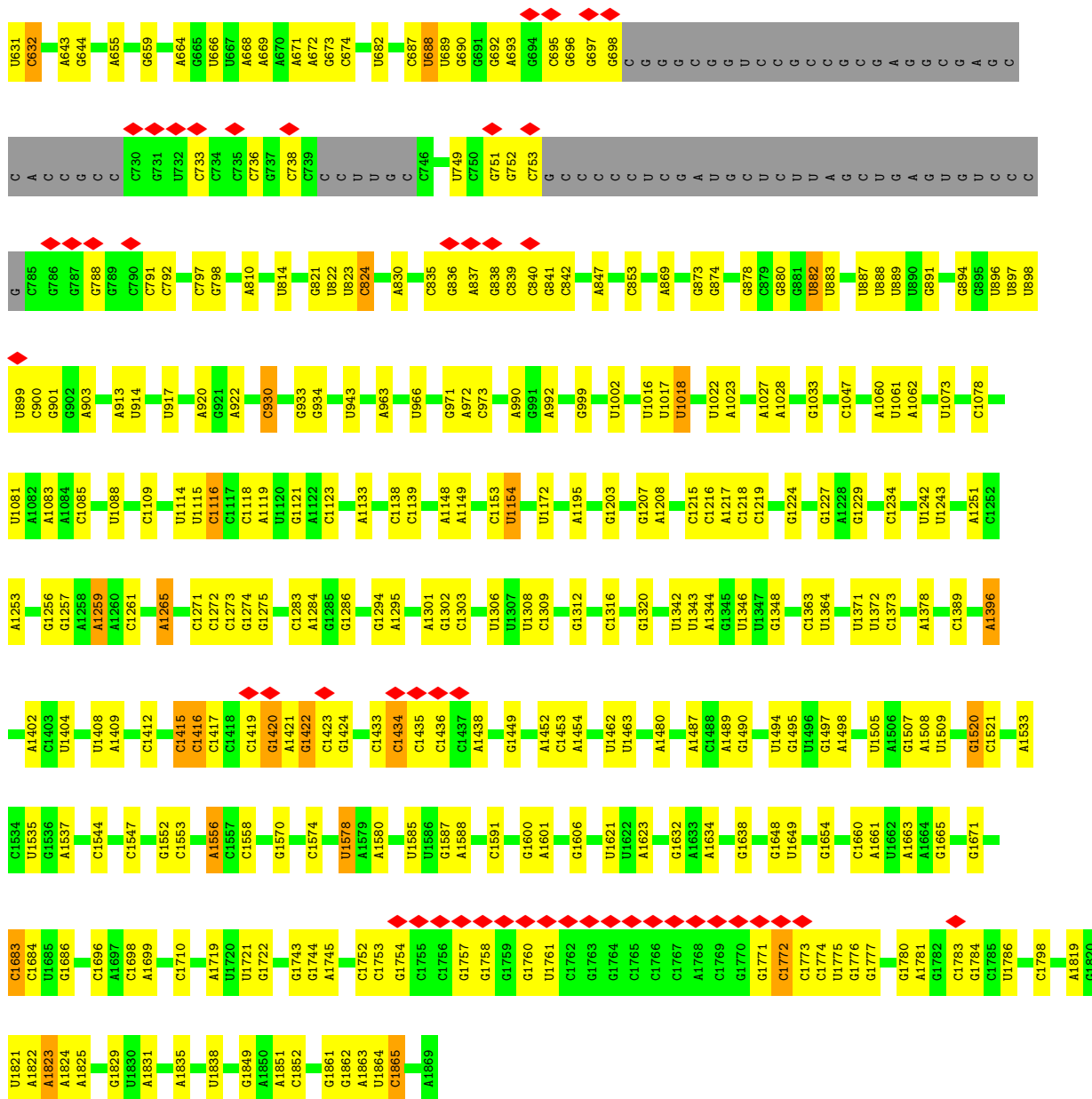


• Molecule 48: 60S ribosomal protein L10a

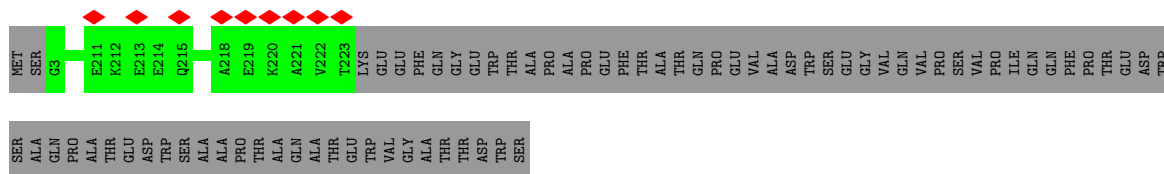
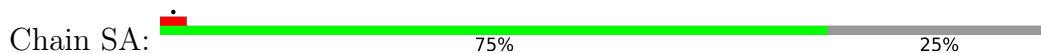


• Molecule 49: 18S ribosomal RNA

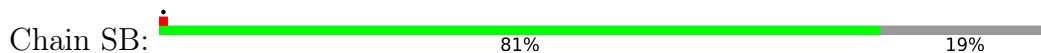


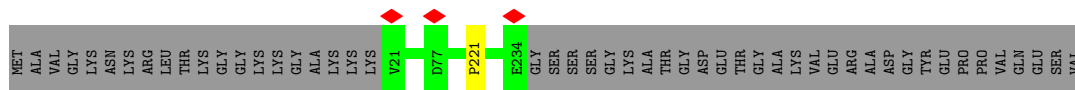


• Molecule 50: 40S ribosomal protein SA

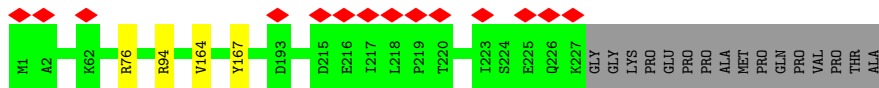
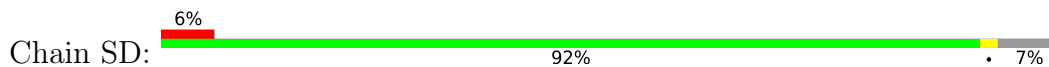


• Molecule 51: 40S ribosomal protein S3a





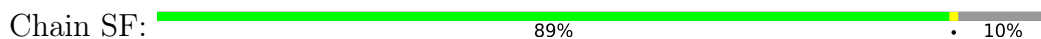
• Molecule 52: 40S ribosomal protein S3



• Molecule 53: 40S ribosomal protein S4, X isoform



• Molecule 54: 40S ribosomal protein S5



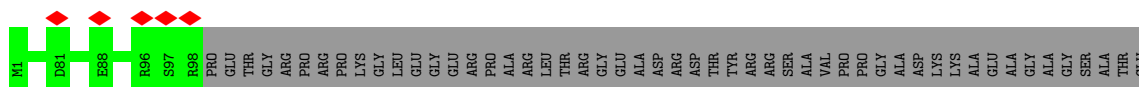
• Molecule 55: 40S ribosomal protein S7



• Molecule 56: 40S ribosomal protein S8

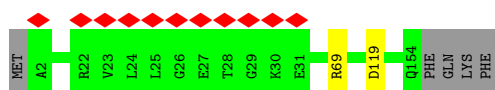


• Molecule 57: 40S ribosomal protein S10

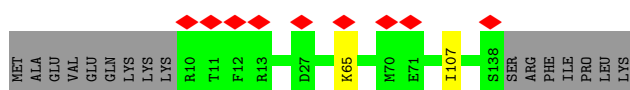
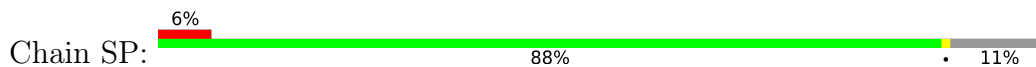


PHE
GLN
PHE
ARG
GLY
GLY
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ARG
GLY
ARG
GLY
GLN
PRO
PRO
GLN

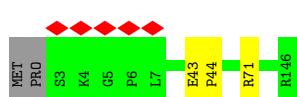
- Molecule 58: 40S ribosomal protein S11



- Molecule 59: 40S ribosomal protein S15



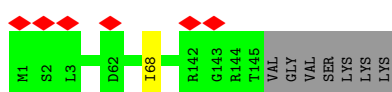
- Molecule 60: 40S ribosomal protein S16



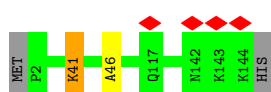
- Molecule 61: 40S ribosomal protein S17



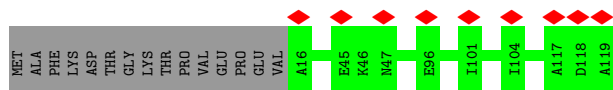
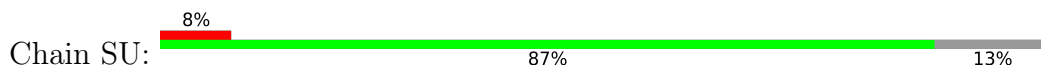
- Molecule 62: 40S ribosomal protein S18



- Molecule 63: 40S ribosomal protein S19



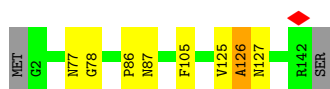
- Molecule 64: 40S ribosomal protein S20



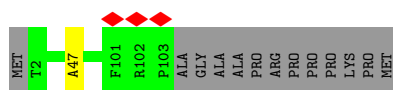
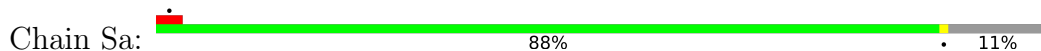
- Molecule 65: 40S ribosomal protein S21



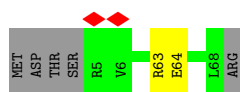
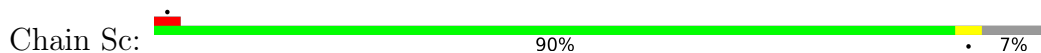
- Molecule 66: 40S ribosomal protein S23



- Molecule 67: 40S ribosomal protein S26



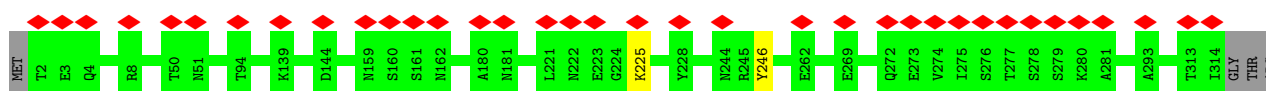
- Molecule 68: 40S ribosomal protein S28

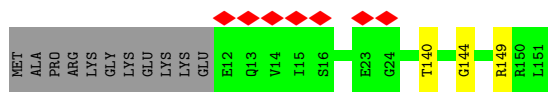


- Molecule 69: 40S ribosomal protein S29

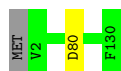


- Molecule 70: Receptor of activated protein C kinase 1

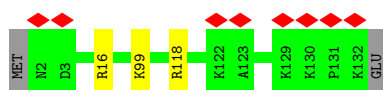




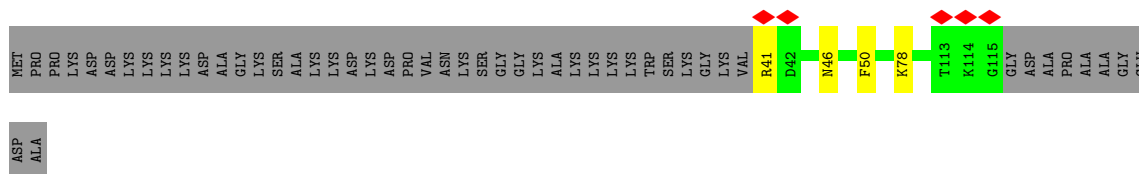
• Molecule 77: 40S ribosomal protein S15a



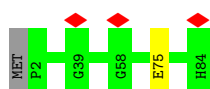
• Molecule 78: 40S ribosomal protein S24



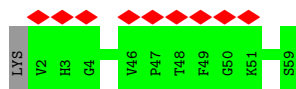
• Molecule 79: 40S ribosomal protein S25



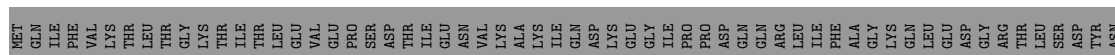
• Molecule 80: 40S ribosomal protein S27

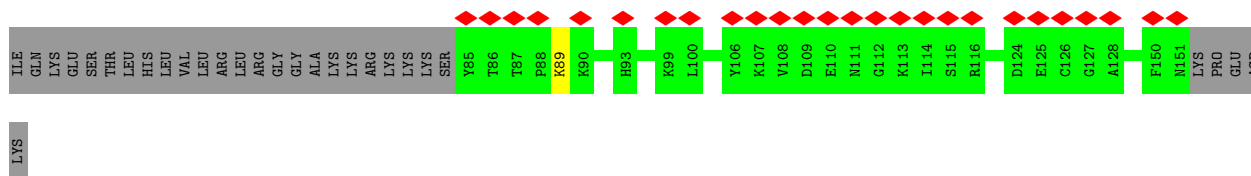


• Molecule 81: 40S ribosomal protein S30

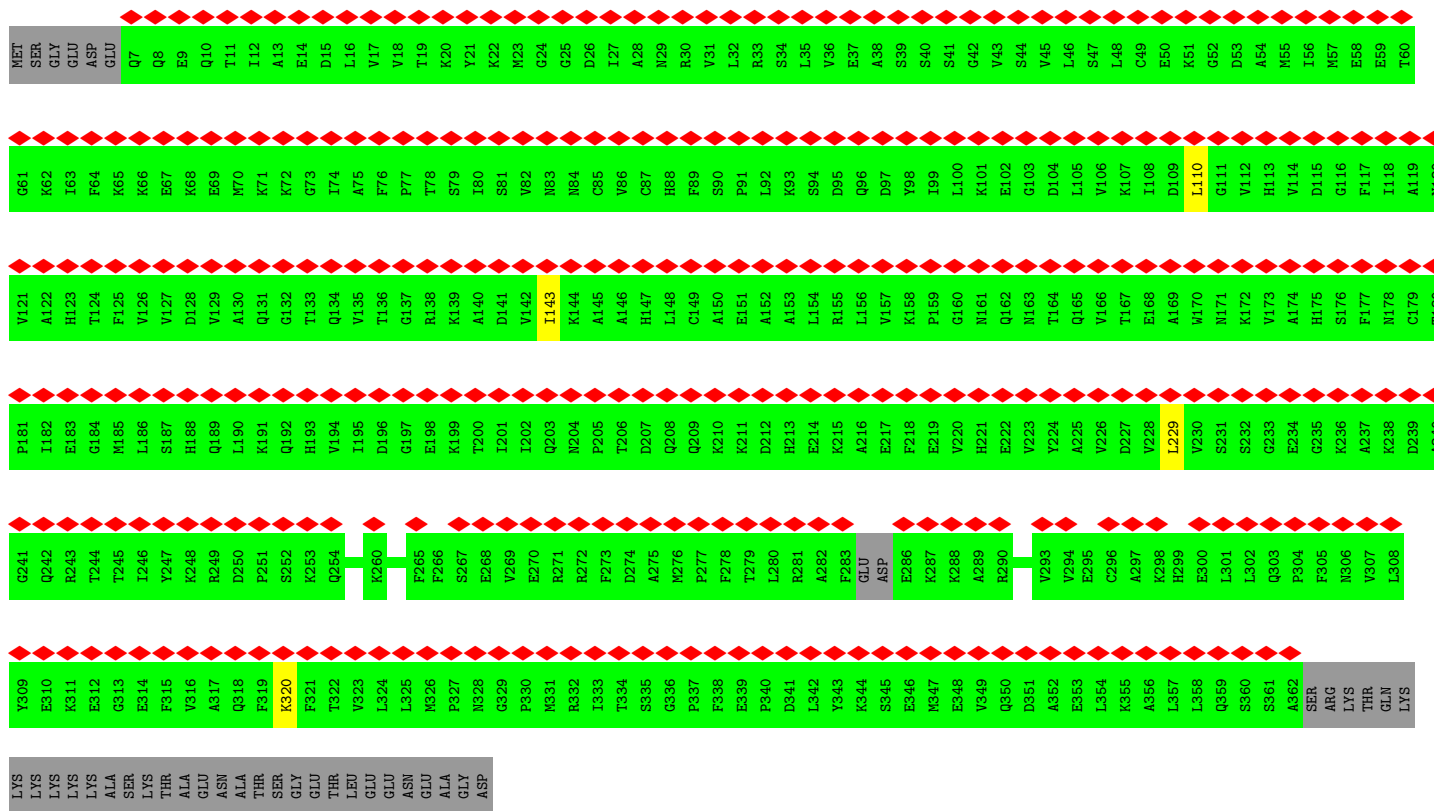
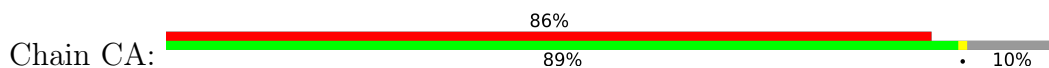


• Molecule 82: Ubiquitin-40S ribosomal protein S27a





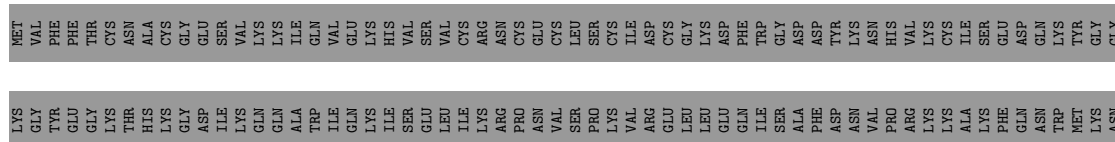
• Molecule 83: Proliferation-associated protein 2G4



• Molecule 84: tRNA



• Molecule 85: Cell growth-regulating nucleolar protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107149	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.518	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	L5	0.85	4/89595 (0.0%)	1.14	572/139686 (0.4%)
2	L7	0.79	0/2861	1.07	10/4459 (0.2%)
3	L8	0.86	0/3701	1.05	10/5766 (0.2%)
4	LA	0.48	0/1936	0.67	1/2596 (0.0%)
5	LB	0.44	0/3306	0.60	1/4424 (0.0%)
6	LC	0.43	0/2981	0.60	2/4002 (0.0%)
7	LD	0.39	0/2428	0.54	0/3252
8	LE	0.36	0/1942	0.58	1/2606 (0.0%)
9	LF	0.44	0/1905	0.57	1/2539 (0.0%)
10	LG	0.40	0/1960	0.59	1/2637 (0.0%)
11	LH	0.41	0/1537	0.54	0/2066
12	LI	0.43	0/1673	0.55	0/2233
13	LJ	0.35	0/1433	0.62	0/1915
14	LL	0.40	0/1732	0.56	0/2315
15	LM	0.41	0/1161	0.60	2/1554 (0.1%)
16	LN	0.47	0/1746	0.60	1/2338 (0.0%)
17	LO	0.42	0/1682	0.52	0/2250
18	LP	0.44	0/1268	0.54	0/1701
19	LQ	0.45	0/1537	0.56	0/2052
20	LR	0.38	0/1582	0.54	0/2091
21	LS	0.44	0/1493	0.53	0/2003
22	LT	0.43	0/1326	0.55	0/1770
23	LU	0.37	0/839	0.62	0/1126
24	LV	0.41	0/993	0.57	0/1332
25	LW	0.38	0/1030	0.57	0/1364
26	LX	0.40	0/1002	0.54	0/1345
27	LY	0.43	0/1132	0.56	0/1504
28	LZ	0.44	0/1130	0.56	0/1507
29	La	0.44	0/1191	0.55	0/1591
30	Lb	0.35	0/889	0.54	0/1175
31	Lc	0.44	0/774	0.59	0/1038
32	Ld	0.42	0/903	0.58	1/1216 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Le	0.45	0/1071	0.60	0/1429
34	Lf	0.46	0/895	0.62	0/1198
35	Lg	0.42	0/916	0.57	0/1220
36	Lh	0.38	0/1023	0.48	0/1351
37	Li	0.36	0/843	0.52	0/1115
38	Lj	0.47	0/720	0.61	0/952
39	Lk	0.37	0/575	0.53	0/761
40	Ll	0.39	0/454	0.54	0/599
41	Lm	0.41	0/435	0.53	0/575
42	Ln	0.37	0/231	0.46	0/294
43	Lo	0.41	0/876	0.56	0/1156
44	Lp	0.43	0/718	0.60	0/953
45	Lr	0.41	0/1017	0.54	0/1364
46	Ls	0.32	0/1519	0.70	2/2052 (0.1%)
47	Lt	0.36	0/1058	0.82	1/1430 (0.1%)
48	Lz	0.31	0/1769	0.68	1/2371 (0.0%)
49	S2	0.75	1/41245 (0.0%)	1.13	252/64265 (0.4%)
50	SA	0.39	0/1778	0.58	0/2416
51	SB	0.37	0/1765	0.56	0/2362
52	SD	0.37	0/1793	0.61	0/2414
53	SE	0.38	0/2118	0.61	2/2849 (0.1%)
54	SF	0.35	0/1481	0.54	0/1988
55	SH	0.36	0/1519	0.63	0/2033
56	SI	0.39	0/1715	0.58	1/2287 (0.0%)
57	SK	0.33	0/851	0.54	0/1147
58	SL	0.42	0/1268	0.59	0/1696
59	SP	0.32	0/1082	0.64	1/1446 (0.1%)
60	SQ	0.35	0/1160	0.61	0/1553
61	SR	0.34	0/1105	0.64	1/1484 (0.1%)
62	SS	0.32	0/1216	0.56	0/1628
63	ST	0.32	0/1131	0.53	0/1515
64	SU	0.33	0/831	0.63	0/1115
65	SV	0.37	0/643	0.63	1/860 (0.1%)
66	SX	0.40	0/1116	0.59	0/1490
67	Sa	0.40	0/836	0.59	0/1121
68	Sc	0.35	0/508	0.62	0/680
69	Sd	0.38	0/470	0.57	0/623
70	Sg	0.33	0/2493	0.65	0/3394
71	SC	0.43	0/1762	0.60	0/2381
72	SG	0.34	0/1946	0.58	1/2590 (0.0%)
73	SJ	0.38	0/1550	0.53	0/2069
74	SM	0.34	0/950	0.79	1/1275 (0.1%)
75	SN	0.39	0/1232	0.53	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SO	0.36	0/1062	0.59	0/1425
77	SW	0.40	0/1051	0.55	0/1406
78	SY	0.35	0/1083	0.53	0/1438
79	SZ	0.31	0/604	0.64	0/810
80	Sb	0.35	0/665	0.56	0/891
81	Se	0.33	0/448	0.54	0/592
82	Sf	0.30	0/560	0.67	0/745
83	CA	0.34	0/2810	0.71	3/3780 (0.1%)
84	CC	0.39	0/1773	1.06	7/2759 (0.3%)
85	CE	0.29	0/613	0.52	0/819
86	i	0.35	0/268	0.48	0/361
All	All	0.67	5/241289 (0.0%)	0.96	877/353636 (0.2%)

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
4	LA	0	2
5	LB	0	2
8	LE	0	1
11	LH	0	2
12	LI	0	1
14	LL	0	1
15	LM	0	2
17	LO	0	1
22	LT	0	3
29	La	0	1
32	Ld	0	1
34	Lf	0	2
36	Lh	0	1
38	Lj	0	1
45	Lr	0	1
46	Ls	0	1
47	Lt	0	6
48	Lz	0	1
51	SB	0	1
52	SD	0	1
54	SF	0	2
55	SH	0	2
60	SQ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
61	SR	0	1
63	ST	0	1
65	SV	0	1
66	SX	0	4
68	Sc	0	1
73	SJ	0	1
79	SZ	0	2
80	Sb	0	1
All	All	0	49

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	1422	G	C6-N1	-6.43	1.35	1.39
1	L5	4764	A	N9-C4	-5.85	1.34	1.37
1	L5	2409	U	C2-O2	-5.46	1.17	1.22
1	L5	5016	A	N9-C4	-5.35	1.34	1.37
1	L5	3775	A	N9-C4	-5.31	1.34	1.37

All (877) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1417	C	N3-C4-N4	-27.21	98.96	118.00
49	S2	1422	G	N1-C6-O6	-26.09	104.24	119.90
49	S2	1422	G	C5-C6-O6	21.91	141.75	128.60
49	S2	1417	C	C5-C4-N4	21.65	135.35	120.20
49	S2	1772	C	N1-C2-O2	15.67	128.30	118.90
49	S2	1772	C	N3-C2-O2	-15.33	111.17	121.90
49	S2	501	C	N1-C2-O2	14.20	127.42	118.90
1	L5	485	C	C2-N1-C1'	14.03	134.23	118.80
49	S2	293	C	N1-C2-O2	13.70	127.12	118.90
49	S2	501	C	C2-N1-C1'	13.61	133.78	118.80
1	L5	2710	C	N1-C2-O2	13.08	126.75	118.90
1	L5	2710	C	C2-N1-C1'	12.62	132.68	118.80
1	L5	2814	C	N1-C2-O2	12.60	126.46	118.90
1	L5	2710	C	N3-C2-O2	-12.27	113.31	121.90
49	S2	501	C	N3-C2-O2	-11.80	113.64	121.90
59	SP	107	ILE	C-N-CA	11.74	151.06	121.70
49	S2	882	U	N1-C2-O2	11.59	130.91	122.80
1	L5	2814	C	N3-C2-O2	-11.14	114.10	121.90
49	S2	1139	C	N3-C2-O2	-11.10	114.13	121.90
49	S2	293	C	C2-N1-C1'	10.63	130.49	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	485	C	N1-C2-O2	10.49	125.20	118.90
1	L5	456	C	O4'-C1'-N1	10.36	116.49	108.20
1	L5	485	C	C6-N1-C1'	-10.35	108.38	120.80
49	S2	293	C	N3-C2-O2	-10.34	114.67	121.90
1	L5	181	C	N1-C2-O2	10.29	125.07	118.90
1	L5	1367	C	N1-C2-O2	10.28	125.07	118.90
49	S2	1772	C	C6-N1-C2	-10.27	116.19	120.30
49	S2	356	C	N1-C2-O2	10.15	124.99	118.90
1	L5	3948	C	N1-C2-O2	10.11	124.97	118.90
49	S2	1139	C	N1-C2-O2	10.10	124.96	118.90
49	S2	1453	C	C2-N1-C1'	9.99	129.79	118.80
1	L5	4923	C	N3-C2-O2	-9.93	114.95	121.90
1	L5	4138	C	N3-C2-O2	-9.84	115.01	121.90
49	S2	882	U	N3-C2-O2	-9.83	115.32	122.20
49	S2	356	C	C2-N1-C1'	9.71	129.49	118.80
1	L5	2018	C	C5-C6-N1	9.69	125.85	121.00
1	L5	1447	C	N3-C2-O2	-9.65	115.15	121.90
1	L5	4921	C	N3-C2-O2	-9.65	115.15	121.90
49	S2	882	U	C2-N1-C1'	9.62	129.24	117.70
49	S2	1772	C	C2-N1-C1'	9.54	129.29	118.80
49	S2	501	C	C6-N1-C1'	-9.54	109.35	120.80
49	S2	118	C	N1-C2-O2	9.52	124.61	118.90
1	L5	417	G	O4'-C1'-N9	9.49	115.80	108.20
1	L5	4557	U	N3-C2-O2	-9.49	115.56	122.20
1	L5	1714	C	N1-C2-O2	9.48	124.59	118.90
1	L5	2710	C	C6-N1-C2	-9.47	116.51	120.30
1	L5	100	C	C2-N1-C1'	9.45	129.20	118.80
1	L5	174	C	N3-C2-O2	-9.39	115.33	121.90
49	S2	1453	C	N1-C2-O2	9.38	124.53	118.90
1	L5	4928	C	C2-N1-C1'	9.25	128.97	118.80
1	L5	1414	C	N3-C2-O2	-9.24	115.43	121.90
1	L5	2709	C	N3-C4-C5	9.24	125.60	121.90
1	L5	516	C	N1-C2-O2	9.22	124.43	118.90
53	SE	93	ASP	CB-CG-OD2	9.20	126.58	118.30
1	L5	753	C	N1-C2-O2	9.20	124.42	118.90
49	S2	427	U	N3-C2-O2	-9.16	115.79	122.20
1	L5	1216	C	C2-N1-C1'	9.15	128.86	118.80
1	L5	4149	C	N3-C2-O2	-9.14	115.50	121.90
1	L5	753	C	N3-C2-O2	-9.13	115.51	121.90
1	L5	4303	C	C6-N1-C2	-9.11	116.66	120.30
1	L5	4926	C	N1-C2-O2	9.07	124.34	118.90
1	L5	4928	C	N1-C2-O2	9.06	124.34	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3948	C	C2-N1-C1'	9.05	128.76	118.80
1	L5	3775	A	N7-C8-N9	9.04	118.32	113.80
1	L5	4926	C	C2-N1-C1'	8.94	128.64	118.80
1	L5	233	U	N3-C2-O2	-8.91	115.96	122.20
1	L5	515	C	N1-C2-O2	8.91	124.24	118.90
49	S2	322	C	N3-C2-O2	-8.89	115.68	121.90
49	S2	1417	C	C4-C5-C6	-8.86	112.97	117.40
49	S2	118	C	C2-N1-C1'	8.84	128.52	118.80
1	L5	4303	C	N3-C2-O2	-8.83	115.72	121.90
1	L5	2018	C	C6-N1-C2	-8.82	116.77	120.30
49	S2	1417	C	N3-C4-C5	8.78	125.41	121.90
1	L5	655	C	N3-C2-O2	-8.76	115.77	121.90
1	L5	4229	U	N3-C2-O2	-8.74	116.08	122.20
74	SM	98	GLY	C-N-CA	8.72	143.50	121.70
49	S2	501	C	C6-N1-C2	-8.61	116.86	120.30
1	L5	1216	C	N1-C2-O2	8.57	124.04	118.90
1	L5	2627	C	C2-N1-C1'	8.55	128.20	118.80
49	S2	356	C	N3-C2-O2	-8.46	115.98	121.90
1	L5	233	U	N1-C2-O2	8.45	128.71	122.80
1	L5	4281	A	N7-C8-N9	8.41	118.01	113.80
1	L5	181	C	N3-C2-O2	-8.40	116.02	121.90
1	L5	4557	U	N1-C2-O2	8.39	128.68	122.80
1	L5	1447	C	C6-N1-C2	-8.33	116.97	120.30
1	L5	2710	C	C6-N1-C1'	-8.32	110.81	120.80
49	S2	118	C	N3-C2-O2	-8.31	116.08	121.90
1	L5	1082	C	O4'-C1'-N1	8.26	114.81	108.20
1	L5	1367	C	N3-C2-O2	-8.26	116.12	121.90
1	L5	3948	C	N3-C2-O2	-8.23	116.14	121.90
49	S2	1139	C	C2-N1-C1'	8.23	127.86	118.80
1	L5	100	C	N3-C2-O2	-8.21	116.16	121.90
1	L5	1714	C	C2-N1-C1'	8.20	127.81	118.80
49	S2	1520	G	C4-N9-C1'	8.19	137.14	126.50
1	L5	1367	C	C2-N1-C1'	8.16	127.78	118.80
84	CC	74	C	C6-N1-C2	-8.16	117.03	120.30
1	L5	3775	A	C2-N3-C4	-8.16	106.52	110.60
1	L5	516	C	N3-C2-O2	-8.14	116.20	121.90
1	L5	1915	C	N3-C2-O2	-8.11	116.23	121.90
1	L5	1252	C	N3-C2-O2	-8.10	116.23	121.90
1	L5	2410	C	C2-N1-C1'	8.09	127.70	118.80
1	L5	4281	A	C8-N9-C4	-8.06	102.58	105.80
1	L5	209	U	C2-N1-C1'	8.05	127.36	117.70
1	L5	4557	U	C2-N1-C1'	8.04	127.34	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1216	C	N3-C2-O2	-8.02	116.28	121.90
1	L5	100	C	C6-N1-C2	-7.99	117.11	120.30
1	L5	181	C	C2-N1-C1'	7.98	127.57	118.80
1	L5	4773	C	N1-C2-O2	7.97	123.68	118.90
3	L8	51	U	N3-C2-O2	-7.96	116.63	122.20
1	L5	499	G	N3-C4-N9	7.94	130.76	126.00
1	L5	4758	U	N1-C2-O2	7.91	128.34	122.80
49	S2	427	U	N1-C2-O2	7.84	128.29	122.80
1	L5	3757	G	O4'-C1'-N9	7.83	114.46	108.20
49	S2	1139	C	C6-N1-C2	-7.80	117.18	120.30
1	L5	4926	C	N3-C2-O2	-7.77	116.46	121.90
49	S2	630	U	C2-N1-C1'	7.77	127.02	117.70
1	L5	2814	C	C2-N1-C1'	7.77	127.34	118.80
3	L8	51	U	N1-C2-O2	7.75	128.23	122.80
1	L5	4709	U	N3-C2-O2	-7.75	116.78	122.20
1	L5	515	C	C2-N1-C1'	7.73	127.31	118.80
1	L5	175	C	N3-C2-O2	-7.72	116.50	121.90
1	L5	2262	G	C4-N9-C1'	7.71	136.52	126.50
1	L5	4758	U	C2-N1-C1'	7.70	126.94	117.70
1	L5	4928	C	N3-C2-O2	-7.69	116.52	121.90
1	L5	1414	C	N1-C2-O2	7.68	123.51	118.90
1	L5	4758	U	N3-C2-O2	-7.67	116.83	122.20
1	L5	115	C	C2-N1-C1'	7.64	127.21	118.80
49	S2	1022	U	C2-N1-C1'	7.63	126.86	117.70
3	L8	64	U	N3-C2-O2	-7.63	116.86	122.20
1	L5	4551	U	N3-C2-O2	-7.61	116.88	122.20
49	S2	1520	G	C8-N9-C1'	-7.60	117.12	127.00
49	S2	593	C	N1-C2-O2	7.60	123.46	118.90
1	L5	1378	C	N1-C2-O2	7.57	123.44	118.90
49	S2	293	C	C6-N1-C1'	-7.56	111.73	120.80
1	L5	2409	U	N1-C2-N3	7.55	119.43	114.90
1	L5	4138	C	C6-N1-C2	-7.53	117.29	120.30
1	L5	4682	U	N3-C2-O2	-7.53	116.93	122.20
1	L5	1714	C	N3-C2-O2	-7.50	116.65	121.90
1	L5	1762	C	C6-N1-C2	-7.49	117.30	120.30
49	S2	1591	C	N1-C2-O2	7.49	123.39	118.90
1	L5	1607	C	C6-N1-C2	-7.49	117.31	120.30
1	L5	3775	A	C5-N7-C8	-7.47	100.16	103.90
1	L5	282	C	C6-N1-C2	-7.46	117.31	120.30
1	L5	4303	C	C2-N1-C1'	7.46	127.01	118.80
49	S2	179	C	N1-C2-O2	7.43	123.36	118.90
1	L5	2351	C	C6-N1-C2	-7.43	117.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	485	C	N3-C2-O2	-7.41	116.71	121.90
1	L5	3775	A	C8-N9-C4	-7.41	102.84	105.80
1	L5	1182	C	N1-C2-O2	7.39	123.33	118.90
1	L5	485	C	C6-N1-C2	-7.38	117.35	120.30
1	L5	4398	C	N1-C2-O2	7.38	123.33	118.90
1	L5	4945	G	C5-C6-O6	-7.36	124.18	128.60
49	S2	1081	U	N3-C2-O2	-7.27	117.11	122.20
1	L5	2528	G	C4-N9-C1'	7.27	135.96	126.50
1	L5	485	C	C5-C6-N1	7.27	124.63	121.00
1	L5	115	C	N1-C2-O2	7.25	123.25	118.90
49	S2	1016	U	N3-C2-O2	-7.25	117.13	122.20
49	S2	1261	C	N1-C2-O2	7.25	123.25	118.90
1	L5	3775	A	N1-C2-N3	7.24	132.92	129.30
1	L5	499	G	C4-N9-C1'	7.24	135.91	126.50
49	S2	1265	A	C2-N3-C4	7.23	114.21	110.60
49	S2	427	U	C2-N1-C1'	7.22	126.37	117.70
1	L5	3693	U	N3-C2-O2	-7.20	117.16	122.20
1	L5	4923	C	N1-C2-O2	7.19	123.22	118.90
1	L5	1344	C	C6-N1-C2	-7.19	117.42	120.30
1	L5	2262	G	N3-C4-N9	7.19	130.31	126.00
1	L5	925	C	N3-C2-O2	-7.18	116.87	121.90
49	S2	1416	C	N3-C2-O2	-7.16	116.89	121.90
1	L5	4281	A	O4'-C1'-N9	7.15	113.92	108.20
49	S2	1865	C	C6-N1-C2	-7.13	117.45	120.30
1	L5	963	G	C4-N9-C1'	7.11	135.74	126.50
1	L5	1182	C	C2-N1-C1'	7.10	126.61	118.80
49	S2	1271	C	N1-C2-O2	7.09	123.16	118.90
49	S2	882	U	C5-C6-N1	7.08	126.24	122.70
1	L5	2262	G	N3-C4-C5	-7.07	125.07	128.60
1	L5	499	G	N3-C4-C5	-7.06	125.07	128.60
48	Lz	194	LEU	CA-CB-CG	7.06	131.53	115.30
1	L5	4709	U	N1-C2-O2	7.06	127.74	122.80
49	S2	1261	C	N3-C2-O2	-7.06	116.96	121.90
49	S2	527	C	N3-C2-O2	-7.05	116.97	121.90
1	L5	2018	C	N1-C2-O2	7.05	123.13	118.90
1	L5	3909	C	C6-N1-C2	-7.05	117.48	120.30
49	S2	1453	C	C6-N1-C1'	-7.04	112.35	120.80
1	L5	2528	G	N3-C4-C5	-6.99	125.11	128.60
72	SG	41	LEU	CA-CB-CG	6.98	131.34	115.30
1	L5	115	C	N3-C2-O2	-6.96	117.03	121.90
1	L5	3948	C	C6-N1-C2	-6.93	117.53	120.30
49	S2	1520	G	N3-C4-N9	6.93	130.16	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3767	C	C5-C6-N1	6.92	124.46	121.00
1	L5	2494	U	N1-C2-O2	6.91	127.64	122.80
1	L5	4229	U	N1-C2-O2	6.91	127.63	122.80
2	L7	39	C	N1-C2-O2	6.90	123.04	118.90
49	S2	1273	C	C6-N1-C2	-6.89	117.55	120.30
1	L5	1241	C	N1-C2-O2	6.88	123.03	118.90
49	S2	356	C	C6-N1-C1'	-6.88	112.54	120.80
49	S2	632	C	C2-N1-C1'	6.88	126.36	118.80
49	S2	1415	C	N1-C2-O2	6.87	123.02	118.90
1	L5	2257	C	C2-N1-C1'	6.87	126.36	118.80
1	L5	1191	C	N3-C2-O2	-6.86	117.10	121.90
1	L5	753	C	C6-N1-C2	-6.86	117.56	120.30
1	L5	1632	A	C2-N3-C4	6.85	114.03	110.60
83	CA	110	LEU	CA-CB-CG	6.85	131.05	115.30
1	L5	2814	C	C6-N1-C2	-6.84	117.56	120.30
1	L5	4398	C	N3-C2-O2	-6.83	117.12	121.90
49	S2	1453	C	N3-C2-O2	-6.83	117.12	121.90
1	L5	100	C	N1-C2-O2	6.82	122.99	118.90
49	S2	1016	U	N1-C2-O2	6.82	127.58	122.80
1	L5	1340	C	C5-C6-N1	6.82	124.41	121.00
1	L5	3772	U	N3-C2-O2	-6.82	117.43	122.20
1	L5	4450	U	N3-C2-O2	-6.82	117.43	122.20
1	L5	1821	G	N3-C4-C5	-6.80	125.20	128.60
49	S2	688	U	P-O3'-C3'	6.80	127.86	119.70
1	L5	3778	U	N1-C2-O2	6.79	127.55	122.80
1	L5	282	C	N3-C2-O2	-6.78	117.16	121.90
1	L5	456	C	N3-C2-O2	-6.78	117.16	121.90
1	L5	1216	C	C6-N1-C2	-6.77	117.59	120.30
1	L5	2760	G	P-O3'-C3'	6.77	127.82	119.70
1	L5	3772	U	C2-N1-C1'	6.76	125.81	117.70
1	L5	516	C	C2-N1-C1'	6.75	126.22	118.80
1	L5	1915	C	N1-C2-O2	6.75	122.95	118.90
1	L5	1241	C	C2-N1-C1'	6.75	126.22	118.80
1	L5	4928	C	C6-N1-C1'	-6.75	112.71	120.80
1	L5	1082	C	P-O3'-C3'	6.74	127.79	119.70
1	L5	2627	C	C6-N1-C2	-6.74	117.60	120.30
1	L5	914	U	P-O3'-C3'	6.73	127.78	119.70
49	S2	494	C	N1-C2-O2	6.71	122.93	118.90
49	S2	579	C	N1-C2-O2	6.70	122.92	118.90
1	L5	1439	C	C2-N1-C1'	6.70	126.17	118.80
1	L5	1309	C	C6-N1-C2	-6.69	117.62	120.30
1	L5	4773	C	N3-C2-O2	-6.69	117.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	220	C	C2-N1-C1'	6.69	126.15	118.80
1	L5	963	G	N3-C4-N9	6.69	130.01	126.00
1	L5	77	U	N3-C2-O2	-6.68	117.52	122.20
1	L5	4945	G	N3-C4-N9	6.68	130.01	126.00
49	S2	178	C	N1-C2-O2	6.68	122.91	118.90
1	L5	1082	C	OP1-P-O3'	6.67	119.88	105.20
1	L5	4682	U	N1-C2-O2	6.67	127.47	122.80
1	L5	1514	U	N3-C2-O2	-6.67	117.53	122.20
49	S2	418	A	O5'-P-OP1	-6.66	99.71	105.70
1	L5	2494	U	N3-C2-O2	-6.64	117.55	122.20
1	L5	4775	C	N1-C2-O2	6.64	122.89	118.90
1	L5	472	C	C2-N1-C1'	6.62	126.09	118.80
1	L5	4476	C	C2-N1-C1'	6.62	126.08	118.80
49	S2	1261	C	C6-N1-C2	-6.62	117.65	120.30
49	S2	325	C	N1-C2-O2	6.61	122.86	118.90
1	L5	1762	C	N3-C2-O2	-6.60	117.28	121.90
1	L5	4456	C	C6-N1-C2	-6.60	117.66	120.30
84	CC	35	U	P-O3'-C3'	6.60	127.62	119.70
1	L5	2410	C	C6-N1-C2	-6.59	117.66	120.30
3	L8	111	U	C2-N1-C1'	6.59	125.60	117.70
49	S2	659	G	C4-N9-C1'	6.58	135.06	126.50
1	L5	3840	U	N3-C2-O2	-6.58	117.59	122.20
2	L7	102	U	N1-C2-O2	6.58	127.41	122.80
1	L5	3693	U	N1-C2-O2	6.58	127.40	122.80
3	L8	51	U	C2-N1-C1'	6.57	125.59	117.70
49	S2	630	U	N1-C2-O2	6.57	127.40	122.80
1	L5	1821	G	N3-C4-N9	6.56	129.94	126.00
1	L5	41	C	C6-N1-C2	-6.56	117.68	120.30
1	L5	499	G	C8-N9-C1'	-6.55	118.48	127.00
1	L5	3637	U	N3-C2-O2	-6.54	117.62	122.20
1	L5	3778	U	N3-C2-O2	-6.53	117.63	122.20
1	L5	453	G	N3-C4-C5	-6.53	125.34	128.60
1	L5	4314	C	N1-C2-O2	6.52	122.81	118.90
1	L5	2675	G	P-O3'-C3'	6.52	127.52	119.70
2	L7	102	U	N3-C2-O2	-6.51	117.64	122.20
1	L5	925	C	N1-C2-O2	6.50	122.80	118.90
1	L5	3892	U	N3-C2-O2	-6.50	117.65	122.20
49	S2	1453	C	C5-C6-N1	6.50	124.25	121.00
1	L5	181	C	C6-N1-C2	-6.49	117.70	120.30
1	L5	498	C	N1-C2-O2	6.48	122.79	118.90
1	L5	4303	C	N1-C2-O2	6.48	122.79	118.90
1	L5	489	C	C2-N1-C1'	6.48	125.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	985	C	C2-N1-C1'	6.47	125.92	118.80
49	S2	814	U	N3-C2-O2	-6.47	117.67	122.20
1	L5	205	C	N3-C2-O2	-6.46	117.37	121.90
1	L5	220	C	C6-N1-C2	-6.46	117.71	120.30
1	L5	4314	C	N3-C2-O2	-6.46	117.38	121.90
1	L5	209	U	C6-N1-C1'	-6.45	112.17	121.20
1	L5	925	C	C6-N1-C2	-6.45	117.72	120.30
1	L5	2018	C	C2-N1-C1'	6.44	125.89	118.80
49	S2	325	C	C2-N1-C1'	6.44	125.89	118.80
1	L5	1853	G	C4-N9-C1'	6.44	134.87	126.50
49	S2	1273	C	N3-C2-O2	-6.44	117.39	121.90
1	L5	233	U	C2-N1-C1'	6.43	125.42	117.70
1	L5	1552	G	O4'-C1'-N9	6.43	113.35	108.20
1	L5	1714	C	C6-N1-C2	-6.43	117.73	120.30
1	L5	4149	C	C6-N1-C2	-6.43	117.73	120.30
1	L5	262	G	N1-C6-O6	-6.42	116.05	119.90
1	L5	963	G	N3-C4-C5	-6.41	125.39	128.60
49	S2	585	C	N1-C1'-C2'	-6.41	104.95	112.00
1	L5	453	G	N3-C4-N9	6.40	129.84	126.00
1	L5	282	C	N1-C2-O2	6.40	122.74	118.90
1	L5	2262	G	C8-N9-C1'	-6.39	118.69	127.00
49	S2	1389	C	C2-N1-C1'	6.38	125.82	118.80
49	S2	632	C	C6-N1-C2	-6.38	117.75	120.30
65	SV	78	ILE	CG1-CB-CG2	-6.37	97.38	111.40
1	L5	2416	G	P-O3'-C3'	6.37	127.34	119.70
1	L5	5016	A	C5-N7-C8	-6.37	100.72	103.90
49	S2	1022	U	N3-C2-O2	-6.36	117.75	122.20
1	L5	1472	C	C2-N1-C1'	6.36	125.79	118.80
1	L5	2018	C	C2-N3-C4	6.35	123.08	119.90
49	S2	1022	U	N1-C2-O2	6.35	127.25	122.80
49	S2	1660	C	N3-C2-O2	-6.35	117.45	121.90
1	L5	1666	C	C6-N1-C2	-6.35	117.76	120.30
1	L5	3930	U	N1-C2-O2	6.34	127.24	122.80
1	L5	2257	C	N1-C2-O2	6.33	122.70	118.90
3	L8	64	U	N1-C2-O2	6.33	127.23	122.80
1	L5	2786	C	C6-N1-C2	-6.32	117.77	120.30
49	S2	293	C	C6-N1-C2	-6.31	117.78	120.30
49	S2	582	U	N1-C1'-C2'	-6.31	105.06	112.00
1	L5	2667	C	N1-C2-O2	6.31	122.69	118.90
49	S2	1415	C	C2-N1-C1'	6.30	125.73	118.80
1	L5	4476	C	N1-C2-O2	6.30	122.68	118.90
49	S2	402	C	C6-N1-C2	-6.29	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2094	G	C4-N9-C1'	6.29	134.68	126.50
1	L5	3771	C	C2-N1-C1'	6.29	125.72	118.80
49	S2	1865	C	N3-C2-O2	-6.29	117.50	121.90
1	L5	4926	C	C6-N1-C2	-6.28	117.79	120.30
49	S2	130	G	C4-N9-C1'	6.27	134.66	126.50
49	S2	1016	U	C2-N1-C1'	6.27	125.22	117.70
1	L5	2048	U	N1-C2-O2	6.27	127.19	122.80
1	L5	4133	C	C2-N1-C1'	6.26	125.69	118.80
1	L5	2528	G	N3-C4-N9	6.25	129.75	126.00
1	L5	3598	C	C2-N1-C1'	6.25	125.67	118.80
1	L5	515	C	C5-C6-N1	6.25	124.12	121.00
1	L5	1082	C	N3-C2-O2	-6.25	117.53	121.90
49	S2	1660	C	C2-N1-C1'	6.24	125.66	118.80
49	S2	1821	U	N3-C2-O2	-6.23	117.84	122.20
1	L5	3594	C	C6-N1-C2	-6.23	117.81	120.30
61	SR	109	LEU	CA-CB-CG	6.22	129.61	115.30
1	L5	257	C	C6-N1-C2	-6.22	117.81	120.30
49	S2	340	C	N1-C2-O2	6.22	122.63	118.90
1	L5	2409	U	C4-C5-C6	6.22	123.43	119.70
1	L5	2033	A	P-O3'-C3'	6.21	127.15	119.70
49	S2	130	G	N3-C4-N9	6.21	129.72	126.00
1	L5	3767	C	C6-N1-C2	-6.20	117.82	120.30
1	L5	4360	U	N3-C2-O2	-6.20	117.86	122.20
49	S2	593	C	C2-N1-C1'	6.20	125.62	118.80
1	L5	5016	A	N7-C8-N9	6.19	116.89	113.80
49	S2	179	C	N3-C2-O2	-6.16	117.59	121.90
1	L5	4913	G	P-O3'-C3'	6.15	127.08	119.70
1	L5	2783	A	C6-N1-C2	6.15	122.29	118.60
49	S2	402	C	C5-C6-N1	6.14	124.07	121.00
1	L5	963	G	C8-N9-C1'	-6.14	119.02	127.00
49	S2	140	U	N1-C1'-C2'	-6.13	105.25	112.00
1	L5	2820	C	N1-C2-O2	6.13	122.58	118.90
1	L5	1703	C	N1-C2-O2	6.13	122.58	118.90
49	S2	1591	C	N3-C2-O2	-6.12	117.61	121.90
1	L5	1762	C	N1-C2-O2	6.12	122.57	118.90
1	L5	4880	C	N1-C2-O2	6.12	122.57	118.90
15	LM	32	ASP	CB-CG-OD1	6.12	123.80	118.30
49	S2	659	G	C8-N9-C1'	-6.11	119.06	127.00
1	L5	4921	C	C6-N1-C2	-6.11	117.86	120.30
49	S2	118	C	C6-N1-C1'	-6.11	113.47	120.80
83	CA	110	LEU	CB-CG-CD2	-6.11	100.62	111.00
49	S2	1453	C	C6-N1-C2	-6.11	117.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1663	C	C5-C6-N1	6.10	124.05	121.00
1	L5	1245	C	C2-N1-C1'	6.10	125.51	118.80
1	L5	2260	C	C2-N1-C1'	6.10	125.51	118.80
1	L5	3631	U	N3-C2-O2	-6.10	117.93	122.20
1	L5	4924	C	N3-C2-O2	-6.10	117.63	121.90
1	L5	2048	U	N3-C2-O2	-6.09	117.94	122.20
49	S2	1696	C	C6-N1-C2	-6.09	117.86	120.30
1	L5	3775	A	O4'-C1'-N9	6.09	113.07	108.20
49	S2	688	U	N3-C2-O2	-6.08	117.94	122.20
1	L5	4945	G	C4-C5-N7	6.08	113.23	110.80
49	S2	4	C	C6-N1-C2	-6.07	117.87	120.30
49	S2	310	C	C2-N1-C1'	6.07	125.48	118.80
1	L5	4281	A	C5-N7-C8	-6.07	100.86	103.90
1	L5	4887	C	N1-C2-O2	6.07	122.54	118.90
1	L5	1378	C	N3-C2-O2	-6.07	117.65	121.90
1	L5	1987	C	C6-N1-C2	-6.07	117.87	120.30
1	L5	4747	C	C2-N1-C1'	6.07	125.47	118.80
1	L5	2560	C	N1-C2-O2	6.05	122.53	118.90
1	L5	4926	C	C6-N1-C1'	-6.05	113.53	120.80
1	L5	1977	C	P-O3'-C3'	6.05	126.96	119.70
1	L5	1216	C	C6-N1-C1'	-6.04	113.55	120.80
1	L5	4476	C	N3-C2-O2	-6.04	117.67	121.90
49	S2	537	C	N1-C2-O2	6.03	122.52	118.90
1	L5	234	G	C4-N9-C1'	6.03	134.33	126.50
1	L5	2560	C	C2-N1-C1'	6.03	125.43	118.80
1	L5	655	C	N1-C2-O2	6.02	122.51	118.90
1	L5	4709	U	C2-N1-C1'	6.01	124.92	117.70
49	S2	322	C	N1-C2-O2	6.01	122.51	118.90
1	L5	3641	U	C5-C6-N1	-6.01	119.69	122.70
49	S2	420	G	P-O3'-C3'	6.01	126.91	119.70
49	S2	1309	C	C2-N1-C1'	6.01	125.41	118.80
1	L5	1182	C	N3-C2-O2	-6.00	117.70	121.90
49	S2	882	U	C6-N1-C1'	-5.99	112.81	121.20
1	L5	2426	U	N3-C2-O2	-5.99	118.01	122.20
49	S2	973	C	N1-C2-O2	5.99	122.49	118.90
49	S2	119	U	N3-C2-O2	-5.99	118.01	122.20
1	L5	4612	C	N1-C2-O2	5.98	122.49	118.90
1	L5	3618	C	C6-N1-C2	-5.98	117.91	120.30
1	L5	3930	U	N3-C2-O2	-5.98	118.02	122.20
1	L5	4450	U	C2-N1-C1'	5.98	124.87	117.70
49	S2	674	C	C6-N1-C2	-5.98	117.91	120.30
1	L5	1929	A	C2-N3-C4	5.97	113.59	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	516	C	C6-N1-C2	-5.97	117.91	120.30
49	S2	501	C	C5-C6-N1	5.97	123.98	121.00
1	L5	2255	C	C2-N1-C1'	5.96	125.35	118.80
1	L5	2627	C	C5-C6-N1	5.96	123.98	121.00
1	L5	4471	U	N3-C2-O2	-5.96	118.03	122.20
1	L5	41	C	C5-C6-N1	5.96	123.98	121.00
5	LB	360	LEU	CA-CB-CG	5.95	128.99	115.30
1	L5	4138	C	N1-C2-O2	5.95	122.47	118.90
49	S2	179	C	C2-N1-C1'	5.95	125.34	118.80
49	S2	824	C	N1-C2-O2	5.95	122.47	118.90
1	L5	100	C	O4'-C1'-N1	5.94	112.95	108.20
1	L5	3680	U	N1-C2-O2	5.94	126.96	122.80
49	S2	293	C	C5-C6-N1	5.94	123.97	121.00
1	L5	3948	C	C6-N1-C1'	-5.94	113.68	120.80
1	L5	4773	C	C2-N1-C1'	5.93	125.33	118.80
1	L5	4399	U	N3-C2-O2	-5.93	118.05	122.20
1	L5	100	C	C6-N1-C1'	-5.93	113.68	120.80
49	S2	1660	C	N1-C2-O2	5.93	122.46	118.90
1	L5	234	G	O4'-C1'-N9	5.92	112.94	108.20
49	S2	563	G	P-O3'-C3'	5.92	126.81	119.70
49	S2	1261	C	C2-N1-C1'	5.92	125.31	118.80
1	L5	2260	C	N1-C2-O2	5.91	122.45	118.90
49	S2	1823	A	OP2-P-O3'	5.91	118.20	105.20
1	L5	2394	G	O4'-C1'-N9	5.90	112.92	108.20
1	L5	1633	G	P-O3'-C3'	5.89	126.77	119.70
1	L5	4107	G	C4-N9-C1'	5.88	134.15	126.50
1	L5	281	U	N3-C2-O2	-5.88	118.08	122.20
49	S2	1219	C	N1-C2-O2	5.88	122.43	118.90
16	LN	134	LEU	CA-CB-CG	5.88	128.81	115.30
49	S2	1434	C	P-O3'-C3'	5.88	126.75	119.70
49	S2	1389	C	C6-N1-C2	-5.87	117.95	120.30
49	S2	1772	C	C5-C6-N1	5.87	123.93	121.00
1	L5	115	C	C6-N1-C2	-5.86	117.95	120.30
1	L5	152	U	N3-C2-O2	-5.86	118.10	122.20
1	L5	1725	U	N3-C2-O2	-5.86	118.10	122.20
49	S2	356	C	C6-N1-C2	-5.86	117.96	120.30
2	L7	28	C	C6-N1-C2	-5.85	117.96	120.30
1	L5	453	G	C4-N9-C1'	5.85	134.10	126.50
1	L5	2786	C	P-O3'-C3'	5.85	126.72	119.70
49	S2	291	G	P-O3'-C3'	5.85	126.72	119.70
49	S2	1417	C	N1-C2-N3	-5.84	115.11	119.20
1	L5	2494	U	C2-N1-C1'	5.84	124.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4775	C	N3-C2-O2	-5.84	117.81	121.90
49	S2	112	U	P-O3'-C3'	5.83	126.70	119.70
49	S2	548	C	N1-C2-O2	5.83	122.40	118.90
1	L5	1083	U	O5'-P-OP1	-5.83	100.46	105.70
49	S2	853	C	C6-N1-C2	-5.82	117.97	120.30
1	L5	4921	C	N1-C2-O2	5.82	122.39	118.90
49	S2	1556	A	C2-N3-C4	5.82	113.51	110.60
1	L5	2096	G	C4-N9-C1'	5.82	134.06	126.50
1	L5	4450	U	N1-C2-O2	5.82	126.87	122.80
1	L5	2627	C	N1-C2-O2	5.81	122.39	118.90
1	L5	3680	U	N3-C2-O2	-5.81	118.14	122.20
1	L5	3948	C	C5-C6-N1	5.80	123.90	121.00
49	S2	322	C	C6-N1-C2	-5.80	117.98	120.30
1	L5	2410	C	N1-C2-O2	5.79	122.38	118.90
1	L5	1514	U	N1-C2-O2	5.79	126.86	122.80
1	L5	1597	G	O4'-C1'-N9	5.79	112.83	108.20
49	S2	130	G	N3-C4-C5	-5.79	125.70	128.60
1	L5	515	C	C6-N1-C2	-5.79	117.98	120.30
1	L5	2820	C	N3-C2-O2	-5.79	117.85	121.90
49	S2	1420	G	C4-N9-C1'	5.78	134.02	126.50
1	L5	4281	A	N1-C2-N3	5.78	132.19	129.30
49	S2	118	C	C6-N1-C2	-5.78	117.99	120.30
1	L5	49	U	N3-C2-O2	-5.77	118.16	122.20
1	L5	220	C	C5-C6-N1	5.77	123.88	121.00
49	S2	973	C	N3-C2-O2	-5.77	117.86	121.90
1	L5	4923	C	C6-N1-C2	-5.76	117.99	120.30
1	L5	2528	G	C8-N9-C1'	-5.76	119.51	127.00
46	Ls	95	LEU	CA-CB-CG	5.76	128.55	115.30
49	S2	1578	U	N3-C2-O2	-5.76	118.17	122.20
1	L5	1405	C	N1-C2-O2	5.76	122.36	118.90
49	S2	592	C	C2-N1-C1'	5.75	125.13	118.80
49	S2	930	C	N1-C2-O2	5.75	122.35	118.90
1	L5	4314	C	C6-N1-C2	-5.75	118.00	120.30
49	S2	25	A	O4'-C1'-N9	5.75	112.80	108.20
1	L5	1996	C	C6-N1-C2	-5.74	118.00	120.30
49	S2	119	U	N1-C2-O2	5.74	126.82	122.80
1	L5	4420	U	N3-C2-O2	-5.73	118.19	122.20
49	S2	630	U	C6-N1-C1'	-5.73	113.18	121.20
49	S2	13	C	C6-N1-C2	-5.73	118.01	120.30
1	L5	4557	U	C6-N1-C1'	-5.73	113.18	121.20
1	L5	2560	C	C5-C6-N1	5.73	123.86	121.00
1	L5	1686	C	C6-N1-C2	-5.72	118.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2709	C	C6-N1-C2	5.71	122.58	120.30
1	L5	4594	U	C2-N1-C1'	5.70	124.54	117.70
83	CA	229	LEU	CA-CB-CG	5.70	128.42	115.30
1	L5	1702	C	C2-N1-C1'	5.70	125.07	118.80
1	L5	3770	U	N1-C2-O2	5.70	126.79	122.80
1	L5	2362	U	N3-C2-O2	-5.70	118.21	122.20
2	L7	39	C	N3-C2-O2	-5.70	117.91	121.90
49	S2	687	C	N1-C2-O2	5.70	122.32	118.90
1	L5	1458	C	N3-C2-O2	-5.69	117.92	121.90
49	S2	4	C	C2-N1-C1'	5.69	125.06	118.80
49	S2	1416	C	C6-N1-C2	-5.69	118.02	120.30
49	S2	1649	U	N3-C2-O2	-5.69	118.22	122.20
1	L5	2464	C	O4'-C1'-N1	5.69	112.75	108.20
49	S2	537	C	C2-N1-C1'	5.69	125.05	118.80
1	L5	3641	U	C4-C5-C6	5.68	123.11	119.70
49	S2	409	C	C6-N1-C2	-5.68	118.03	120.30
1	L5	4420	U	N1-C2-O2	5.68	126.78	122.80
53	SE	139	LEU	CA-CB-CG	5.68	128.36	115.30
49	S2	632	C	C5-C6-N1	5.68	123.84	121.00
84	CC	74	C	C5-C6-N1	5.67	123.84	121.00
1	L5	3762	U	N1-C2-O2	5.67	126.77	122.80
1	L5	2011	C	N1-C2-O2	5.67	122.30	118.90
49	S2	1364	U	N3-C2-O2	-5.66	118.24	122.20
1	L5	4594	U	N3-C2-O2	-5.65	118.24	122.20
1	L5	1762	C	C2-N1-C1'	5.65	125.02	118.80
1	L5	406	C	C6-N1-C2	-5.65	118.04	120.30
1	L5	4215	C	N1-C2-O2	5.65	122.29	118.90
49	S2	814	U	N1-C2-O2	5.65	126.75	122.80
1	L5	4572	U	C2-N1-C1'	5.64	124.47	117.70
1	L5	2802	C	C6-N1-C2	-5.64	118.05	120.30
49	S2	1265	A	N3-C4-N9	5.64	131.91	127.40
49	S2	1364	U	N1-C2-O2	5.64	126.75	122.80
1	L5	96	U	N3-C2-O2	-5.63	118.26	122.20
1	L5	234	G	C8-N9-C1'	-5.63	119.69	127.00
1	L5	1644	C	C5-C6-N1	5.62	123.81	121.00
1	L5	3598	C	C6-N1-C2	-5.62	118.05	120.30
56	SI	129	LEU	CA-CB-CG	5.62	128.23	115.30
1	L5	3882	C	C6-N1-C2	-5.62	118.05	120.30
1	L5	2627	C	C6-N1-C1'	-5.61	114.06	120.80
1	L5	1173	G	N3-C4-N9	-5.61	122.63	126.00
1	L5	1367	C	C6-N1-C1'	-5.61	114.07	120.80
1	L5	4895	C	N1-C2-O2	5.60	122.26	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	CC	74	C	C2'-C3'-O3'	5.60	122.67	113.70
1	L5	2708	U	C2-N1-C1'	5.60	124.42	117.70
49	S2	1271	C	N3-C2-O2	-5.59	117.98	121.90
1	L5	654	C	N1-C2-O2	5.59	122.25	118.90
1	L5	5035	U	N3-C2-O2	-5.59	118.29	122.20
1	L5	1217	G	N3-C4-N9	5.59	129.35	126.00
1	L5	1458	C	N1-C2-O2	5.59	122.25	118.90
1	L5	3636	C	C6-N1-C2	-5.58	118.07	120.30
49	S2	178	C	N3-C2-O2	-5.58	117.99	121.90
1	L5	205	C	N1-C2-O2	5.58	122.25	118.90
1	L5	3636	C	N3-C2-O2	-5.58	117.99	121.90
1	L5	4352	U	N3-C2-O2	-5.58	118.30	122.20
1	L5	3657	U	N3-C2-O2	-5.57	118.30	122.20
49	S2	1578	U	N1-C2-O2	5.57	126.70	122.80
49	S2	1047	C	C6-N1-C2	-5.56	118.08	120.30
1	L5	3598	C	C5-C6-N1	5.56	123.78	121.00
1	L5	3673	C	P-O3'-C3'	5.56	126.37	119.70
1	L5	498	C	N3-C2-O2	-5.56	118.01	121.90
1	L5	2860	C	C6-N1-C2	-5.56	118.08	120.30
1	L5	2892	C	C2-N1-C1'	5.55	124.91	118.80
49	S2	593	C	N3-C2-O2	-5.55	118.01	121.90
1	L5	4662	C	C6-N1-C2	-5.55	118.08	120.30
1	L5	294	G	N3-C4-N9	5.55	129.33	126.00
1	L5	1378	C	C2-N1-C1'	5.55	124.91	118.80
1	L5	3909	C	N3-C2-O2	-5.55	118.01	121.90
1	L5	4612	C	N3-C2-O2	-5.55	118.02	121.90
1	L5	112	C	C2-N1-C1'	5.54	124.90	118.80
1	L5	2255	C	N1-C2-O2	5.54	122.23	118.90
1	L5	257	C	C5-C6-N1	5.54	123.77	121.00
1	L5	1821	G	C4-N9-C1'	5.54	133.70	126.50
1	L5	4775	C	C2-N1-C1'	5.54	124.89	118.80
49	S2	580	U	N3-C2-O2	-5.54	118.32	122.20
1	L5	86	U	N3-C2-O2	-5.54	118.32	122.20
49	S2	579	C	N3-C2-O2	-5.54	118.03	121.90
49	S2	1591	C	C2-N1-C1'	5.53	124.89	118.80
1	L5	653	U	N1-C2-O2	5.53	126.67	122.80
1	L5	712	C	C6-N1-C2	-5.53	118.09	120.30
1	L5	1709	C	N1-C2-O2	5.53	122.22	118.90
49	S2	1018	U	N3-C2-O2	-5.53	118.33	122.20
49	S2	1821	U	N1-C2-O2	5.53	126.67	122.80
2	L7	34	C	N1-C2-O2	5.53	122.22	118.90
1	L5	136	C	N1-C2-O2	5.52	122.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	325	C	N3-C2-O2	-5.52	118.03	121.90
49	S2	1408	U	C5-C6-N1	5.52	125.46	122.70
1	L5	985	C	C6-N1-C2	-5.51	118.09	120.30
1	L5	1344	C	C5-C6-N1	5.51	123.75	121.00
1	L5	3892	U	N1-C2-O2	5.51	126.66	122.80
1	L5	3771	C	C6-N1-C2	-5.51	118.10	120.30
49	S2	1649	U	N1-C2-O2	5.50	126.65	122.80
1	L5	209	U	N1-C2-O2	5.50	126.65	122.80
1	L5	4703	U	N3-C2-O2	-5.50	118.35	122.20
49	S2	1265	A	N3-C4-C5	-5.50	122.95	126.80
1	L5	515	C	N3-C2-O2	-5.50	118.05	121.90
49	S2	1149	A	C2-N3-C4	5.50	113.35	110.60
49	S2	494	C	N3-C2-O2	-5.50	118.05	121.90
1	L5	294	G	N3-C4-C5	-5.49	125.85	128.60
49	S2	1632	G	O4'-C1'-N9	5.49	112.59	108.20
1	L5	4137	C	N1-C2-O2	5.49	122.19	118.90
1	L5	174	C	N1-C2-O2	5.49	122.19	118.90
1	L5	263	G	C5-C6-O6	5.49	131.89	128.60
49	S2	331	C	N1-C2-O2	5.49	122.19	118.90
49	S2	323	C	N3-C2-O2	-5.48	118.06	121.90
1	L5	740	G	N3-C4-N9	-5.48	122.71	126.00
1	L5	4447	C	C2-N1-C1'	-5.48	112.77	118.80
1	L5	4398	C	C6-N1-C2	-5.48	118.11	120.30
49	S2	1865	C	N1-C2-O2	5.48	122.19	118.90
1	L5	2351	C	C2-N1-C1'	5.47	124.82	118.80
1	L5	1853	G	C8-N9-C1'	-5.47	119.89	127.00
1	L5	2508	U	N3-C2-O2	-5.47	118.37	122.20
1	L5	294	G	C2-N3-C4	5.47	114.63	111.90
1	L5	3584	C	N1-C2-O2	5.46	122.18	118.90
1	L5	36	U	N3-C2-O2	-5.46	118.38	122.20
1	L5	406	C	P-O3'-C3'	5.46	126.25	119.70
49	S2	14	C	C6-N1-C2	-5.46	118.12	120.30
49	S2	1396	A	C2-N3-C4	5.45	113.33	110.60
1	L5	1726	U	N3-C2-O2	-5.45	118.39	122.20
1	L5	1809	C	C2-N1-C1'	5.45	124.79	118.80
1	L5	4507	A	O4'-C1'-N9	5.45	112.56	108.20
49	S2	179	C	C6-N1-C2	-5.45	118.12	120.30
49	S2	1154	U	C2-N1-C1'	5.45	124.24	117.70
1	L5	2899	C	C2-N1-C1'	5.45	124.79	118.80
1	L5	2710	C	C5-C6-N1	5.44	123.72	121.00
1	L5	3785	A	O4'-C1'-N9	5.44	112.55	108.20
49	S2	1865	C	C2-N1-C1'	5.44	124.78	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3778	U	C2-N1-C1'	5.43	124.22	117.70
9	LF	33	LEU	CA-CB-CG	5.43	127.78	115.30
49	S2	687	C	N3-C2-O2	-5.42	118.11	121.90
1	L5	278	G	O4'-C1'-N9	-5.42	103.86	108.20
49	S2	581	U	C2-N1-C1'	5.42	124.20	117.70
49	S2	630	U	N3-C2-O2	-5.42	118.41	122.20
1	L5	262	G	C5-C6-O6	5.41	131.84	128.60
49	S2	853	C	N1-C2-O2	5.41	122.14	118.90
49	S2	1218	C	C5-C6-N1	5.41	123.70	121.00
1	L5	449	C	N1-C2-O2	5.40	122.14	118.90
1	L5	904	C	N3-C2-O2	-5.40	118.12	121.90
1	L5	2094	G	C8-N9-C1'	-5.39	119.99	127.00
1	L5	3838	U	N3-C2-O2	-5.39	118.42	122.20
32	Ld	46	LEU	CA-CB-CG	-5.39	102.90	115.30
1	L5	53	C	C6-N1-C2	-5.39	118.14	120.30
1	L5	1367	C	C6-N1-C2	-5.39	118.15	120.30
49	S2	527	C	N1-C2-O2	5.39	122.13	118.90
1	L5	1309	C	C5-C6-N1	5.38	123.69	121.00
10	LG	265	LEU	CA-CB-CG	5.38	127.69	115.30
84	CC	34	U	C2-N1-C1'	5.38	124.16	117.70
1	L5	1439	C	C6-N1-C2	-5.38	118.15	120.30
1	L5	653	U	N3-C2-O2	-5.38	118.43	122.20
1	L5	500	G	N3-C2-N2	5.38	123.66	119.90
1	L5	2867	C	C6-N1-C2	-5.37	118.15	120.30
1	L5	4447	C	C6-N1-C1'	5.37	127.25	120.80
49	S2	542	U	N1-C2-O2	5.37	126.56	122.80
49	S2	116	U	C5-C6-N1	5.37	125.39	122.70
1	L5	971	U	C2-N1-C1'	5.37	124.14	117.70
49	S2	130	G	C8-N9-C1'	-5.36	120.03	127.00
1	L5	4613	C	N1-C2-O2	5.36	122.11	118.90
1	L5	1714	C	C6-N1-C1'	-5.36	114.37	120.80
1	L5	1893	C	C6-N1-C2	-5.36	118.16	120.30
1	L5	4898	G	N1-C6-O6	-5.36	116.69	119.90
49	S2	688	U	N1-C2-O2	5.36	126.55	122.80
49	S2	824	C	N3-C2-O2	-5.36	118.15	121.90
49	S2	1172	U	N1-C2-O2	5.36	126.55	122.80
49	S2	1520	G	N3-C4-C5	-5.36	125.92	128.60
1	L5	4714	C	N1-C2-O2	5.35	122.11	118.90
1	L5	4261	C	C5-C6-N1	5.35	123.68	121.00
1	L5	228	C	C6-N1-C2	-5.35	118.16	120.30
1	L5	274	C	C2-N1-C1'	5.35	124.68	118.80
1	L5	365	U	N3-C2-O2	-5.35	118.46	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	985	C	C5-C6-N1	5.34	123.67	121.00
1	L5	1315	C	C6-N1-C2	-5.34	118.16	120.30
1	L5	1252	C	C6-N1-C2	-5.34	118.16	120.30
1	L5	2409	U	N3-C2-O2	-5.33	118.47	122.20
1	L5	4771	C	C5-C6-N1	5.33	123.67	121.00
6	LC	260	LEU	CB-CG-CD1	-5.33	101.95	111.00
2	L7	34	C	C6-N1-C2	-5.32	118.17	120.30
6	LC	352	ASP	CB-CG-OD1	5.32	123.09	118.30
1	L5	4147	G	N1-C6-O6	-5.32	116.71	119.90
49	S2	105	U	N3-C2-O2	-5.32	118.47	122.20
1	L5	4594	U	N1-C2-O2	5.32	126.53	122.80
1	L5	2532	C	C2-N1-C1'	5.32	124.65	118.80
1	L5	504	G	C2-N3-C4	5.31	114.56	111.90
49	S2	1346	U	N3-C2-O2	-5.31	118.48	122.20
1	L5	3637	U	N1-C2-O2	5.31	126.52	122.80
1	L5	365	U	N1-C2-O2	5.31	126.51	122.80
1	L5	1582	U	N3-C2-O2	-5.31	118.49	122.20
1	L5	2560	C	C6-N1-C2	-5.30	118.18	120.30
1	L5	1929	A	C4-N9-C1'	5.30	135.84	126.30
49	S2	1420	G	N3-C4-C5	-5.30	125.95	128.60
1	L5	2304	U	N3-C2-O2	-5.30	118.49	122.20
1	L5	1714	C	C5-C6-N1	5.30	123.65	121.00
1	L5	5028	G	N3-C4-N9	5.30	129.18	126.00
1	L5	2850	A	C8-N9-C4	-5.29	103.68	105.80
2	L7	39	C	C2-N1-C1'	5.29	124.62	118.80
8	LE	50	LEU	CA-CB-CG	5.29	127.48	115.30
49	S2	340	C	N3-C2-O2	-5.29	118.19	121.90
1	L5	4766	C	C2-N1-C1'	5.29	124.62	118.80
49	S2	570	C	N1-C2-O2	5.29	122.08	118.90
1	L5	175	C	C6-N1-C1'	5.29	127.15	120.80
1	L5	1731	C	C6-N1-C2	-5.29	118.19	120.30
49	S2	196	C	N1-C2-O2	5.29	122.07	118.90
1	L5	5016	A	O4'-C1'-N9	5.29	112.43	108.20
49	S2	1420	G	N3-C4-N9	5.29	129.17	126.00
1	L5	1720	C	C6-N1-C2	-5.29	118.19	120.30
1	L5	3762	U	N3-C2-O2	-5.28	118.50	122.20
49	S2	1408	U	C2-N1-C1'	5.28	124.04	117.70
49	S2	1772	C	C6-N1-C1'	-5.28	114.46	120.80
1	L5	1644	C	C6-N1-C2	-5.28	118.19	120.30
1	L5	1405	C	C6-N1-C2	-5.28	118.19	120.30
1	L5	3911	C	C5-C6-N1	5.28	123.64	121.00
1	L5	1439	C	N1-C2-O2	5.27	122.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1405	C	N3-C2-O2	-5.27	118.21	121.90
1	L5	4147	G	C5-C6-O6	5.27	131.76	128.60
49	S2	1116	C	N1-C2-O2	5.27	122.06	118.90
49	S2	1259	A	C2-N3-C4	5.27	113.23	110.60
49	S2	1022	U	C6-N1-C1'	-5.27	113.83	121.20
1	L5	2856	C	N3-C2-O2	-5.26	118.22	121.90
49	S2	218	U	N3-C2-O2	-5.26	118.52	122.20
49	S2	222	U	N3-C2-O2	-5.26	118.52	122.20
1	L5	972	C	N1-C2-O2	5.26	122.06	118.90
49	S2	1412	C	C2-N1-C1'	5.26	124.59	118.80
1	L5	2257	C	C6-N1-C1'	-5.26	114.49	120.80
1	L5	1861	U	N3-C2-O2	-5.26	118.52	122.20
1	L5	3767	C	C2-N1-C1'	5.26	124.58	118.80
3	L8	101	C	C6-N1-C2	-5.26	118.20	120.30
1	L5	2791	C	C6-N1-C2	-5.25	118.20	120.30
1	L5	2860	C	N3-C2-O2	-5.25	118.22	121.90
1	L5	3667	C	O5'-P-OP1	-5.25	100.97	105.70
49	S2	1172	U	N3-C2-O2	-5.25	118.53	122.20
1	L5	456	C	C6-N1-C2	-5.25	118.20	120.30
49	S2	682	U	N3-C2-O2	-5.25	118.53	122.20
49	S2	1060	A	O4'-C1'-N9	5.25	112.40	108.20
1	L5	2281	U	N1-C2-O2	5.25	126.47	122.80
1	L5	2416	G	OP2-P-O3'	5.25	116.74	105.20
1	L5	1882	U	C5-C4-O4	-5.24	122.75	125.90
3	L8	111	U	N1-C2-O2	5.24	126.47	122.80
1	L5	2018	C	N3-C4-C5	-5.24	119.80	121.90
1	L5	4920	C	N1-C2-O2	5.24	122.05	118.90
1	L5	757	G	N3-C4-N9	5.24	129.14	126.00
1	L5	3770	U	N3-C2-O2	-5.24	118.53	122.20
1	L5	175	C	C6-N1-C2	-5.24	118.20	120.30
1	L5	753	C	C2-N1-C1'	5.24	124.56	118.80
1	L5	4254	G	N3-C4-C5	-5.23	125.98	128.60
1	L5	1251	C	N1-C2-O2	5.23	122.04	118.90
1	L5	977	C	C2-N1-C1'	5.23	124.56	118.80
1	L5	2410	C	C6-N1-C1'	-5.23	114.53	120.80
1	L5	2709	C	N3-C4-N4	-5.22	114.34	118.00
49	S2	1272	C	N1-C2-O2	5.22	122.03	118.90
49	S2	1591	C	C6-N1-C2	-5.22	118.21	120.30
1	L5	4112	C	N3-C2-O2	-5.21	118.25	121.90
1	L5	1607	C	N3-C2-O2	-5.21	118.25	121.90
1	L5	2351	C	C5-C6-N1	5.21	123.60	121.00
1	L5	4162	C	N1-C2-O2	5.21	122.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4399	U	N1-C2-O2	5.21	126.44	122.80
1	L5	1540	C	C6-N1-C2	-5.20	118.22	120.30
49	S2	531	A	OP1-P-O3'	5.20	116.64	105.20
49	S2	570	C	N3-C2-O2	-5.20	118.26	121.90
1	L5	493	G	P-O3'-C3'	5.20	125.94	119.70
49	S2	578	C	N1-C2-O2	5.20	122.02	118.90
1	L5	2532	C	C5-C6-N1	5.19	123.59	121.00
1	L5	180	C	C6-N1-C2	-5.19	118.22	120.30
49	S2	1271	C	C2-N1-C1'	5.19	124.51	118.80
1	L5	1417	C	C2-N1-C1'	5.18	124.50	118.80
49	S2	966	U	N3-C2-O2	-5.18	118.57	122.20
1	L5	3622	C	C5-C6-N1	5.18	123.59	121.00
1	L5	2607	C	C6-N1-C2	-5.18	118.23	120.30
1	L5	297	U	C5-C6-N1	5.18	125.29	122.70
1	L5	498	C	C2-N1-C1'	5.18	124.50	118.80
1	L5	3870	C	C5-C6-N1	5.18	123.59	121.00
1	L5	672	C	N1-C2-O2	5.18	122.01	118.90
1	L5	3772	U	N1-C2-O2	5.18	126.42	122.80
1	L5	904	C	N1-C2-O2	5.17	122.00	118.90
1	L5	1996	C	C5-C6-N1	5.17	123.59	121.00
1	L5	3967	G	N3-C4-C5	-5.17	126.01	128.60
4	LA	55	GLY	C-N-CA	5.17	134.64	121.70
1	L5	4764	A	C6-N1-C2	5.17	121.70	118.60
1	L5	3911	C	C6-N1-C2	-5.17	118.23	120.30
1	L5	1447	C	N1-C2-O2	5.17	122.00	118.90
1	L5	1446	C	N1-C2-O2	5.16	122.00	118.90
2	L7	102	U	C2-N1-C1'	5.16	123.90	117.70
49	S2	1556	A	N3-C4-N9	5.16	131.53	127.40
1	L5	3789	C	C6-N1-C2	-5.16	118.23	120.30
1	L5	4766	C	C6-N1-C2	-5.16	118.24	120.30
49	S2	151	C	C6-N1-C2	-5.16	118.24	120.30
1	L5	3638	G	C2-N3-C4	5.16	114.48	111.90
49	S2	1415	C	N3-C2-O2	-5.16	118.29	121.90
84	CC	74	C	P-O3'-C3'	5.16	125.89	119.70
1	L5	4747	C	C6-N1-C2	-5.15	118.24	120.30
1	L5	4078	C	C6-N1-C2	-5.15	118.24	120.30
1	L5	181	C	C6-N1-C1'	-5.15	114.62	120.80
1	L5	4601	U	N3-C2-O2	-5.15	118.59	122.20
47	Lt	80	LEU	CA-CB-CG	5.15	127.15	115.30
49	S2	853	C	N3-C2-O2	-5.15	118.30	121.90
1	L5	4527	G	O4'-C1'-N9	5.15	112.32	108.20
1	L5	4572	U	C5-C6-N1	5.15	125.27	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4532	U	N3-C2-O2	-5.15	118.60	122.20
49	S2	321	C	N1-C2-O2	5.15	121.99	118.90
49	S2	1309	C	N1-C2-O2	5.15	121.99	118.90
84	CC	74	C	C6-N1-C1'	5.15	126.98	120.80
1	L5	180	C	C5-C6-N1	5.14	123.57	121.00
49	S2	559	G	O4'-C1'-N9	5.14	112.31	108.20
1	L5	1893	C	C2-N1-C1'	5.14	124.45	118.80
1	L5	4926	C	O4'-C1'-N1	5.14	112.31	108.20
1	L5	2856	C	N1-C2-O2	5.13	121.98	118.90
1	L5	4973	U	N3-C2-O2	-5.13	118.61	122.20
46	Ls	105	ASN	C-N-CA	5.13	134.52	121.70
1	L5	262	G	C8-N9-C4	-5.12	104.35	106.40
1	L5	2492	C	C6-N1-C2	-5.12	118.25	120.30
1	L5	4402	C	N1-C2-O2	5.12	121.97	118.90
1	L5	4945	G	N9-C4-C5	-5.12	103.35	105.40
1	L5	1577	G	C5-C6-O6	5.12	131.67	128.60
49	S2	666	U	C2-N1-C1'	5.12	123.84	117.70
1	L5	412	G	C4-C5-N7	5.12	112.85	110.80
1	L5	4758	U	C6-N1-C1'	-5.12	114.03	121.20
1	L5	4107	G	N3-C4-N9	5.12	129.07	126.00
49	S2	118	C	O4'-C1'-N1	5.11	112.29	108.20
49	S2	151	C	C2-N1-C1'	5.11	124.42	118.80
1	L5	712	C	C5-C6-N1	5.11	123.56	121.00
49	S2	1683	C	N1-C2-O2	5.11	121.97	118.90
1	L5	2094	G	N3-C4-N9	5.11	129.06	126.00
1	L5	4880	C	C2-N1-C1'	5.11	124.42	118.80
49	S2	559	G	C5-C6-O6	5.11	131.66	128.60
1	L5	4254	G	N3-C4-N9	5.10	129.06	126.00
49	S2	1002	U	N1-C2-O2	5.10	126.37	122.80
1	L5	1632	A	C8-N9-C4	-5.10	103.76	105.80
49	S2	1234	C	C6-N1-C2	-5.10	118.26	120.30
1	L5	2528	G	C8-N9-C4	-5.09	104.36	106.40
49	S2	1073	U	N3-C2-O2	-5.09	118.64	122.20
1	L5	1792	U	N3-C2-O2	-5.09	118.64	122.20
1	L5	4281	A	C2-N3-C4	-5.09	108.06	110.60
49	S2	577	U	N3-C2-O2	-5.09	118.64	122.20
49	S2	882	U	C6-N1-C2	-5.09	117.95	121.00
1	L5	515	C	C6-N1-C1'	-5.08	114.71	120.80
1	L5	1702	C	N1-C2-O2	5.08	121.95	118.90
49	S2	1316	C	N1-C2-O2	5.08	121.95	118.90
1	L5	4215	C	N3-C2-O2	-5.08	118.35	121.90
1	L5	4387	C	N1-C2-O2	5.08	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	402	C	C2-N3-C4	5.07	122.44	119.90
49	S2	1018	U	N1-C2-O2	5.07	126.35	122.80
1	L5	1632	A	C4-N9-C1'	5.07	135.43	126.30
3	L8	111	U	N3-C2-O2	-5.07	118.65	122.20
1	L5	1241	C	N3-C2-O2	-5.07	118.35	121.90
1	L5	4171	C	N1-C2-O2	5.07	121.94	118.90
49	S2	1710	C	N1-C2-O2	5.07	121.94	118.90
1	L5	1687	U	N3-C2-O2	-5.07	118.65	122.20
49	S2	1218	C	C6-N1-C2	-5.07	118.27	120.30
1	L5	2783	A	N1-C2-N3	-5.06	126.77	129.30
1	L5	4985	U	N3-C2-O2	-5.06	118.66	122.20
1	L5	453	G	C2-N3-C4	5.06	114.43	111.90
1	L5	1517	G	C2-N3-C4	5.06	114.43	111.90
1	L5	472	C	N1-C2-O2	5.06	121.94	118.90
1	L5	1340	C	C6-N1-C2	-5.06	118.28	120.30
1	L5	1439	C	C5-C6-N1	5.06	123.53	121.00
1	L5	1735	U	N1-C2-O2	5.05	126.34	122.80
49	S2	417	C	O4'-C1'-N1	5.05	112.24	108.20
1	L5	152	U	N1-C2-O2	5.05	126.33	122.80
1	L5	1726	U	N1-C2-O2	5.05	126.33	122.80
15	LM	87	ALA	C-N-CA	5.05	134.33	121.70
49	S2	323	C	N1-C2-O2	5.05	121.93	118.90
1	L5	1182	C	C6-N1-C2	-5.05	118.28	120.30
49	S2	548	C	N3-C2-O2	-5.05	118.37	121.90
1	L5	3631	U	N1-C2-O2	5.05	126.33	122.80
49	S2	571	U	N3-C2-O2	-5.05	118.67	122.20
1	L5	4289	U	N1-C2-O2	5.04	126.33	122.80
1	L5	5016	A	C2-N3-C4	-5.04	108.08	110.60
1	L5	3639	U	N3-C2-O2	-5.04	118.67	122.20
1	L5	4714	C	N3-C2-O2	-5.04	118.37	121.90
1	L5	4898	G	C5-C6-O6	5.04	131.62	128.60
1	L5	504	G	N3-C2-N2	-5.04	116.38	119.90
1	L5	3930	U	C2-N1-C1'	5.04	123.74	117.70
3	L8	32	C	N1-C2-O2	5.04	121.92	118.90
49	S2	1219	C	N3-C2-O2	-5.03	118.38	121.90
1	L5	1395	U	N3-C2-O2	-5.03	118.68	122.20
49	S2	314	U	N3-C2-O2	-5.03	118.68	122.20
1	L5	4241	C	C2-N1-C1'	5.03	124.33	118.80
1	L5	4708	A	C2-N3-C4	5.03	113.11	110.60
49	S2	494	C	C6-N1-C2	-5.03	118.29	120.30
49	S2	1556	A	C4-N9-C1'	5.03	135.35	126.30
1	L5	4476	C	C6-N1-C2	-5.02	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	469	C	N1-C2-O2	5.02	121.91	118.90
1	L5	1494	U	N3-C2-O2	-5.02	118.69	122.20
49	S2	1684	C	N1-C2-O2	5.02	121.91	118.90
2	L7	78	C	C6-N1-C2	-5.01	118.29	120.30
1	L5	3866	C	C6-N1-C2	-5.01	118.30	120.30
1	L5	4107	G	N3-C4-C5	-5.01	126.09	128.60
49	S2	1229	G	N7-C8-N9	5.01	115.61	113.10
1	L5	155	C	N3-C2-O2	-5.01	118.39	121.90
1	L5	672	C	C2-N1-C1'	5.01	124.31	118.80
1	L5	906	C	N3-C2-O2	-5.01	118.39	121.90
1	L5	1596	U	P-O3'-C3'	5.01	125.71	119.70
1	L5	4183	G	N3-C4-N9	5.01	129.00	126.00
1	L5	1259	G	N1-C6-O6	-5.00	116.90	119.90
1	L5	4402	C	N3-C2-O2	-5.00	118.40	121.90
1	L5	740	G	C8-N9-C1'	5.00	133.50	127.00
49	S2	178	C	C2-N1-C1'	5.00	124.30	118.80
49	S2	494	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	LA	110	GLY	Peptide
4	LA	54	ARG	Peptide
5	LB	17	LEU	Peptide
5	LB	258	HIS	Peptide
8	LE	129	GLY	Peptide
11	LH	106	GLN	Peptide
11	LH	173	ARG	Peptide
12	LI	54	SER	Peptide
14	LL	154	VAL	Peptide
15	LM	87	ALA	Peptide
15	LM	88	ALA	Peptide
17	LO	110	PRO	Peptide
22	LT	135	PRO	Peptide
22	LT	136	ARG	Peptide
22	LT	80	VAL	Peptide
29	La	22	ILE	Peptide
32	Ld	59	THR	Peptide
34	Lf	103	VAL	Peptide
34	Lf	106	TYR	Peptide
36	Lh	86	LYS	Peptide

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Mol	Chain	Res	Type	Group
38	Lj	39	TYR	Peptide
45	Lr	20	ARG	Peptide
46	Ls	149	ARG	Peptide
47	Lt	140	GLY	Peptide
47	Lt	141	CYS	Peptide
47	Lt	147	HIS	Peptide
47	Lt	148	PRO	Peptide
47	Lt	53	TRP	Peptide
47	Lt	9	GLU	Peptide
48	Lz	183	ILE	Peptide
51	SB	221	PRO	Peptide
52	SD	164	VAL	Peptide
54	SF	126	THR	Peptide
54	SF	78	MET	Peptide
55	SH	13	GLY	Peptide
55	SH	15	LYS	Peptide
73	SJ	137	VAL	Peptide
60	SQ	43	GLU	Peptide
61	SR	84	TYR	Peptide
63	ST	46	ALA	Peptide
65	SV	78	ILE	Peptide
66	SX	125	VAL	Peptide
66	SX	126	ALA	Peptide
66	SX	77	ASN	Peptide
66	SX	86	PRO	Peptide
79	SZ	46	ASN	Peptide
79	SZ	78	LYS	Peptide
80	Sb	75	GLU	Peptide
68	Sc	63	ARG	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	225 (92%)	20 (8%)	1 (0%)	34	57
5	LB	400/403 (99%)	380 (95%)	17 (4%)	3 (1%)	19	39
6	LC	366/427 (86%)	341 (93%)	25 (7%)	0	100	100
7	LD	291/297 (98%)	267 (92%)	24 (8%)	0	100	100
8	LE	232/288 (81%)	211 (91%)	21 (9%)	0	100	100
9	LF	223/248 (90%)	214 (96%)	9 (4%)	0	100	100
10	LG	239/266 (90%)	224 (94%)	15 (6%)	0	100	100
11	LH	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
12	LI	198/214 (92%)	183 (92%)	14 (7%)	1 (0%)	29	52
13	LJ	174/178 (98%)	157 (90%)	16 (9%)	1 (1%)	25	47
14	LL	208/211 (99%)	191 (92%)	17 (8%)	0	100	100
15	LM	137/215 (64%)	130 (95%)	6 (4%)	1 (1%)	22	43
16	LN	201/204 (98%)	191 (95%)	8 (4%)	2 (1%)	15	32
17	LO	199/203 (98%)	189 (95%)	10 (5%)	0	100	100
18	LP	151/184 (82%)	140 (93%)	10 (7%)	1 (1%)	22	43
19	LQ	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
20	LR	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
21	LS	173/176 (98%)	161 (93%)	12 (7%)	0	100	100
22	LT	157/160 (98%)	148 (94%)	8 (5%)	1 (1%)	25	47
23	LU	99/128 (77%)	86 (87%)	13 (13%)	0	100	100
24	LV	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
25	LW	122/157 (78%)	111 (91%)	11 (9%)	0	100	100
26	LX	118/156 (76%)	116 (98%)	2 (2%)	0	100	100
27	LY	132/145 (91%)	123 (93%)	9 (7%)	0	100	100
28	LZ	133/136 (98%)	123 (92%)	10 (8%)	0	100	100
29	La	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
30	Lb	105/159 (66%)	98 (93%)	7 (7%)	0	100	100
31	Lc	96/115 (84%)	90 (94%)	6 (6%)	0	100	100
32	Ld	105/125 (84%)	97 (92%)	8 (8%)	0	100	100
33	Le	126/135 (93%)	119 (94%)	6 (5%)	1 (1%)	19	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Lf	107/110 (97%)	99 (92%)	6 (6%)	2 (2%)	8	15
35	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
36	Lh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
37	Li	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
38	Lj	84/97 (87%)	75 (89%)	8 (10%)	1 (1%)	13	27
39	Lk	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
40	Ll	48/51 (94%)	48 (100%)	0	0	100	100
41	Lm	50/128 (39%)	50 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
44	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
45	Lr	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
46	Ls	194/317 (61%)	166 (86%)	27 (14%)	1 (0%)	29	52
47	Lt	137/165 (83%)	100 (73%)	33 (24%)	4 (3%)	4	7
48	Lz	215/217 (99%)	160 (74%)	55 (26%)	0	100	100
50	SA	219/295 (74%)	202 (92%)	17 (8%)	0	100	100
51	SB	212/264 (80%)	201 (95%)	11 (5%)	0	100	100
52	SD	225/243 (93%)	201 (89%)	24 (11%)	0	100	100
53	SE	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
54	SF	180/204 (88%)	164 (91%)	16 (9%)	0	100	100
55	SH	182/194 (94%)	161 (88%)	21 (12%)	0	100	100
56	SI	204/208 (98%)	196 (96%)	8 (4%)	0	100	100
57	SK	96/165 (58%)	85 (88%)	11 (12%)	0	100	100
58	SL	151/158 (96%)	140 (93%)	11 (7%)	0	100	100
59	SP	127/145 (88%)	119 (94%)	8 (6%)	0	100	100
60	SQ	142/146 (97%)	128 (90%)	13 (9%)	1 (1%)	22	43
61	SR	133/135 (98%)	116 (87%)	16 (12%)	1 (1%)	19	39
62	SS	143/152 (94%)	131 (92%)	12 (8%)	0	100	100
63	ST	141/145 (97%)	130 (92%)	10 (7%)	1 (1%)	22	43
64	SU	102/119 (86%)	93 (91%)	9 (9%)	0	100	100
65	SV	81/83 (98%)	74 (91%)	5 (6%)	2 (2%)	5	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	SX	139/143 (97%)	131 (94%)	4 (3%)	4 (3%)	4	7
67	Sa	100/115 (87%)	92 (92%)	7 (7%)	1 (1%)	15	32
68	Sc	62/69 (90%)	52 (84%)	9 (14%)	1 (2%)	9	19
69	Sd	53/56 (95%)	50 (94%)	2 (4%)	1 (2%)	8	15
70	Sg	311/317 (98%)	269 (86%)	41 (13%)	1 (0%)	41	64
71	SC	220/293 (75%)	205 (93%)	15 (7%)	0	100	100
72	SG	235/249 (94%)	222 (94%)	13 (6%)	0	100	100
73	SJ	183/194 (94%)	169 (92%)	12 (7%)	2 (1%)	14	30
74	SM	120/132 (91%)	109 (91%)	11 (9%)	0	100	100
75	SN	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
76	SO	138/151 (91%)	127 (92%)	9 (6%)	2 (1%)	11	22
77	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
78	SY	129/133 (97%)	123 (95%)	6 (5%)	0	100	100
79	SZ	73/125 (58%)	60 (82%)	13 (18%)	0	100	100
80	Sb	81/84 (96%)	71 (88%)	10 (12%)	0	100	100
81	Se	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
82	Sf	65/156 (42%)	55 (85%)	10 (15%)	0	100	100
83	CA	350/394 (89%)	328 (94%)	22 (6%)	0	100	100
85	CE	70/379 (18%)	67 (96%)	3 (4%)	0	100	100
86	i	31/180 (17%)	29 (94%)	2 (6%)	0	100	100
All	All	12323/14340 (86%)	11364 (92%)	922 (8%)	37 (0%)	44	64

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	LN	124	ASP
47	Lt	147	HIS
66	SX	127	ASN
47	Lt	142	ASN
47	Lt	148	PRO
63	ST	41	LYS
65	SV	79	VAL
68	Sc	64	GLU
5	LB	302	ASN
5	LB	360	LEU

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Mol	Chain	Res	Type
15	LM	88	ALA
33	Le	73	GLY
66	SX	78	GLY
67	Sa	47	ALA
34	Lf	80	ASN
34	Lf	107	PRO
60	SQ	44	PRO
66	SX	126	ALA
69	Sd	14	PHE
73	SJ	138	ARG
5	LB	18	PRO
13	LJ	18	ARG
16	LN	83	LYS
22	LT	137	GLU
61	SR	94	GLU
76	SO	140	THR
38	Lj	40	PRO
47	Lt	9	GLU
66	SX	87	ASN
70	Sg	246	TYR
12	LI	15	LYS
65	SV	78	ILE
4	LA	55	GLY
76	SO	144	GLY
18	LP	77	GLY
46	Ls	150	GLY
73	SJ	123	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/199 (96%)	189 (100%)	1 (0%)	88	96
5	LB	348/349 (100%)	345 (99%)	3 (1%)	78	91
6	LC	306/348 (88%)	304 (99%)	2 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	LD	246/250 (98%)	244 (99%)	2 (1%)	81	92
8	LE	209/252 (83%)	208 (100%)	1 (0%)	88	96
9	LF	194/215 (90%)	192 (99%)	2 (1%)	76	90
10	LG	203/223 (91%)	201 (99%)	2 (1%)	76	90
11	LH	169/171 (99%)	169 (100%)	0	100	100
12	LI	172/181 (95%)	172 (100%)	0	100	100
13	LJ	148/149 (99%)	148 (100%)	0	100	100
14	LL	176/177 (99%)	175 (99%)	1 (1%)	86	95
15	LM	118/161 (73%)	117 (99%)	1 (1%)	81	92
16	LN	171/172 (99%)	171 (100%)	0	100	100
17	LO	173/174 (99%)	172 (99%)	1 (1%)	86	95
18	LP	134/163 (82%)	133 (99%)	1 (1%)	84	94
19	LQ	164/165 (99%)	163 (99%)	1 (1%)	86	95
20	LR	166/175 (95%)	163 (98%)	3 (2%)	59	80
21	LS	156/157 (99%)	156 (100%)	0	100	100
22	LT	139/140 (99%)	137 (99%)	2 (1%)	67	85
23	LU	91/115 (79%)	90 (99%)	1 (1%)	73	88
24	LV	101/107 (94%)	100 (99%)	1 (1%)	76	90
25	LW	103/126 (82%)	102 (99%)	1 (1%)	76	90
26	LX	108/133 (81%)	108 (100%)	0	100	100
27	LY	124/135 (92%)	123 (99%)	1 (1%)	81	92
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	120/121 (99%)	120 (100%)	0	100	100
30	Lb	88/126 (70%)	88 (100%)	0	100	100
31	Lc	83/97 (86%)	83 (100%)	0	100	100
32	Ld	98/110 (89%)	98 (100%)	0	100	100
33	Le	114/121 (94%)	114 (100%)	0	100	100
34	Lf	88/89 (99%)	87 (99%)	1 (1%)	73	88
35	Lg	98/100 (98%)	96 (98%)	2 (2%)	55	78
36	Lh	109/110 (99%)	109 (100%)	0	100	100
37	Li	86/89 (97%)	85 (99%)	1 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Lj	73/80 (91%)	73 (100%)	0	100	100
39	Lk	64/65 (98%)	64 (100%)	0	100	100
40	Ll	47/48 (98%)	46 (98%)	1 (2%)	53	77
41	Lm	48/116 (41%)	48 (100%)	0	100	100
42	Ln	23/24 (96%)	23 (100%)	0	100	100
43	Lo	93/94 (99%)	93 (100%)	0	100	100
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/121 (90%)	109 (100%)	0	100	100
46	Ls	162/258 (63%)	159 (98%)	3 (2%)	57	79
47	Lt	112/137 (82%)	110 (98%)	2 (2%)	59	80
48	Lz	195/196 (100%)	193 (99%)	2 (1%)	76	90
50	SA	183/243 (75%)	183 (100%)	0	100	100
51	SB	195/231 (84%)	195 (100%)	0	100	100
52	SD	190/202 (94%)	187 (98%)	3 (2%)	62	82
53	SE	224/225 (100%)	224 (100%)	0	100	100
54	SF	156/170 (92%)	156 (100%)	0	100	100
55	SH	166/174 (95%)	161 (97%)	5 (3%)	41	67
56	SI	178/180 (99%)	176 (99%)	2 (1%)	73	88
57	SK	89/136 (65%)	89 (100%)	0	100	100
58	SL	137/142 (96%)	135 (98%)	2 (2%)	65	83
59	SP	115/130 (88%)	114 (99%)	1 (1%)	78	91
60	SQ	119/121 (98%)	118 (99%)	1 (1%)	81	92
61	SR	122/122 (100%)	121 (99%)	1 (1%)	81	92
62	SS	126/132 (96%)	125 (99%)	1 (1%)	81	92
63	ST	113/115 (98%)	112 (99%)	1 (1%)	78	91
64	SU	94/107 (88%)	94 (100%)	0	100	100
65	SV	67/67 (100%)	67 (100%)	0	100	100
66	SX	113/115 (98%)	112 (99%)	1 (1%)	78	91
67	Sa	89/98 (91%)	89 (100%)	0	100	100
68	Sc	57/62 (92%)	57 (100%)	0	100	100
69	Sd	48/49 (98%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	Sg	272/275 (99%)	271 (100%)	1 (0%)	91	97
71	SC	188/225 (84%)	185 (98%)	3 (2%)	62	82
72	SG	207/218 (95%)	205 (99%)	2 (1%)	76	90
73	SJ	161/168 (96%)	159 (99%)	2 (1%)	71	87
74	SM	102/108 (94%)	98 (96%)	4 (4%)	32	58
75	SN	130/131 (99%)	129 (99%)	1 (1%)	81	92
76	SO	110/119 (92%)	109 (99%)	1 (1%)	78	91
77	SW	112/113 (99%)	111 (99%)	1 (1%)	78	91
78	SY	113/115 (98%)	110 (97%)	3 (3%)	44	71
79	SZ	66/103 (64%)	64 (97%)	2 (3%)	41	67
80	Sb	75/76 (99%)	75 (100%)	0	100	100
81	Se	43/48 (90%)	43 (100%)	0	100	100
82	Sf	60/140 (43%)	59 (98%)	1 (2%)	60	81
83	CA	303/336 (90%)	301 (99%)	2 (1%)	84	94
85	CE	68/338 (20%)	68 (100%)	0	100	100
86	i	28/151 (18%)	28 (100%)	0	100	100
All	All	10729/12217 (88%)	10649 (99%)	80 (1%)	84	94

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	207	VAL
5	LB	162	VAL
5	LB	223	THR
5	LB	337	VAL
6	LC	257	PHE
6	LC	364	LYS
7	LD	37	VAL
7	LD	85	LYS
8	LE	56	ARG
9	LF	29	LYS
9	LF	248	ASN
10	LG	26	LYS
10	LG	121	LYS
14	LL	70	VAL
15	LM	38	VAL

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Mol	Chain	Res	Type
17	LO	27	VAL
18	LP	24	VAL
19	LQ	83	VAL
20	LR	177	LEU
20	LR	180	LYS
20	LR	181	LYS
22	LT	107	LYS
22	LT	117	LYS
23	LU	97	ARG
24	LV	48	ARG
25	LW	110	ARG
27	LY	79	VAL
34	Lf	33	VAL
35	Lg	54	ARG
35	Lg	63	VAL
37	Li	29	ARG
40	Ll	36	ARG
46	Ls	26	LYS
46	Ls	35	VAL
46	Ls	89	VAL
47	Lt	121	LEU
47	Lt	147	HIS
48	Lz	7	ARG
48	Lz	173	LYS
52	SD	76	ARG
52	SD	94	ARG
52	SD	167	TYR
55	SH	29	GLU
55	SH	32	MET
55	SH	57	ARG
55	SH	69	LEU
55	SH	118	ARG
56	SI	154	LYS
56	SI	205	ARG
58	SL	69	ARG
58	SL	119	ASP
59	SP	65	LYS
60	SQ	71	ARG
61	SR	78	ARG
62	SS	68	ILE
63	ST	41	LYS
66	SX	105	PHE

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Mol	Chain	Res	Type
70	Sg	225	LYS
71	SC	64	THR
71	SC	112	VAL
71	SC	137	VAL
72	SG	98	ARG
72	SG	119	LYS
73	SJ	5	ARG
73	SJ	116	LYS
74	SM	18	LEU
74	SM	42	LEU
74	SM	125	GLU
74	SM	129	LYS
75	SN	133	ARG
76	SO	149	ARG
77	SW	80	ASP
78	SY	16	ARG
78	SY	99	LYS
78	SY	118	ARG
79	SZ	41	ARG
79	SZ	50	PHE
82	Sf	89	LYS
83	CA	143	ILE
83	CA	320	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	97	ASN
4	LA	132	ASN
5	LB	42	HIS
5	LB	213	GLN
6	LC	38	ASN
6	LC	119	GLN
6	LC	178	ASN
6	LC	231	ASN
7	LD	191	ASN
7	LD	282	GLN
8	LE	190	HIS
9	LF	39	GLN
9	LF	63	GLN
9	LF	206	ASN
10	LG	38	ASN

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Mol	Chain	Res	Type
11	LH	42	ASN
14	LL	19	GLN
16	LN	196	ASN
18	LP	21	ASN
18	LP	25	HIS
18	LP	34	GLN
18	LP	56	GLN
18	LP	97	ASN
18	LP	116	HIS
19	LQ	21	GLN
19	LQ	44	ASN
19	LQ	125	GLN
20	LR	39	GLN
20	LR	86	ASN
20	LR	130	ASN
22	LT	90	ASN
27	LY	4	ASN
27	LY	14	ASN
27	LY	66	GLN
28	LZ	78	ASN
29	La	28	HIS
29	La	85	GLN
30	Lb	19	ASN
31	Lc	15	ASN
33	Le	107	ASN
33	Le	117	GLN
34	Lf	56	ASN
34	Lf	80	ASN
35	Lg	100	GLN
38	Lj	66	HIS
38	Lj	76	HIS
43	Lo	45	GLN
43	Lo	51	GLN
44	Lp	56	HIS
45	Lr	100	ASN
46	Ls	85	ASN
46	Ls	191	GLN
47	Lt	70	GLN
47	Lt	149	HIS
48	Lz	19	HIS
48	Lz	21	ASN
48	Lz	35	GLN

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Mol	Chain	Res	Type
48	Lz	197	ASN
48	Lz	200	ASN
50	SA	141	ASN
51	SB	179	ASN
51	SB	186	ASN
53	SE	98	ASN
53	SE	138	HIS
53	SE	188	ASN
54	SF	31	ASN
54	SF	148	ASN
55	SH	114	GLN
56	SI	35	ASN
56	SI	84	ASN
56	SI	138	ASN
56	SI	155	ASN
56	SI	165	GLN
57	SK	39	ASN
57	SK	44	HIS
60	SQ	80	GLN
61	SR	31	ASN
62	SS	101	ASN
63	ST	128	GLN
64	SU	28	ASN
64	SU	81	GLN
66	SX	61	GLN
69	Sd	26	ASN
70	Sg	14	HIS
70	Sg	117	ASN
71	SC	113	GLN
72	SG	110	ASN
72	SG	163	ASN
73	SJ	125	HIS
74	SM	15	ASN
74	SM	19	GLN
75	SN	49	GLN
77	SW	90	GLN
77	SW	91	ASN
79	SZ	45	ASN
79	SZ	64	ASN
80	Sb	26	GLN
83	CA	134	GLN
83	CA	161	ASN

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Mol	Chain	Res	Type
83	CA	204	ASN
83	CA	306	ASN
85	CE	310	ASN
86	i	158	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3706/5066 (73%)	830 (22%)	18 (0%)
2	L7	119/121 (98%)	11 (9%)	0
3	L8	155/157 (98%)	27 (17%)	0
49	S2	1717/1869 (91%)	408 (23%)	11 (0%)
84	CC	74/75 (98%)	23 (31%)	2 (2%)
All	All	5771/7288 (79%)	1299 (22%)	31 (0%)

All (1299) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	2	G
1	L5	17	A
1	L5	30	C
1	L5	39	A
1	L5	42	A
1	L5	48	G
1	L5	56	A
1	L5	59	A
1	L5	64	A
1	L5	65	A
1	L5	66	A
1	L5	69	A
1	L5	72	C
1	L5	73	A
1	L5	74	G
1	L5	91	G
1	L5	98	A
1	L5	104	G
1	L5	108	A
1	L5	109	G
1	L5	110	C
1	L5	119	G
1	L5	120	A

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Mol	Chain	Res	Type
1	L5	132	G
1	L5	133	C
1	L5	134	G
1	L5	135	G
1	L5	136	C
1	L5	137	G
1	L5	145	G
1	L5	152	U
1	L5	159	C
1	L5	165	A
1	L5	181	C
1	L5	182	G
1	L5	183	C
1	L5	184	U
1	L5	185	C
1	L5	188	G
1	L5	189	G
1	L5	200	U
1	L5	209	U
1	L5	216	C
1	L5	218	A
1	L5	219	G
1	L5	233	U
1	L5	234	G
1	L5	255	C
1	L5	256	G
1	L5	261	G
1	L5	265	C
1	L5	266	C
1	L5	267	G
1	L5	269	G
1	L5	280	G
1	L5	297	U
1	L5	306	A
1	L5	315	G
1	L5	316	U
1	L5	340	C
1	L5	350	C
1	L5	373	G
1	L5	387	G
1	L5	388	A
1	L5	398	A

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Mol	Chain	Res	Type
1	L5	401	G
1	L5	407	A
1	L5	408	A
1	L5	409	G
1	L5	410	A
1	L5	411	G
1	L5	412	G
1	L5	413	G
1	L5	431	G
1	L5	432	U
1	L5	449	C
1	L5	450	G
1	L5	452	A
1	L5	453	G
1	L5	454	U
1	L5	456	C
1	L5	457	G
1	L5	467	U
1	L5	468	U
1	L5	484	U
1	L5	485	C
1	L5	486	C
1	L5	489	C
1	L5	493	G
1	L5	494	U
1	L5	497	G
1	L5	498	C
1	L5	499	G
1	L5	500	G
1	L5	502	C
1	L5	503	C
1	L5	504	G
1	L5	505	G
1	L5	509	A
1	L5	510	U
1	L5	512	U
1	L5	513	U
1	L5	514	U
1	L5	515	C
1	L5	516	C
1	L5	517	C
1	L5	518	G

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Mol	Chain	Res	Type
1	L5	643	C
1	L5	646	G
1	L5	656	C
1	L5	657	C
1	L5	659	G
1	L5	665	C
1	L5	666	G
1	L5	667	A
1	L5	668	C
1	L5	669	C
1	L5	673	C
1	L5	685	C
1	L5	686	A
1	L5	687	U
1	L5	688	U
1	L5	696	C
1	L5	703	G
1	L5	704	C
1	L5	708	G
1	L5	730	G
1	L5	731	G
1	L5	738	C
1	L5	739	G
1	L5	740	G
1	L5	742	G
1	L5	744	G
1	L5	746	A
1	L5	753	C
1	L5	758	G
1	L5	759	G
1	L5	760	G
1	L5	904	C
1	L5	913	U
1	L5	914	U
1	L5	915	A
1	L5	916	C
1	L5	917	A
1	L5	918	G
1	L5	923	C
1	L5	924	C
1	L5	926	G
1	L5	932	A

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Mol	Chain	Res	Type
1	L5	933	G
1	L5	934	C
1	L5	935	A
1	L5	936	C
1	L5	937	U
1	L5	943	A
1	L5	945	U
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	962	C
1	L5	965	G
1	L5	967	C
1	L5	970	G
1	L5	971	U
1	L5	977	C
1	L5	982	U
1	L5	984	C
1	L5	985	C
1	L5	989	U
1	L5	990	C
1	L5	992	C
1	L5	993	G
1	L5	995	C
1	L5	996	G
1	L5	1048	G
1	L5	1049	C
1	L5	1050	C
1	L5	1051	G
1	L5	1070	G
1	L5	1072	C
1	L5	1074	G
1	L5	1075	G
1	L5	1082	C
1	L5	1083	U
1	L5	1095	A
1	L5	1168	G
1	L5	1169	G
1	L5	1170	G
1	L5	1171	G
1	L5	1172	C
1	L5	1173	G

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Mol	Chain	Res	Type
1	L5	1178	G
1	L5	1180	C
1	L5	1181	C
1	L5	1182	C
1	L5	1183	C
1	L5	1202	C
1	L5	1203	G
1	L5	1204	C
1	L5	1210	C
1	L5	1211	G
1	L5	1214	C
1	L5	1215	C
1	L5	1217	G
1	L5	1218	G
1	L5	1219	G
1	L5	1222	A
1	L5	1235	G
1	L5	1241	C
1	L5	1246	G
1	L5	1253	G
1	L5	1254	A
1	L5	1257	A
1	L5	1258	G
1	L5	1266	G
1	L5	1267	C
1	L5	1269	G
1	L5	1270	A
1	L5	1271	G
1	L5	1272	C
1	L5	1273	G
1	L5	1274	A
1	L5	1275	G
1	L5	1277	G
1	L5	1280	C
1	L5	1284	G
1	L5	1285	U
1	L5	1287	G
1	L5	1294	A
1	L5	1295	C
1	L5	1301	C
1	L5	1312	A
1	L5	1324	A

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Mol	Chain	Res	Type
1	L5	1326	A
1	L5	1337	A
1	L5	1344	C
1	L5	1354	A
1	L5	1358	G
1	L5	1359	G
1	L5	1365	C
1	L5	1367	C
1	L5	1377	G
1	L5	1378	C
1	L5	1387	A
1	L5	1393	G
1	L5	1394	G
1	L5	1397	A
1	L5	1398	A
1	L5	1404	G
1	L5	1405	C
1	L5	1407	C
1	L5	1409	C
1	L5	1410	U
1	L5	1411	C
1	L5	1414	C
1	L5	1420	A
1	L5	1435	G
1	L5	1437	C
1	L5	1439	C
1	L5	1440	U
1	L5	1441	C
1	L5	1443	A
1	L5	1446	C
1	L5	1447	C
1	L5	1482	G
1	L5	1483	C
1	L5	1493	G
1	L5	1497	A
1	L5	1498	G
1	L5	1502	G
1	L5	1514	U
1	L5	1517	G
1	L5	1525	A
1	L5	1534	A
1	L5	1547	A

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Mol	Chain	Res	Type
1	L5	1562	G
1	L5	1566	C
1	L5	1578	U
1	L5	1591	U
1	L5	1596	U
1	L5	1624	G
1	L5	1625	G
1	L5	1631	A
1	L5	1633	G
1	L5	1634	A
1	L5	1638	A
1	L5	1640	C
1	L5	1654	G
1	L5	1661	C
1	L5	1676	C
1	L5	1677	U
1	L5	1678	C
1	L5	1697	G
1	L5	1699	A
1	L5	1700	G
1	L5	1703	C
1	L5	1704	C
1	L5	1705	G
1	L5	1707	C
1	L5	1715	C
1	L5	1716	G
1	L5	1717	C
1	L5	1718	C
1	L5	1719	A
1	L5	1726	U
1	L5	1734	G
1	L5	1735	U
1	L5	1740	C
1	L5	1741	G
1	L5	1742	A
1	L5	1745	G
1	L5	1750	G
1	L5	1755	C
1	L5	1757	U
1	L5	1758	G
1	L5	1760	G
1	L5	1761	G

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Mol	Chain	Res	Type
1	L5	1762	C
1	L5	1763	C
1	L5	1764	G
1	L5	1765	A
1	L5	1766	A
1	L5	1768	C
1	L5	1770	A
1	L5	1771	U
1	L5	1775	A
1	L5	1785	C
1	L5	1787	A
1	L5	1797	G
1	L5	1804	A
1	L5	1810	G
1	L5	1815	G
1	L5	1820	C
1	L5	1821	G
1	L5	1822	U
1	L5	1834	U
1	L5	1836	G
1	L5	1837	A
1	L5	1842	G
1	L5	1843	A
1	L5	1855	G
1	L5	1869	G
1	L5	1882	U
1	L5	1897	A
1	L5	1918	U
1	L5	1919	G
1	L5	1920	C
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G
1	L5	1931	C
1	L5	1932	A
1	L5	1936	C
1	L5	1940	G
1	L5	1948	G
1	L5	1951	G
1	L5	1959	U
1	L5	1960	A
1	L5	1961	G

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Mol	Chain	Res	Type
1	L5	1962	A
1	L5	1974	U
1	L5	1975	G
1	L5	1978	C
1	L5	1980	U
1	L5	1983	A
1	L5	1984	A
1	L5	1985	G
1	L5	1986	U
1	L5	1987	C
1	L5	1988	G
1	L5	1990	A
1	L5	1991	A
1	L5	1992	U
1	L5	1993	C
1	L5	1997	U
1	L5	1998	A
1	L5	2001	G
1	L5	2002	A
1	L5	2014	C
1	L5	2017	A
1	L5	2018	C
1	L5	2024	G
1	L5	2025	A
1	L5	2026	A
1	L5	2034	G
1	L5	2046	G
1	L5	2048	U
1	L5	2055	G
1	L5	2056	G
1	L5	2062	C
1	L5	2069	A
1	L5	2084	C
1	L5	2085	G
1	L5	2089	G
1	L5	2092	G
1	L5	2093	A
1	L5	2095	A
1	L5	2096	G
1	L5	2097	U
1	L5	2098	G
1	L5	2101	C

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Mol	Chain	Res	Type
1	L5	2102	G
1	L5	2108	G
1	L5	2112	G
1	L5	2113	G
1	L5	2250	C
1	L5	2252	G
1	L5	2253	A
1	L5	2256	C
1	L5	2258	C
1	L5	2260	C
1	L5	2289	C
1	L5	2300	A
1	L5	2301	G
1	L5	2306	G
1	L5	2313	A
1	L5	2332	A
1	L5	2333	G
1	L5	2348	G
1	L5	2351	C
1	L5	2360	A
1	L5	2369	U
1	L5	2383	C
1	L5	2395	A
1	L5	2397	G
1	L5	2417	A
1	L5	2418	A
1	L5	2421	G
1	L5	2425	U
1	L5	2441	C
1	L5	2447	U
1	L5	2450	G
1	L5	2453	A
1	L5	2464	C
1	L5	2465	C
1	L5	2467	U
1	L5	2469	C
1	L5	2471	G
1	L5	2474	G
1	L5	2475	G
1	L5	2478	C
1	L5	2479	G
1	L5	2483	G

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Mol	Chain	Res	Type
1	L5	2484	A
1	L5	2485	U
1	L5	2487	G
1	L5	2488	C
1	L5	2489	C
1	L5	2490	U
1	L5	2491	C
1	L5	2494	U
1	L5	2495	U
1	L5	2503	G
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G
1	L5	2513	A
1	L5	2519	U
1	L5	2537	A
1	L5	2544	G
1	L5	2546	G
1	L5	2547	G
1	L5	2554	U
1	L5	2559	G
1	L5	2560	C
1	L5	2565	A
1	L5	2573	A
1	L5	2583	C
1	L5	2587	A
1	L5	2589	C
1	L5	2601	A
1	L5	2611	A
1	L5	2627	C
1	L5	2638	G
1	L5	2652	G
1	L5	2653	C
1	L5	2662	G
1	L5	2669	C
1	L5	2670	C
1	L5	2675	G
1	L5	2676	A
1	L5	2687	U
1	L5	2695	A
1	L5	2696	A
1	L5	2703	G

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Mol	Chain	Res	Type
1	L5	2707	U
1	L5	2708	U
1	L5	2709	C
1	L5	2710	C
1	L5	2711	G
1	L5	2721	G
1	L5	2724	G
1	L5	2726	G
1	L5	2739	C
1	L5	2742	G
1	L5	2743	A
1	L5	2746	A
1	L5	2756	G
1	L5	2759	G
1	L5	2761	U
1	L5	2763	U
1	L5	2764	A
1	L5	2769	U
1	L5	2770	C
1	L5	2787	A
1	L5	2788	U
1	L5	2790	U
1	L5	2815	A
1	L5	2826	U
1	L5	2827	G
1	L5	2838	G
1	L5	2848	G
1	L5	2855	G
1	L5	2867	C
1	L5	2877	G
1	L5	2892	C
1	L5	2900	U
1	L5	2902	G
1	L5	2903	G
1	L5	2904	U
1	L5	2905	C
1	L5	2906	G
1	L5	2908	U
1	L5	3585	G
1	L5	3586	G
1	L5	3587	C
1	L5	3590	G

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Mol	Chain	Res	Type
1	L5	3591	C
1	L5	3594	C
1	L5	3595	U
1	L5	3596	A
1	L5	3597	G
1	L5	3604	A
1	L5	3615	G
1	L5	3616	U
1	L5	3618	C
1	L5	3626	G
1	L5	3630	A
1	L5	3635	A
1	L5	3644	U
1	L5	3646	A
1	L5	3662	A
1	L5	3673	C
1	L5	3674	G
1	L5	3711	A
1	L5	3713	U
1	L5	3714	G
1	L5	3727	A
1	L5	3729	U
1	L5	3748	A
1	L5	3750	G
1	L5	3753	G
1	L5	3757	G
1	L5	3758	U
1	L5	3759	A
1	L5	3760	A
1	L5	3771	C
1	L5	3775	A
1	L5	3776	G
1	L5	3777	G
1	L5	3784	A
1	L5	3786	U
1	L5	3802	U
1	L5	3811	G
1	L5	3812	C
1	L5	3814	U
1	L5	3817	A
1	L5	3818	U
1	L5	3819	G

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Mol	Chain	Res	Type
1	L5	3838	U
1	L5	3839	G
1	L5	3840	U
1	L5	3851	U
1	L5	3867	A
1	L5	3877	A
1	L5	3878	C
1	L5	3879	G
1	L5	3885	G
1	L5	3887	C
1	L5	3892	U
1	L5	3897	G
1	L5	3898	G
1	L5	3901	A
1	L5	3906	A
1	L5	3907	G
1	L5	3908	A
1	L5	3915	U
1	L5	3938	G
1	L5	3942	A
1	L5	3943	A
1	L5	3944	G
1	L5	3947	A
1	L5	3948	C
1	L5	3949	A
1	L5	3950	U
1	L5	3953	G
1	L5	3955	G
1	L5	3956	G
1	L5	3957	U
1	L5	3958	G
1	L5	3959	U
1	L5	3961	G
1	L5	3962	A
1	L5	3963	A
1	L5	3964	U
1	L5	3965	A
1	L5	3966	A
1	L5	3969	G
1	L5	3970	G
1	L5	3971	G
1	L5	3973	G

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Mol	Chain	Res	Type
1	L5	3974	G
1	L5	3977	C
1	L5	4034	G
1	L5	4035	G
1	L5	4036	G
1	L5	4038	C
1	L5	4039	G
1	L5	4041	C
1	L5	4042	G
1	L5	4043	G
1	L5	4045	G
1	L5	4046	A
1	L5	4048	A
1	L5	4049	U
1	L5	4051	C
1	L5	4052	C
1	L5	4053	A
1	L5	4054	C
1	L5	4055	U
1	L5	4056	A
1	L5	4057	C
1	L5	4058	U
1	L5	4059	C
1	L5	4062	A
1	L5	4063	U
1	L5	4064	C
1	L5	4065	G
1	L5	4076	G
1	L5	4084	G
1	L5	4086	G
1	L5	4096	C
1	L5	4097	G
1	L5	4099	G
1	L5	4101	C
1	L5	4102	C
1	L5	4103	C
1	L5	4104	G
1	L5	4107	G
1	L5	4108	G
1	L5	4111	U
1	L5	4112	C
1	L5	4113	U

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Mol	Chain	Res	Type
1	L5	4114	C
1	L5	4115	G
1	L5	4116	C
1	L5	4117	U
1	L5	4119	C
1	L5	4122	G
1	L5	4127	A
1	L5	4140	C
1	L5	4141	G
1	L5	4142	C
1	L5	4143	G
1	L5	4144	C
1	L5	4146	G
1	L5	4162	C
1	L5	4163	U
1	L5	4168	G
1	L5	4170	A
1	L5	4177	C
1	L5	4183	G
1	L5	4184	G
1	L5	4191	G
1	L5	4196	G
1	L5	4203	A
1	L5	4222	G
1	L5	4228	G
1	L5	4229	U
1	L5	4233	A
1	L5	4237	C
1	L5	4249	G
1	L5	4251	A
1	L5	4254	G
1	L5	4257	A
1	L5	4265	U
1	L5	4268	A
1	L5	4273	A
1	L5	4281	A
1	L5	4291	G
1	L5	4295	U
1	L5	4304	A
1	L5	4305	G
1	L5	4306	U
1	L5	4314	C

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Mol	Chain	Res	Type
1	L5	4319	C
1	L5	4329	G
1	L5	4330	G
1	L5	4332	C
1	L5	4349	C
1	L5	4354	U
1	L5	4373	G
1	L5	4376	A
1	L5	4377	G
1	L5	4378	A
1	L5	4379	A
1	L5	4380	A
1	L5	4387	C
1	L5	4391	G
1	L5	4394	A
1	L5	4405	G
1	L5	4422	A
1	L5	4426	C
1	L5	4448	G
1	L5	4449	A
1	L5	4453	C
1	L5	4464	A
1	L5	4475	G
1	L5	4488	A
1	L5	4500	U
1	L5	4512	U
1	L5	4513	A
1	L5	4519	C
1	L5	4524	G
1	L5	4531	U
1	L5	4545	G
1	L5	4548	A
1	L5	4549	G
1	L5	4557	U
1	L5	4560	C
1	L5	4567	G
1	L5	4573	G
1	L5	4575	G
1	L5	4589	A
1	L5	4590	A
1	L5	4600	G
1	L5	4617	G

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Mol	Chain	Res	Type
1	L5	4636	U
1	L5	4637	G
1	L5	4656	A
1	L5	4670	C
1	L5	4672	A
1	L5	4679	G
1	L5	4684	A
1	L5	4687	A
1	L5	4694	G
1	L5	4695	C
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4719	G
1	L5	4720	C
1	L5	4731	G
1	L5	4733	C
1	L5	4734	A
1	L5	4740	G
1	L5	4741	C
1	L5	4742	G
1	L5	4745	G
1	L5	4754	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G
1	L5	4764	A
1	L5	4765	G
1	L5	4771	C
1	L5	4772	C
1	L5	4775	C
1	L5	4859	C
1	L5	4863	G
1	L5	4870	G
1	L5	4871	C
1	L5	4875	G
1	L5	4881	U
1	L5	4882	U
1	L5	4883	C
1	L5	4888	U
1	L5	4889	G
1	L5	4895	C

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Mol	Chain	Res	Type
1	L5	4896	G
1	L5	4900	C
1	L5	4901	G
1	L5	4902	C
1	L5	4910	A
1	L5	4912	G
1	L5	4914	C
1	L5	4922	C
1	L5	4923	C
1	L5	4925	U
1	L5	4927	G
1	L5	4928	C
1	L5	4934	A
1	L5	4940	C
1	L5	4941	G
1	L5	4943	A
1	L5	4944	C
1	L5	4951	G
1	L5	4955	A
1	L5	4960	G
1	L5	4961	G
1	L5	4963	G
1	L5	4966	A
1	L5	4976	U
1	L5	4979	A
1	L5	4988	U
1	L5	4989	U
1	L5	4990	C
1	L5	4991	U
1	L5	5007	A
1	L5	5013	C
1	L5	5014	A
1	L5	5017	G
1	L5	5022	U
1	L5	5023	C
1	L5	5024	C
1	L5	5025	C
1	L5	5026	U
1	L5	5028	G
1	L5	5029	C
1	L5	5031	G
1	L5	5034	A

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Mol	Chain	Res	Type
1	L5	5041	G
1	L5	5047	C
1	L5	5050	C
1	L5	5053	U
1	L5	5054	C
1	L5	5055	G
1	L5	5058	A
1	L5	5061	A
1	L5	5069	U
2	L7	4	U
2	L7	33	U
2	L7	38	U
2	L7	42	A
2	L7	53	U
2	L7	63	C
2	L7	64	G
2	L7	100	A
2	L7	102	U
2	L7	110	G
2	L7	111	C
3	L8	2	G
3	L8	25	G
3	L8	34	U
3	L8	35	C
3	L8	48	A
3	L8	59	A
3	L8	60	G
3	L8	62	A
3	L8	63	U
3	L8	82	A
3	L8	83	C
3	L8	84	A
3	L8	85	U
3	L8	86	U
3	L8	87	G
3	L8	94	G
3	L8	103	A
3	L8	105	C
3	L8	110	U
3	L8	111	U
3	L8	114	G
3	L8	123	U

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Mol	Chain	Res	Type
3	L8	124	U
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	156	U
49	S2	4	C
49	S2	17	C
49	S2	23	G
49	S2	33	G
49	S2	41	G
49	S2	44	U
49	S2	45	A
49	S2	46	A
49	S2	56	G
49	S2	58	C
49	S2	59	U
49	S2	64	A
49	S2	67	C
49	S2	68	A
49	S2	72	C
49	S2	73	C
49	S2	74	G
49	S2	76	U
49	S2	92	A
49	S2	99	A
49	S2	103	A
49	S2	113	G
49	S2	114	G
49	S2	115	U
49	S2	121	U
49	S2	126	G
49	S2	129	C
49	S2	130	G
49	S2	139	C
49	S2	140	U
49	S2	143	U
49	S2	158	A
49	S2	159	A
49	S2	160	U
49	S2	162	C
49	S2	170	A
49	S2	175	A

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Mol	Chain	Res	Type
49	S2	179	C
49	S2	190	G
49	S2	191	A
49	S2	196	C
49	S2	197	U
49	S2	198	U
49	S2	199	C
49	S2	200	G
49	S2	203	G
49	S2	204	G
49	S2	206	G
49	S2	208	G
49	S2	211	G
49	S2	212	C
49	S2	214	U
49	S2	290	U
49	S2	291	G
49	S2	292	A
49	S2	293	C
49	S2	295	C
49	S2	302	A
49	S2	306	C
49	S2	307	G
49	S2	308	G
49	S2	309	G
49	S2	311	C
49	S2	318	A
49	S2	319	C
49	S2	323	C
49	S2	324	C
49	S2	325	C
49	S2	326	C
49	S2	327	G
49	S2	328	U
49	S2	329	G
49	S2	332	G
49	S2	335	G
49	S2	338	G
49	S2	339	A
49	S2	360	A
49	S2	362	C
49	S2	363	A

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Mol	Chain	Res	Type
49	S2	364	A
49	S2	368	U
49	S2	369	C
49	S2	370	G
49	S2	374	G
49	S2	385	G
49	S2	386	C
49	S2	408	A
49	S2	409	C
49	S2	417	C
49	S2	418	A
49	S2	421	G
49	S2	429	C
49	S2	438	G
49	S2	448	A
49	S2	449	A
49	S2	450	C
49	S2	452	G
49	S2	464	A
49	S2	465	A
49	S2	466	G
49	S2	471	G
49	S2	472	C
49	S2	473	A
49	S2	474	G
49	S2	482	G
49	S2	487	U
49	S2	488	U
49	S2	492	C
49	S2	493	A
49	S2	502	C
49	S2	516	A
49	S2	517	C
49	S2	525	A
49	S2	529	A
49	S2	531	A
49	S2	532	C
49	S2	533	A
49	S2	536	A
49	S2	537	C
49	S2	540	U
49	S2	542	U

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Mol	Chain	Res	Type
49	S2	545	A
49	S2	546	G
49	S2	547	G
49	S2	551	U
49	S2	554	A
49	S2	556	U
49	S2	557	U
49	S2	558	G
49	S2	559	G
49	S2	560	A
49	S2	563	G
49	S2	564	A
49	S2	566	U
49	S2	576	A
49	S2	582	U
49	S2	583	A
49	S2	584	A
49	S2	587	A
49	S2	589	G
49	S2	590	A
49	S2	591	U
49	S2	596	U
49	S2	597	G
49	S2	600	G
49	S2	604	A
49	S2	607	U
49	S2	608	C
49	S2	614	C
49	S2	627	U
49	S2	628	A
49	S2	631	U
49	S2	632	C
49	S2	643	A
49	S2	644	G
49	S2	655	A
49	S2	664	A
49	S2	668	A
49	S2	669	A
49	S2	671	A
49	S2	672	A
49	S2	673	G
49	S2	688	U

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Mol	Chain	Res	Type
49	S2	689	U
49	S2	690	G
49	S2	692	G
49	S2	693	A
49	S2	695	C
49	S2	696	G
49	S2	697	G
49	S2	698	G
49	S2	733	C
49	S2	736	C
49	S2	738	C
49	S2	749	U
49	S2	751	G
49	S2	752	G
49	S2	753	C
49	S2	788	G
49	S2	791	C
49	S2	792	C
49	S2	797	C
49	S2	798	G
49	S2	810	A
49	S2	821	G
49	S2	822	U
49	S2	823	U
49	S2	824	C
49	S2	830	A
49	S2	835	C
49	S2	836	G
49	S2	837	A
49	S2	838	G
49	S2	839	C
49	S2	840	C
49	S2	841	G
49	S2	842	C
49	S2	847	A
49	S2	869	A
49	S2	873	G
49	S2	874	G
49	S2	878	G
49	S2	880	G
49	S2	882	U
49	S2	883	U

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Mol	Chain	Res	Type
49	S2	887	U
49	S2	888	U
49	S2	889	U
49	S2	891	G
49	S2	894	G
49	S2	896	U
49	S2	897	U
49	S2	898	U
49	S2	899	U
49	S2	900	C
49	S2	901	G
49	S2	903	A
49	S2	913	A
49	S2	914	U
49	S2	917	U
49	S2	920	A
49	S2	922	A
49	S2	930	C
49	S2	933	G
49	S2	934	G
49	S2	943	U
49	S2	963	A
49	S2	971	G
49	S2	972	A
49	S2	990	A
49	S2	992	A
49	S2	999	G
49	S2	1017	U
49	S2	1018	U
49	S2	1023	A
49	S2	1027	A
49	S2	1028	A
49	S2	1033	G
49	S2	1061	U
49	S2	1062	A
49	S2	1078	C
49	S2	1083	A
49	S2	1085	C
49	S2	1088	U
49	S2	1109	C
49	S2	1114	U
49	S2	1115	U

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Mol	Chain	Res	Type
49	S2	1116	C
49	S2	1118	C
49	S2	1119	A
49	S2	1121	G
49	S2	1123	C
49	S2	1133	A
49	S2	1138	C
49	S2	1148	A
49	S2	1153	C
49	S2	1154	U
49	S2	1195	A
49	S2	1203	G
49	S2	1207	G
49	S2	1208	A
49	S2	1215	C
49	S2	1216	C
49	S2	1217	A
49	S2	1224	G
49	S2	1227	G
49	S2	1242	U
49	S2	1243	U
49	S2	1251	A
49	S2	1253	A
49	S2	1256	G
49	S2	1257	G
49	S2	1259	A
49	S2	1265	A
49	S2	1274	G
49	S2	1275	G
49	S2	1283	C
49	S2	1284	A
49	S2	1286	G
49	S2	1294	G
49	S2	1295	A
49	S2	1301	A
49	S2	1302	G
49	S2	1303	C
49	S2	1306	U
49	S2	1308	U
49	S2	1312	G
49	S2	1320	G
49	S2	1342	U

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Mol	Chain	Res	Type
49	S2	1343	U
49	S2	1344	A
49	S2	1348	G
49	S2	1363	C
49	S2	1371	U
49	S2	1372	U
49	S2	1373	C
49	S2	1378	A
49	S2	1396	A
49	S2	1402	A
49	S2	1404	U
49	S2	1409	A
49	S2	1415	C
49	S2	1416	C
49	S2	1419	C
49	S2	1420	G
49	S2	1421	A
49	S2	1422	G
49	S2	1423	C
49	S2	1424	G
49	S2	1433	C
49	S2	1435	C
49	S2	1436	C
49	S2	1438	A
49	S2	1449	G
49	S2	1452	A
49	S2	1454	A
49	S2	1462	U
49	S2	1463	U
49	S2	1480	A
49	S2	1487	A
49	S2	1489	A
49	S2	1490	G
49	S2	1494	U
49	S2	1495	G
49	S2	1497	G
49	S2	1498	A
49	S2	1505	U
49	S2	1507	G
49	S2	1508	A
49	S2	1509	U
49	S2	1520	G

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Mol	Chain	Res	Type
49	S2	1521	C
49	S2	1533	A
49	S2	1535	U
49	S2	1537	A
49	S2	1544	C
49	S2	1547	C
49	S2	1552	G
49	S2	1553	C
49	S2	1556	A
49	S2	1558	C
49	S2	1570	G
49	S2	1574	C
49	S2	1578	U
49	S2	1580	A
49	S2	1585	U
49	S2	1587	G
49	S2	1588	A
49	S2	1600	G
49	S2	1601	A
49	S2	1606	G
49	S2	1621	U
49	S2	1623	A
49	S2	1634	A
49	S2	1638	G
49	S2	1648	G
49	S2	1654	G
49	S2	1661	A
49	S2	1663	A
49	S2	1665	G
49	S2	1671	G
49	S2	1683	C
49	S2	1686	G
49	S2	1698	C
49	S2	1699	A
49	S2	1719	A
49	S2	1721	U
49	S2	1722	G
49	S2	1743	G
49	S2	1744	G
49	S2	1745	A
49	S2	1752	C
49	S2	1753	C

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Mol	Chain	Res	Type
49	S2	1754	G
49	S2	1757	G
49	S2	1758	G
49	S2	1760	G
49	S2	1761	U
49	S2	1771	G
49	S2	1772	C
49	S2	1773	C
49	S2	1774	C
49	S2	1775	U
49	S2	1776	G
49	S2	1777	G
49	S2	1780	G
49	S2	1781	A
49	S2	1783	C
49	S2	1784	G
49	S2	1786	U
49	S2	1798	C
49	S2	1819	A
49	S2	1822	A
49	S2	1823	A
49	S2	1824	A
49	S2	1825	A
49	S2	1829	G
49	S2	1831	A
49	S2	1835	A
49	S2	1838	U
49	S2	1849	G
49	S2	1851	A
49	S2	1852	C
49	S2	1861	G
49	S2	1862	G
49	S2	1863	A
49	S2	1864	U
49	S2	1865	C
84	CC	16	C
84	CC	17	G
84	CC	18	G
84	CC	19	C
84	CC	20	U
84	CC	28	C
84	CC	31	G

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Mol	Chain	Res	Type
84	CC	32	C
84	CC	33	U
84	CC	35	U
84	CC	36	C
84	CC	37	A
84	CC	38	C
84	CC	39	C
84	CC	45	G
84	CC	46	A
84	CC	47	C
84	CC	48	C
84	CC	51	G
84	CC	57	A
84	CC	59	U
84	CC	72	G
84	CC	75	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	406	C
1	L5	493	G
1	L5	914	U
1	L5	955	G
1	L5	1082	C
1	L5	1633	G
1	L5	1977	C
1	L5	2033	A
1	L5	2416	G
1	L5	2675	G
1	L5	2760	G
1	L5	2786	C
1	L5	3614	G
1	L5	3673	C
1	L5	3876	A
1	L5	4378	A
1	L5	4699	U
1	L5	4913	G
49	S2	60	G
49	S2	92	A
49	S2	112	U
49	S2	158	A

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Mol	Chain	Res	Type
49	S2	291	G
49	S2	417	C
49	S2	420	G
49	S2	563	G
49	S2	668	A
49	S2	688	U
49	S2	1434	C
84	CC	35	U
84	CC	74	C

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 264 ligands modelled in this entry, 264 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

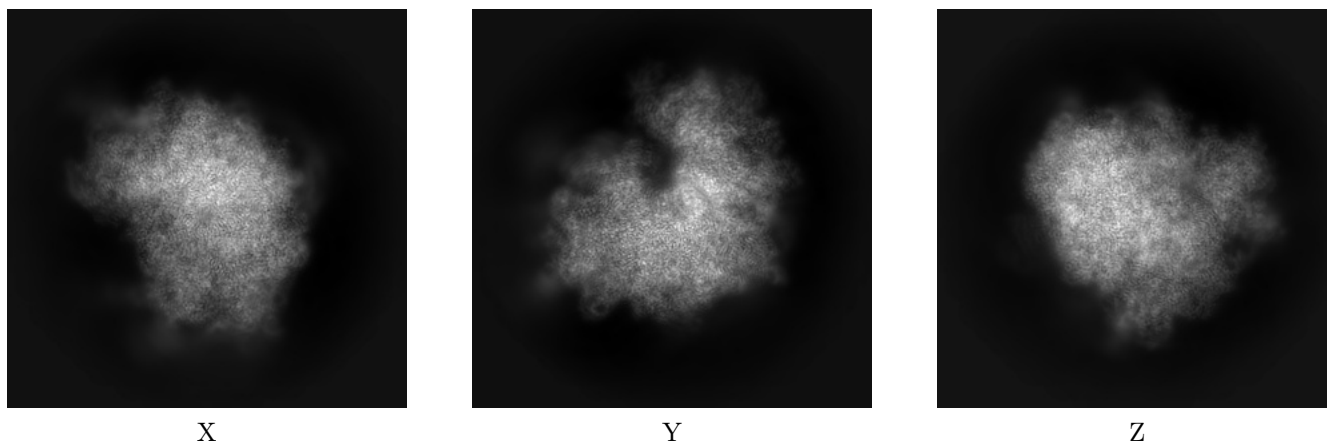
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11292. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

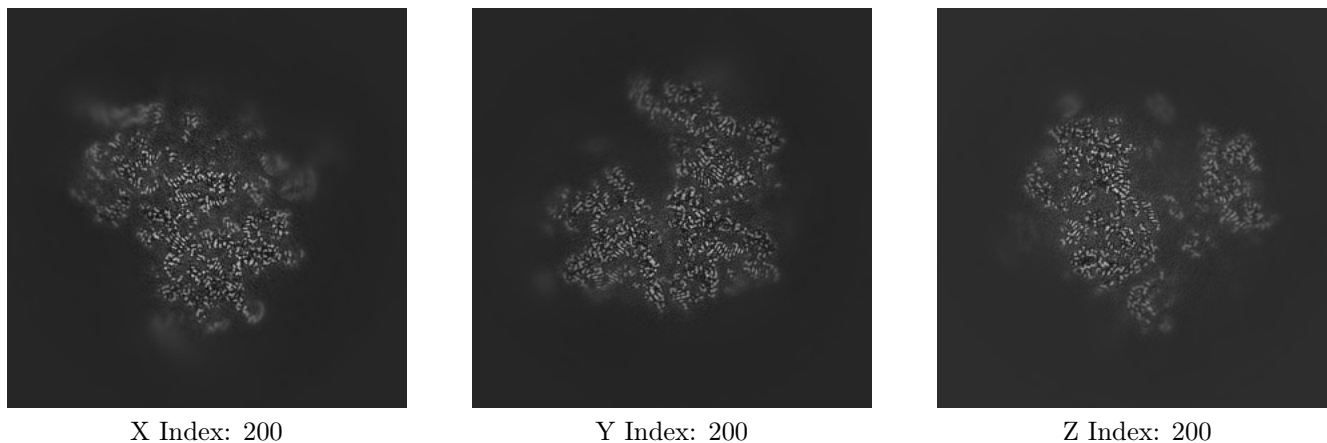
6.1.1 Primary map



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

6.2 Central slices [i](#)

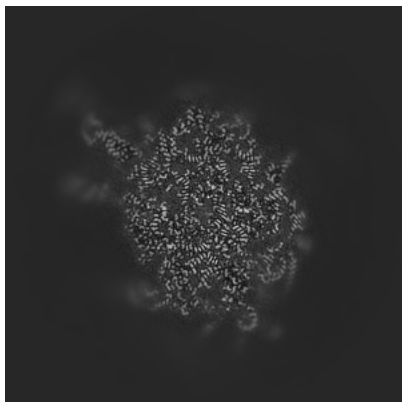
6.2.1 Primary map



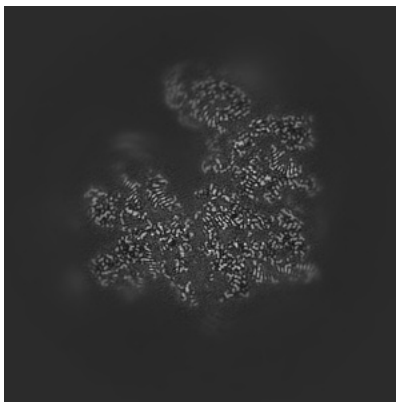
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

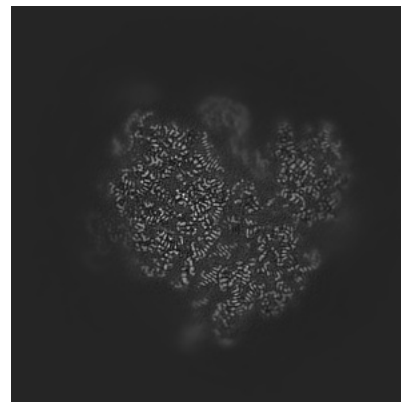
6.3.1 Primary map



X Index: 178



Y Index: 194

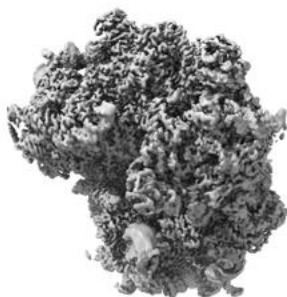


Z Index: 224

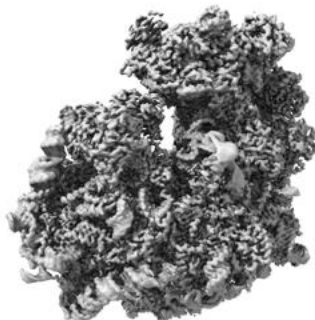
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

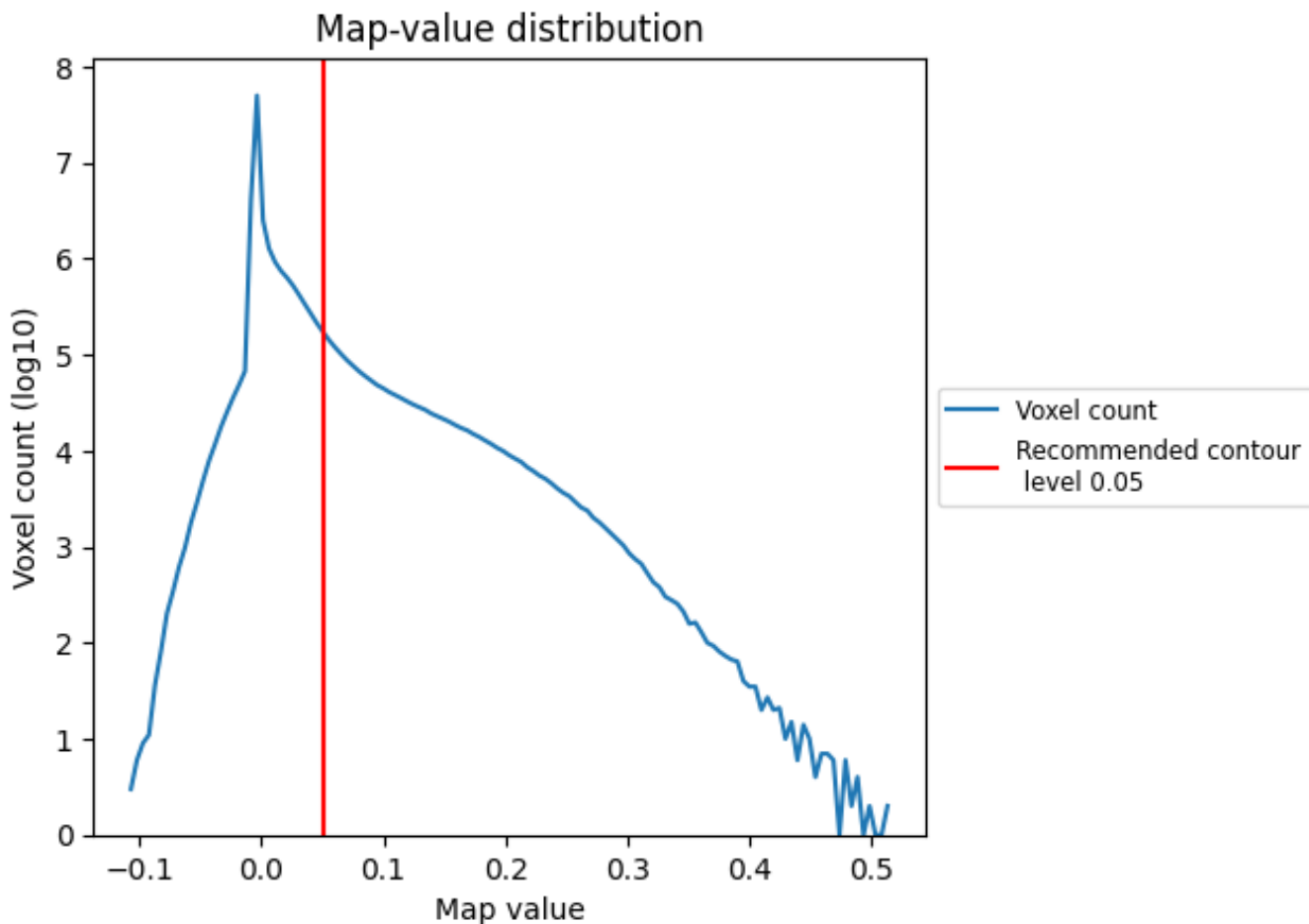
6.5 Mask visualisation

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

7 Map analysis [i](#)

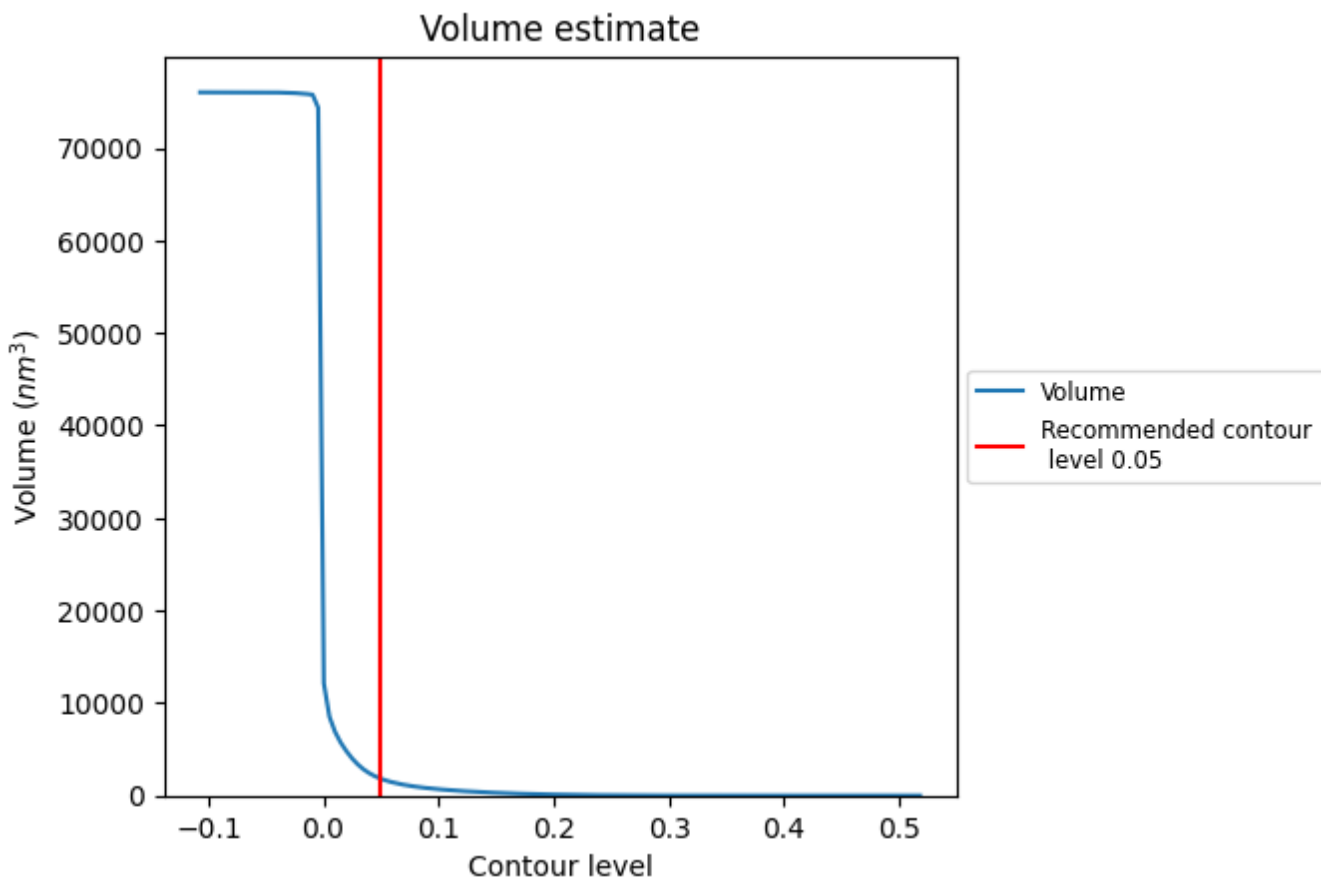
This section contains the results of statistical analysis of the map.

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.

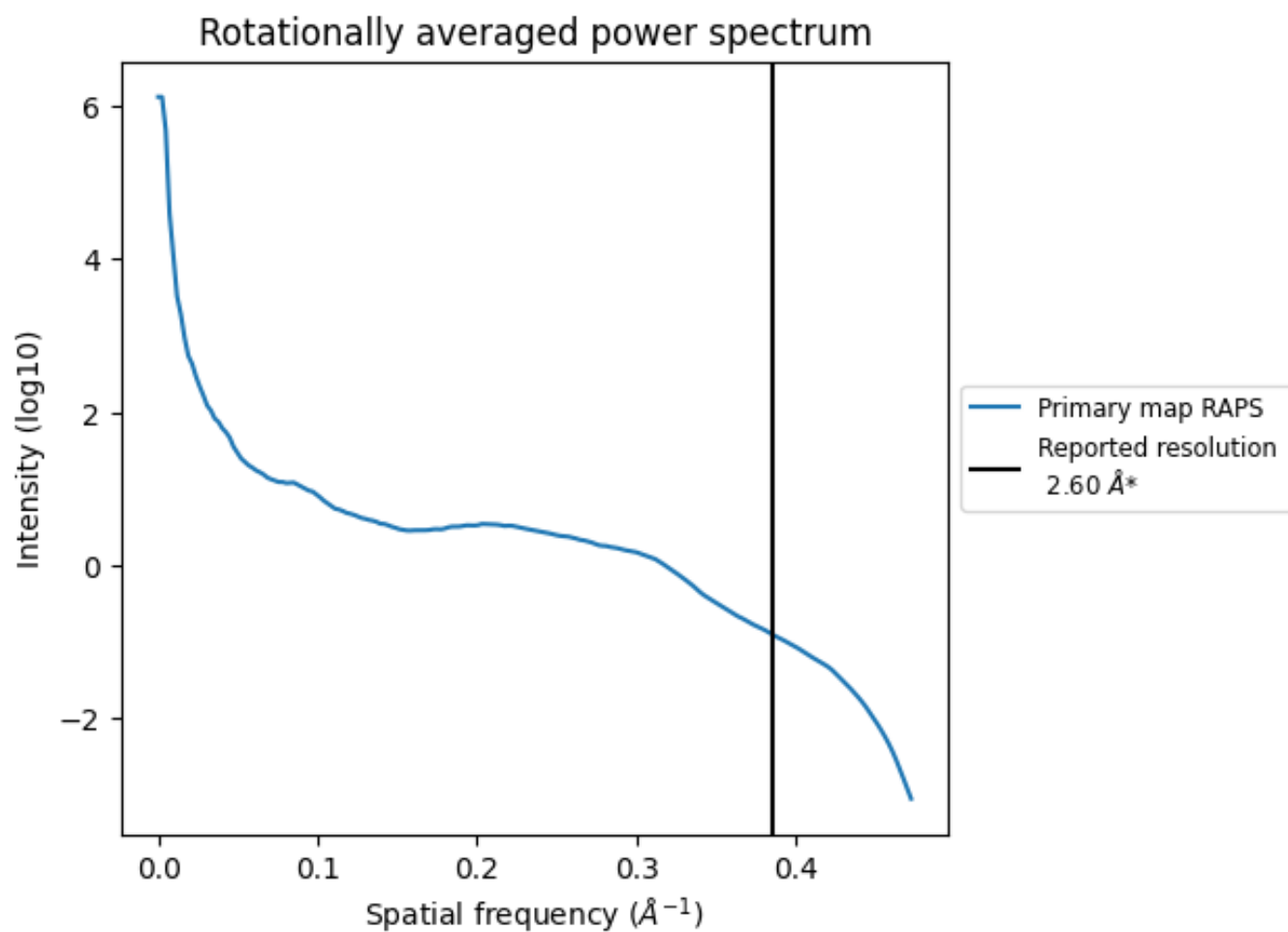
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1822 nm³; this corresponds to an approximate mass of 1646 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

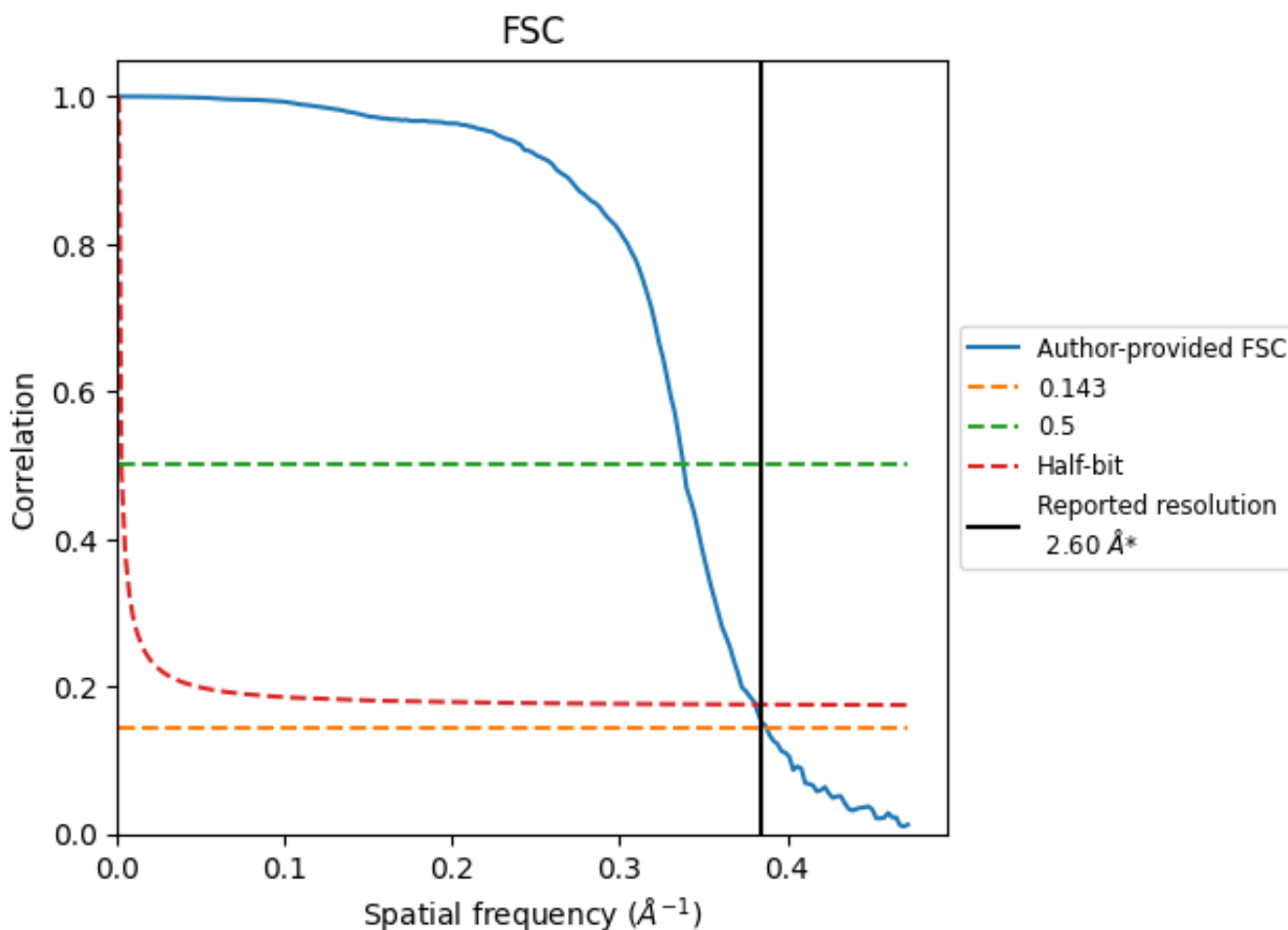


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

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

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

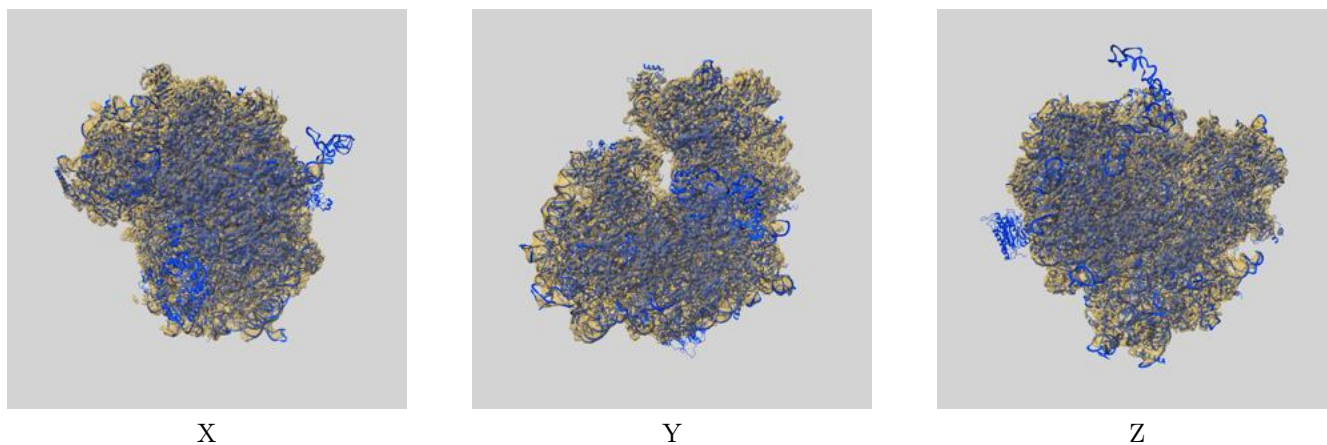
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.58	2.96	2.63
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

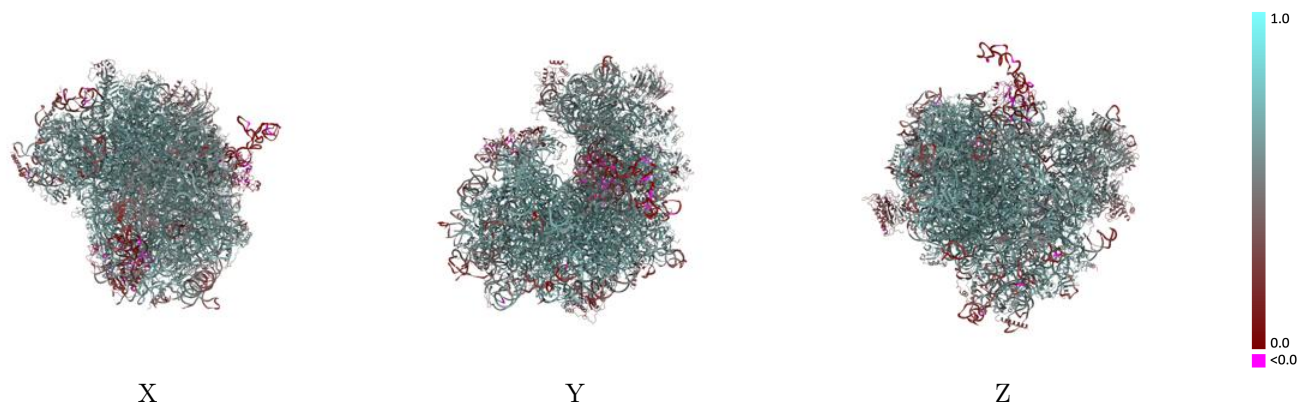
This section contains information regarding the fit between EMDB map EMD-11292 and PDB model 6ZMI. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



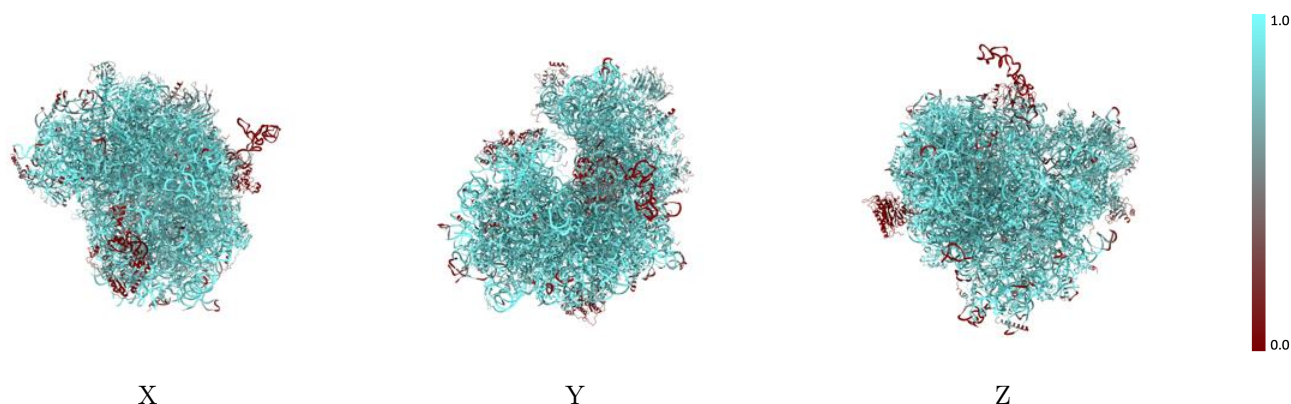
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



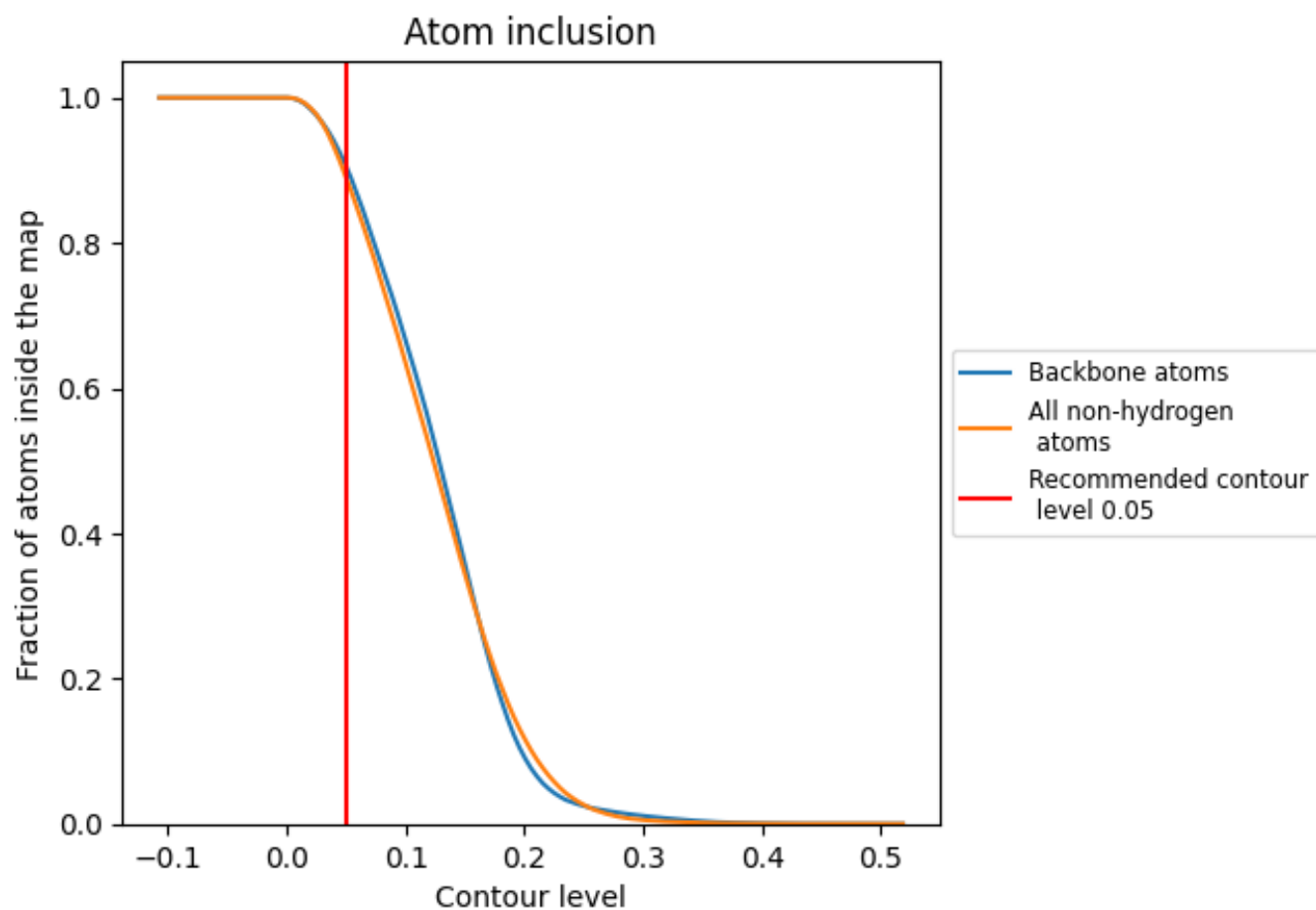
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8899	 0.5750
CA	 0.0385	 0.3190
CC	 0.8402	 0.3510
CE	 0.7735	 0.5450
L5	 0.9304	 0.5890
L7	 0.9930	 0.6360
L8	 0.9665	 0.6210
LA	 0.9869	 0.6800
LB	 0.9412	 0.6450
LC	 0.9449	 0.6340
LD	 0.9100	 0.5870
LE	 0.8535	 0.5600
LF	 0.9635	 0.6440
LG	 0.8452	 0.5730
LH	 0.9318	 0.6090
LI	 0.9471	 0.6230
LJ	 0.8181	 0.5110
LL	 0.8972	 0.6040
LM	 0.9359	 0.6020
LN	 0.9938	 0.6820
LO	 0.9574	 0.6500
LP	 0.9611	 0.6610
LQ	 0.9765	 0.6630
LR	 0.8913	 0.6040
LS	 0.9786	 0.6520
LT	 0.9367	 0.6170
LU	 0.8426	 0.5310
LV	 0.9656	 0.6550
LW	 0.7010	 0.4780
LX	 0.9311	 0.6250
LY	 0.9258	 0.6210
LZ	 0.9385	 0.6170
La	 0.9708	 0.6630
Lb	 0.8619	 0.5650
Lc	 0.9304	 0.6230






















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Chain	Atom inclusion	Q-score
Ld	 0.9207	 0.6190
Le	 0.9774	 0.6620
Lf	 0.9810	 0.6610
Lg	 0.9265	 0.6430
Lh	 0.9266	 0.6080
Li	 0.9223	 0.6050
Lj	 0.9822	 0.6680
Lk	 0.8474	 0.5640
Ll	 0.9764	 0.6380
Lm	 0.9279	 0.6240
Ln	 0.9856	 0.6670
Lo	 0.9307	 0.6350
Lp	 0.9594	 0.6680
Lr	 0.9595	 0.6310
Ls	 0.1436	 0.1380
Lt	 0.0350	 0.0940
Lz	 0.1307	 0.1510
S2	 0.9433	 0.5820
SA	 0.8888	 0.5810
SB	 0.9122	 0.5940
SC	 0.9373	 0.6100
SD	 0.8386	 0.5240
SE	 0.9289	 0.5940
SF	 0.8917	 0.5370
SG	 0.7925	 0.5060
SH	 0.7537	 0.4980
SI	 0.8974	 0.5850
SJ	 0.9058	 0.5760
SK	 0.7913	 0.4830
SL	 0.8944	 0.6120
SM	 0.3125	 0.2690
SN	 0.9573	 0.6320
SO	 0.8990	 0.5910
SP	 0.7809	 0.4850
SQ	 0.8644	 0.5450
SR	 0.8066	 0.5240
SS	 0.8135	 0.5060
ST	 0.8614	 0.5300
SU	 0.7788	 0.4950
SV	 0.9148	 0.5870
SW	 0.9644	 0.6400
SX	 0.9514	 0.6340

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Chain	Atom inclusion	Q-score
SY	 0.8174	 0.5290
SZ	 0.7273	 0.4700
Sa	 0.9214	 0.6060
Sb	 0.8858	 0.5710
Sc	 0.8169	 0.5250
Sd	 0.9457	 0.5890
Se	 0.8061	 0.5460
Sf	 0.4719	 0.3380
Sg	 0.6880	 0.4630
i	 0.9261	 0.6210