Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 10:15 pm GMT

PDB ID	:	6ZME
EMDB ID	:	EMD-11289
Title	:	SARS-CoV-2 Nsp1 bound to the human CCDC124-80S-eERF1 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	:	3.00 Å(reported)

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

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

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

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

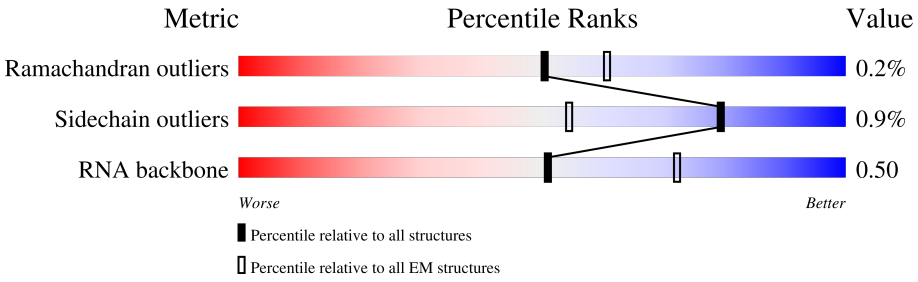
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	L5	5066	53% 19% 26%
2	L7	121	86% 13%
3	L8	157	78% 21%
4	LA	257	95%
5	LB	403	98%
6	LC	427	84% 14%
7	LD	297	98%
8	LE	288	9% 81% 18%

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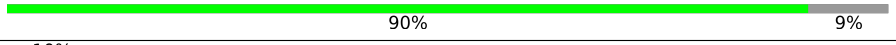
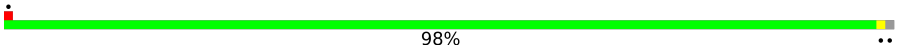
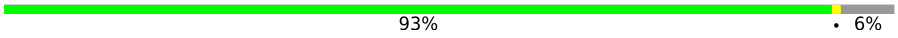
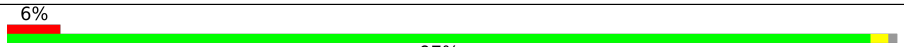
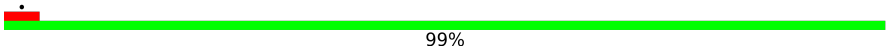
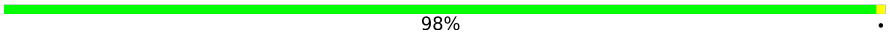
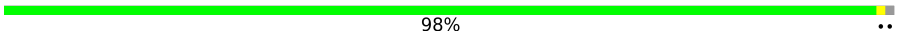
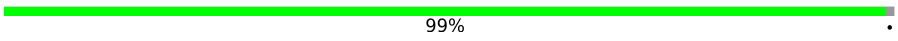
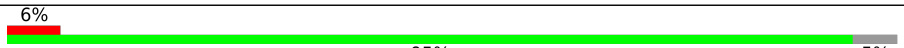
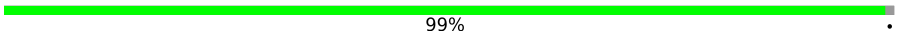
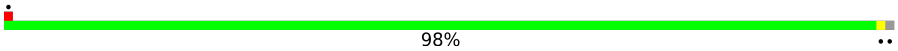
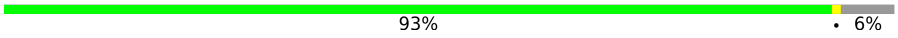
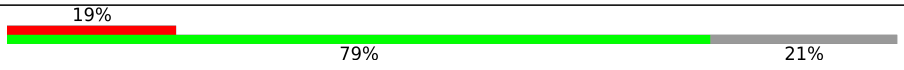
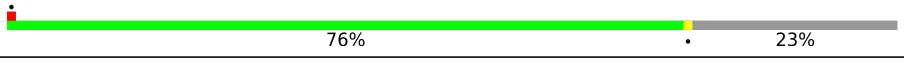
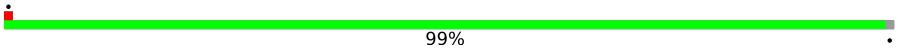
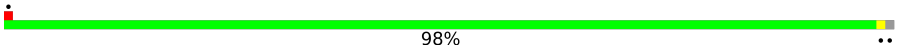
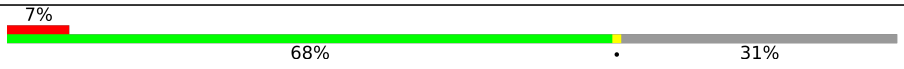
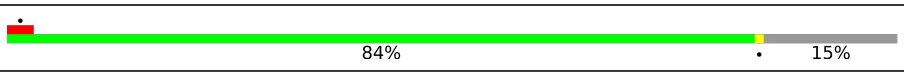
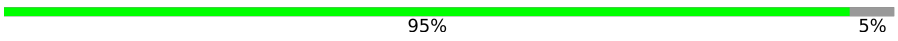
Mol	Chain	Length	Quality of chain
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	

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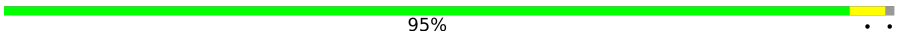
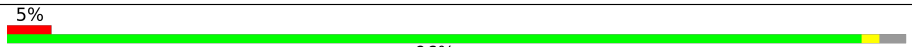
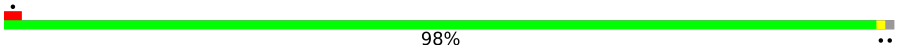
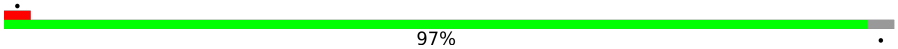
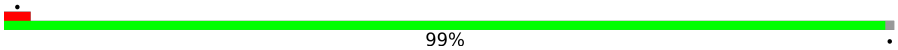
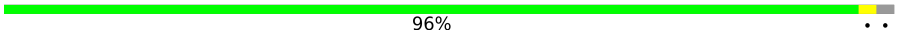
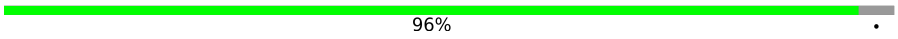
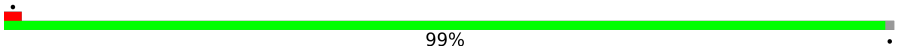
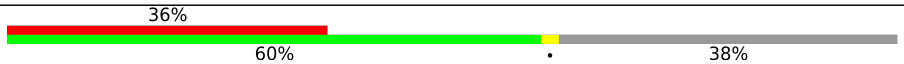
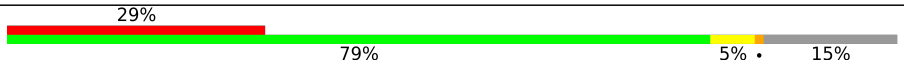
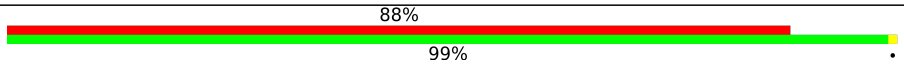
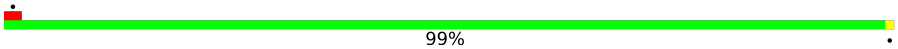
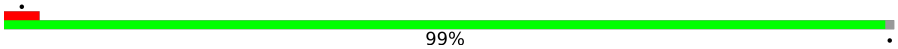
Mol	Chain	Length	Quality of chain
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	Ls	317	
47	Lt	165	
48	Lz	217	
49	S2	1869	
50	SA	295	
51	SB	264	
52	SD	243	
53	SE	263	
54	SF	204	
55	SH	194	
56	SI	208	
57	SK	165	
58	SL	158	

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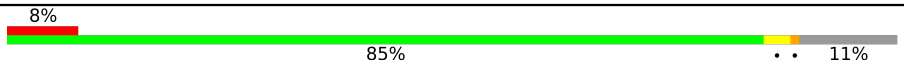
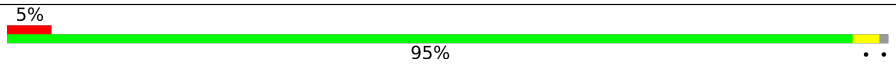
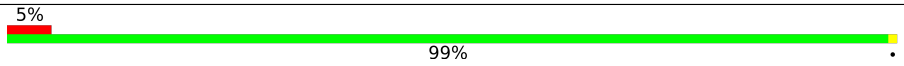
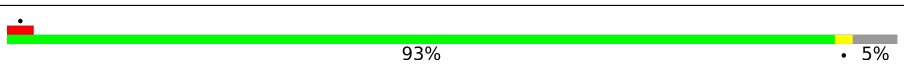
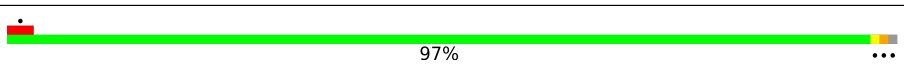
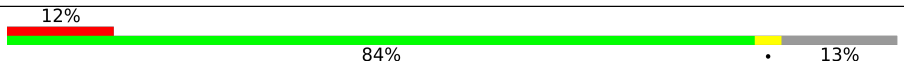
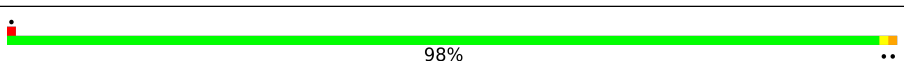
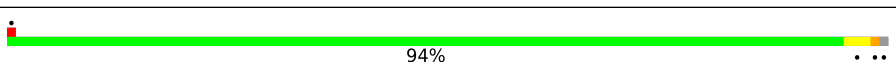
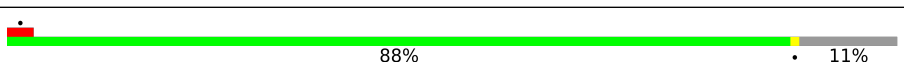
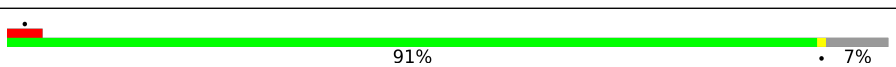
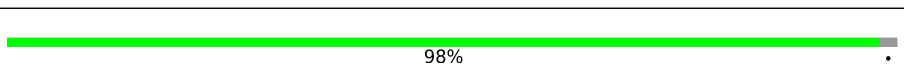
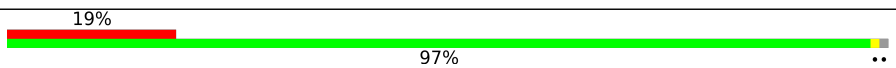
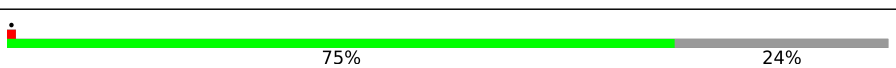
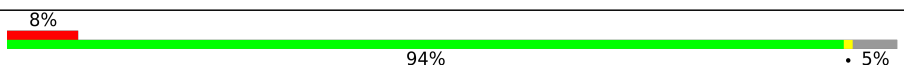
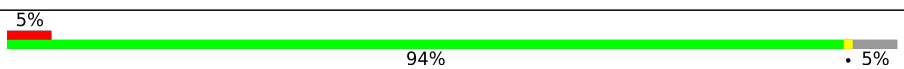
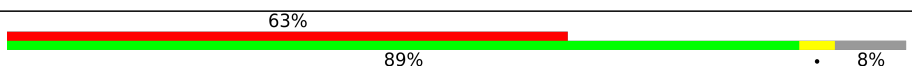
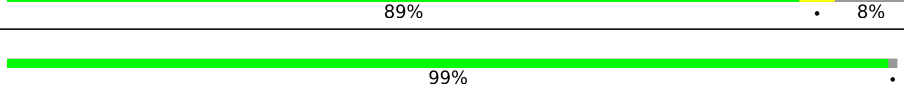
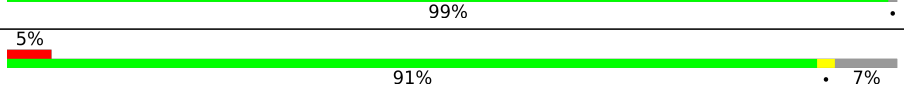
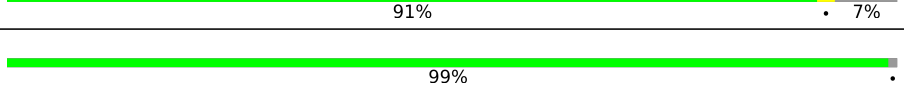
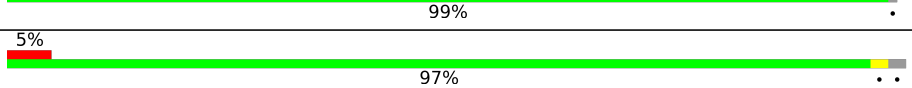
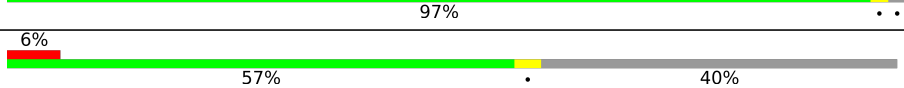
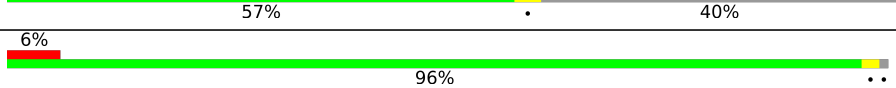
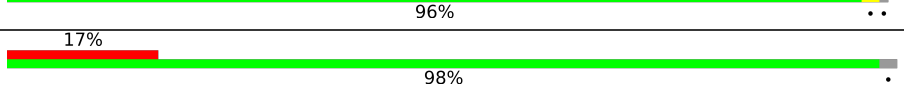
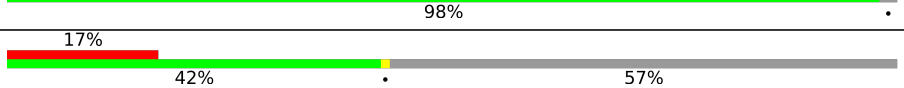
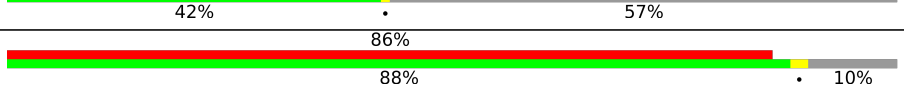
Mol	Chain	Length	Quality of chain
59	SP	145	
60	SQ	146	
61	SR	135	
62	SS	152	
63	ST	145	
64	SU	119	
65	SV	83	
66	SX	143	
67	Sa	115	
68	Sc	69	
69	Sd	56	
70	Sg	317	
71	SC	293	
72	SG	249	
73	SJ	194	
74	SM	132	
75	SN	151	
76	SO	151	
77	SW	130	
78	SY	133	
79	SZ	125	
80	Sb	84	
81	Se	59	
82	Sf	156	
83	CA	394	

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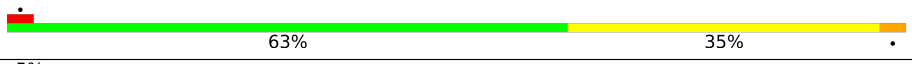
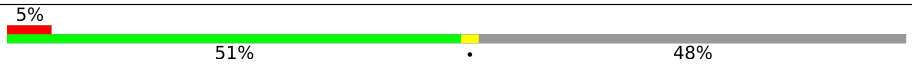
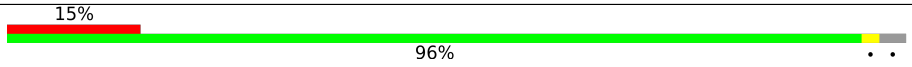
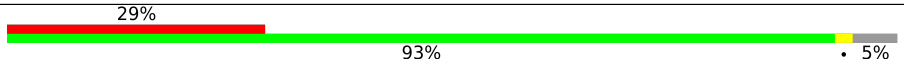
Mol	Chain	Length	Quality of chain
84	CC	75	
85	CE	223	
86	CF	180	
87	CI	599	
88	CH	437	

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 233375 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
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

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

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

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

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

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

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

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

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

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

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

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

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

- 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
21	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
49	S2	1740	Total	C	N	O	P	0	0
			36899	16459	6598	12103	1739		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
70	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			439	268	97	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
84	CC	75	Total	C	N	O	P	0	0
			1589	710	279	525	75		

- Molecule 85 is a protein called Coiled-coil domain-containing protein 124.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	CE	117	Total	C	N	O	S	0	0
			998	611	199	184	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
86	CF	29	Total	C	N	O	S	0	0
			239	145	43	50	1		

- Molecule 87 is a protein called ATP-binding cassette sub-family E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	CI	582	Total	C	N	O	S	0	0
			4586	2931	785	839	31		

- Molecule 88 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	CH	415	Total	C	N	O	S	0	0
			3257	2073	556	617	11		

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	L5	210	Total	Mg	0
			210	210	
89	L7	3	Total	Mg	0
			3	3	
89	L8	4	Total	Mg	0
			4	4	
89	LA	1	Total	Mg	0
			1	1	
89	LB	1	Total	Mg	0
			1	1	
89	LI	1	Total	Mg	0
			1	1	

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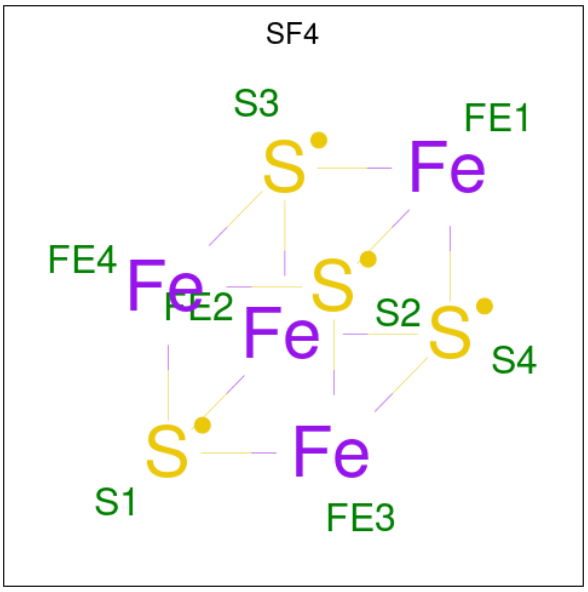
Mol	Chain	Residues	Atoms	AltConf
89	LP	1	Total Mg 1 1	0
89	LV	1	Total Mg 1 1	0
89	LX	1	Total Mg 1 1	0
89	Le	2	Total Mg 2 2	0
89	Lg	1	Total Mg 1 1	0
89	S2	29	Total Mg 29 29	0
89	SG	1	Total Mg 1 1	0

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

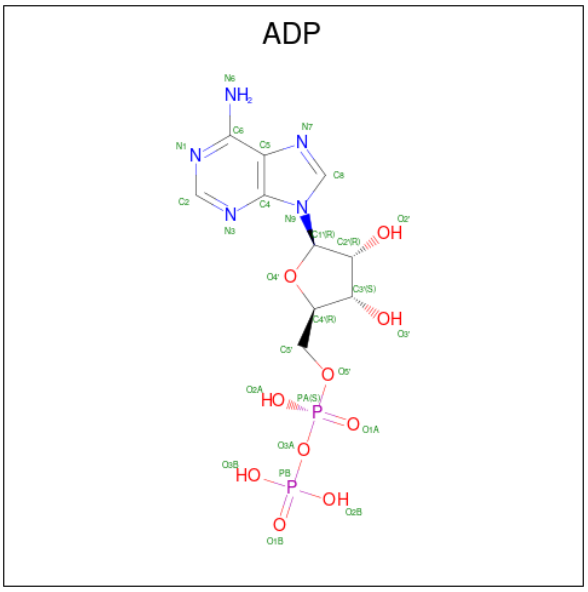
Mol	Chain	Residues	Atoms	AltConf
90	Lg	1	Total Zn 1 1	0
90	Lj	1	Total Zn 1 1	0
90	Lm	1	Total Zn 1 1	0
90	Lo	1	Total Zn 1 1	0
90	Lp	1	Total Zn 1 1	0
90	Sa	1	Total Zn 1 1	0
90	Sd	1	Total Zn 1 1	0
90	Sf	1	Total Zn 1 1	0

- Molecule 91 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
91	CI	1	Total	Fe	S	0
			16	8	8	
91	CI	1	Total	Fe	S	0
			16	8	8	

- Molecule 92 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



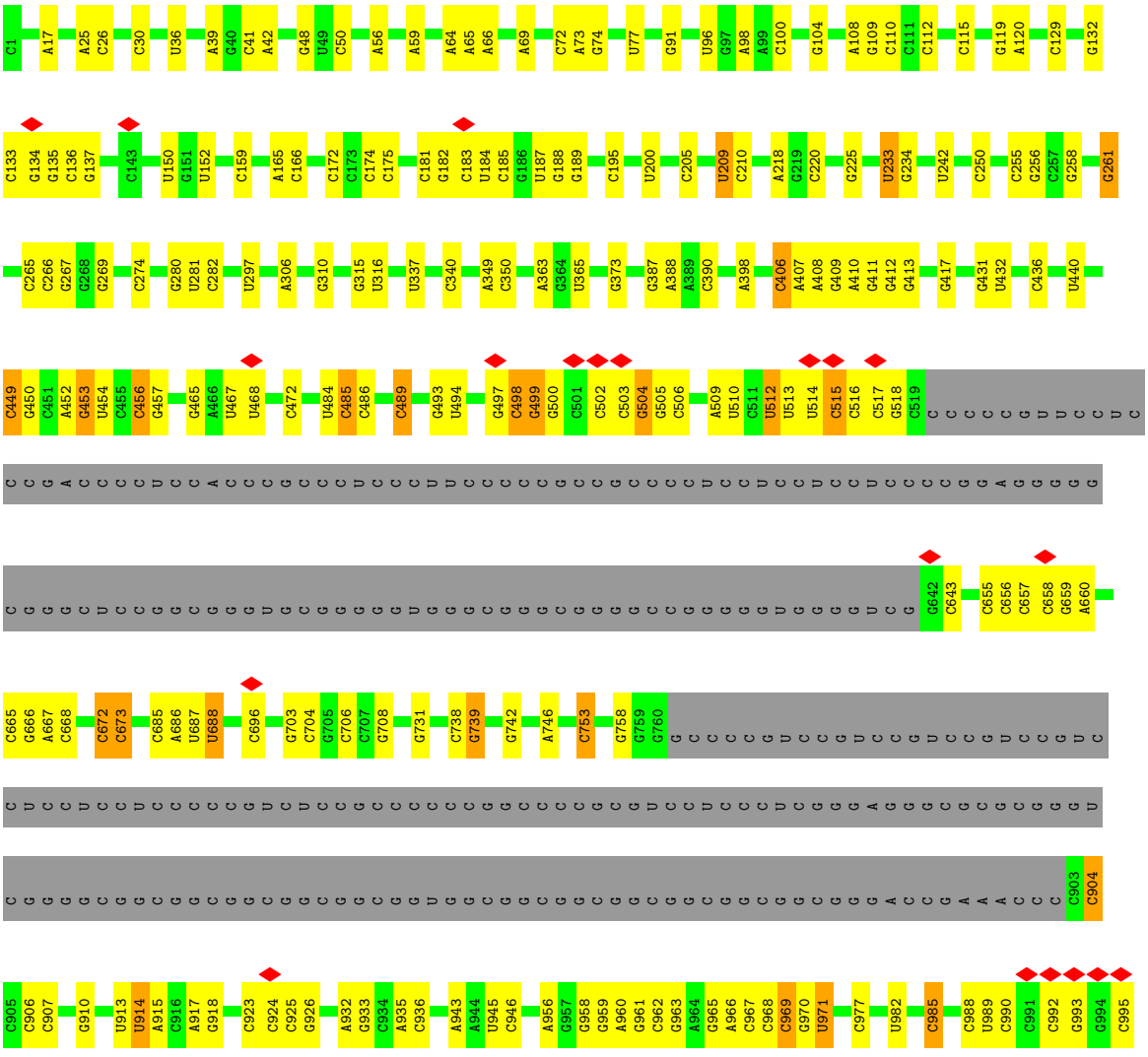
Mol	Chain	Residues	Atoms					AltConf
92	CI	1	Total	C	N	O	P	0
			27	10	5	10	2	

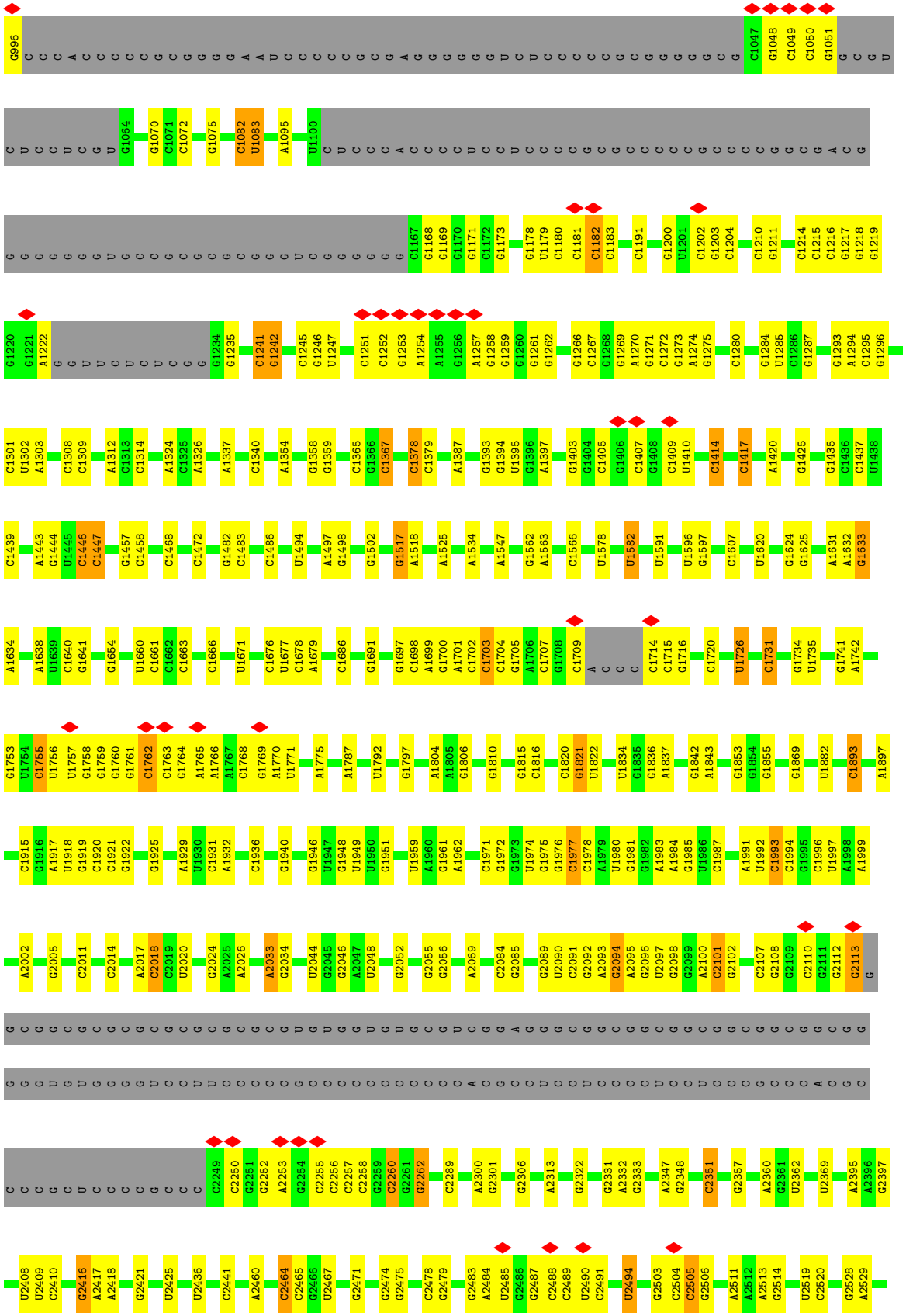
3 Residue-property plots (i)

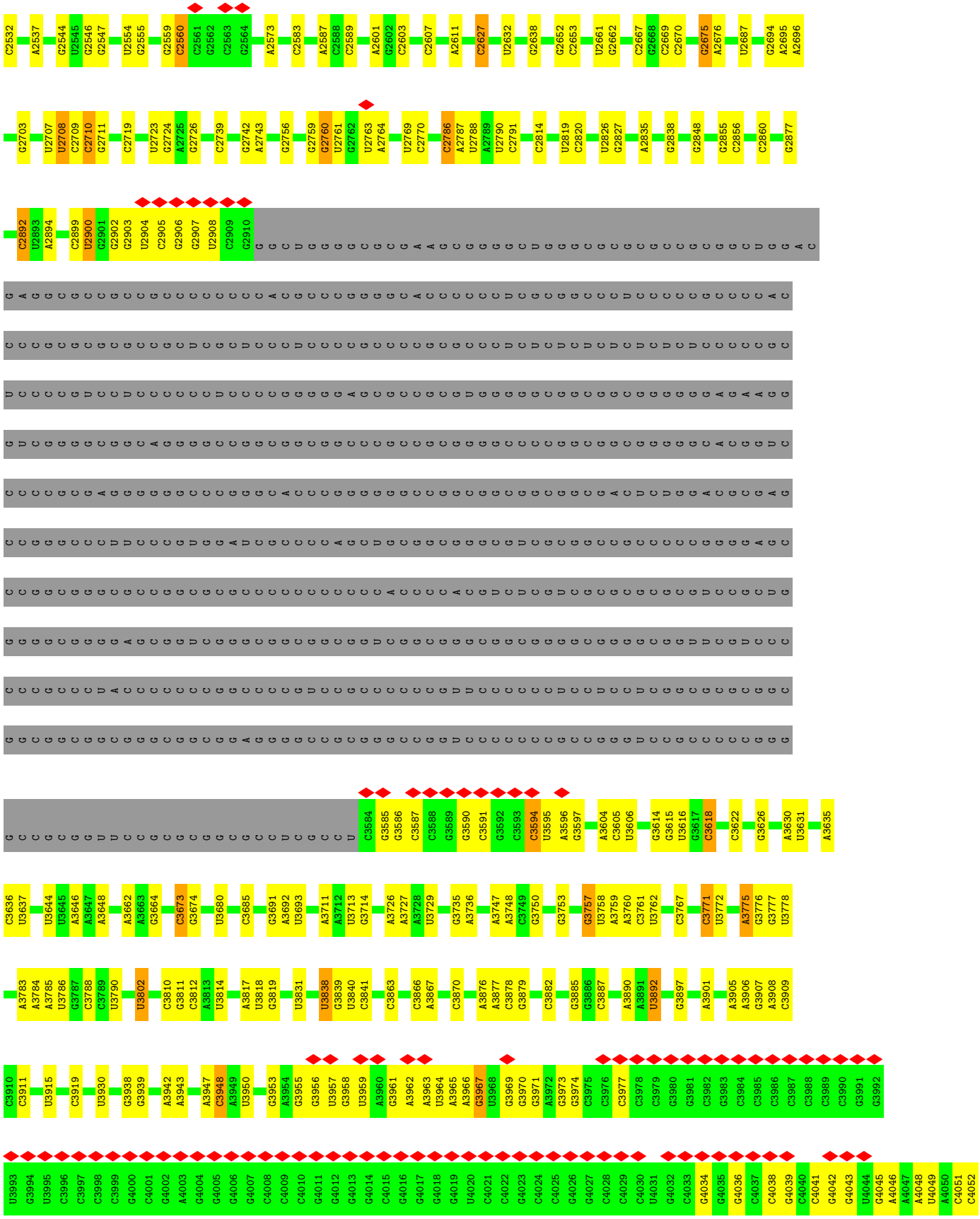
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

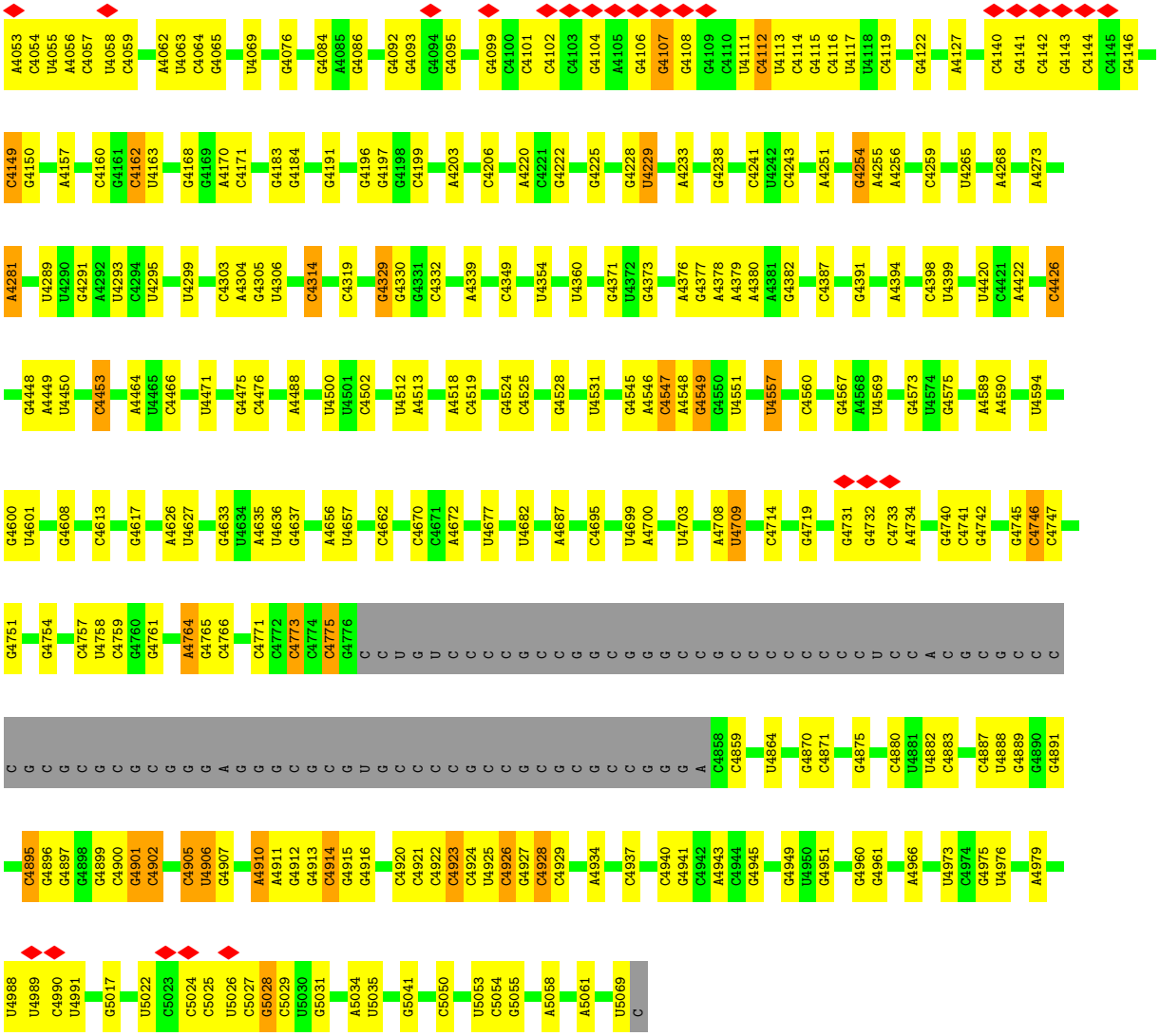
- Molecule 1: 28S ribosomal RNA

Chain L5:



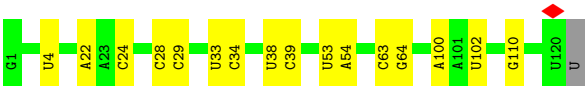



C2532 A2537 G2544 U2545 G2546 G2547 U2554 G2555 G2559 C2560 C2561 G2562 C2563 G2564 A2573 C2583 A2587 C2588 C2589 A2601 G2602 C2603 C2607 A2611 C2627 U2632 G2638 G2652 C2653 U2661 G2662 C2667 G2668 C2669 C2670 G2675 A2676 U2687 G2694 A2695 A2696
G2703 U2707 U2708 C2709 C2710 G2711 C2719 U2723 G2724 A2725 G2726 C2739 G2742 A2743 G2756 G2759 G2760 U2761 G2762 U2763 A2764 U2769 C2770 C2786 A2787 U2788 A2789 U2790 C2791 C2814 U2819 C2820 U2826 G2827 A2835 G2838 G2848 G2855 C2856 C2860 G2877
C2892 U2893 A2894 C2899 U2900 G2901 G2902 G2903 U2904 C2905 G2906 G2907 U2908 C2909 G2910
C3584 G3585 G3586 C3587 C3588 G3589 G3590 C3591 G3592 C3593 C3594 U3595 A3596 G3597 A3604 C3605 U3606 G3614 G3615 U3616 G3617 C3618 C3622 G3626 A3630 U3631 A3635
C3636 U3637 U3644 U3645 A3646 A3647 A3648 A3662 A3663 G3664 C3673 G3674 U3680 C3685 G3691 A3692 U3693 A3711 A3712 U3713 G3714 A3726 A3727 A3728 U3729 G3735 A3736 A3747 A3748 C3749 G3750 G3753 G3757 U3758 A3759 A3760 C3761 U3762 C3767 C3771 U3772 A3775 G3776 G3777 U3778
A3783 A3784 A3785 U3786 G3787 C3788 C3789 U3790 U3802 C3810 G3811 C3812 A3813 U3814 A3817 U3818 G3819 U3831 U3838 G3839 U3840 C3841 C3863 C3866 A3867 C3870 A3876 A3877 C3878 G3879 C3882 G3885 G3886 C3887 A3890 A3891 U3892 G3897 A3901 A3905 A3906 G3907 A3908 C3909
C3910 C3911 U3915 C3919 U3930 G3938 G3939 A3942 A3943 A3947 C3948 A3949 U3950 G3953 A3954 G3955 G3956 U3957 G3958 U3959 A3960 G3961 A3962 A3963 U3964 A3965 A3966 G3967 U3968 G3969 G3970 G3971 A3972 G3973 G3974 G3975 G3976 C3977 C3978 C3979 G3980 G3981 C3982 G3983 C3984 C3985 C3986 C3987 C3988 C3989 C3990 G3991 G3992
U3993 G3994 U3995 C3996 C3997 C3998 C3999 G4000 C4001 G4002 A4003 G4004 G4005 G4006 C4007 C4008 C4009 C4010 G4011 G4012 G4013 G4014 C4015 G4016 G4017 G4018 G4019 U4020 C4021 C4022 G4023 C4024 C4025 G4026 G4027 C4028 C4029 C4030 U4031 G4032 C4033 G4034 G4035 G4036 C4037 C4038 G4039 C4040 C4041 G4042 G4043 U4044 G4045 A4046 A4047 A4048 U4049 A4050 C4051 C4052



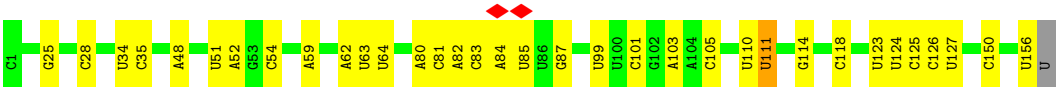
• Molecule 2: 5S ribosomal RNA

Chain L7:



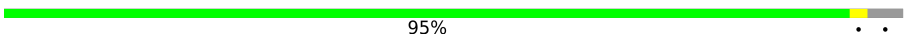
• Molecule 3: 5.8S ribosomal RNA

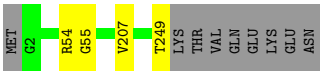
Chain L8:



• Molecule 4: 60S ribosomal protein L8

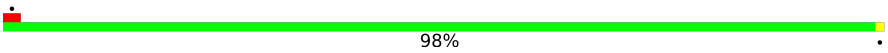
Chain LA:

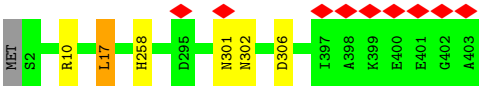




• Molecule 5: 60S ribosomal protein L3

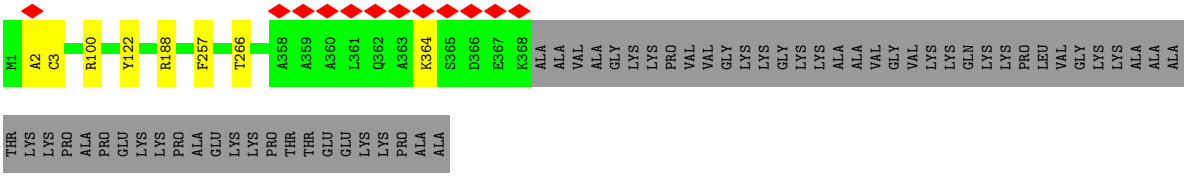
Chain LB:





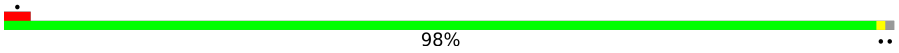
• Molecule 6: 60S ribosomal protein L4

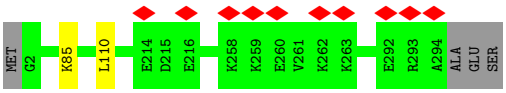
Chain LC:



• Molecule 7: 60S ribosomal protein L5

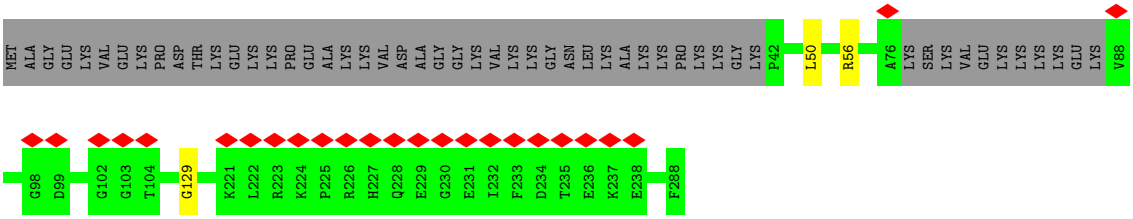
Chain LD:





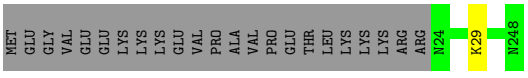
• Molecule 8: 60S ribosomal protein L6

Chain LE:



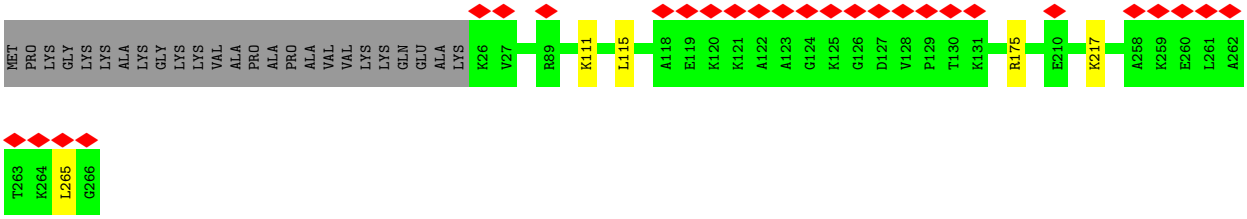
• Molecule 9: 60S ribosomal protein L7

Chain LF:



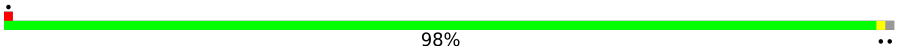
• Molecule 10: 60S ribosomal protein L7a

Chain LG:



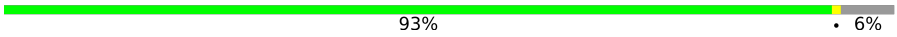
• Molecule 11: 60S ribosomal protein L9

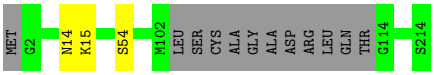
Chain LH:



• Molecule 12: 60S ribosomal protein L10-like

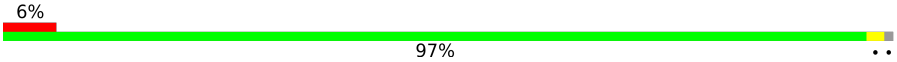
Chain LI:

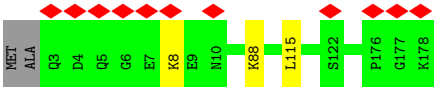




• Molecule 13: 60S ribosomal protein L11

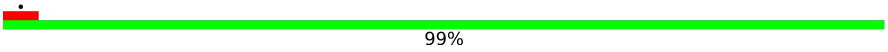
Chain LJ:

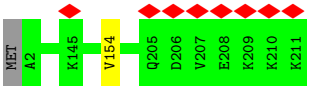




• Molecule 14: 60S ribosomal protein L13

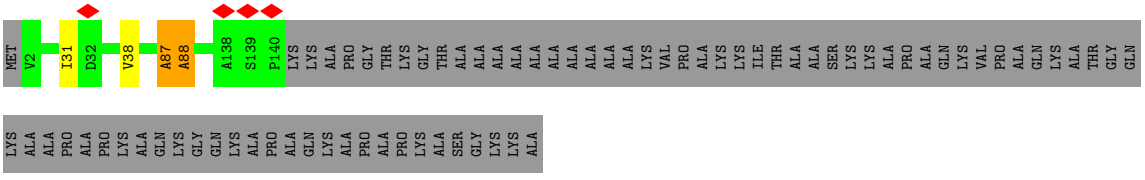
Chain LL:





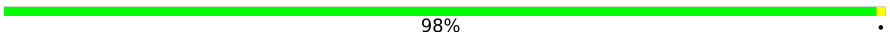
• Molecule 15: 60S ribosomal protein L14

Chain LM:



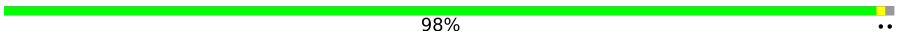
• Molecule 16: 60S ribosomal protein L15

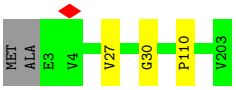
Chain LN:



• Molecule 17: 60S ribosomal protein L13a

Chain LO:



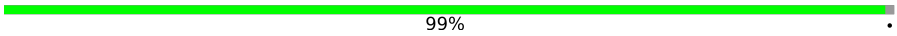


• Molecule 18: 60S ribosomal protein L17

Chain LP:

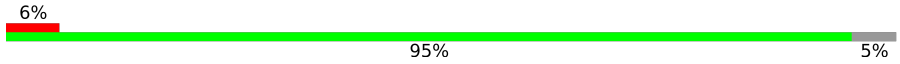
• Molecule 19: 60S ribosomal protein L18

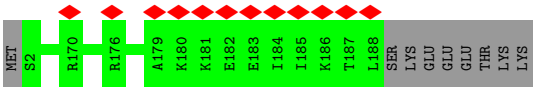
Chain LQ:



• Molecule 20: 60S ribosomal protein L19

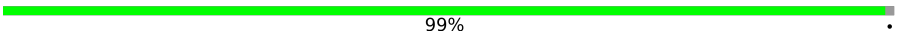
Chain LR:





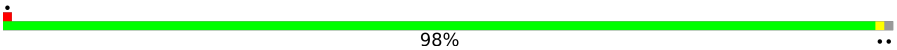
• Molecule 21: 60S ribosomal protein L18a

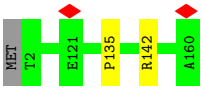
Chain LS:



• Molecule 22: 60S ribosomal protein L21

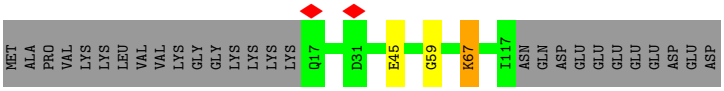
Chain LT:





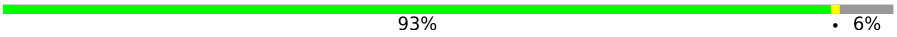
• Molecule 23: 60S ribosomal protein L22

Chain LU:



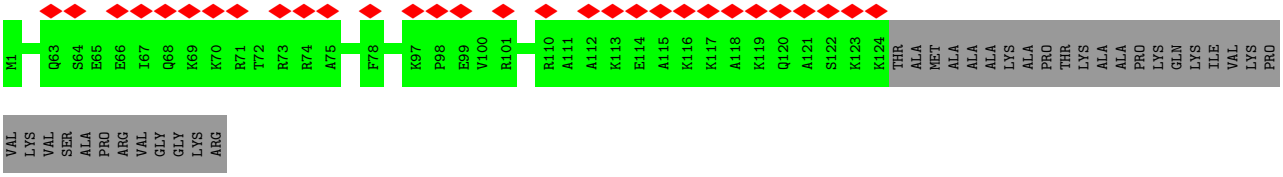
• Molecule 24: 60S ribosomal protein L23

Chain LV:



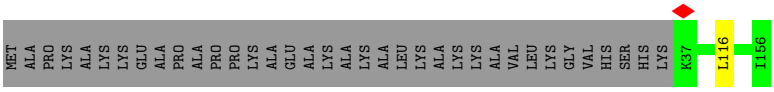
• Molecule 25: 60S ribosomal protein L24

Chain LW:



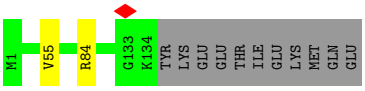
• Molecule 26: 60S ribosomal protein L23a

Chain LX:



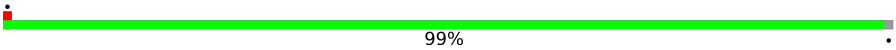
• Molecule 27: 60S ribosomal protein L26

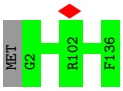
Chain LY:



• Molecule 28: 60S ribosomal protein L27

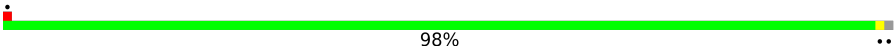
Chain LZ:

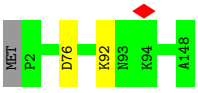




• Molecule 29: 60S ribosomal protein L27a

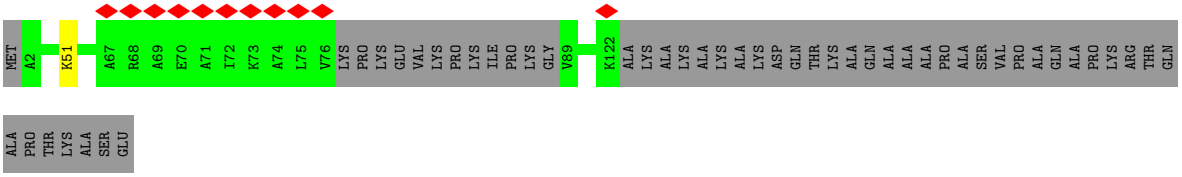
Chain La:





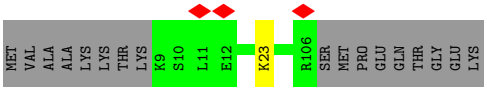
• Molecule 30: 60S ribosomal protein L29

Chain Lb:



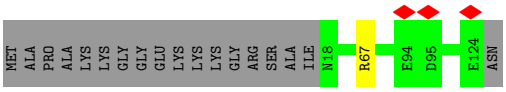
• Molecule 31: 60S ribosomal protein L30

Chain Lc:



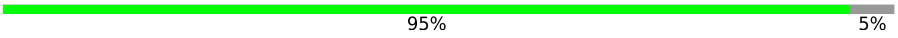
• Molecule 32: 60S ribosomal protein L31

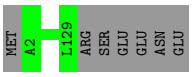
Chain Ld:



• Molecule 33: 60S ribosomal protein L32

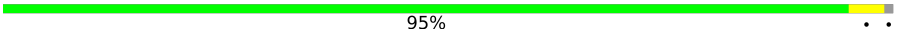
Chain Le:

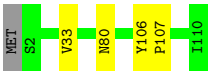




• Molecule 34: 60S ribosomal protein L35a

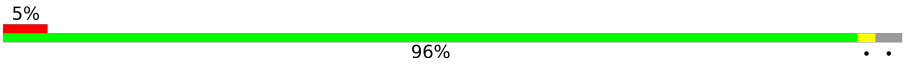
Chain Lf:

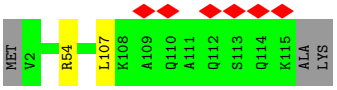




• Molecule 35: 60S ribosomal protein L34

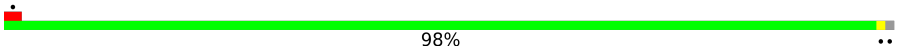
Chain Lg:

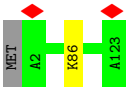




• Molecule 36: 60S ribosomal protein L35

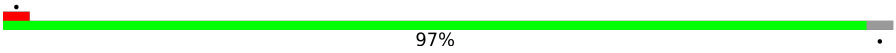
Chain Lh:

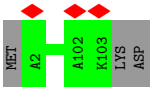




• Molecule 37: 60S ribosomal protein L36

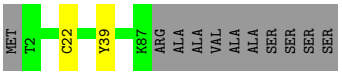
Chain Li:





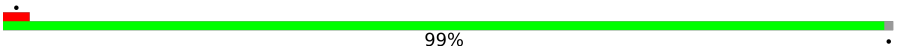
• Molecule 38: 60S ribosomal protein L37

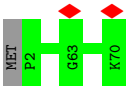
Chain Lj:



• Molecule 39: 60S ribosomal protein L38

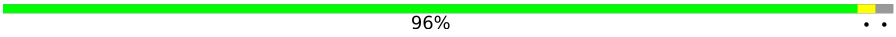
Chain Lk:





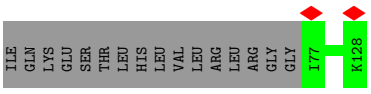
• Molecule 40: 60S ribosomal protein L39

Chain Ll:



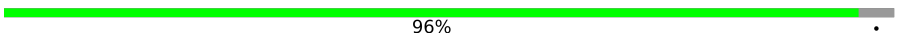
• Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:



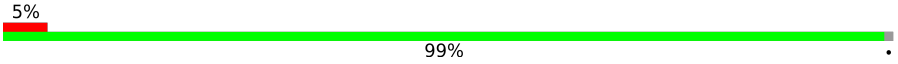
• Molecule 42: 60S ribosomal protein L41

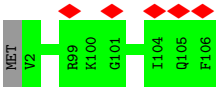
Chain Ln:



• Molecule 43: 60S ribosomal protein L36a

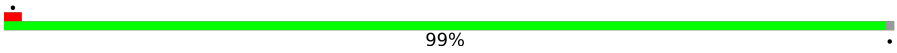
Chain Lo:

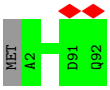




• Molecule 44: 60S ribosomal protein L37a

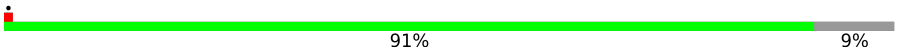
Chain Lp:

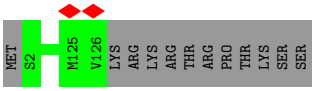




• Molecule 45: 60S ribosomal protein L28

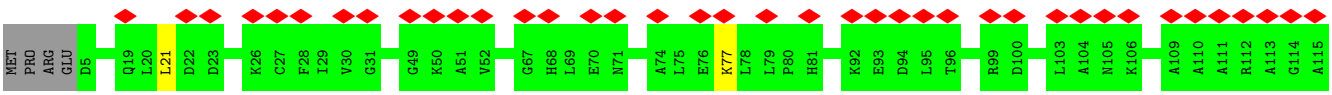
Chain Lr:

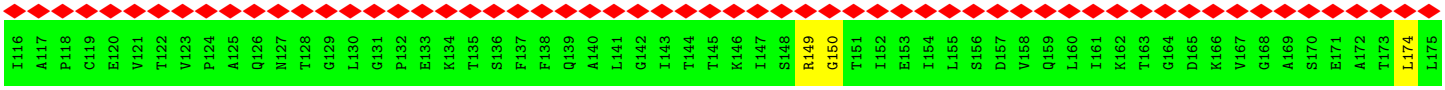


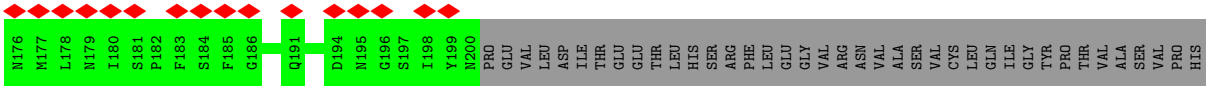


• Molecule 46: 60S acidic ribosomal protein P0

Chain Ls:

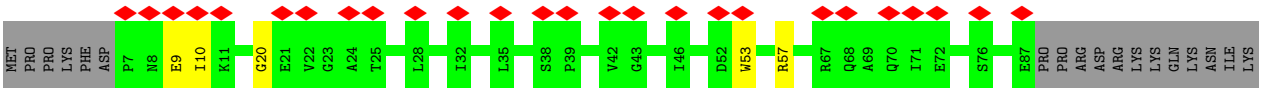


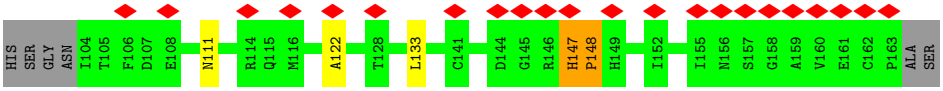




• Molecule 47: 60S ribosomal protein L12

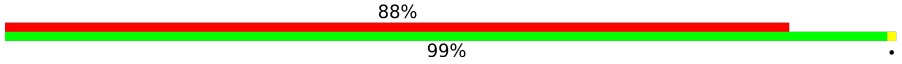
Chain Lt:

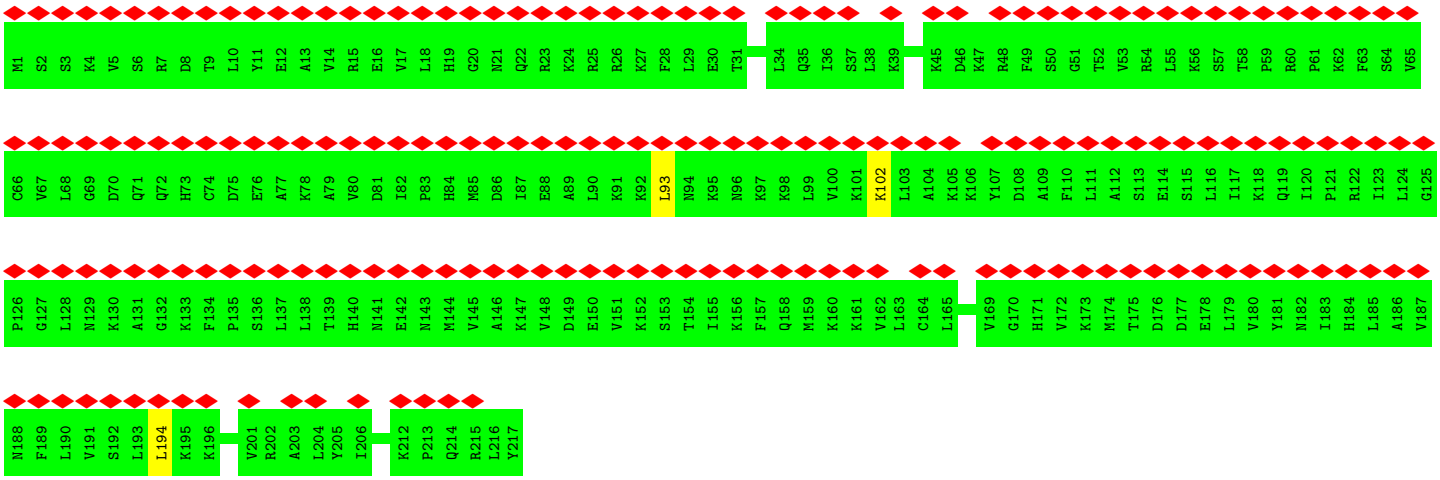




• Molecule 48: 60S ribosomal protein L10a

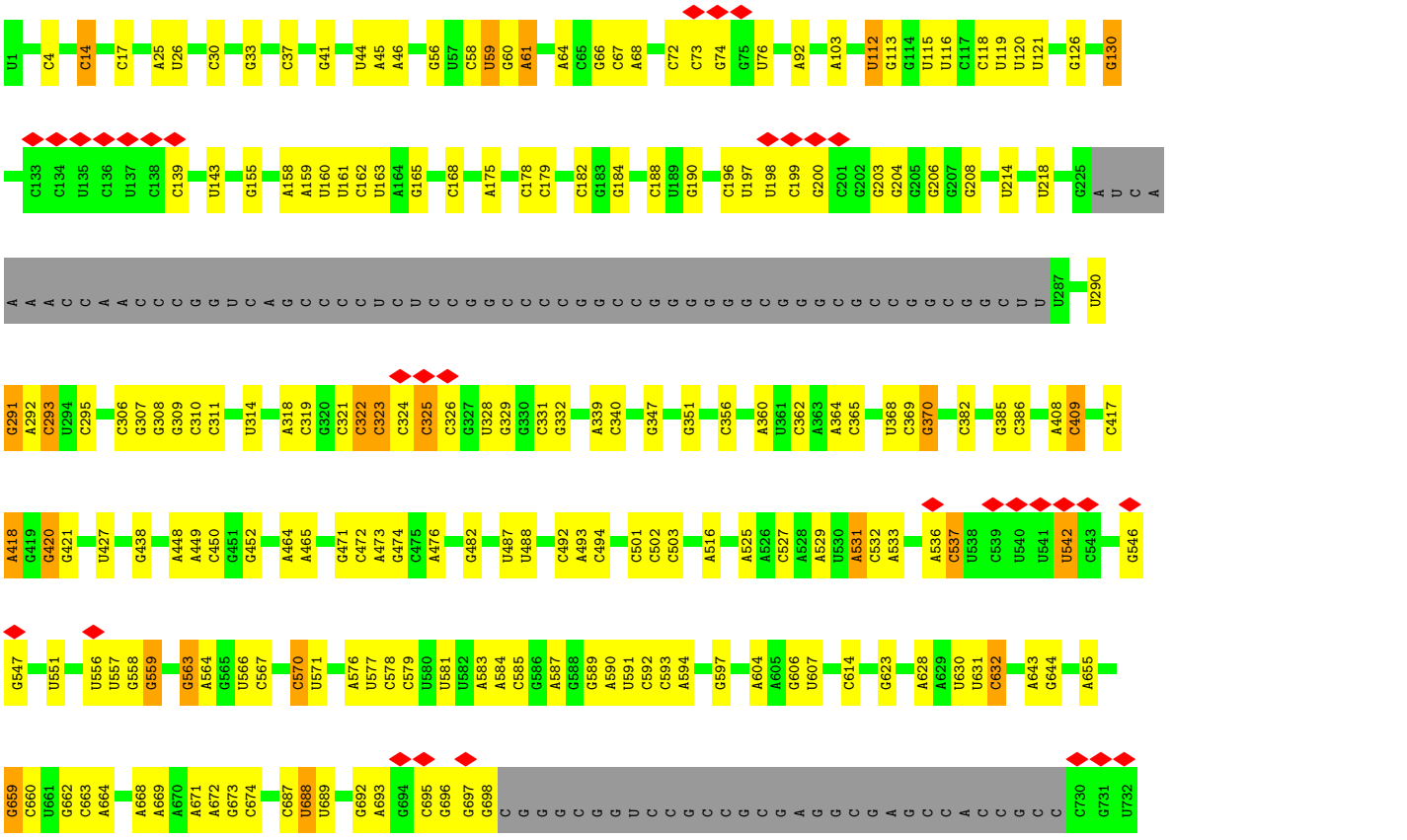
Chain Lz:

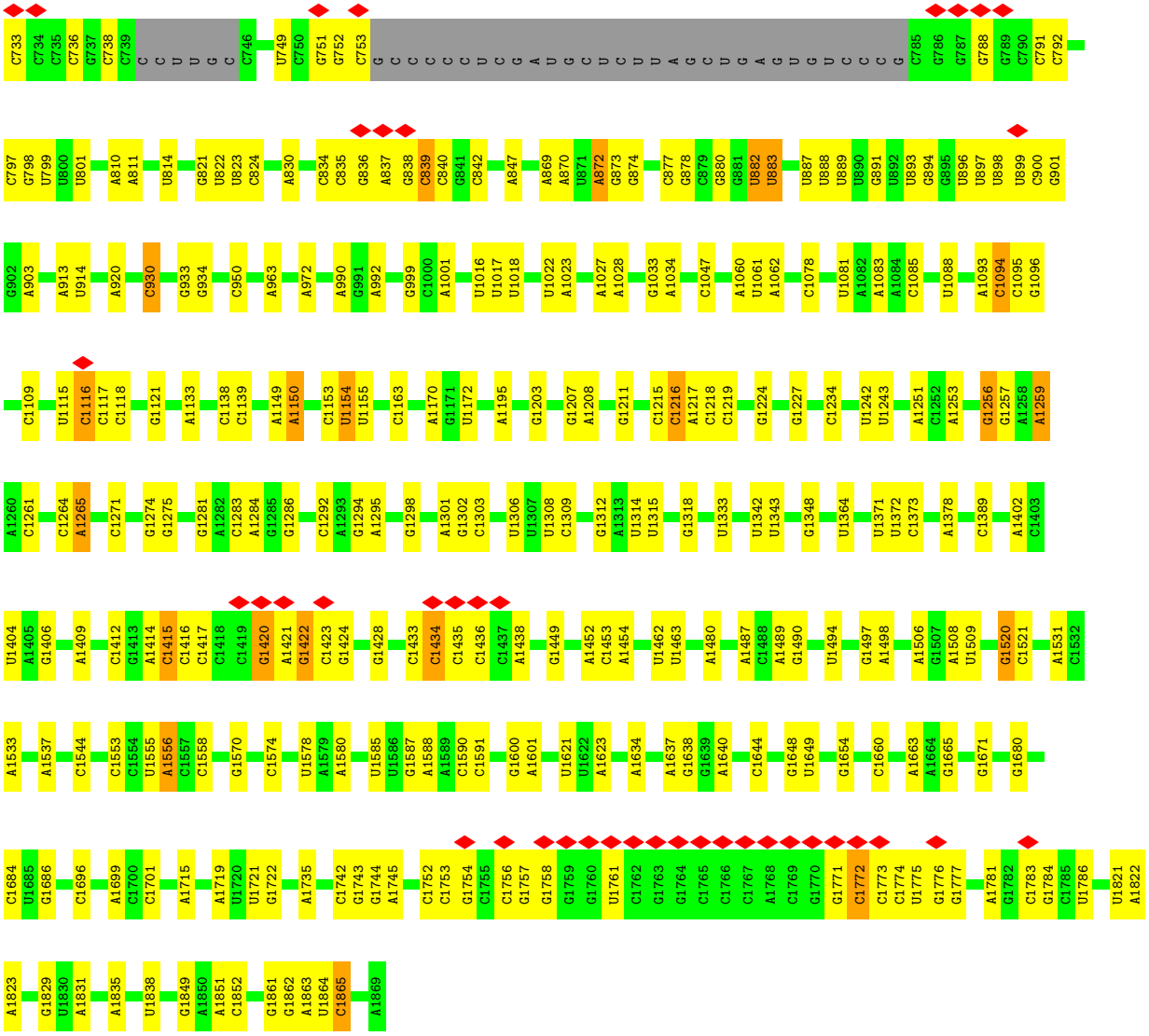




• Molecule 49: 18S ribosomal RNA

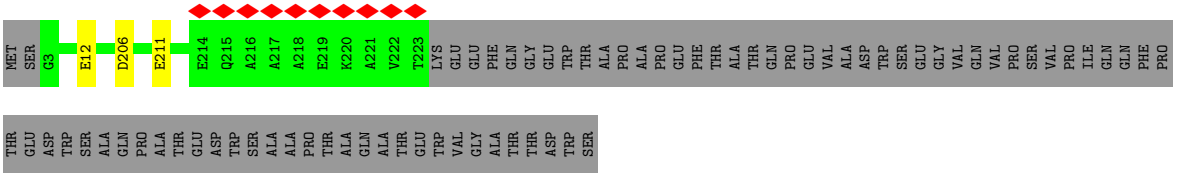
Chain S2:





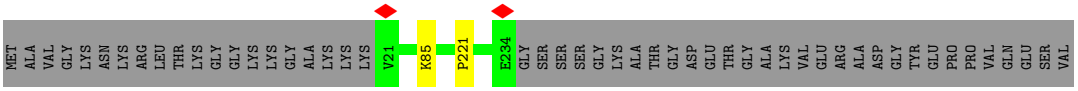
• Molecule 50: 40S ribosomal protein SA

Chain SA:



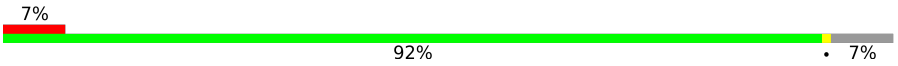
• Molecule 51: 40S ribosomal protein S3a

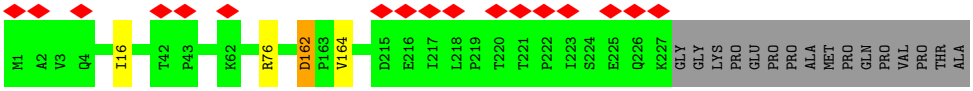
Chain SB:



• Molecule 52: 40S ribosomal protein S3

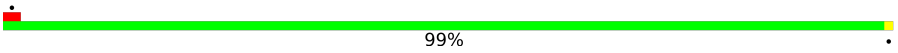
Chain SD:

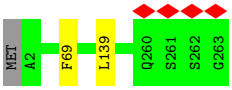




• Molecule 53: 40S ribosomal protein S4, X isoform

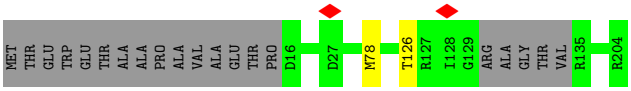
Chain SE:





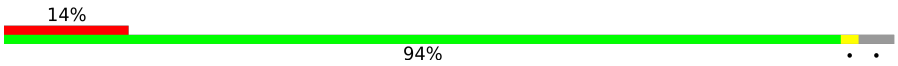
• Molecule 54: 40S ribosomal protein S5

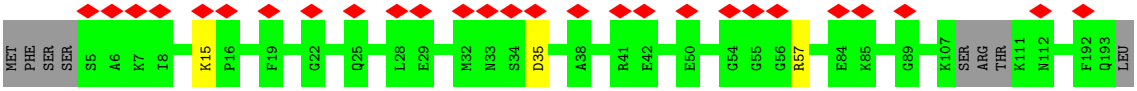
Chain SF:



• Molecule 55: 40S ribosomal protein S7

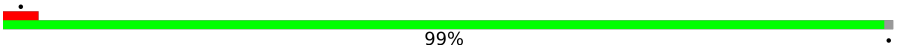
Chain SH:

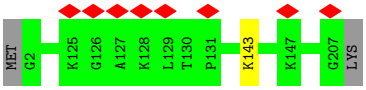




• Molecule 56: 40S ribosomal protein S8

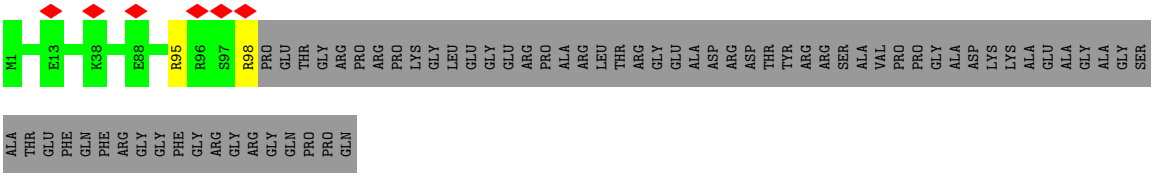
Chain SI:





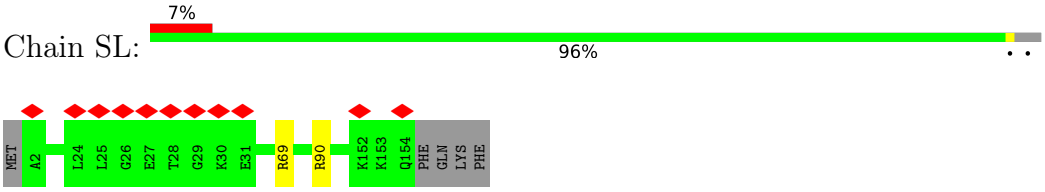
• Molecule 57: 40S ribosomal protein S10

Chain SK:



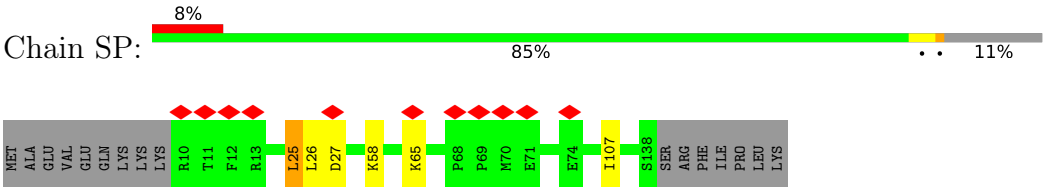
• Molecule 58: 40S ribosomal protein S11

Chain SL:



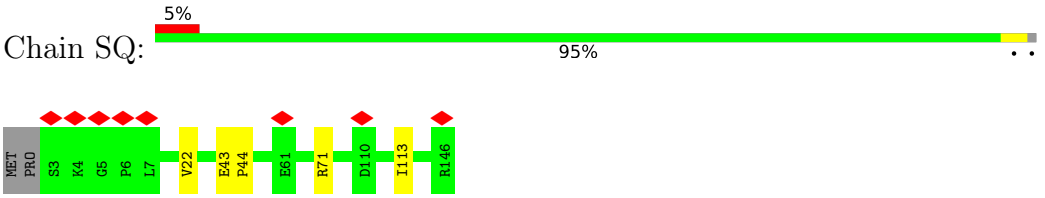
• Molecule 59: 40S ribosomal protein S15

Chain SP:



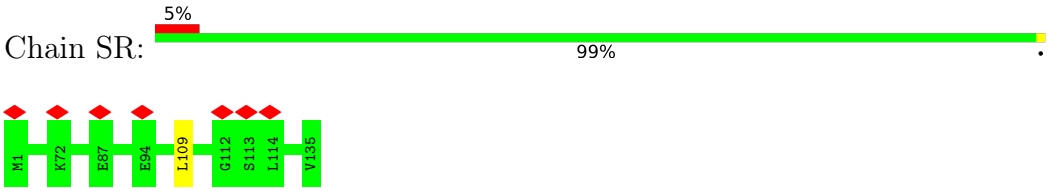
• Molecule 60: 40S ribosomal protein S16

Chain SQ:



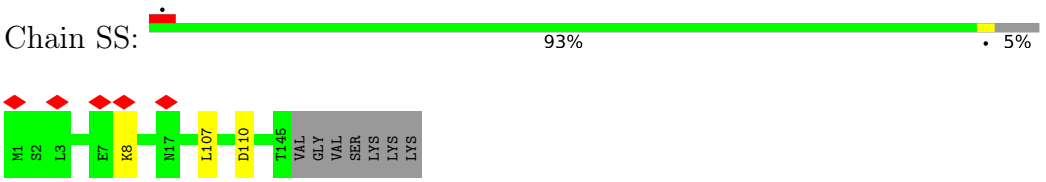
• Molecule 61: 40S ribosomal protein S17

Chain SR:



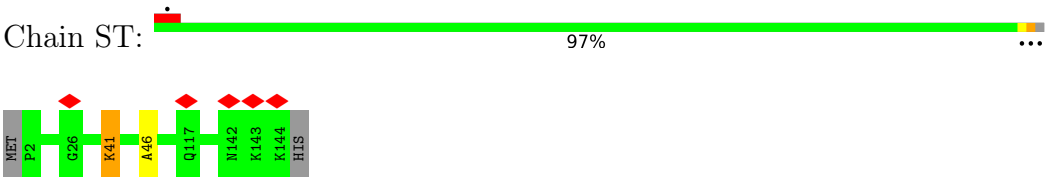
• Molecule 62: 40S ribosomal protein S18

Chain SS:



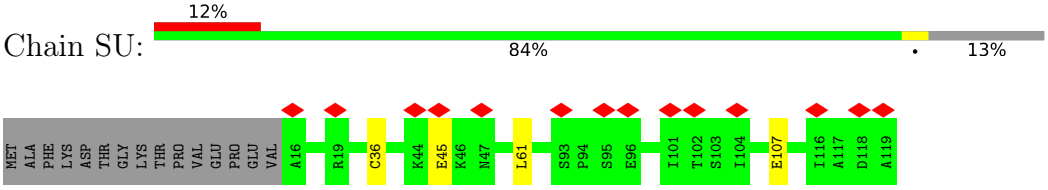
• Molecule 63: 40S ribosomal protein S19

Chain ST:



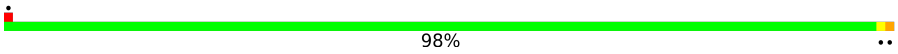
• Molecule 64: 40S ribosomal protein S20

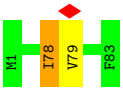
Chain SU:



• Molecule 65: 40S ribosomal protein S21

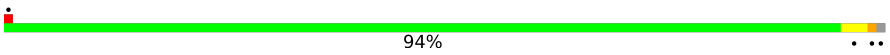
Chain SV:

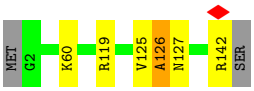




• Molecule 66: 40S ribosomal protein S23

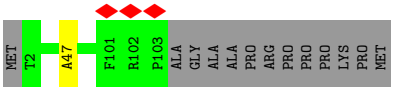
Chain SX:





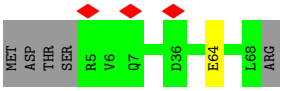
• Molecule 67: 40S ribosomal protein S26

Chain Sa:



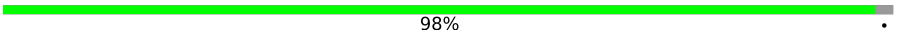
• Molecule 68: 40S ribosomal protein S28

Chain Sc:



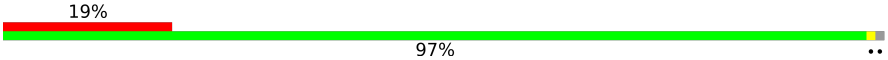
• Molecule 69: 40S ribosomal protein S29

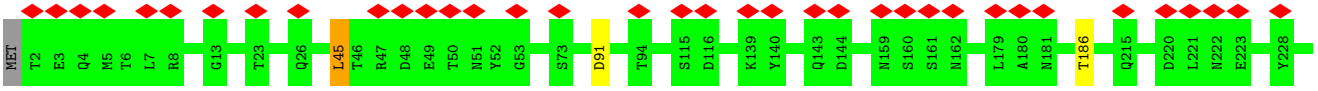
Chain Sd:

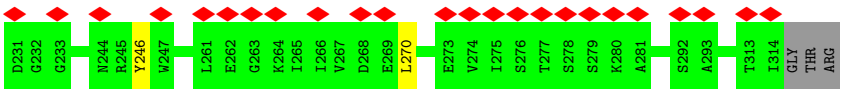


• Molecule 70: Receptor of activated protein C kinase 1

Chain Sg:

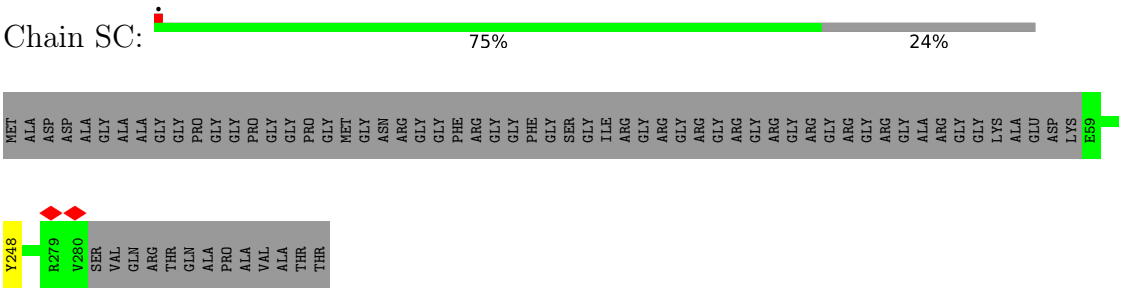






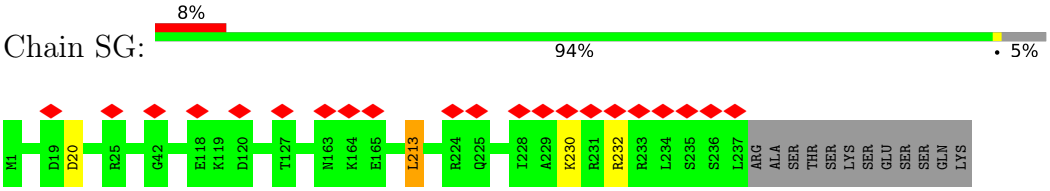
• Molecule 71: 40S ribosomal protein S2

Chain SC:



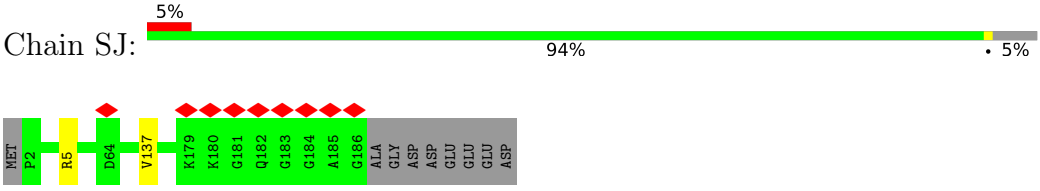
• Molecule 72: 40S ribosomal protein S6

Chain SG:



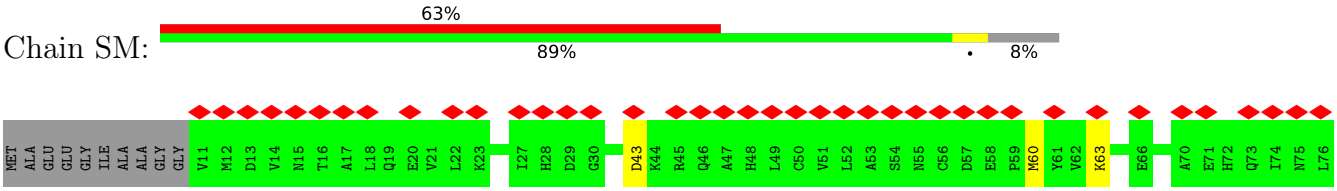
• Molecule 73: 40S ribosomal protein S9

Chain SJ:



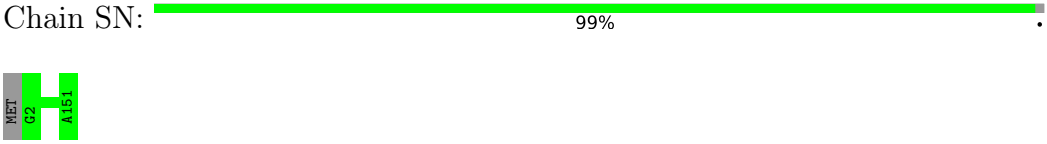
• Molecule 74: 40S ribosomal protein S12

Chain SM:



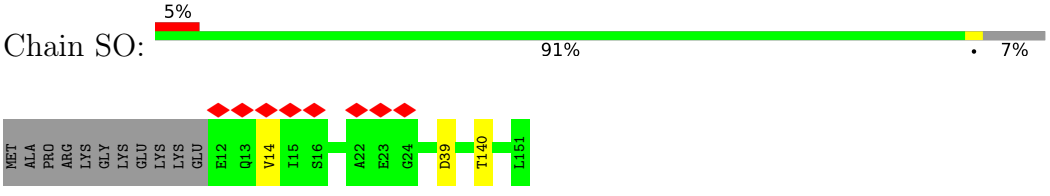
• Molecule 75: 40S ribosomal protein S13

Chain SN:



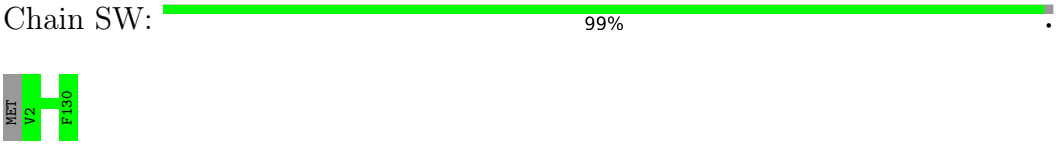
• Molecule 76: 40S ribosomal protein S14

Chain SO:



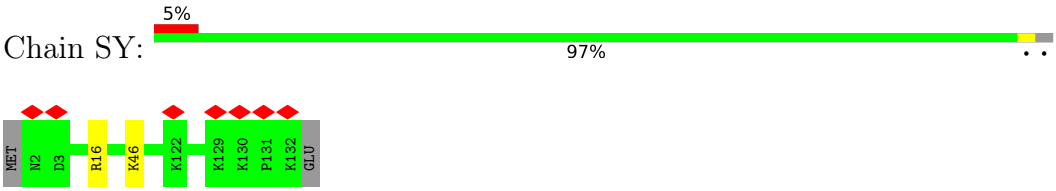
• Molecule 77: 40S ribosomal protein S15a

Chain SW:



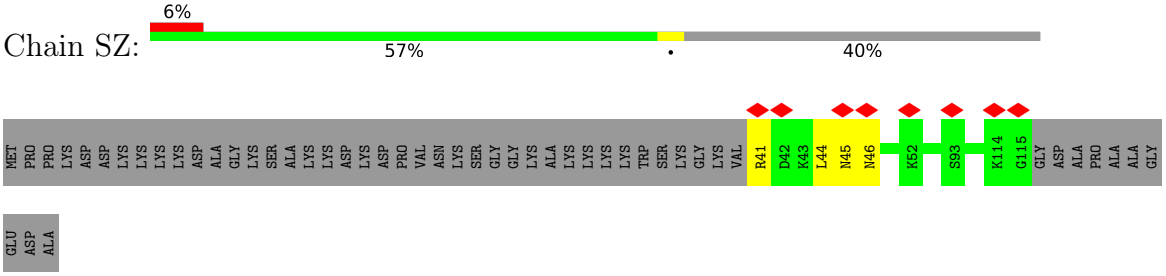
• Molecule 78: 40S ribosomal protein S24

Chain SY:



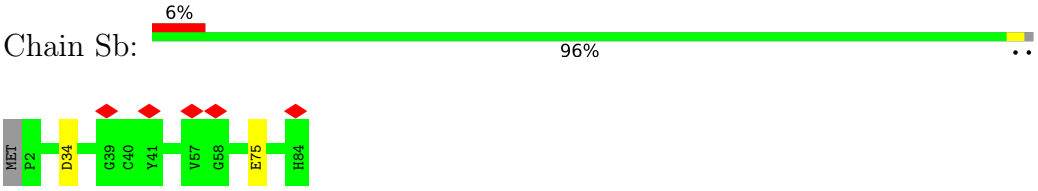
• Molecule 79: 40S ribosomal protein S25

Chain SZ:



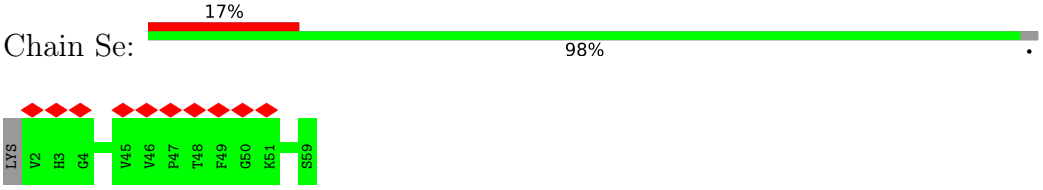
• Molecule 80: 40S ribosomal protein S27

Chain Sb:



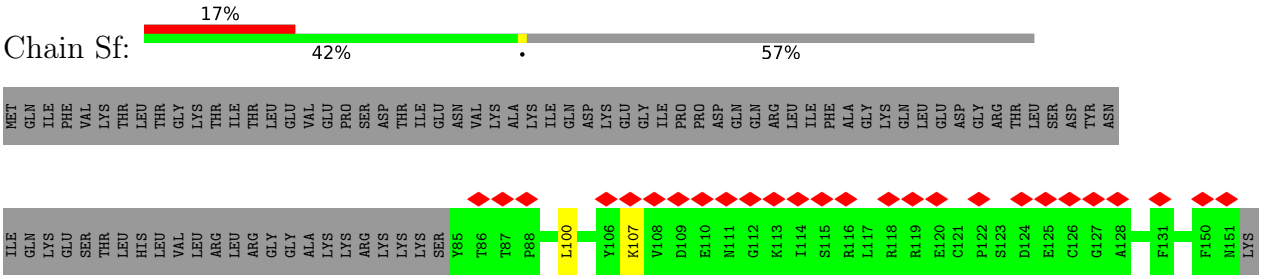
• Molecule 81: 40S ribosomal protein S30

Chain Se:



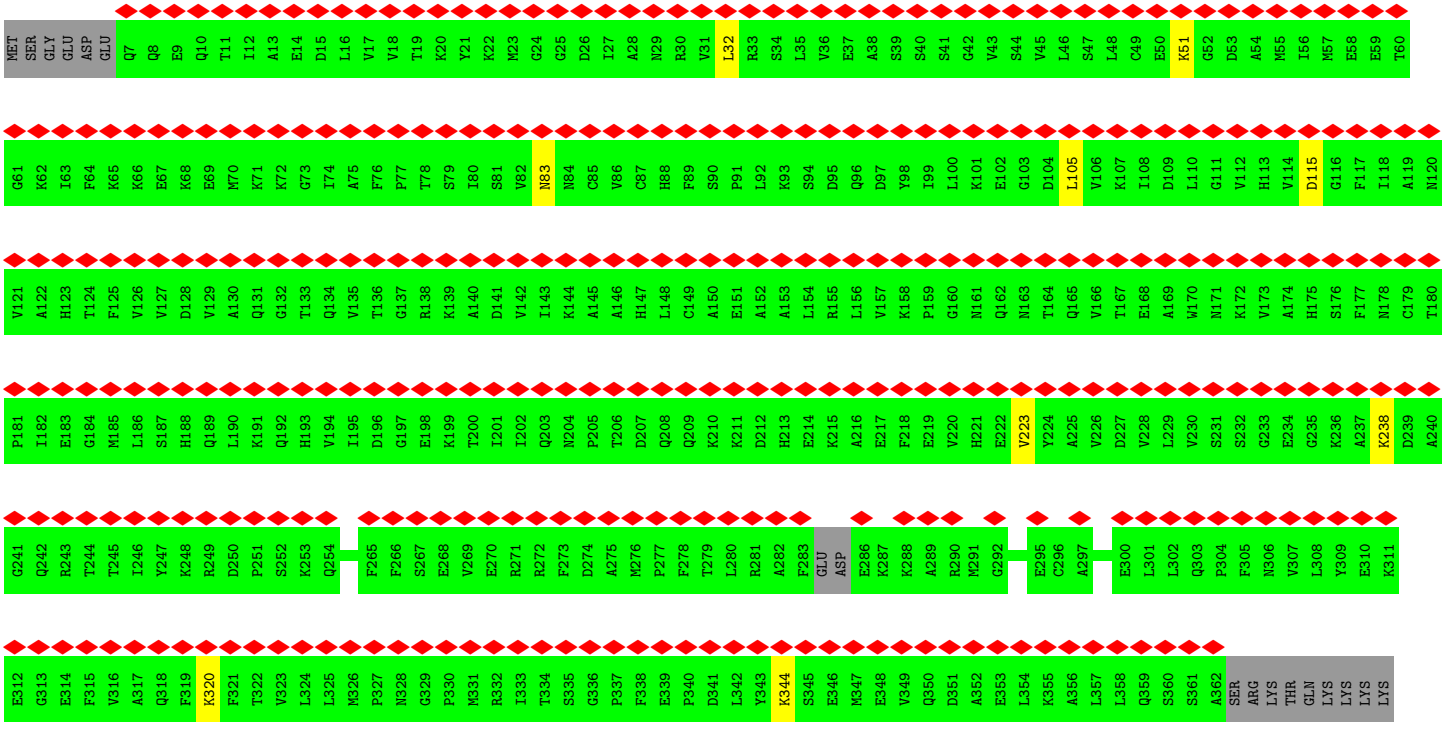
• Molecule 82: Ubiquitin-40S ribosomal protein S27a

Chain Sf:



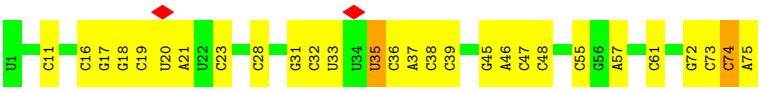
• Molecule 83: Proliferation-associated protein 2G4

Chain CA:



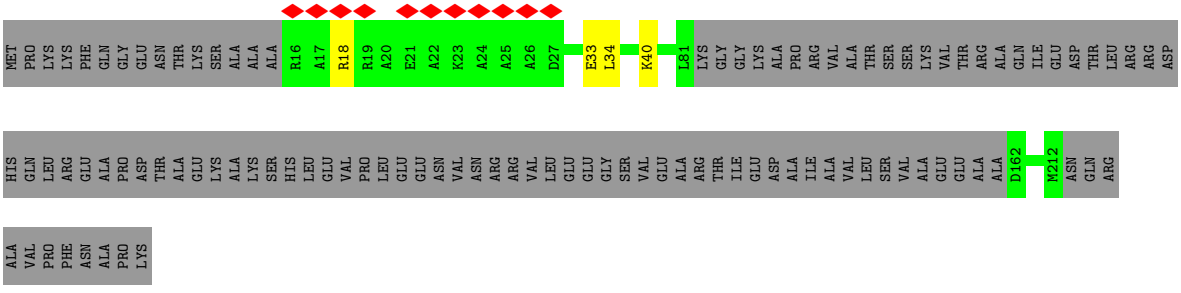
• Molecule 84: tRNA

Chain CC:



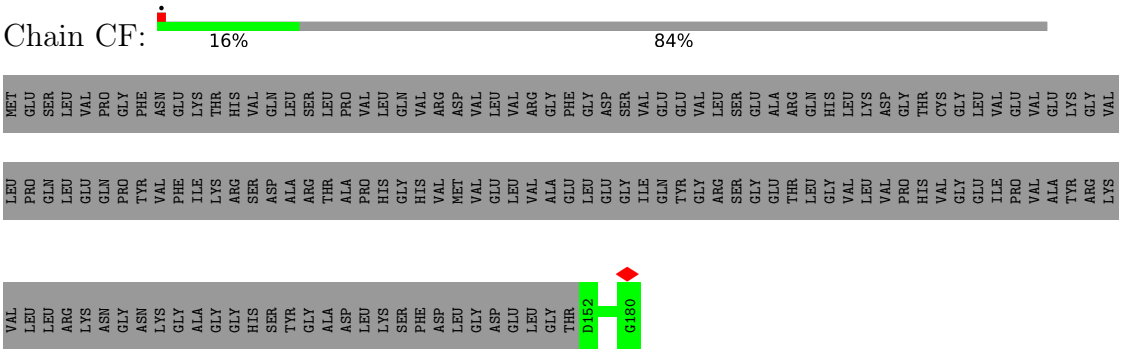
• Molecule 85: Coiled-coil domain-containing protein 124

Chain CE:



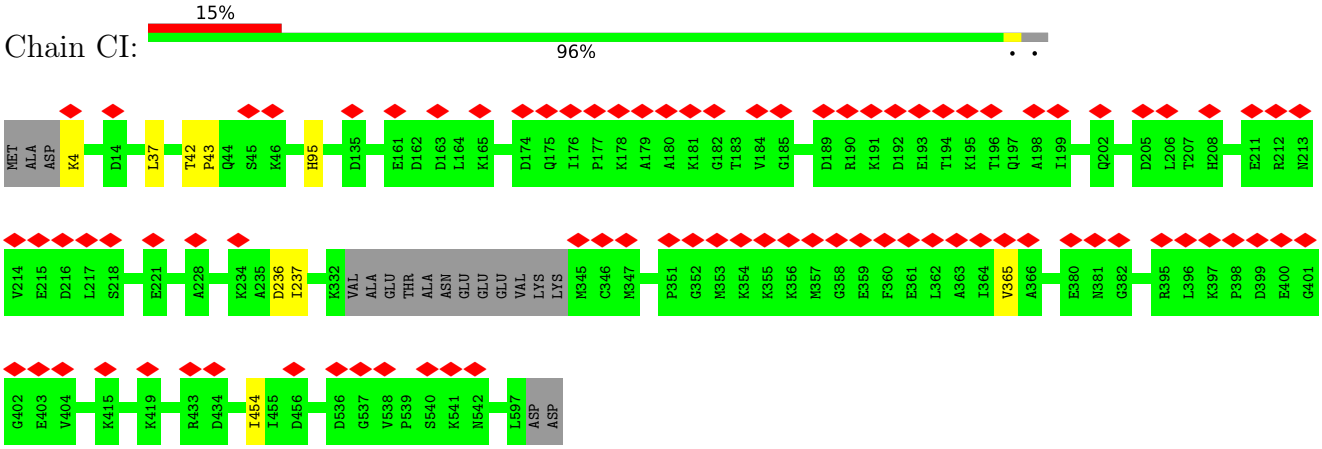
• Molecule 86: Non-structural protein 1

Chain CF:



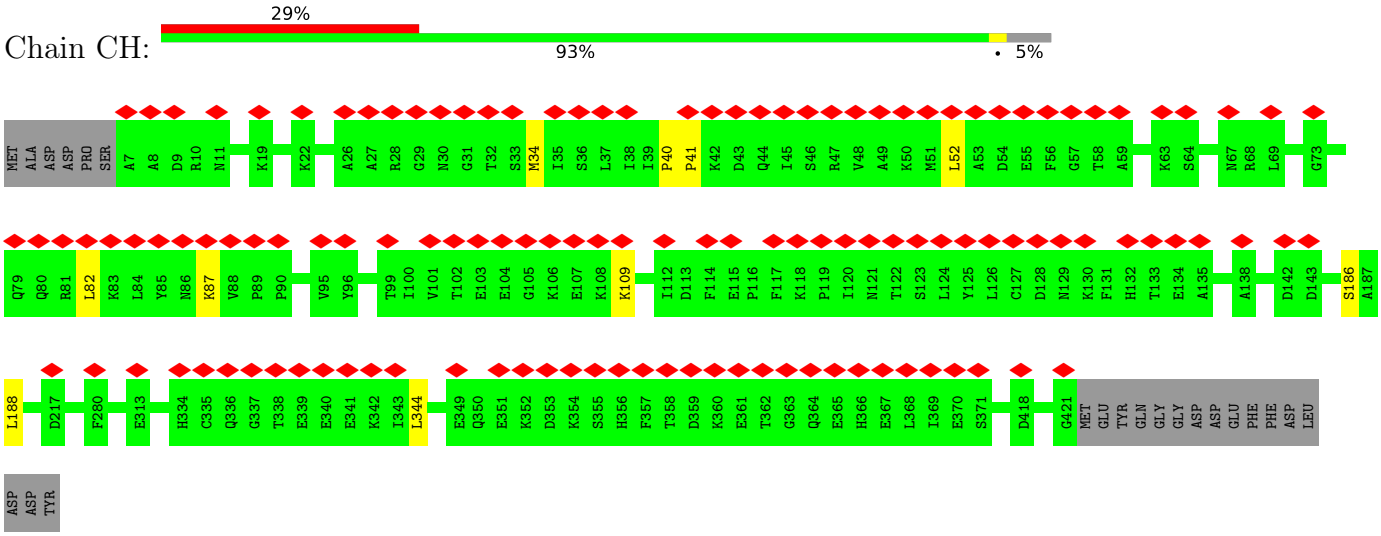
• Molecule 87: ATP-binding cassette sub-family E member 1

Chain CI:



• Molecule 88: Eukaryotic peptide chain release factor subunit 1

Chain CH:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13337	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	0.457	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.004	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP, MG, SF4

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	0.68	3/89595 (0.0%)	1.12	547/139686 (0.4%)
2	L7	0.61	0/2861	1.06	13/4459 (0.3%)
3	L8	0.66	0/3701	1.02	13/5766 (0.2%)
4	LA	0.43	0/1936	0.63	0/2596
5	LB	0.38	0/3306	0.60	2/4424 (0.0%)
6	LC	0.38	0/2981	0.59	2/4002 (0.0%)
7	LD	0.34	0/2428	0.54	1/3252 (0.0%)
8	LE	0.32	0/1942	0.57	1/2606 (0.0%)
9	LF	0.40	0/1905	0.55	0/2539
10	LG	0.34	0/1960	0.56	1/2637 (0.0%)
11	LH	0.35	0/1537	0.55	0/2066
12	LI	0.36	0/1673	0.54	0/2233
13	LJ	0.32	0/1433	0.61	1/1915 (0.1%)
14	LL	0.35	0/1732	0.54	0/2315
15	LM	0.36	0/1161	0.55	1/1554 (0.1%)
16	LN	0.41	0/1746	0.57	1/2338 (0.0%)
17	LO	0.38	0/1682	0.50	0/2250
18	LP	0.39	0/1268	0.50	0/1701
19	LQ	0.39	0/1537	0.51	0/2052
20	LR	0.34	0/1582	0.53	0/2091
21	LS	0.38	0/1493	0.50	0/2003
22	LT	0.39	0/1326	0.57	0/1770
23	LU	0.35	0/839	0.64	0/1126
24	LV	0.37	0/993	0.57	0/1332
25	LW	0.36	0/1030	0.55	0/1364
26	LX	0.34	0/1002	0.53	1/1345 (0.1%)
27	LY	0.35	0/1132	0.53	0/1504
28	LZ	0.37	0/1130	0.50	0/1507
29	La	0.38	0/1191	0.52	0/1591
30	Lb	0.30	0/889	0.52	0/1175
31	Lc	0.38	0/774	0.54	0/1038
32	Ld	0.36	0/903	0.55	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Le	0.40	0/1071	0.55	0/1429
34	Lf	0.41	0/895	0.57	0/1198
35	Lg	0.38	0/916	0.56	1/1220 (0.1%)
36	Lh	0.31	0/1023	0.49	0/1351
37	Li	0.31	0/843	0.49	0/1115
38	Lj	0.41	0/720	0.59	0/952
39	Lk	0.33	0/575	0.52	0/761
40	Ll	0.34	0/454	0.54	0/599
41	Lm	0.36	0/435	0.51	0/575
42	Ln	0.36	0/231	0.44	0/294
43	Lo	0.35	0/876	0.49	0/1156
44	Lp	0.40	0/718	0.56	0/953
45	Lr	0.35	0/1017	0.51	0/1364
46	Ls	0.32	0/1519	0.65	0/2052
47	Lt	0.34	0/1058	0.79	1/1430 (0.1%)
48	Lz	0.31	0/1769	0.69	2/2371 (0.1%)
49	S2	0.62	6/41245 (0.0%)	1.12	272/64265 (0.4%)
50	SA	0.34	0/1778	0.57	0/2416
51	SB	0.32	0/1765	0.55	0/2362
52	SD	0.32	0/1793	0.59	0/2414
53	SE	0.34	0/2118	0.56	1/2849 (0.0%)
54	SF	0.30	0/1481	0.54	0/1988
55	SH	0.32	0/1519	0.62	1/2033 (0.0%)
56	SI	0.34	0/1715	0.56	0/2287
57	SK	0.31	0/851	0.57	0/1147
58	SL	0.39	0/1268	0.55	0/1696
59	SP	0.29	0/1082	0.66	4/1446 (0.3%)
60	SQ	0.32	0/1160	0.62	0/1553
61	SR	0.30	0/1105	0.60	1/1484 (0.1%)
62	SS	0.31	0/1216	0.62	2/1628 (0.1%)
63	ST	0.32	0/1131	0.51	0/1515
64	SU	0.32	0/831	0.60	0/1115
65	SV	0.33	0/643	0.62	1/860 (0.1%)
66	SX	0.39	0/1116	0.58	0/1490
67	Sa	0.38	0/836	0.61	0/1121
68	Sc	0.31	0/508	0.61	0/680
69	Sd	0.35	0/470	0.55	0/623
70	Sg	0.32	0/2493	0.71	2/3394 (0.1%)
71	SC	0.38	0/1762	0.60	0/2381
72	SG	0.30	0/1946	0.57	1/2590 (0.0%)
73	SJ	0.34	0/1550	0.53	0/2069
74	SM	0.32	0/950	0.64	0/1275
75	SN	0.33	0/1232	0.50	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	SO	0.34	0/1062	0.61	0/1425
77	SW	0.38	0/1051	0.54	0/1406
78	SY	0.33	0/1083	0.51	0/1438
79	SZ	0.30	0/604	0.73	1/810 (0.1%)
80	Sb	0.32	0/665	0.55	0/891
81	Se	0.30	0/444	0.58	0/588
82	Sf	0.29	0/560	0.63	1/745 (0.1%)
83	CA	0.34	0/2810	0.75	4/3780 (0.1%)
84	CC	0.33	0/1773	1.00	4/2759 (0.1%)
85	CE	0.28	0/1010	0.54	1/1339 (0.1%)
86	CF	0.31	0/244	0.44	0/328
87	CI	0.31	0/4672	0.57	1/6308 (0.0%)
88	CH	0.34	0/3309	0.62	3/4450 (0.1%)
All	All	0.54	9/249639 (0.0%)	0.93	888/364877 (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	1
5	LB	0	3
8	LE	0	1
11	LH	0	1
12	LI	0	3
14	LL	0	1
15	LM	0	3
17	LO	0	2
22	LT	0	1
34	Lf	0	1
36	Lh	0	1
38	Lj	0	1
46	Ls	0	1
47	Lt	0	6
51	SB	0	1
52	SD	0	2
54	SF	0	2
55	SH	0	1
60	SQ	0	1
63	ST	0	1
64	SU	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
65	SV	0	1
66	SX	0	3
73	SJ	0	1
74	SM	0	1
76	SO	0	1
79	SZ	0	1
80	Sb	0	1
87	CI	0	5
88	CH	0	1
All	All	0	51

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	61	A	O3'-P	-8.05	1.51	1.61
1	L5	4546	A	O3'-P	-6.98	1.52	1.61
1	L5	2113	G	C1'-N9	-6.71	1.37	1.46
49	S2	59	U	O3'-P	-6.53	1.53	1.61
49	S2	1093	A	O3'-P	-6.38	1.53	1.61
49	S2	1422	G	C6-N1	-5.45	1.35	1.39
49	S2	1265	A	N9-C4	5.29	1.41	1.37
49	S2	1095	C	O3'-P	-5.17	1.54	1.61
1	L5	4764	A	N9-C4	-5.16	1.34	1.37

All (888) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1417	C	N3-C4-N4	-25.06	100.46	118.00
49	S2	1422	G	N1-C6-O6	-23.97	105.52	119.90
49	S2	1422	G	C5-C6-O6	21.36	141.42	128.60
49	S2	1417	C	C5-C4-N4	19.22	133.65	120.20
49	S2	1772	C	N1-C2-O2	15.49	128.19	118.90
49	S2	1772	C	N3-C2-O2	-14.81	111.54	121.90
1	L5	485	C	C2-N1-C1'	14.24	134.47	118.80
49	S2	501	C	N1-C2-O2	13.80	127.18	118.90
1	L5	2710	C	C2-N1-C1'	13.33	133.46	118.80
1	L5	2710	C	N1-C2-O2	13.24	126.85	118.90
49	S2	501	C	C2-N1-C1'	12.87	132.96	118.80
49	S2	293	C	N1-C2-O2	12.80	126.58	118.90
49	S2	883	U	N3-C2-O2	-11.53	114.13	122.20
49	S2	501	C	N3-C2-O2	-11.36	113.95	121.90
49	S2	882	U	N1-C2-O2	11.29	130.70	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	233	U	C2-N1-C1'	11.28	131.24	117.70
1	L5	2710	C	N3-C2-O2	-10.74	114.38	121.90
1	L5	485	C	C6-N1-C1'	-10.64	108.03	120.80
1	L5	969	C	N1-C2-O2	10.60	125.26	118.90
49	S2	293	C	C2-N1-C1'	10.39	130.23	118.80
49	S2	882	U	N3-C2-O2	-10.37	114.94	122.20
49	S2	1453	C	C2-N1-C1'	10.25	130.08	118.80
1	L5	4907	G	N9-C1'-C2'	-10.18	100.77	114.00
1	L5	2018	C	C5-C6-N1	10.15	126.07	121.00
1	L5	4549	G	N9-C1'-C2'	-10.15	100.81	114.00
49	S2	1453	C	N1-C2-O2	10.09	124.95	118.90
49	S2	1772	C	C6-N1-C2	-10.05	116.28	120.30
49	S2	293	C	N3-C2-O2	-10.04	114.87	121.90
49	S2	1772	C	C2-N1-C1'	9.96	129.76	118.80
49	S2	118	C	N1-C2-O2	9.96	124.87	118.90
1	L5	1447	C	N3-C2-O2	-9.94	114.94	121.90
1	L5	4921	C	N3-C2-O2	-9.82	115.02	121.90
1	L5	1714	C	N1-C2-O2	9.78	124.77	118.90
1	L5	753	C	N1-C2-O2	9.76	124.75	118.90
1	L5	4149	C	N3-C2-O2	-9.70	115.11	121.90
1	L5	100	C	C2-N1-C1'	9.63	129.39	118.80
49	S2	1417	C	C4-C5-C6	-9.61	112.59	117.40
1	L5	181	C	N1-C2-O2	9.60	124.66	118.90
1	L5	2710	C	C6-N1-C1'	-9.51	109.39	120.80
49	S2	882	U	C2-N1-C1'	9.46	129.05	117.70
1	L5	485	C	N1-C2-O2	9.45	124.57	118.90
1	L5	906	C	N3-C2-O2	-9.22	115.44	121.90
1	L5	4926	C	N1-C2-O2	9.19	124.42	118.90
1	L5	4928	C	N1-C2-O2	9.17	124.40	118.90
49	S2	1096	G	N9-C1'-C2'	-9.16	101.93	112.00
1	L5	1414	C	N3-C2-O2	-9.13	115.51	121.90
1	L5	4923	C	N3-C2-O2	-9.13	115.51	121.90
49	S2	1139	C	N3-C2-O2	-9.13	115.51	121.90
1	L5	417	G	O4'-C1'-N9	9.10	115.48	108.20
1	L5	115	C	N1-C2-O2	9.04	124.33	118.90
49	S2	1139	C	C2-N1-C1'	9.03	128.73	118.80
1	L5	4928	C	C2-N1-C1'	9.03	128.73	118.80
49	S2	1261	C	N1-C2-O2	8.98	124.29	118.90
49	S2	1417	C	N3-C4-C5	8.98	125.49	121.90
49	S2	322	C	N3-C2-O2	-8.97	115.62	121.90
1	L5	449	C	N1-C2-O2	8.93	124.26	118.90
1	L5	233	U	N1-C2-O2	8.93	129.05	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	456	C	O4'-C1'-N1	8.89	115.32	108.20
49	S2	356	C	C2-N1-C1'	8.88	128.57	118.80
49	S2	1139	C	N1-C2-O2	8.86	124.22	118.90
1	L5	4916	G	N9-C1'-C2'	-8.85	102.26	112.00
49	S2	501	C	C6-N1-C1'	-8.84	110.20	120.80
1	L5	753	C	N3-C2-O2	-8.82	115.72	121.90
49	S2	1416	C	N3-C2-O2	-8.82	115.73	121.90
49	S2	501	C	C6-N1-C2	-8.76	116.79	120.30
1	L5	456	C	N3-C2-O2	-8.74	115.78	121.90
49	S2	118	C	C2-N1-C1'	8.74	128.41	118.80
49	S2	118	C	N3-C2-O2	-8.73	115.79	121.90
1	L5	4926	C	C2-N1-C1'	8.70	128.37	118.80
1	L5	4557	U	C2-N1-C1'	8.68	128.12	117.70
1	L5	4557	U	N3-C2-O2	-8.68	116.12	122.20
3	L8	64	U	N3-C2-O2	-8.53	116.23	122.20
1	L5	1252	C	N3-C2-O2	-8.50	115.95	121.90
1	L5	969	C	C2-N1-C1'	8.49	128.14	118.80
1	L5	2018	C	C6-N1-C2	-8.47	116.91	120.30
1	L5	969	C	N3-C2-O2	-8.46	115.98	121.90
49	S2	1016	U	N3-C2-O2	-8.45	116.28	122.20
1	L5	233	U	C6-N1-C1'	-8.45	109.38	121.20
1	L5	4914	C	N1-C1'-C2'	-8.41	102.75	112.00
1	L5	4303	C	C2-N1-C1'	8.36	128.00	118.80
1	L5	115	C	C2-N1-C1'	8.34	127.97	118.80
1	L5	3948	C	N1-C2-O2	8.27	123.86	118.90
1	L5	2410	C	C2-N1-C1'	8.26	127.89	118.80
1	L5	1714	C	C2-N1-C1'	8.26	127.88	118.80
49	S2	427	U	C2-N1-C1'	8.20	127.54	117.70
49	S2	356	C	N1-C2-O2	8.20	123.82	118.90
49	S2	179	C	N1-C2-O2	8.17	123.80	118.90
49	S2	579	C	N1-C2-O2	8.17	123.80	118.90
1	L5	2627	C	C2-N1-C1'	8.16	127.78	118.80
1	L5	2814	C	N1-C2-O2	8.16	123.80	118.90
49	S2	168	C	N1-C2-O2	8.16	123.80	118.90
1	L5	115	C	N3-C2-O2	-8.16	116.19	121.90
1	L5	2710	C	C6-N1-C2	-8.15	117.04	120.30
49	S2	1016	U	N1-C2-O2	8.13	128.49	122.80
1	L5	4398	C	N1-C2-O2	8.11	123.77	118.90
83	CA	223	VAL	CG1-CB-CG2	-8.08	97.97	110.90
5	LB	17	LEU	CA-CB-CG	8.08	133.88	115.30
49	S2	427	U	N3-C2-O2	-8.07	116.55	122.20
1	L5	77	U	N3-C2-O2	-8.06	116.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	100	C	N3-C2-O2	-8.06	116.26	121.90
49	S2	1022	U	C2-N1-C1'	8.05	127.36	117.70
1	L5	1216	C	C2-N1-C1'	7.95	127.55	118.80
49	S2	1139	C	C6-N1-C2	-7.93	117.13	120.30
1	L5	4557	U	N1-C2-O2	7.91	128.34	122.80
1	L5	1714	C	N3-C2-O2	-7.89	116.38	121.90
1	L5	906	C	C6-N1-C2	-7.87	117.15	120.30
49	S2	310	C	C2-N1-C1'	7.86	127.44	118.80
1	L5	971	U	C2-N1-C1'	7.84	127.11	117.70
1	L5	1447	C	C6-N1-C2	-7.81	117.18	120.30
1	L5	4915	G	N9-C1'-C2'	-7.79	103.43	112.00
1	L5	4926	C	N3-C2-O2	-7.78	116.46	121.90
1	L5	516	C	N1-C2-O2	7.77	123.56	118.90
1	L5	963	G	C4-N9-C1'	7.77	136.60	126.50
1	L5	4229	U	N3-C2-O2	-7.74	116.78	122.20
49	S2	1271	C	N1-C2-O2	7.73	123.54	118.90
1	L5	181	C	N3-C2-O2	-7.71	116.51	121.90
49	S2	1261	C	N3-C2-O2	-7.64	116.55	121.90
1	L5	4905	C	N1-C1'-C2'	-7.62	103.61	112.00
1	L5	233	U	N3-C2-O2	-7.62	116.87	122.20
49	S2	1520	G	C4-N9-C1'	7.61	136.39	126.50
49	S2	427	U	N1-C2-O2	7.60	128.12	122.80
49	S2	322	C	N1-C2-O2	7.60	123.46	118.90
49	S2	630	U	C2-N1-C1'	7.59	126.81	117.70
1	L5	181	C	C2-N1-C1'	7.59	127.15	118.80
1	L5	1414	C	N1-C2-O2	7.59	123.45	118.90
1	L5	753	C	C6-N1-C2	-7.58	117.27	120.30
1	L5	175	C	N3-C2-O2	-7.58	116.59	121.90
1	L5	100	C	N1-C2-O2	7.56	123.44	118.90
49	S2	1591	C	N1-C2-O2	7.55	123.43	118.90
49	S2	1453	C	N3-C2-O2	-7.52	116.64	121.90
1	L5	2627	C	C6-N1-C2	-7.52	117.29	120.30
49	S2	1420	G	C4-N9-C1'	7.50	136.25	126.50
1	L5	220	C	C2-N1-C1'	7.49	127.04	118.80
1	L5	4928	C	N3-C2-O2	-7.48	116.67	121.90
1	L5	925	C	N1-C2-O2	7.46	123.38	118.90
49	S2	1520	G	N3-C4-N9	7.44	130.47	126.00
1	L5	1241	C	N1-C2-O2	7.44	123.36	118.90
49	S2	1117	C	N1-C2-O2	7.43	123.36	118.90
49	S2	178	C	N1-C2-O2	7.43	123.36	118.90
1	L5	129	C	N3-C2-O2	-7.42	116.70	121.90
1	L5	449	C	C2-N1-C1'	7.42	126.96	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	925	C	N3-C2-O2	-7.42	116.71	121.90
1	L5	753	C	C2-N1-C1'	7.42	126.96	118.80
1	L5	2094	G	C4-N9-C1'	7.42	136.14	126.50
1	L5	4303	C	N3-C2-O2	-7.41	116.71	121.90
1	L5	4303	C	N1-C2-O2	7.38	123.33	118.90
49	S2	1265	A	C2-N3-C4	7.38	114.29	110.60
49	S2	293	C	C6-N1-C1'	-7.36	111.97	120.80
49	S2	1453	C	C6-N1-C1'	-7.36	111.97	120.80
3	L8	51	U	N1-C2-O2	7.34	127.94	122.80
49	S2	527	C	N3-C2-O2	-7.34	116.76	121.90
1	L5	2627	C	N1-C2-O2	7.32	123.29	118.90
1	L5	2262	G	C4-N9-C1'	7.30	136.00	126.50
3	L8	51	U	N3-C2-O2	-7.30	117.09	122.20
1	L5	3685	C	C6-N1-C2	-7.30	117.38	120.30
49	S2	688	U	N3-C2-O2	-7.30	117.09	122.20
49	S2	1094	C	C1'-C2'-O2'	-7.29	88.74	110.60
1	L5	100	C	C6-N1-C2	-7.29	117.39	120.30
1	L5	485	C	C5-C6-N1	7.27	124.64	121.00
49	S2	1016	U	C2-N1-C1'	7.23	126.37	117.70
49	S2	168	C	N3-C2-O2	-7.22	116.84	121.90
1	L5	485	C	C6-N1-C2	-7.20	117.42	120.30
49	S2	883	U	N1-C2-O2	7.19	127.84	122.80
1	L5	2262	G	N3-C4-N9	7.18	130.31	126.00
1	L5	453	G	C4-N9-C1'	7.18	135.83	126.50
1	L5	1182	C	N1-C2-O2	7.17	123.20	118.90
1	L5	963	G	N3-C4-N9	7.17	130.30	126.00
49	S2	1261	C	C2-N1-C1'	7.17	126.68	118.80
1	L5	2262	G	N3-C4-C5	-7.15	125.03	128.60
5	LB	306	ASP	CB-CG-OD1	7.15	124.73	118.30
49	S2	1315	U	N1-C2-O2	7.14	127.80	122.80
1	L5	1517	G	N3-C4-N9	7.13	130.28	126.00
1	L5	1216	C	N1-C2-O2	7.13	123.18	118.90
1	L5	4746	C	C2-N1-C1'	7.13	126.64	118.80
1	L5	4905	C	C1'-C2'-O2'	-7.13	89.22	110.60
1	L5	4926	C	C6-N1-C2	-7.12	117.45	120.30
1	L5	969	C	C6-N1-C2	-7.10	117.46	120.30
1	L5	4149	C	N1-C2-O2	7.08	123.15	118.90
1	L5	4923	C	N1-C2-O2	7.08	123.15	118.90
1	L5	1182	C	C2-N1-C1'	7.08	126.59	118.80
49	S2	1389	C	C2-N1-C1'	7.07	126.58	118.80
1	L5	4929	C	N3-C2-O2	-7.05	116.97	121.90
1	L5	209	U	C2-N1-C1'	7.03	126.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1094	C	C4'-C3'-O3'	7.02	127.05	113.00
1	L5	971	U	N1-C2-O2	7.01	127.71	122.80
1	L5	4547	C	N1-C1'-C2'	-7.01	104.28	112.00
49	S2	570	C	N1-C2-O2	7.01	123.10	118.90
1	L5	1714	C	C6-N1-C2	-7.00	117.50	120.30
49	S2	118	C	C6-N1-C2	-6.99	117.50	120.30
49	S2	356	C	N3-C2-O2	-6.96	117.02	121.90
49	S2	883	U	C6-N1-C2	-6.96	116.83	121.00
3	L8	51	U	C2-N1-C1'	6.95	126.04	117.70
1	L5	1340	C	C5-C6-N1	6.94	124.47	121.00
1	L5	4709	U	N1-C2-O2	6.94	127.66	122.80
1	L5	963	G	N3-C4-C5	-6.93	125.13	128.60
1	L5	3772	U	C2-N1-C1'	6.93	126.02	117.70
1	L5	3757	G	O4'-C1'-N9	6.93	113.74	108.20
1	L5	453	G	N3-C4-N9	6.91	130.14	126.00
1	L5	453	G	N3-C4-C5	-6.89	125.16	128.60
1	L5	3778	U	N1-C2-O2	6.88	127.61	122.80
1	L5	2786	C	C6-N1-C2	-6.87	117.55	120.30
1	L5	2819	U	N3-C2-O2	-6.87	117.39	122.20
1	L5	2107	C	N3-C2-O2	-6.86	117.10	121.90
1	L5	3778	U	N3-C2-O2	-6.86	117.40	122.20
1	L5	1762	C	C6-N1-C2	-6.86	117.56	120.30
49	S2	579	C	N3-C2-O2	-6.85	117.11	121.90
1	L5	1082	C	OP1-P-O3'	6.83	120.24	105.20
1	L5	4905	C	C4'-C3'-O3'	6.83	126.67	113.00
49	S2	1149	A	C4'-C3'-O3'	-6.83	95.05	109.40
49	S2	1420	G	N3-C4-C5	-6.83	125.19	128.60
1	L5	3636	C	C6-N1-C2	-6.83	117.57	120.30
1	L5	3772	U	N3-C2-O2	-6.82	117.42	122.20
1	L5	963	G	C8-N9-C1'	-6.81	118.15	127.00
1	L5	449	C	N3-C2-O2	-6.80	117.14	121.90
1	L5	3948	C	N3-C2-O2	-6.80	117.14	121.90
49	S2	1416	C	C6-N1-C2	-6.80	117.58	120.30
1	L5	50	C	N1-C2-O2	6.79	122.98	118.90
1	L5	2528	G	C4-N9-C1'	6.79	135.32	126.50
49	S2	168	C	C6-N1-C2	-6.79	117.59	120.30
49	S2	882	U	C5-C6-N1	6.79	126.09	122.70
1	L5	2760	G	P-O3'-C3'	6.78	127.84	119.70
1	L5	655	C	N3-C2-O2	-6.78	117.15	121.90
1	L5	2814	C	C2-N1-C1'	6.78	126.25	118.80
1	L5	4924	C	N3-C2-O2	-6.78	117.16	121.90
49	S2	688	U	P-O3'-C3'	6.78	127.83	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	1378	C	N1-C2-O2	6.78	122.97	118.90
1	L5	3767	C	C5-C6-N1	6.78	124.39	121.00
49	S2	1219	C	N1-C2-O2	6.77	122.96	118.90
49	S2	1520	G	C8-N9-C1'	-6.77	118.20	127.00
1	L5	1082	C	P-O3'-C3'	6.77	127.82	119.70
1	L5	1082	C	O4'-C1'-N1	6.76	113.61	108.20
1	L5	914	U	P-O3'-C3'	6.76	127.81	119.70
1	L5	2667	C	N1-C2-O2	6.74	122.95	118.90
1	L5	2410	C	C5-C6-N1	6.74	124.37	121.00
49	S2	1364	U	N1-C2-O2	6.74	127.52	122.80
1	L5	4709	U	C2-N1-C1'	6.74	125.78	117.70
1	L5	673	C	C2-N1-C1'	6.73	126.20	118.80
1	L5	2710	C	C5-C6-N1	6.72	124.36	121.00
1	L5	1458	C	N1-C2-O2	6.71	122.92	118.90
1	L5	1686	C	C6-N1-C2	-6.70	117.62	120.30
49	S2	814	U	N3-C2-O2	-6.69	117.52	122.20
1	L5	4945	G	N3-C4-N9	6.69	130.01	126.00
3	L8	64	U	N1-C2-O2	6.67	127.47	122.80
1	L5	4398	C	N3-C2-O2	-6.67	117.23	121.90
49	S2	1315	U	N3-C2-O2	-6.64	117.55	122.20
1	L5	4420	U	N1-C2-O2	6.64	127.45	122.80
49	S2	1591	C	N3-C2-O2	-6.64	117.25	121.90
1	L5	41	C	C6-N1-C2	-6.63	117.65	120.30
1	L5	4502	C	N1-C2-O2	6.63	122.88	118.90
1	L5	4112	C	N3-C2-O2	-6.63	117.26	121.90
49	S2	1150	A	C4'-C3'-O3'	-6.62	95.49	109.40
49	S2	1420	G	N3-C4-N9	6.62	129.97	126.00
59	SP	107	ILE	C-N-CA	6.62	138.24	121.70
49	S2	1261	C	C6-N1-C2	-6.62	117.65	120.30
1	L5	115	C	C6-N1-C2	-6.61	117.66	120.30
1	L5	4420	U	N3-C2-O2	-6.59	117.59	122.20
49	S2	659	G	C4-N9-C1'	6.59	135.06	126.50
1	L5	4551	U	N3-C2-O2	-6.58	117.59	122.20
1	L5	925	C	C6-N1-C2	-6.57	117.67	120.30
1	L5	1367	C	N1-C2-O2	6.57	122.84	118.90
1	L5	3771	C	C2-N1-C1'	6.56	126.02	118.80
1	L5	516	C	N3-C2-O2	-6.55	117.31	121.90
1	L5	4709	U	N3-C2-O2	-6.55	117.61	122.20
1	L5	3948	C	C2-N1-C1'	6.54	125.99	118.80
49	S2	1578	U	N3-C2-O2	-6.54	117.62	122.20
1	L5	1191	C	N3-C2-O2	-6.53	117.33	121.90
49	S2	1756	C	N1-C2-O2	6.52	122.81	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1095	C	N1-C1'-C2'	-6.52	104.83	112.00
1	L5	220	C	C6-N1-C2	-6.51	117.70	120.30
49	S2	1271	C	C2-N1-C1'	6.51	125.96	118.80
49	S2	179	C	N3-C2-O2	-6.51	117.35	121.90
72	SG	213	LEU	CA-CB-CG	6.50	130.26	115.30
1	L5	1241	C	C2-N1-C1'	6.48	125.93	118.80
1	L5	4880	C	N1-C2-O2	6.47	122.78	118.90
1	L5	3693	U	N3-C2-O2	-6.47	117.67	122.20
49	S2	1415	C	N1-C2-O2	6.46	122.78	118.90
84	CC	35	U	P-O3'-C3'	6.46	127.45	119.70
1	L5	4682	U	N1-C2-O2	6.45	127.32	122.80
1	L5	4887	C	N1-C2-O2	6.45	122.77	118.90
1	L5	2107	C	N1-C2-O2	6.44	122.77	118.90
49	S2	179	C	C2-N1-C1'	6.43	125.87	118.80
49	S2	314	U	N3-C2-O2	-6.43	117.70	122.20
1	L5	515	C	N1-C2-O2	6.42	122.75	118.90
49	S2	1520	G	N3-C4-C5	-6.42	125.39	128.60
1	L5	96	U	N3-C2-O2	-6.42	117.71	122.20
1	L5	1731	C	C6-N1-C2	-6.42	117.73	120.30
1	L5	4662	C	C6-N1-C2	-6.41	117.74	120.30
49	S2	1389	C	C6-N1-C2	-6.41	117.74	120.30
1	L5	4682	U	N3-C2-O2	-6.41	117.72	122.20
1	L5	2094	G	C8-N9-C1'	-6.40	118.67	127.00
49	S2	1022	U	N1-C2-O2	6.40	127.28	122.80
1	L5	2410	C	N1-C2-O2	6.40	122.74	118.90
1	L5	4864	U	N1-C2-O2	6.40	127.28	122.80
1	L5	4303	C	C6-N1-C2	-6.39	117.74	120.30
1	L5	3767	C	C6-N1-C2	-6.39	117.74	120.30
49	S2	883	U	C2-N1-C1'	6.36	125.33	117.70
2	L7	102	U	N1-C2-O2	6.35	127.24	122.80
49	S2	4	C	C6-N1-C2	-6.35	117.76	120.30
2	L7	34	C	N1-C2-O2	6.34	122.70	118.90
1	L5	1245	C	C2-N1-C1'	6.34	125.77	118.80
49	S2	494	C	N1-C2-O2	6.34	122.70	118.90
49	S2	1309	C	C2-N1-C1'	6.34	125.77	118.80
1	L5	100	C	C6-N1-C1'	-6.34	113.20	120.80
49	S2	814	U	N1-C2-O2	6.33	127.23	122.80
3	L8	101	C	C6-N1-C2	-6.33	117.77	120.30
49	S2	501	C	C5-C6-N1	6.32	124.16	121.00
49	S2	1364	U	N3-C2-O2	-6.32	117.78	122.20
1	L5	2410	C	C6-N1-C2	-6.31	117.78	120.30
1	L5	2675	G	P-O3'-C3'	6.30	127.27	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	174	C	N3-C2-O2	-6.30	117.49	121.90
47	Lt	133	LEU	CA-CB-CG	6.29	129.77	115.30
49	S2	1420	G	C8-N9-C1'	-6.28	118.84	127.00
1	L5	2667	C	N3-C2-O2	-6.27	117.51	121.90
1	L5	1996	C	C6-N1-C2	-6.26	117.80	120.30
1	L5	3911	C	C6-N1-C2	-6.26	117.80	120.30
49	S2	1292	C	N1-C2-O2	6.26	122.66	118.90
1	L5	688	U	N1-C2-O2	6.26	127.18	122.80
1	L5	2094	G	N3-C4-N9	6.25	129.75	126.00
49	S2	293	C	C6-N1-C2	-6.25	117.80	120.30
1	L5	515	C	C2-N1-C1'	6.23	125.66	118.80
1	L5	4915	G	C1'-C2'-O2'	-6.23	91.90	110.60
1	L5	1447	C	N1-C2-O2	6.23	122.64	118.90
84	CC	74	C	C6-N1-C2	-6.22	117.81	120.30
1	L5	1632	A	C2-N3-C4	6.22	113.71	110.60
16	LN	134	LEU	CA-CB-CG	6.21	129.59	115.30
1	L5	2018	C	C2-N1-C1'	6.21	125.63	118.80
1	L5	4928	C	C6-N1-C1'	-6.20	113.36	120.80
1	L5	516	C	C2-N1-C1'	6.20	125.62	118.80
1	L5	3772	U	N1-C2-O2	6.20	127.14	122.80
3	L8	111	U	C2-N1-C1'	6.19	125.13	117.70
1	L5	2900	U	N1-C2-O2	6.19	127.13	122.80
49	S2	630	U	N1-C2-O2	6.19	127.13	122.80
1	L5	2494	U	N1-C2-O2	6.18	127.13	122.80
1	L5	2627	C	C5-C6-N1	6.18	124.09	121.00
49	S2	1865	C	C6-N1-C2	-6.17	117.83	120.30
1	L5	2820	C	N1-C2-O2	6.17	122.60	118.90
79	SZ	44	LEU	CA-CB-CG	6.17	129.50	115.30
1	L5	985	C	C2-N1-C1'	6.17	125.59	118.80
1	L5	3930	U	N1-C2-O2	6.17	127.12	122.80
49	S2	1417	C	N1-C2-N3	-6.17	114.88	119.20
88	CH	52	LEU	CA-CB-CG	6.17	129.49	115.30
2	L7	102	U	N3-C2-O2	-6.16	117.89	122.20
1	L5	1853	G	C4-N9-C1'	6.16	134.50	126.50
1	L5	4907	G	C4'-C3'-O3'	6.16	125.31	113.00
49	S2	1022	U	N3-C2-O2	-6.16	117.89	122.20
1	L5	4069	U	N1-C2-O2	6.15	127.11	122.80
1	L5	112	C	C2-N1-C1'	6.15	125.57	118.80
1	L5	2033	A	P-O3'-C3'	6.15	127.08	119.70
1	L5	2860	C	C6-N1-C2	-6.14	117.84	120.30
1	L5	4915	G	C4'-C3'-O3'	6.14	125.29	113.00
49	S2	168	C	C2-N1-C1'	6.14	125.56	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1772	C	C5-C6-N1	6.14	124.07	121.00
1	L5	3892	U	N3-C2-O2	-6.14	117.90	122.20
1	L5	2262	G	C8-N9-C1'	-6.13	119.03	127.00
49	S2	356	C	C6-N1-C1'	-6.13	113.45	120.80
1	L5	2819	U	N1-C2-O2	6.12	127.09	122.80
1	L5	1083	U	O5'-P-OP1	-6.12	100.19	105.70
1	L5	1472	C	C2-N1-C1'	6.12	125.53	118.80
1	L5	2362	U	N3-C2-O2	-6.12	117.92	122.20
1	L5	4112	C	C6-N1-C2	-6.12	117.85	120.30
49	S2	1865	C	C2-N1-C1'	6.12	125.53	118.80
1	L5	2627	C	N3-C2-O2	-6.12	117.62	121.90
1	L5	1182	C	N3-C2-O2	-6.11	117.62	121.90
49	S2	1590	C	N1-C2-O2	6.11	122.57	118.90
1	L5	4450	U	N3-C2-O2	-6.11	117.92	122.20
49	S2	365	C	C2-N1-C1'	6.11	125.52	118.80
49	S2	570	C	N3-C2-O2	-6.11	117.62	121.90
1	L5	4476	C	C2-N1-C1'	6.10	125.51	118.80
1	L5	904	C	C5-C6-N1	6.10	124.05	121.00
49	S2	1078	C	C2-N1-C1'	6.09	125.50	118.80
59	SP	25	LEU	CA-CB-CG	6.09	129.31	115.30
1	L5	1417	C	C6-N1-C2	-6.08	117.87	120.30
1	L5	4398	C	C6-N1-C2	-6.08	117.87	120.30
1	L5	3594	C	C6-N1-C2	-6.07	117.87	120.30
1	L5	977	C	C2-N1-C1'	6.07	125.48	118.80
1	L5	3693	U	N1-C2-O2	6.07	127.05	122.80
1	L5	1367	C	C2-N1-C1'	6.06	125.47	118.80
1	L5	1241	C	N3-C2-O2	-6.05	117.66	121.90
49	S2	1696	C	N1-C2-O2	6.05	122.53	118.90
1	L5	453	G	C8-N9-C1'	-6.04	119.16	127.00
1	L5	1666	C	C6-N1-C2	-6.03	117.89	120.30
1	L5	4928	C	C6-N1-C2	-6.03	117.89	120.30
49	S2	1315	U	C2-N1-C1'	6.03	124.94	117.70
49	S2	1649	U	N1-C2-O2	6.02	127.01	122.80
1	L5	5022	U	N1-C2-O2	6.01	127.01	122.80
1	L5	4502	C	C6-N1-C2	-6.01	117.89	120.30
49	S2	119	U	N3-C2-O2	-6.01	117.99	122.20
1	L5	1663	C	C2-N1-C1'	6.01	125.41	118.80
1	L5	3911	C	C5-C6-N1	6.00	124.00	121.00
1	L5	181	C	C6-N1-C2	-6.00	117.90	120.30
1	L5	4281	A	O4'-C1'-N9	6.00	113.00	108.20
49	S2	178	C	N3-C2-O2	-6.00	117.70	121.90
1	L5	4450	U	C2-N1-C1'	6.00	124.89	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	3930	U	N3-C2-O2	-5.99	118.01	122.20
1	L5	489	C	C2-N1-C1'	5.98	125.38	118.80
1	L5	485	C	N3-C2-O2	-5.98	117.71	121.90
1	L5	1731	C	C2-N1-C1'	5.98	125.38	118.80
1	L5	4243	C	C6-N1-C2	-5.98	117.91	120.30
1	L5	1517	G	N3-C4-C5	-5.98	125.61	128.60
1	L5	4864	U	N3-C2-O2	-5.98	118.02	122.20
49	S2	1219	C	C2-N1-C1'	5.98	125.37	118.80
1	L5	2528	G	C8-N9-C1'	-5.97	119.23	127.00
49	S2	1150	A	O5'-P-OP1	-5.97	100.32	105.70
1	L5	2011	C	N1-C2-O2	5.97	122.48	118.90
1	L5	3948	C	C6-N1-C2	-5.97	117.91	120.30
1	L5	220	C	C5-C6-N1	5.96	123.98	121.00
1	L5	2900	U	N3-C2-O2	-5.96	118.03	122.20
1	L5	1417	C	C5-C6-N1	5.95	123.98	121.00
1	L5	4914	C	C4'-C3'-O3'	5.95	124.90	113.00
49	S2	537	C	N1-C2-O2	5.95	122.47	118.90
49	S2	1117	C	N3-C2-O2	-5.94	117.74	121.90
1	L5	3631	U	N3-C2-O2	-5.94	118.04	122.20
1	L5	4594	U	N3-C2-O2	-5.94	118.04	122.20
1	L5	1582	U	N3-C2-O2	-5.93	118.05	122.20
1	L5	1216	C	N3-C2-O2	-5.93	117.75	121.90
1	L5	2900	U	C2-N1-C1'	5.93	124.82	117.70
59	SP	26	LEU	CA-CB-CG	5.93	128.95	115.30
1	L5	4910	A	P-O3'-C3'	5.93	126.81	119.70
1	L5	1395	U	N3-C2-O2	-5.93	118.05	122.20
1	L5	1417	C	C2-N1-C1'	5.92	125.31	118.80
1	L5	672	C	C2-N1-C1'	5.92	125.31	118.80
55	SH	35	ASP	CB-CG-OD1	5.91	123.62	118.30
49	S2	1434	C	P-O3'-C3'	5.91	126.79	119.70
1	L5	971	U	N3-C2-O2	-5.90	118.07	122.20
1	L5	1720	C	C6-N1-C2	-5.90	117.94	120.30
1	L5	2899	C	C2-N1-C1'	5.90	125.29	118.80
1	L5	3771	C	C6-N1-C2	-5.90	117.94	120.30
1	L5	4945	G	C5-C6-O6	-5.90	125.06	128.60
1	L5	1893	C	C2-N1-C1'	5.89	125.28	118.80
1	L5	1726	U	N3-C2-O2	-5.89	118.08	122.20
48	Lz	194	LEU	CA-CB-CG	5.89	128.84	115.30
1	L5	4594	U	C2-N1-C1'	5.89	124.76	117.70
49	S2	325	C	C2-N1-C1'	5.89	125.28	118.80
49	S2	356	C	C6-N1-C2	-5.89	117.94	120.30
1	L5	1996	C	C5-C6-N1	5.88	123.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	3841	C	C2-N1-C1'	5.88	125.27	118.80
1	L5	406	C	P-O3'-C3'	5.87	126.74	119.70
1	L5	2528	G	N3-C4-N9	5.87	129.52	126.00
49	S2	1094	C	N1-C1'-C2'	-5.87	105.54	112.00
49	S2	1453	C	C6-N1-C2	-5.87	117.95	120.30
1	L5	1417	C	N1-C2-O2	5.86	122.42	118.90
49	S2	130	G	C4-N9-C1'	5.86	134.12	126.50
1	L5	1977	C	P-O3'-C3'	5.85	126.72	119.70
1	L5	4547	C	C1'-C2'-O2'	-5.85	93.05	110.60
1	L5	4613	C	N1-C2-O2	5.84	122.41	118.90
1	L5	5035	U	N3-C2-O2	-5.84	118.11	122.20
49	S2	1271	C	N3-C2-O2	-5.84	117.81	121.90
1	L5	1582	U	N1-C2-O2	5.84	126.89	122.80
1	L5	4471	U	N3-C2-O2	-5.84	118.11	122.20
1	L5	4682	U	C2-N1-C1'	5.83	124.70	117.70
49	S2	291	G	P-O3'-C3'	5.83	126.70	119.70
1	L5	1703	C	N1-C2-O2	5.83	122.40	118.90
1	L5	2409	U	N1-C2-N3	5.83	118.40	114.90
49	S2	1219	C	N3-C2-O2	-5.83	117.82	121.90
1	L5	4594	U	N1-C2-O2	5.83	126.88	122.80
1	L5	1633	G	P-O3'-C3'	5.82	126.68	119.70
1	L5	3838	U	N1-C2-O2	5.81	126.87	122.80
49	S2	310	C	C6-N1-C1'	-5.81	113.83	120.80
49	S2	1116	C	N1-C2-O2	5.81	122.38	118.90
49	S2	688	U	N1-C2-O2	5.81	126.86	122.80
49	S2	632	C	C6-N1-C2	-5.80	117.98	120.30
1	L5	4162	C	N1-C2-O2	5.79	122.38	118.90
1	L5	205	C	N3-C2-O2	-5.79	117.84	121.90
1	L5	1702	C	C2-N1-C1'	5.79	125.17	118.80
1	L5	4887	C	C2-N1-C1'	5.79	125.17	118.80
49	S2	418	A	O5'-P-OP1	-5.79	100.49	105.70
1	L5	4758	U	C2-N1-C1'	5.78	124.64	117.70
1	L5	1251	C	N1-C2-O2	5.78	122.37	118.90
2	L7	39	C	N1-C2-O2	5.78	122.37	118.90
1	L5	77	U	N1-C2-O2	5.78	126.84	122.80
1	L5	4420	U	C2-N1-C1'	5.77	124.62	117.70
49	S2	1117	C	C2-N1-C1'	5.77	125.15	118.80
1	L5	2362	U	N1-C2-O2	5.77	126.84	122.80
1	L5	1726	U	N1-C2-O2	5.76	126.84	122.80
1	L5	3622	C	C5-C6-N1	5.76	123.88	121.00
1	L5	4241	C	C2-N1-C1'	5.76	125.14	118.80
1	L5	4714	C	N1-C2-O2	5.76	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1216	C	N1-C2-O2	5.76	122.36	118.90
1	L5	4557	U	C6-N1-C1'	-5.76	113.14	121.20
1	L5	904	C	C6-N1-C2	-5.76	118.00	120.30
1	L5	50	C	N3-C2-O2	-5.76	117.87	121.90
49	S2	559	G	O4'-C1'-N9	5.76	112.81	108.20
1	L5	2708	U	C2-N1-C1'	5.75	124.60	117.70
1	L5	2786	C	P-O3'-C3'	5.75	126.61	119.70
1	L5	988	C	N1-C2-O2	5.75	122.35	118.90
1	L5	1517	G	C4-N9-C1'	5.75	133.98	126.50
1	L5	2505	C	N1-C2-O2	5.75	122.35	118.90
1	L5	2257	C	C2-N1-C1'	5.75	125.12	118.80
1	L5	988	C	C2-N1-C1'	5.75	125.12	118.80
49	S2	409	C	C6-N1-C2	-5.74	118.00	120.30
49	S2	1772	C	C6-N1-C1'	-5.74	113.91	120.80
87	CI	37	LEU	CA-CB-CG	5.74	128.51	115.30
1	L5	5028	G	N3-C4-N9	5.74	129.44	126.00
1	L5	1915	C	N3-C2-O2	-5.74	117.89	121.90
1	L5	4399	U	N1-C2-O2	5.74	126.81	122.80
2	L7	102	U	C2-N1-C1'	5.73	124.57	117.70
1	L5	2255	C	C2-N1-C1'	5.73	125.10	118.80
49	S2	1578	U	N1-C2-O2	5.73	126.81	122.80
1	L5	673	C	C6-N1-C2	-5.72	118.01	120.30
1	L5	4901	G	N1-C6-O6	-5.72	116.47	119.90
49	S2	112	U	P-O3'-C3'	5.72	126.56	119.70
1	L5	3909	C	C6-N1-C2	-5.72	118.01	120.30
49	S2	14	C	C6-N1-C2	-5.72	118.01	120.30
49	S2	178	C	C2-N1-C1'	5.71	125.09	118.80
49	S2	527	C	N1-C2-O2	5.71	122.33	118.90
49	S2	1865	C	N3-C2-O2	-5.71	117.90	121.90
1	L5	36	U	N1-C2-O2	5.71	126.79	122.80
1	L5	1458	C	N3-C2-O2	-5.71	117.91	121.90
49	S2	1696	C	N3-C2-O2	-5.71	117.91	121.90
49	S2	1821	U	N3-C2-O2	-5.71	118.21	122.20
1	L5	969	C	C5-C6-N1	5.70	123.85	121.00
49	S2	1218	C	C5-C6-N1	5.70	123.85	121.00
49	S2	37	C	C6-N1-C2	-5.69	118.02	120.30
49	S2	1453	C	C5-C6-N1	5.69	123.84	121.00
1	L5	1755	C	N1-C2-O2	5.68	122.31	118.90
1	L5	4069	U	N3-C2-O2	-5.68	118.22	122.20
49	S2	632	C	C2-N1-C1'	5.68	125.05	118.80
1	L5	4502	C	N3-C2-O2	-5.67	117.93	121.90
1	L5	1340	C	C6-N1-C2	-5.67	118.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	4880	C	N3-C2-O2	-5.67	117.93	121.90
49	S2	310	C	N1-C2-O2	5.67	122.30	118.90
1	L5	2416	G	P-O3'-C3'	5.67	126.50	119.70
59	SP	27	ASP	CB-CG-OD1	5.67	123.40	118.30
1	L5	2820	C	N3-C2-O2	-5.67	117.93	121.90
1	L5	1726	U	C2-N1-C1'	5.66	124.50	117.70
1	L5	4921	C	N1-C2-O2	5.66	122.30	118.90
1	L5	2094	G	N3-C4-C5	-5.66	125.77	128.60
6	LC	3	CYS	CA-CB-SG	5.65	124.17	114.00
49	S2	1234	C	C2-N1-C1'	5.65	125.01	118.80
49	S2	882	U	C6-N1-C2	-5.64	117.61	121.00
49	S2	531	A	C2-N3-C4	5.64	113.42	110.60
49	S2	61	A	N9-C1'-C2'	-5.64	105.80	112.00
49	S2	130	G	N3-C4-N9	5.64	129.38	126.00
1	L5	673	C	C5-C6-N1	5.64	123.82	121.00
49	S2	322	C	C6-N1-C2	-5.64	118.05	120.30
1	L5	4921	C	C6-N1-C2	-5.63	118.05	120.30
49	S2	179	C	C6-N1-C2	-5.63	118.05	120.30
49	S2	120	U	N3-C2-O2	-5.63	118.26	122.20
1	L5	985	C	C5-C6-N1	5.63	123.82	121.00
49	S2	1756	C	N3-C2-O2	-5.63	117.96	121.90
49	S2	1660	C	C2-N1-C1'	5.63	124.99	118.80
49	S2	427	U	C6-N1-C1'	-5.63	113.32	121.20
49	S2	1139	C	C6-N1-C1'	-5.63	114.05	120.80
1	L5	41	C	C5-C6-N1	5.62	123.81	121.00
49	S2	1821	U	N1-C2-O2	5.62	126.74	122.80
1	L5	250	C	C2-N1-C1'	5.62	124.98	118.80
1	L5	4314	C	C6-N1-C2	-5.62	118.05	120.30
1	L5	3788	C	N1-C2-O2	5.62	122.27	118.90
49	S2	882	U	C6-N1-C1'	-5.62	113.34	121.20
1	L5	4360	U	N3-C2-O2	-5.61	118.27	122.20
1	L5	4775	C	N1-C2-O2	5.61	122.27	118.90
1	L5	4880	C	C2-N1-C1'	5.61	124.97	118.80
49	S2	632	C	C5-C6-N1	5.61	123.80	121.00
1	L5	1714	C	C5-C6-N1	5.61	123.80	121.00
1	L5	4426	C	C2-N1-C1'	5.61	124.97	118.80
49	S2	118	C	C6-N1-C1'	-5.61	114.07	120.80
1	L5	3775	A	O4'-C1'-N9	5.60	112.68	108.20
1	L5	4864	U	C2-N1-C1'	5.60	124.42	117.70
1	L5	1517	G	C8-N9-C1'	-5.59	119.73	127.00
1	L5	4112	C	N1-C2-O2	5.59	122.26	118.90
1	L5	4926	C	C5-C6-N1	5.59	123.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	1494	U	N3-C2-O2	-5.59	118.28	122.20
84	CC	74	C	P-O3'-C3'	5.59	126.41	119.70
1	L5	498	C	N1-C2-O2	5.59	122.25	118.90
1	L5	3685	C	C5-C6-N1	5.59	123.80	121.00
1	L5	2494	U	N3-C2-O2	-5.59	118.29	122.20
1	L5	4171	C	N1-C2-O2	5.59	122.25	118.90
49	S2	872	A	O4'-C1'-N9	5.58	112.67	108.20
8	LE	50	LEU	CA-CB-CG	5.58	128.12	115.30
49	S2	119	U	N1-C2-O2	5.57	126.70	122.80
1	L5	3838	U	N3-C2-O2	-5.57	118.30	122.20
1	L5	4895	C	N1-C2-O2	5.57	122.24	118.90
1	L5	5022	U	N3-C2-O2	-5.57	118.30	122.20
1	L5	2362	U	C2-N1-C1'	5.56	124.37	117.70
1	L5	3762	U	N1-C2-O2	5.56	126.69	122.80
49	S2	930	C	N1-C2-O2	5.56	122.23	118.90
1	L5	985	C	C6-N1-C2	-5.55	118.08	120.30
1	L5	282	C	N3-C2-O2	-5.55	118.02	121.90
49	S2	659	G	C8-N9-C1'	-5.55	119.79	127.00
49	S2	581	U	C2-N1-C1'	5.55	124.36	117.70
1	L5	1494	U	N1-C2-O2	5.54	126.68	122.80
1	L5	4254	G	C4-N9-C1'	5.54	133.70	126.50
1	L5	3622	C	C6-N1-C2	-5.54	118.08	120.30
49	S2	1649	U	N3-C2-O2	-5.54	118.32	122.20
49	S2	188	C	C2-N1-C1'	5.54	124.89	118.80
1	L5	3673	C	P-O3'-C3'	5.53	126.34	119.70
49	S2	531	A	C4-N9-C1'	5.53	136.26	126.30
49	S2	630	U	N3-C2-O2	-5.53	118.33	122.20
48	Lz	93	LEU	CA-CB-CG	5.53	128.02	115.30
49	S2	420	G	P-O3'-C3'	5.53	126.34	119.70
49	S2	1415	C	C2-N1-C1'	5.53	124.88	118.80
1	L5	456	C	N1-C2-O2	5.53	122.22	118.90
1	L5	1252	C	C6-N1-C2	-5.53	118.09	120.30
1	L5	2814	C	N3-C2-O2	-5.53	118.03	121.90
1	L5	4259	C	C5-C6-N1	5.53	123.76	121.00
1	L5	4926	C	C6-N1-C1'	-5.53	114.17	120.80
1	L5	2494	U	C2-N1-C1'	5.53	124.33	117.70
49	S2	61	A	C1'-C2'-O2'	-5.53	94.02	110.60
1	L5	4773	C	N1-C2-O2	5.52	122.21	118.90
1	L5	337	U	N3-C2-O2	-5.52	118.34	122.20
1	L5	4149	C	C6-N1-C2	-5.51	118.10	120.30
49	S2	1590	C	N3-C2-O2	-5.51	118.04	121.90
1	L5	2410	C	C6-N1-C1'	-5.51	114.19	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	1309	C	C6-N1-C2	-5.50	118.10	120.30
1	L5	4229	U	N1-C2-O2	5.50	126.65	122.80
49	S2	1660	C	N1-C2-O2	5.50	122.20	118.90
49	S2	331	C	C2-N1-C1'	5.50	124.85	118.80
1	L5	242	U	N3-C2-O2	-5.49	118.36	122.20
1	L5	512	U	N1-C2-O2	5.49	126.64	122.80
1	L5	1929	A	C2-N3-C4	5.49	113.34	110.60
1	L5	2347	A	O4'-C1'-N9	-5.48	103.81	108.20
1	L5	1816	C	C6-N1-C2	-5.48	118.11	120.30
49	S2	1265	A	N3-C4-N9	5.48	131.78	127.40
1	L5	1216	C	C6-N1-C1'	-5.47	114.23	120.80
1	L5	3637	U	N3-C2-O2	-5.47	118.37	122.20
1	L5	205	C	N1-C2-O2	5.47	122.18	118.90
49	S2	4	C	C2-N1-C1'	5.47	124.82	118.80
1	L5	282	C	N1-C2-O2	5.46	122.18	118.90
1	L5	655	C	N1-C2-O2	5.46	122.18	118.90
1	L5	2464	C	O4'-C1'-N1	5.46	112.57	108.20
88	CH	344	LEU	CA-CB-CG	5.46	127.85	115.30
1	L5	3785	A	O4'-C1'-N9	5.46	112.56	108.20
83	CA	32	LEU	CA-CB-CG	5.45	127.84	115.30
1	L5	4303	C	C6-N1-C1'	-5.45	114.26	120.80
1	L5	4775	C	C2-N1-C1'	5.45	124.80	118.80
1	L5	100	C	O4'-C1'-N1	5.45	112.56	108.20
1	L5	2260	C	N1-C2-O2	5.45	122.17	118.90
49	S2	687	C	C2-N1-C1'	5.45	124.79	118.80
1	L5	4399	U	N3-C2-O2	-5.44	118.39	122.20
49	S2	1172	U	N1-C2-O2	5.44	126.61	122.80
1	L5	499	G	N3-C4-C5	-5.44	125.88	128.60
1	L5	3919	C	C6-N1-C2	-5.44	118.12	120.30
1	L5	969	C	C6-N1-C1'	-5.44	114.28	120.80
1	L5	96	U	N1-C2-O2	5.44	126.61	122.80
1	L5	1242	G	C4-N9-C1'	5.43	133.56	126.50
1	L5	1929	A	C4-N9-C1'	5.43	136.08	126.30
1	L5	4453	C	C6-N1-C2	-5.43	118.13	120.30
49	S2	30	C	C6-N1-C2	-5.43	118.13	120.30
1	L5	209	U	C6-N1-C1'	-5.43	113.60	121.20
35	Lg	107	LEU	CA-CB-CG	5.42	127.78	115.30
1	L5	1994	C	N3-C2-O2	-5.42	118.10	121.90
1	L5	274	C	C2-N1-C1'	5.42	124.76	118.80
1	L5	282	C	C6-N1-C2	-5.42	118.13	120.30
1	L5	504	G	N3-C4-C5	-5.42	125.89	128.60
1	L5	4329	G	C4-N9-C1'	5.42	133.54	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	4	C	C5-C6-N1	5.42	123.71	121.00
1	L5	1976	G	C4-N9-C1'	5.42	133.54	126.50
2	L7	34	C	C6-N1-C2	-5.42	118.13	120.30
49	S2	1333	U	N3-C2-O2	-5.42	118.41	122.20
49	S2	1234	C	C6-N1-C2	-5.41	118.13	120.30
49	S2	1271	C	C6-N1-C2	-5.41	118.14	120.30
1	L5	1709	C	N1-C2-O2	5.40	122.14	118.90
1	L5	4303	C	O4'-C1'-N1	5.40	112.52	108.20
1	L5	337	U	N1-C2-O2	5.40	126.58	122.80
1	L5	504	G	C2-N3-C4	5.40	114.60	111.90
1	L5	4093	G	C4-N9-C1'	5.40	133.52	126.50
49	S2	1172	U	N3-C2-O2	-5.40	118.42	122.20
1	L5	1182	C	C6-N1-C2	-5.40	118.14	120.30
49	S2	323	C	N3-C2-O2	-5.40	118.12	121.90
1	L5	115	C	C6-N1-C1'	-5.40	114.33	120.80
1	L5	1472	C	C6-N1-C2	-5.40	118.14	120.30
49	S2	370	G	O5'-P-OP1	-5.40	100.84	105.70
1	L5	2014	C	N1-C2-O2	5.39	122.14	118.90
1	L5	516	C	C6-N1-C2	-5.39	118.14	120.30
1	L5	3930	U	C5-C6-N1	5.39	125.39	122.70
1	L5	985	C	N1-C2-O2	5.38	122.13	118.90
13	LJ	115	LEU	CA-CB-CG	5.38	127.69	115.30
1	L5	4887	C	N3-C2-O2	-5.38	118.13	121.90
49	S2	1265	A	N3-C4-C5	-5.38	123.03	126.80
1	L5	1821	G	N3-C4-N9	5.38	129.22	126.00
1	L5	4199	C	N1-C2-O2	5.38	122.13	118.90
1	L5	688	U	N3-C2-O2	-5.37	118.44	122.20
1	L5	4901	G	C5-C6-O6	5.37	131.82	128.60
1	L5	4206	C	N1-C2-O2	5.36	122.12	118.90
49	S2	1556	A	C2-N3-C4	5.36	113.28	110.60
1	L5	4254	G	N3-C4-C5	-5.36	125.92	128.60
1	L5	3802	U	C2-N1-C1'	5.36	124.13	117.70
1	L5	4476	C	N1-C2-O2	5.35	122.11	118.90
49	S2	542	U	N1-C2-O2	5.35	126.55	122.80
1	L5	4206	C	C2-N1-C1'	5.35	124.68	118.80
49	S2	1022	U	C6-N1-C1'	-5.34	113.72	121.20
1	L5	904	C	N1-C2-O2	5.34	122.11	118.90
49	S2	839	C	N1-C2-O2	5.34	122.11	118.90
1	L5	971	U	C6-N1-C1'	-5.34	113.72	121.20
49	S2	1417	C	C2-N3-C4	5.34	122.57	119.90
53	SE	139	LEU	CA-CB-CG	5.33	127.57	115.30
1	L5	472	C	C2-N1-C1'	5.33	124.67	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	3882	C	C2-N1-C1'	5.33	124.67	118.80
49	S2	365	C	C6-N1-C2	-5.33	118.17	120.30
2	L7	33	U	N1-C2-O2	5.32	126.53	122.80
1	L5	390	C	C6-N1-C2	-5.31	118.18	120.30
1	L5	4906	U	C3'-C2'-C1'	5.31	105.75	101.50
2	L7	34	C	N3-C2-O2	-5.31	118.19	121.90
1	L5	4945	G	C4-C5-N7	5.31	112.92	110.80
49	S2	1389	C	N1-C2-O2	5.31	122.08	118.90
49	S2	537	C	C2-N1-C1'	5.30	124.63	118.80
1	L5	1607	C	N3-C2-O2	-5.30	118.19	121.90
1	L5	4254	G	N3-C4-N9	5.30	129.18	126.00
1	L5	2532	C	C2-N1-C1'	5.30	124.63	118.80
49	S2	178	C	C6-N1-C2	-5.30	118.18	120.30
1	L5	3775	A	N7-C8-N9	5.29	116.45	113.80
1	L5	2020	U	N3-C2-O2	-5.29	118.50	122.20
6	LC	2	ALA	C-N-CA	5.29	134.92	121.70
49	S2	1219	C	C6-N1-C2	-5.29	118.19	120.30
49	S2	1292	C	C6-N1-C2	-5.29	118.19	120.30
85	CE	34	LEU	CA-CB-CG	5.29	127.46	115.30
49	S2	839	C	N3-C2-O2	-5.29	118.20	121.90
49	S2	325	C	N1-C2-O2	5.28	122.07	118.90
49	S2	218	U	N3-C2-O2	-5.28	118.51	122.20
1	L5	4766	C	C2-N1-C1'	5.27	124.60	118.80
10	LG	265	LEU	CA-CB-CG	5.27	127.43	115.30
49	S2	1259	A	C2-N3-C4	5.27	113.24	110.60
1	L5	4293	U	N3-C2-O2	-5.27	118.51	122.20
1	L5	5022	U	C2-N1-C1'	5.27	124.02	117.70
49	S2	688	U	C6-N1-C2	-5.27	117.84	121.00
1	L5	1731	C	C5-C6-N1	5.27	123.63	121.00
1	L5	3930	U	C2-N1-C1'	5.27	124.02	117.70
49	S2	606	G	C6-C5-N7	-5.27	127.24	130.40
1	L5	2351	C	C2-N1-C1'	5.26	124.59	118.80
49	S2	950	C	C6-N1-C2	-5.26	118.20	120.30
1	L5	1994	C	N1-C2-O2	5.26	122.05	118.90
1	L5	4549	G	O5'-P-OP1	-5.26	100.97	105.70
49	S2	563	G	P-O3'-C3'	5.25	126.01	119.70
1	L5	1245	C	C5-C6-N1	5.25	123.63	121.00
1	L5	2791	C	C2-N1-C1'	5.25	124.58	118.80
1	L5	4746	C	N1-C2-O2	5.25	122.05	118.90
49	S2	687	C	N1-C2-O2	5.25	122.05	118.90
49	S2	1154	U	C2-N1-C1'	5.24	123.99	117.70
1	L5	3967	G	N3-C4-C5	-5.24	125.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	321	C	N1-C2-O2	5.24	122.04	118.90
1	L5	1446	C	N1-C2-O2	5.24	122.04	118.90
1	L5	3788	C	C2-N1-C1'	5.24	124.56	118.80
1	L5	4293	U	N1-C2-O2	5.24	126.47	122.80
49	S2	1163	C	C6-N1-C2	-5.24	118.20	120.30
1	L5	499	G	C4-N9-C1'	5.24	133.31	126.50
1	L5	5028	G	C4-N9-C1'	5.23	133.30	126.50
1	L5	449	C	C6-N1-C1'	-5.23	114.52	120.80
1	L5	261	G	N3-C4-N9	5.23	129.14	126.00
1	L5	3771	C	N1-C2-O2	5.22	122.03	118.90
1	L5	4281	A	C8-N9-C4	-5.22	103.71	105.80
49	S2	1756	C	C2-N1-C1'	5.22	124.55	118.80
1	L5	925	C	C5-C6-N1	5.22	123.61	121.00
1	L5	1671	U	N3-C2-O2	-5.22	118.55	122.20
49	S2	1139	C	O4'-C1'-N1	5.22	112.38	108.20
1	L5	1714	C	C6-N1-C1'	-5.21	114.54	120.80
1	L5	1720	C	C5-C6-N1	5.21	123.61	121.00
49	S2	1256	G	C4-N9-C1'	5.21	133.28	126.50
1	L5	1993	C	C6-N1-C2	-5.21	118.22	120.30
1	L5	2257	C	N1-C2-O2	5.21	122.03	118.90
70	Sg	91	ASP	CB-CG-OD1	5.21	122.99	118.30
1	L5	2532	C	C5-C6-N1	5.21	123.60	121.00
3	L8	111	U	N1-C2-O2	5.21	126.45	122.80
1	L5	673	C	N1-C2-O2	5.21	122.02	118.90
1	L5	1597	G	O4'-C1'-N9	5.21	112.36	108.20
49	S2	578	C	N1-C2-O2	5.21	122.02	118.90
88	CH	82	LEU	CA-CB-CG	5.21	127.28	115.30
1	L5	4398	C	C2-N1-C1'	5.21	124.53	118.80
2	L7	24	C	C6-N1-C2	-5.21	118.22	120.30
62	SS	110	ASP	CB-CG-OD1	5.21	122.98	118.30
1	L5	1216	C	C6-N1-C2	-5.20	118.22	120.30
49	S2	1060	A	O4'-C1'-N9	5.20	112.36	108.20
1	L5	2528	G	N3-C4-C5	-5.20	126.00	128.60
49	S2	593	C	N1-C2-O2	5.20	122.02	118.90
49	S2	323	C	N1-C2-O2	5.20	122.02	118.90
49	S2	331	C	N1-C2-O2	5.20	122.02	118.90
1	L5	4162	C	N3-C2-O2	-5.19	118.27	121.90
49	S2	1271	C	C5-C6-N1	5.18	123.59	121.00
83	CA	115	ASP	CB-CG-OD1	5.18	122.96	118.30
1	L5	4199	C	N3-C2-O2	-5.18	118.28	121.90
26	LX	116	LEU	CA-CB-CG	5.18	127.21	115.30
1	L5	1755	C	C2-N1-C1'	5.18	124.49	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	1976	G	N3-C4-N9	5.18	129.11	126.00
49	S2	1591	C	C6-N1-C2	-5.18	118.23	120.30
1	L5	4920	C	N1-C2-O2	5.17	122.00	118.90
2	L7	24	C	N1-C2-O2	5.17	122.00	118.90
1	L5	1308	C	C6-N1-C2	-5.17	118.23	120.30
1	L5	4703	U	N3-C2-O2	-5.17	118.58	122.20
1	L5	3882	C	C6-N1-C2	-5.17	118.23	120.30
3	L8	118	C	C2-N1-C1'	5.17	124.48	118.80
49	S2	130	G	N3-C4-C5	-5.17	126.02	128.60
1	L5	112	C	C6-N1-C2	-5.16	118.24	120.30
1	L5	3771	C	C5-C6-N1	5.16	123.58	121.00
49	S2	1081	U	N3-C2-O2	-5.16	118.59	122.20
1	L5	2416	G	OP2-P-O3'	5.16	116.54	105.20
49	S2	165	G	C4-N9-C1'	5.16	133.20	126.50
1	L5	1245	C	N1-C2-O2	5.15	121.99	118.90
1	L5	2607	C	C6-N1-C2	-5.15	118.24	120.30
2	L7	33	U	N3-C2-O2	-5.15	118.59	122.20
1	L5	195	C	C6-N1-C2	-5.15	118.24	120.30
1	L5	390	C	C2-N1-C1'	5.15	124.46	118.80
1	L5	1378	C	N3-C2-O2	-5.15	118.30	121.90
1	L5	4746	C	C6-N1-C1'	-5.14	114.63	120.80
1	L5	1472	C	C5-C6-N1	5.14	123.57	121.00
49	S2	630	U	C6-N1-C1'	-5.14	114.01	121.20
49	S2	1389	C	C5-C6-N1	5.14	123.57	121.00
1	L5	1762	C	N3-C2-O2	-5.13	118.31	121.90
1	L5	2560	C	C5-C6-N1	5.13	123.56	121.00
1	L5	4880	C	C6-N1-C2	-5.13	118.25	120.30
2	L7	28	C	N1-C2-O2	5.13	121.98	118.90
1	L5	36	U	N3-C2-O2	-5.13	118.61	122.20
1	L5	3863	C	C5-C6-N1	5.13	123.56	121.00
1	L5	456	C	C6-N1-C2	-5.13	118.25	120.30
1	L5	1245	C	C6-N1-C2	-5.13	118.25	120.30
1	L5	2632	U	N3-C2-O2	-5.13	118.61	122.20
1	L5	2892	C	C2-N1-C1'	5.13	124.44	118.80
1	L5	3831	U	N3-C2-O2	-5.13	118.61	122.20
3	L8	99	U	C2-N1-C1'	5.12	123.85	117.70
49	S2	409	C	C5-C6-N1	5.12	123.56	121.00
61	SR	109	LEU	CA-CB-CG	5.12	127.07	115.30
62	SS	107	LEU	CA-CB-CG	5.12	127.07	115.30
1	L5	977	C	N1-C2-O2	5.12	121.97	118.90
1	L5	3618	C	C6-N1-C2	-5.12	118.25	120.30
1	L5	4450	U	N1-C2-O2	5.12	126.38	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	4973	U	N3-C2-O2	-5.11	118.62	122.20
49	S2	571	U	N3-C2-O2	-5.11	118.62	122.20
1	L5	2101	C	C6-N1-C1'	5.11	126.93	120.80
1	L5	205	C	C6-N1-C2	-5.11	118.26	120.30
1	L5	904	C	C2-N1-C1'	5.10	124.41	118.80
15	LM	87	ALA	C-N-CA	5.10	134.44	121.70
49	S2	1684	C	N1-C2-O2	5.10	121.96	118.90
1	L5	3841	C	C6-N1-C2	-5.09	118.26	120.30
82	Sf	100	LEU	CA-CB-CG	5.09	127.00	115.30
1	L5	4773	C	N3-C2-O2	-5.08	118.34	121.90
1	L5	1663	C	C6-N1-C2	-5.08	118.27	120.30
1	L5	2255	C	N1-C2-O2	5.08	121.95	118.90
7	LD	110	LEU	CA-CB-CG	5.08	126.98	115.30
49	S2	1292	C	N3-C2-O2	-5.08	118.34	121.90
1	L5	3911	C	C2-N1-C1'	5.08	124.39	118.80
1	L5	4299	U	N3-C2-O2	-5.08	118.65	122.20
1	L5	3870	C	C2-N1-C1'	5.08	124.38	118.80
3	L8	111	U	N3-C2-O2	-5.08	118.65	122.20
1	L5	2409	U	C4-C5-C6	5.07	122.75	119.70
1	L5	2856	C	N1-C2-O2	5.07	121.94	118.90
49	S2	26	U	C5-C6-N1	5.07	125.24	122.70
49	S2	674	C	C6-N1-C2	-5.07	118.27	120.30
83	CA	105	LEU	CA-CB-CG	5.07	126.97	115.30
1	L5	4289	U	N3-C2-O2	-5.07	118.65	122.20
1	L5	4766	C	C6-N1-C2	-5.07	118.27	120.30
3	L8	28	C	C6-N1-C2	-5.07	118.27	120.30
1	L5	3802	U	N3-C2-O2	-5.07	118.65	122.20
49	S2	130	G	C8-N9-C1'	-5.06	120.42	127.00
1	L5	515	C	C5-C6-N1	5.06	123.53	121.00
1	L5	1607	C	N1-C2-O2	5.06	121.94	118.90
1	L5	2260	C	C2-N1-C1'	5.06	124.36	118.80
1	L5	2505	C	C2-N1-C1'	5.06	124.37	118.80
1	L5	4709	U	C5-C6-N1	5.06	125.23	122.70
1	L5	4945	G	C6-C5-N7	-5.06	127.36	130.40
49	S2	577	U	N3-C2-O2	-5.06	118.66	122.20
49	S2	1292	C	C2-N1-C1'	5.06	124.36	118.80
70	Sg	45	LEU	CA-CB-CG	5.06	126.93	115.30
1	L5	1620	U	N3-C2-O2	-5.05	118.66	122.20
1	L5	4107	G	C4-N9-C1'	5.05	133.07	126.50
49	S2	1315	U	C5-C6-N1	5.05	125.23	122.70
84	CC	74	C	C2'-C3'-O3'	5.05	121.78	113.70
1	L5	753	C	C5-C6-N1	5.05	123.52	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	606	G	C4-N9-C1'	5.04	133.06	126.50
49	S2	120	U	N1-C2-O2	5.04	126.33	122.80
1	L5	281	U	N3-C2-O2	-5.04	118.67	122.20
1	L5	1367	C	N3-C2-O2	-5.04	118.37	121.90
1	L5	3909	C	C2-N1-C1'	5.04	124.35	118.80
65	SV	78	ILE	CG1-CB-CG2	-5.04	100.31	111.40
1	L5	914	U	C5-C4-O4	-5.04	122.88	125.90
49	S2	1314	U	C5-C6-N1	5.04	125.22	122.70
1	L5	3909	C	N3-C2-O2	-5.04	118.37	121.90
1	L5	4476	C	N3-C2-O2	-5.04	118.38	121.90
1	L5	2708	U	N1-C2-O2	5.03	126.32	122.80
49	S2	1216	C	C6-N1-C2	-5.03	118.29	120.30
49	S2	688	U	C2-N1-C1'	5.03	123.74	117.70
1	L5	365	U	N1-C2-O2	5.03	126.32	122.80
1	L5	1259	G	N1-C6-O6	-5.03	116.88	119.90
3	L8	54	C	N1-C2-O2	5.03	121.92	118.90
1	L5	4206	C	C5-C6-N1	5.03	123.51	121.00
49	S2	606	G	N3-C4-N9	5.03	129.02	126.00
1	L5	3866	C	C5-C6-N1	5.02	123.51	121.00
49	S2	494	C	N3-C2-O2	-5.02	118.39	121.90
49	S2	592	C	N1-C2-O2	5.02	121.91	118.90
49	S2	1591	C	C2-N1-C1'	5.02	124.32	118.80
49	S2	592	C	C2-N1-C1'	5.01	124.31	118.80
1	L5	1468	C	C6-N1-C2	-5.01	118.30	120.30
49	S2	578	C	C6-N1-C2	-5.01	118.30	120.30
49	S2	1309	C	C6-N1-C2	-5.01	118.30	120.30
49	S2	1309	C	N1-C2-O2	5.01	121.91	118.90
1	L5	4902	C	C5-C6-N1	5.01	123.50	121.00
49	S2	883	U	N1-C2-N3	5.01	117.91	114.90
1	L5	4289	U	C2-N1-C1'	5.01	123.71	117.70
1	L5	739	G	N3-C4-N9	5.00	129.00	126.00
2	L7	29	C	C2-N1-C1'	5.00	124.30	118.80
1	L5	2018	C	C2-N3-C4	5.00	122.40	119.90

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
88	CH	40	PRO	Peptide
87	CI	236	ASP	Peptide
87	CI	365	VAL	Peptide
87	CI	42	THR	Peptide

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Mol	Chain	Res	Type	Group
87	CI	454	ILE	Peptide
87	CI	95	HIS	Peptide
4	LA	54	ARG	Peptide
5	LB	17	LEU	Peptide
5	LB	258	HIS	Peptide
5	LB	301	ASN	Peptide
8	LE	129	GLY	Peptide
11	LH	106	GLN	Peptide
12	LI	14	ASN	Peptide
12	LI	15	LYS	Peptide
12	LI	54	SER	Peptide
14	LL	154	VAL	Peptide
15	LM	31	ILE	Peptide
15	LM	87	ALA	Peptide
15	LM	88	ALA	Peptide
17	LO	110	PRO	Peptide
17	LO	30	GLY	Peptide
22	LT	135	PRO	Peptide
34	Lf	106	TYR	Peptide
36	Lh	86	LYS	Peptide
38	Lj	39	TYR	Peptide
46	Ls	149	ARG	Peptide
47	Lt	122	ALA	Peptide
47	Lt	147	HIS	Peptide
47	Lt	148	PRO	Peptide
47	Lt	20	GLY	Peptide
47	Lt	53	TRP	Peptide
47	Lt	9	GLU	Peptide
51	SB	221	PRO	Peptide
52	SD	162	ASP	Peptide
52	SD	164	VAL	Peptide
54	SF	126	THR	Peptide
54	SF	78	MET	Peptide
55	SH	15	LYS	Peptide
73	SJ	137	VAL	Peptide
74	SM	43	ASP	Peptide
76	SO	14	VAL	Peptide
60	SQ	43	GLU	Peptide
63	ST	46	ALA	Peptide
64	SU	107	GLU	Peptide
64	SU	61	LEU	Peptide
65	SV	78	ILE	Peptide

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Mol	Chain	Res	Type	Group
66	SX	125	VAL	Peptide
66	SX	126	ALA	Peptide
66	SX	60	LYS	Peptide
79	SZ	46	ASN	Peptide
80	Sb	75	GLU	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	223 (91%)	22 (9%)	1 (0%)	34	72
5	LB	400/403 (99%)	374 (94%)	25 (6%)	1 (0%)	41	76
6	LC	366/427 (86%)	337 (92%)	29 (8%)	0	100	100
7	LD	291/297 (98%)	266 (91%)	25 (9%)	0	100	100
8	LE	232/288 (81%)	212 (91%)	20 (9%)	0	100	100
9	LF	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
10	LG	239/266 (90%)	223 (93%)	16 (7%)	0	100	100
11	LH	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
12	LI	198/214 (92%)	182 (92%)	16 (8%)	0	100	100
13	LJ	174/178 (98%)	154 (88%)	20 (12%)	0	100	100
14	LL	208/211 (99%)	190 (91%)	18 (9%)	0	100	100
15	LM	137/215 (64%)	125 (91%)	11 (8%)	1 (1%)	22	60
16	LN	201/204 (98%)	191 (95%)	8 (4%)	2 (1%)	15	53
17	LO	199/203 (98%)	186 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	LP	151/184 (82%)	141 (93%)	10 (7%)	0	100	100
19	LQ	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
20	LR	185/196 (94%)	176 (95%)	9 (5%)	0	100	100
21	LS	173/176 (98%)	163 (94%)	10 (6%)	0	100	100
22	LT	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
23	LU	99/128 (77%)	84 (85%)	13 (13%)	2 (2%)	7	34
24	LV	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
25	LW	122/157 (78%)	113 (93%)	9 (7%)	0	100	100
26	LX	118/156 (76%)	113 (96%)	5 (4%)	0	100	100
27	LY	132/145 (91%)	123 (93%)	9 (7%)	0	100	100
28	LZ	133/136 (98%)	124 (93%)	9 (7%)	0	100	100
29	La	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
30	Lb	105/159 (66%)	97 (92%)	8 (8%)	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%)	117 (93%)	9 (7%)	0	100	100
34	Lf	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	8	36
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%)	96 (96%)	4 (4%)	0	100	100
38	Lj	84/97 (87%)	76 (90%)	8 (10%)	0	100	100
39	Lk	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
40	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
41	Lm	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
44	Lp	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
45	Lr	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
46	Ls	194/317 (61%)	173 (89%)	20 (10%)	1 (0%)	29	68
47	Lt	137/165 (83%)	107 (78%)	27 (20%)	3 (2%)	6	31
48	Lz	215/217 (99%)	159 (74%)	56 (26%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
50	SA	219/295 (74%)	194 (89%)	24 (11%)	1 (0%)	29 68
51	SB	212/264 (80%)	199 (94%)	13 (6%)	0	100 100
52	SD	225/243 (93%)	200 (89%)	25 (11%)	0	100 100
53	SE	260/263 (99%)	242 (93%)	18 (7%)	0	100 100
54	SF	180/204 (88%)	163 (91%)	17 (9%)	0	100 100
55	SH	182/194 (94%)	157 (86%)	25 (14%)	0	100 100
56	SI	204/208 (98%)	194 (95%)	10 (5%)	0	100 100
57	SK	96/165 (58%)	86 (90%)	10 (10%)	0	100 100
58	SL	151/158 (96%)	140 (93%)	11 (7%)	0	100 100
59	SP	127/145 (88%)	116 (91%)	11 (9%)	0	100 100
60	SQ	142/146 (97%)	124 (87%)	17 (12%)	1 (1%)	22 60
61	SR	133/135 (98%)	117 (88%)	16 (12%)	0	100 100
62	SS	143/152 (94%)	132 (92%)	11 (8%)	0	100 100
63	ST	141/145 (97%)	129 (92%)	11 (8%)	1 (1%)	22 60
64	SU	102/119 (86%)	89 (87%)	13 (13%)	0	100 100
65	SV	81/83 (98%)	72 (89%)	8 (10%)	1 (1%)	13 48
66	SX	139/143 (97%)	130 (94%)	7 (5%)	2 (1%)	11 43
67	Sa	100/115 (87%)	90 (90%)	9 (9%)	1 (1%)	15 53
68	Sc	62/69 (90%)	49 (79%)	12 (19%)	1 (2%)	9 40
69	Sd	53/56 (95%)	48 (91%)	5 (9%)	0	100 100
70	Sg	311/317 (98%)	269 (86%)	41 (13%)	1 (0%)	41 76
71	SC	220/293 (75%)	206 (94%)	14 (6%)	0	100 100
72	SG	235/249 (94%)	219 (93%)	16 (7%)	0	100 100
73	SJ	183/194 (94%)	171 (93%)	12 (7%)	0	100 100
74	SM	120/132 (91%)	109 (91%)	11 (9%)	0	100 100
75	SN	148/151 (98%)	141 (95%)	7 (5%)	0	100 100
76	SO	138/151 (91%)	126 (91%)	11 (8%)	1 (1%)	22 60
77	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100 100
78	SY	129/133 (97%)	122 (95%)	7 (5%)	0	100 100
79	SZ	73/125 (58%)	59 (81%)	13 (18%)	1 (1%)	11 43
80	Sb	81/84 (96%)	72 (89%)	9 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
81	Se	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
82	Sf	65/156 (42%)	54 (83%)	11 (17%)	0	100	100
83	CA	350/394 (89%)	331 (95%)	18 (5%)	1 (0%)	41	76
85	CE	113/223 (51%)	109 (96%)	4 (4%)	0	100	100
86	CF	27/180 (15%)	26 (96%)	1 (4%)	0	100	100
87	CI	578/599 (96%)	537 (93%)	39 (7%)	2 (0%)	41	76
88	CH	413/437 (94%)	388 (94%)	24 (6%)	1 (0%)	47	82
All	All	13353/15220 (88%)	12258 (92%)	1067 (8%)	28 (0%)	50	82

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	LN	124	ASP
66	SX	127	ASN
15	LM	88	ALA
23	LU	59	GLY
47	Lt	10	ILE
47	Lt	148	PRO
63	ST	41	LYS
67	Sa	47	ALA
79	SZ	45	ASN
83	CA	83	ASN
34	Lf	80	ASN
46	Ls	150	GLY
47	Lt	147	HIS
66	SX	126	ALA
76	SO	140	THR
4	LA	55	GLY
5	LB	302	ASN
50	SA	12	GLU
68	Sc	64	GLU
87	CI	43	PRO
34	Lf	107	PRO
70	Sg	246	TYR
16	LN	83	LYS
23	LU	67	LYS
60	SQ	44	PRO
88	CH	41	PRO
65	SV	79	VAL
87	CI	237	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%)	188 (99%)	2 (1%)	73 90
5	LB	348/349 (100%)	347 (100%)	1 (0%)	92 97
6	LC	306/348 (88%)	300 (98%)	6 (2%)	55 83
7	LD	246/250 (98%)	245 (100%)	1 (0%)	91 97
8	LE	209/252 (83%)	208 (100%)	1 (0%)	88 96
9	LF	194/215 (90%)	193 (100%)	1 (0%)	88 96
10	LG	203/223 (91%)	199 (98%)	4 (2%)	55 83
11	LH	169/171 (99%)	168 (99%)	1 (1%)	86 95
12	LI	172/181 (95%)	172 (100%)	0	100 100
13	LJ	148/149 (99%)	146 (99%)	2 (1%)	67 88
14	LL	176/177 (99%)	176 (100%)	0	100 100
15	LM	118/161 (73%)	117 (99%)	1 (1%)	81 93
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%)	134 (100%)	0	100 100
19	LQ	164/165 (99%)	164 (100%)	0	100 100
20	LR	166/175 (95%)	166 (100%)	0	100 100
21	LS	156/157 (99%)	156 (100%)	0	100 100
22	LT	139/140 (99%)	138 (99%)	1 (1%)	84 94
23	LU	91/115 (79%)	89 (98%)	2 (2%)	52 81
24	LV	101/107 (94%)	100 (99%)	1 (1%)	76 91
25	LW	103/126 (82%)	103 (100%)	0	100 100
26	LX	108/133 (81%)	108 (100%)	0	100 100
27	LY	124/135 (92%)	122 (98%)	2 (2%)	62 86
28	LZ	117/118 (99%)	117 (100%)	0	100 100
29	La	120/121 (99%)	118 (98%)	2 (2%)	60 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	Lb	88/126 (70%)	87 (99%)	1 (1%)	73 90
31	Lc	83/97 (86%)	82 (99%)	1 (1%)	71 90
32	Ld	98/110 (89%)	97 (99%)	1 (1%)	76 91
33	Le	114/121 (94%)	114 (100%)	0	100 100
34	Lf	88/89 (99%)	87 (99%)	1 (1%)	73 90
35	Lg	98/100 (98%)	97 (99%)	1 (1%)	76 91
36	Lh	109/110 (99%)	109 (100%)	0	100 100
37	Li	86/89 (97%)	86 (100%)	0	100 100
38	Lj	73/80 (91%)	72 (99%)	1 (1%)	67 88
39	Lk	64/65 (98%)	64 (100%)	0	100 100
40	Ll	47/48 (98%)	46 (98%)	1 (2%)	53 82
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 84
47	Lt	112/137 (82%)	110 (98%)	2 (2%)	59 85
48	Lz	195/196 (100%)	194 (100%)	1 (0%)	88 96
50	SA	183/243 (75%)	181 (99%)	2 (1%)	73 90
51	SB	195/231 (84%)	194 (100%)	1 (0%)	88 96
52	SD	190/202 (94%)	187 (98%)	3 (2%)	62 86
53	SE	224/225 (100%)	223 (100%)	1 (0%)	91 97
54	SF	156/170 (92%)	156 (100%)	0	100 100
55	SH	166/174 (95%)	165 (99%)	1 (1%)	86 95
56	SI	178/180 (99%)	177 (99%)	1 (1%)	86 95
57	SK	89/136 (65%)	87 (98%)	2 (2%)	52 81
58	SL	137/142 (96%)	135 (98%)	2 (2%)	65 87
59	SP	115/130 (88%)	112 (97%)	3 (3%)	46 78
60	SQ	119/121 (98%)	116 (98%)	3 (2%)	47 79
61	SR	122/122 (100%)	122 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
62	SS	126/132 (96%)	125 (99%)	1 (1%)	81 93
63	ST	113/115 (98%)	112 (99%)	1 (1%)	78 92
64	SU	94/107 (88%)	92 (98%)	2 (2%)	53 82
65	SV	67/67 (100%)	67 (100%)	0	100 100
66	SX	113/115 (98%)	111 (98%)	2 (2%)	59 85
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
70	Sg	272/275 (99%)	269 (99%)	3 (1%)	73 90
71	SC	188/225 (84%)	187 (100%)	1 (0%)	88 96
72	SG	207/218 (95%)	203 (98%)	4 (2%)	57 84
73	SJ	161/168 (96%)	160 (99%)	1 (1%)	86 95
74	SM	102/108 (94%)	98 (96%)	4 (4%)	32 69
75	SN	130/131 (99%)	130 (100%)	0	100 100
76	SO	110/119 (92%)	109 (99%)	1 (1%)	78 92
77	SW	112/113 (99%)	112 (100%)	0	100 100
78	SY	113/115 (98%)	111 (98%)	2 (2%)	59 85
79	SZ	66/103 (64%)	65 (98%)	1 (2%)	65 87
80	Sb	75/76 (99%)	74 (99%)	1 (1%)	69 89
81	Se	42/48 (88%)	42 (100%)	0	100 100
82	Sf	60/140 (43%)	59 (98%)	1 (2%)	60 85
83	CA	303/336 (90%)	299 (99%)	4 (1%)	69 89
85	CE	104/190 (55%)	101 (97%)	3 (3%)	42 76
86	CF	26/151 (17%)	26 (100%)	0	100 100
87	CI	511/526 (97%)	510 (100%)	1 (0%)	93 98
88	CH	353/376 (94%)	348 (99%)	5 (1%)	67 88
All	All	11626/12971 (90%)	11527 (99%)	99 (1%)	79 92

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	207	VAL
4	LA	249	THR

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Mol	Chain	Res	Type
5	LB	10	ARG
6	LC	100	ARG
6	LC	122	TYR
6	LC	188	ARG
6	LC	257	PHE
6	LC	266	THR
6	LC	364	LYS
7	LD	85	LYS
8	LE	56	ARG
9	LF	29	LYS
10	LG	111	LYS
10	LG	115	LEU
10	LG	175	ARG
10	LG	217	LYS
11	LH	187	VAL
13	LJ	8	LYS
13	LJ	88	LYS
15	LM	38	VAL
17	LO	27	VAL
22	LT	142	ARG
23	LU	45	GLU
23	LU	67	LYS
24	LV	48	ARG
27	LY	55	VAL
27	LY	84	ARG
29	La	76	ASP
29	La	92	LYS
30	Lb	51	LYS
31	Lc	23	LYS
32	Ld	67	ARG
34	Lf	33	VAL
35	Lg	54	ARG
38	Lj	22	CYS
40	Ll	36	ARG
46	Ls	21	LEU
46	Ls	77	LYS
46	Ls	174	LEU
47	Lt	57	ARG
47	Lt	111	ASN
48	Lz	102	LYS
50	SA	206	ASP
50	SA	211	GLU

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Mol	Chain	Res	Type
51	SB	85	LYS
52	SD	16	ILE
52	SD	76	ARG
52	SD	162	ASP
53	SE	69	PHE
55	SH	57	ARG
56	SI	143	LYS
57	SK	95	ARG
57	SK	98	ARG
58	SL	69	ARG
58	SL	90	ARG
59	SP	25	LEU
59	SP	58	LYS
59	SP	65	LYS
60	SQ	22	VAL
60	SQ	71	ARG
60	SQ	113	ILE
62	SS	8	LYS
63	ST	41	LYS
64	SU	36	CYS
64	SU	45	GLU
66	SX	119	ARG
66	SX	142	ARG
70	Sg	45	LEU
70	Sg	186	THR
70	Sg	270	LEU
71	SC	248	TYR
72	SG	20	ASP
72	SG	213	LEU
72	SG	230	LYS
72	SG	232	ARG
73	SJ	5	ARG
74	SM	60	MET
74	SM	63	LYS
74	SM	84	LYS
74	SM	93	LYS
76	SO	39	ASP
78	SY	16	ARG
78	SY	46	LYS
79	SZ	41	ARG
80	Sb	34	ASP
82	Sf	107	LYS

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Mol	Chain	Res	Type
83	CA	51	LYS
83	CA	238	LYS
83	CA	320	LYS
83	CA	344	LYS
85	CE	18	ARG
85	CE	33	GLU
85	CE	40	LYS
87	CI	4	LYS
88	CH	34	MET
88	CH	87	LYS
88	CH	109	LYS
88	CH	186	SER
88	CH	188	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	132	ASN
4	LA	215	ASN
5	LB	301	ASN
6	LC	346	ASN
7	LD	9	ASN
7	LD	111	ASN
9	LF	24	ASN
10	LG	149	ASN
10	LG	153	GLN
10	LG	236	HIS
12	LI	203	HIS
13	LJ	42	GLN
14	LL	205	GLN
16	LN	149	GLN
16	LN	196	ASN
17	LO	180	GLN
18	LP	80	GLN
18	LP	97	ASN
19	LQ	21	GLN
19	LQ	44	ASN
19	LQ	188	ASN
20	LR	34	ASN
20	LR	86	ASN
21	LS	37	HIS
24	LV	27	ASN

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Mol	Chain	Res	Type
27	LY	14	ASN
29	La	66	ASN
29	La	67	GLN
31	Lc	15	ASN
33	Le	107	ASN
34	Lf	56	ASN
37	Li	80	HIS
38	Lj	66	HIS
41	Lm	117	HIS
43	Lo	19	GLN
43	Lo	45	GLN
43	Lo	51	GLN
45	Lr	70	GLN
45	Lr	100	ASN
46	Ls	72	ASN
46	Ls	176	ASN
47	Lt	70	GLN
47	Lt	115	GLN
47	Lt	156	ASN
48	Lz	21	ASN
48	Lz	35	GLN
48	Lz	200	ASN
50	SA	141	ASN
51	SB	92	GLN
51	SB	179	ASN
51	SB	202	GLN
53	SE	138	HIS
53	SE	157	ASN
53	SE	188	ASN
53	SE	260	GLN
54	SF	148	ASN
56	SI	84	ASN
57	SK	50	GLN
57	SK	73	ASN
58	SL	11	GLN
58	SL	83	GLN
60	SQ	86	GLN
61	SR	48	ASN
61	SR	62	GLN
61	SR	118	GLN
62	SS	76	GLN
62	SS	105	ASN

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Mol	Chain	Res	Type
63	ST	12	GLN
63	ST	128	GLN
66	SX	61	GLN
66	SX	77	ASN
68	Sc	7	GLN
70	Sg	14	HIS
70	Sg	51	ASN
70	Sg	64	HIS
72	SG	13	GLN
72	SG	81	HIS
72	SG	110	ASN
74	SM	82	ASN
76	SO	32	HIS
80	Sb	9	HIS
80	Sb	26	GLN
83	CA	10	GLN
83	CA	134	GLN
83	CA	193	HIS
83	CA	209	GLN
85	CE	45	HIS
85	CE	180	GLN
87	CI	85	HIS
87	CI	251	GLN
87	CI	520	HIS
87	CI	556	ASN
87	CI	561	GLN
88	CH	11	ASN
88	CH	121	ASN
88	CH	129	ASN
88	CH	265	ASN
88	CH	277	ASN
88	CH	364	GLN
88	CH	380	ASN
88	CH	381	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3706/5066 (73%)	904 (24%)	20 (0%)
2	L7	119/121 (98%)	9 (7%)	0
3	L8	155/157 (98%)	27 (17%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	S2	1717/1869 (91%)	404 (23%)	12 (0%)
84	CC	74/75 (98%)	26 (35%)	2 (2%)
All	All	5771/7288 (79%)	1370 (23%)	34 (0%)

All (1370) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	17	A
1	L5	25	A
1	L5	26	C
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
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	150	U
1	L5	152	U
1	L5	159	C
1	L5	165	A
1	L5	166	C

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Mol	Chain	Res	Type
1	L5	172	C
1	L5	182	G
1	L5	183	C
1	L5	184	U
1	L5	185	C
1	L5	187	U
1	L5	188	G
1	L5	189	G
1	L5	200	U
1	L5	209	U
1	L5	210	C
1	L5	218	A
1	L5	225	G
1	L5	233	U
1	L5	234	G
1	L5	255	C
1	L5	256	G
1	L5	258	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	310	G
1	L5	315	G
1	L5	316	U
1	L5	340	C
1	L5	349	A
1	L5	350	C
1	L5	363	A
1	L5	373	G
1	L5	387	G
1	L5	388	A
1	L5	398	A
1	L5	407	A
1	L5	408	A
1	L5	409	G
1	L5	410	A
1	L5	411	G

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Mol	Chain	Res	Type
1	L5	412	G
1	L5	413	G
1	L5	431	G
1	L5	432	U
1	L5	436	C
1	L5	440	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	465	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	506	C
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	517	C
1	L5	518	G
1	L5	643	C
1	L5	656	C
1	L5	657	C

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Mol	Chain	Res	Type
1	L5	658	C
1	L5	659	G
1	L5	660	A
1	L5	665	C
1	L5	666	G
1	L5	667	A
1	L5	668	C
1	L5	672	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	706	C
1	L5	708	G
1	L5	731	G
1	L5	738	C
1	L5	739	G
1	L5	742	G
1	L5	746	A
1	L5	753	C
1	L5	758	G
1	L5	904	C
1	L5	907	C
1	L5	910	G
1	L5	913	U
1	L5	914	U
1	L5	915	A
1	L5	917	A
1	L5	918	G
1	L5	923	C
1	L5	924	C
1	L5	926	G
1	L5	932	A
1	L5	933	G
1	L5	935	A
1	L5	936	C
1	L5	943	A
1	L5	945	U

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Mol	Chain	Res	Type
1	L5	946	C
1	L5	956	A
1	L5	958	G
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	962	C
1	L5	965	G
1	L5	966	A
1	L5	967	C
1	L5	968	C
1	L5	969	C
1	L5	970	G
1	L5	971	U
1	L5	982	U
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	1075	G
1	L5	1082	C
1	L5	1083	U
1	L5	1095	A
1	L5	1168	G
1	L5	1169	G
1	L5	1171	G
1	L5	1173	G
1	L5	1178	G
1	L5	1179	U
1	L5	1180	C
1	L5	1181	C
1	L5	1182	C
1	L5	1183	C

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Mol	Chain	Res	Type
1	L5	1200	G
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	1242	G
1	L5	1246	G
1	L5	1247	U
1	L5	1253	G
1	L5	1254	A
1	L5	1257	A
1	L5	1258	G
1	L5	1261	G
1	L5	1262	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	1280	C
1	L5	1284	G
1	L5	1285	U
1	L5	1287	G
1	L5	1293	G
1	L5	1294	A
1	L5	1295	C
1	L5	1296	G
1	L5	1301	C
1	L5	1302	U

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Mol	Chain	Res	Type
1	L5	1303	A
1	L5	1312	A
1	L5	1314	C
1	L5	1324	A
1	L5	1326	A
1	L5	1337	A
1	L5	1354	A
1	L5	1358	G
1	L5	1359	G
1	L5	1365	C
1	L5	1367	C
1	L5	1378	C
1	L5	1379	C
1	L5	1387	A
1	L5	1393	G
1	L5	1394	G
1	L5	1397	A
1	L5	1403	G
1	L5	1405	C
1	L5	1407	C
1	L5	1409	C
1	L5	1410	U
1	L5	1414	C
1	L5	1417	C
1	L5	1420	A
1	L5	1425	G
1	L5	1435	G
1	L5	1437	C
1	L5	1439	C
1	L5	1443	A
1	L5	1444	G
1	L5	1446	C
1	L5	1447	C
1	L5	1457	G
1	L5	1482	G
1	L5	1483	C
1	L5	1486	C
1	L5	1497	A
1	L5	1498	G
1	L5	1502	G
1	L5	1517	G
1	L5	1518	A

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Mol	Chain	Res	Type
1	L5	1525	A
1	L5	1534	A
1	L5	1547	A
1	L5	1562	G
1	L5	1563	A
1	L5	1566	C
1	L5	1578	U
1	L5	1582	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	1641	G
1	L5	1654	G
1	L5	1660	U
1	L5	1661	C
1	L5	1676	C
1	L5	1677	U
1	L5	1678	C
1	L5	1679	A
1	L5	1691	G
1	L5	1697	G
1	L5	1698	C
1	L5	1699	A
1	L5	1700	G
1	L5	1701	A
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	1726	U
1	L5	1731	C
1	L5	1734	G
1	L5	1735	U
1	L5	1741	G

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Mol	Chain	Res	Type
1	L5	1742	A
1	L5	1753	G
1	L5	1755	C
1	L5	1756	U
1	L5	1757	U
1	L5	1758	G
1	L5	1759	G
1	L5	1760	G
1	L5	1761	G
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	1769	G
1	L5	1770	A
1	L5	1771	U
1	L5	1775	A
1	L5	1787	A
1	L5	1792	U
1	L5	1797	G
1	L5	1804	A
1	L5	1806	G
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	1893	C
1	L5	1897	A
1	L5	1917	A
1	L5	1918	U
1	L5	1919	G

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Mol	Chain	Res	Type
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	1946	G
1	L5	1948	G
1	L5	1949	U
1	L5	1951	G
1	L5	1959	U
1	L5	1961	G
1	L5	1962	A
1	L5	1971	C
1	L5	1972	G
1	L5	1974	U
1	L5	1975	G
1	L5	1978	C
1	L5	1980	U
1	L5	1981	G
1	L5	1983	A
1	L5	1984	A
1	L5	1985	G
1	L5	1987	C
1	L5	1991	A
1	L5	1992	U
1	L5	1993	C
1	L5	1997	U
1	L5	1999	A
1	L5	2002	A
1	L5	2005	G
1	L5	2017	A
1	L5	2018	C
1	L5	2024	G
1	L5	2026	A
1	L5	2034	G
1	L5	2044	U
1	L5	2046	G
1	L5	2048	U
1	L5	2052	G

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Mol	Chain	Res	Type
1	L5	2055	G
1	L5	2056	G
1	L5	2069	A
1	L5	2084	C
1	L5	2085	G
1	L5	2089	G
1	L5	2090	U
1	L5	2091	C
1	L5	2092	G
1	L5	2093	A
1	L5	2094	G
1	L5	2095	A
1	L5	2096	G
1	L5	2097	U
1	L5	2098	G
1	L5	2100	A
1	L5	2101	C
1	L5	2102	G
1	L5	2108	G
1	L5	2110	C
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	2262	G
1	L5	2289	C
1	L5	2300	A
1	L5	2301	G
1	L5	2306	G
1	L5	2313	A
1	L5	2322	G
1	L5	2331	G
1	L5	2332	A
1	L5	2333	G
1	L5	2348	G
1	L5	2351	C
1	L5	2357	G
1	L5	2360	A

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Mol	Chain	Res	Type
1	L5	2369	U
1	L5	2395	A
1	L5	2397	G
1	L5	2408	U
1	L5	2417	A
1	L5	2418	A
1	L5	2421	G
1	L5	2425	U
1	L5	2436	U
1	L5	2441	C
1	L5	2460	A
1	L5	2464	C
1	L5	2465	C
1	L5	2467	U
1	L5	2471	G
1	L5	2474	G
1	L5	2475	G
1	L5	2478	C
1	L5	2479	G
1	L5	2483	G
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	2503	G
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G
1	L5	2511	A
1	L5	2513	A
1	L5	2514	G
1	L5	2519	U
1	L5	2520	C
1	L5	2529	A
1	L5	2537	A
1	L5	2544	G
1	L5	2546	G
1	L5	2547	G

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Mol	Chain	Res	Type
1	L5	2554	U
1	L5	2555	G
1	L5	2559	G
1	L5	2560	C
1	L5	2573	A
1	L5	2583	C
1	L5	2587	A
1	L5	2589	C
1	L5	2601	A
1	L5	2603	C
1	L5	2611	A
1	L5	2627	C
1	L5	2638	G
1	L5	2652	G
1	L5	2653	C
1	L5	2661	U
1	L5	2662	G
1	L5	2669	C
1	L5	2670	C
1	L5	2676	A
1	L5	2687	U
1	L5	2694	G
1	L5	2695	A
1	L5	2696	A
1	L5	2703	G
1	L5	2707	U
1	L5	2708	U
1	L5	2709	C
1	L5	2710	C
1	L5	2711	G
1	L5	2719	C
1	L5	2723	U
1	L5	2724	G
1	L5	2726	G
1	L5	2739	C
1	L5	2742	G
1	L5	2743	A
1	L5	2756	G
1	L5	2759	G
1	L5	2761	U
1	L5	2763	U
1	L5	2764	A

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Mol	Chain	Res	Type
1	L5	2769	U
1	L5	2770	C
1	L5	2787	A
1	L5	2788	U
1	L5	2790	U
1	L5	2826	U
1	L5	2827	G
1	L5	2835	A
1	L5	2838	G
1	L5	2848	G
1	L5	2855	G
1	L5	2877	G
1	L5	2892	C
1	L5	2894	A
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	2907	G
1	L5	2908	U
1	L5	3585	G
1	L5	3586	G
1	L5	3587	C
1	L5	3590	G
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	3605	C
1	L5	3606	U
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

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Mol	Chain	Res	Type
1	L5	3648	A
1	L5	3662	A
1	L5	3664	G
1	L5	3673	C
1	L5	3674	G
1	L5	3680	U
1	L5	3691	G
1	L5	3692	A
1	L5	3711	A
1	L5	3713	U
1	L5	3714	G
1	L5	3726	A
1	L5	3727	A
1	L5	3729	U
1	L5	3735	G
1	L5	3736	A
1	L5	3747	A
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	3761	C
1	L5	3771	C
1	L5	3775	A
1	L5	3776	G
1	L5	3777	G
1	L5	3783	A
1	L5	3784	A
1	L5	3786	U
1	L5	3790	U
1	L5	3802	U
1	L5	3810	C
1	L5	3811	G
1	L5	3812	C
1	L5	3814	U
1	L5	3817	A
1	L5	3818	U
1	L5	3819	G
1	L5	3838	U

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Mol	Chain	Res	Type
1	L5	3839	G
1	L5	3840	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	3890	A
1	L5	3892	U
1	L5	3897	G
1	L5	3901	A
1	L5	3905	A
1	L5	3906	A
1	L5	3907	G
1	L5	3908	A
1	L5	3915	U
1	L5	3938	G
1	L5	3939	G
1	L5	3942	A
1	L5	3943	A
1	L5	3947	A
1	L5	3948	C
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	3967	G
1	L5	3969	G
1	L5	3970	G
1	L5	3971	G
1	L5	3973	G
1	L5	3974	G

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Mol	Chain	Res	Type
1	L5	3977	C
1	L5	4034	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	4092	G
1	L5	4095	G
1	L5	4099	G
1	L5	4101	C
1	L5	4102	C
1	L5	4104	G
1	L5	4106	G
1	L5	4107	G
1	L5	4108	G
1	L5	4111	U
1	L5	4112	C
1	L5	4113	U
1	L5	4114	C
1	L5	4115	G

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Mol	Chain	Res	Type
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	4149	C
1	L5	4150	G
1	L5	4157	A
1	L5	4160	C
1	L5	4162	C
1	L5	4163	U
1	L5	4168	G
1	L5	4170	A
1	L5	4183	G
1	L5	4184	G
1	L5	4191	G
1	L5	4196	G
1	L5	4197	G
1	L5	4203	A
1	L5	4220	A
1	L5	4222	G
1	L5	4225	G
1	L5	4228	G
1	L5	4229	U
1	L5	4233	A
1	L5	4238	G
1	L5	4251	A
1	L5	4254	G
1	L5	4255	A
1	L5	4256	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

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Mol	Chain	Res	Type
1	L5	4304	A
1	L5	4305	G
1	L5	4306	U
1	L5	4314	C
1	L5	4319	C
1	L5	4329	G
1	L5	4330	G
1	L5	4332	C
1	L5	4339	A
1	L5	4349	C
1	L5	4354	U
1	L5	4371	G
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	4382	G
1	L5	4387	C
1	L5	4391	G
1	L5	4394	A
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	4466	C
1	L5	4475	G
1	L5	4488	A
1	L5	4500	U
1	L5	4512	U
1	L5	4513	A
1	L5	4518	A
1	L5	4519	C
1	L5	4524	G
1	L5	4525	C
1	L5	4528	G
1	L5	4531	U
1	L5	4545	G
1	L5	4547	C

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Mol	Chain	Res	Type
1	L5	4548	A
1	L5	4549	G
1	L5	4557	U
1	L5	4560	C
1	L5	4567	G
1	L5	4569	U
1	L5	4573	G
1	L5	4575	G
1	L5	4589	A
1	L5	4590	A
1	L5	4600	G
1	L5	4601	U
1	L5	4608	G
1	L5	4617	G
1	L5	4626	A
1	L5	4627	U
1	L5	4633	G
1	L5	4635	A
1	L5	4636	U
1	L5	4637	G
1	L5	4656	A
1	L5	4657	U
1	L5	4670	C
1	L5	4672	A
1	L5	4677	U
1	L5	4687	A
1	L5	4695	C
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4719	G
1	L5	4731	G
1	L5	4732	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	4746	C
1	L5	4747	C
1	L5	4751	G

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Mol	Chain	Res	Type
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	4773	C
1	L5	4775	C
1	L5	4859	C
1	L5	4870	G
1	L5	4871	C
1	L5	4875	G
1	L5	4882	U
1	L5	4883	C
1	L5	4888	U
1	L5	4889	G
1	L5	4891	G
1	L5	4895	C
1	L5	4896	G
1	L5	4897	G
1	L5	4899	G
1	L5	4900	C
1	L5	4901	G
1	L5	4902	C
1	L5	4905	C
1	L5	4906	U
1	L5	4910	A
1	L5	4911	A
1	L5	4912	G
1	L5	4914	C
1	L5	4922	C
1	L5	4923	C
1	L5	4925	U
1	L5	4926	C
1	L5	4927	G
1	L5	4928	C
1	L5	4934	A
1	L5	4937	C
1	L5	4940	C
1	L5	4941	G
1	L5	4943	A

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Mol	Chain	Res	Type
1	L5	4949	G
1	L5	4951	G
1	L5	4960	G
1	L5	4961	G
1	L5	4966	A
1	L5	4975	G
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	5017	G
1	L5	5024	C
1	L5	5025	C
1	L5	5026	U
1	L5	5027	C
1	L5	5028	G
1	L5	5029	C
1	L5	5031	G
1	L5	5034	A
1	L5	5041	G
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	22	A
2	L7	38	U
2	L7	53	U
2	L7	54	A
2	L7	63	C
2	L7	64	G
2	L7	100	A
2	L7	110	G
3	L8	25	G
3	L8	34	U
3	L8	35	C
3	L8	48	A

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Mol	Chain	Res	Type
3	L8	52	A
3	L8	59	A
3	L8	62	A
3	L8	63	U
3	L8	80	A
3	L8	81	C
3	L8	82	A
3	L8	83	C
3	L8	84	A
3	L8	85	U
3	L8	87	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
3	L8	124	U
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	150	C
3	L8	156	U
49	S2	14	C
49	S2	17	C
49	S2	25	A
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	61	A
49	S2	64	A
49	S2	66	G
49	S2	67	C
49	S2	68	A
49	S2	72	C
49	S2	73	C
49	S2	74	G

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Mol	Chain	Res	Type
49	S2	76	U
49	S2	92	A
49	S2	103	A
49	S2	113	G
49	S2	115	U
49	S2	116	U
49	S2	121	U
49	S2	126	G
49	S2	130	G
49	S2	139	C
49	S2	143	U
49	S2	155	G
49	S2	158	A
49	S2	159	A
49	S2	160	U
49	S2	161	U
49	S2	162	C
49	S2	163	U
49	S2	175	A
49	S2	182	C
49	S2	184	G
49	S2	190	G
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	214	U
49	S2	290	U
49	S2	292	A
49	S2	293	C
49	S2	295	C
49	S2	306	C
49	S2	307	G
49	S2	308	G
49	S2	309	G
49	S2	311	C
49	S2	318	A

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Mol	Chain	Res	Type
49	S2	319	C
49	S2	322	C
49	S2	323	C
49	S2	324	C
49	S2	325	C
49	S2	326	C
49	S2	328	U
49	S2	329	G
49	S2	332	G
49	S2	339	A
49	S2	340	C
49	S2	347	G
49	S2	351	G
49	S2	360	A
49	S2	362	C
49	S2	364	A
49	S2	368	U
49	S2	369	C
49	S2	370	G
49	S2	382	C
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	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	471	G
49	S2	472	C
49	S2	473	A
49	S2	474	G
49	S2	476	A
49	S2	482	G
49	S2	487	U
49	S2	488	U

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Mol	Chain	Res	Type
49	S2	492	C
49	S2	493	A
49	S2	502	C
49	S2	503	C
49	S2	516	A
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	542	U
49	S2	546	G
49	S2	547	G
49	S2	551	U
49	S2	556	U
49	S2	557	U
49	S2	558	G
49	S2	559	G
49	S2	563	G
49	S2	564	A
49	S2	566	U
49	S2	567	C
49	S2	570	C
49	S2	576	A
49	S2	583	A
49	S2	584	A
49	S2	585	C
49	S2	587	A
49	S2	589	G
49	S2	590	A
49	S2	591	U
49	S2	594	A
49	S2	597	G
49	S2	604	A
49	S2	607	U
49	S2	614	C
49	S2	623	G
49	S2	628	A
49	S2	631	U
49	S2	632	C

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Mol	Chain	Res	Type
49	S2	643	A
49	S2	644	G
49	S2	655	A
49	S2	659	G
49	S2	660	C
49	S2	662	G
49	S2	663	C
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
49	S2	689	U
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	798	G
49	S2	799	U
49	S2	801	U
49	S2	810	A
49	S2	811	A
49	S2	821	G
49	S2	822	U
49	S2	823	U
49	S2	824	C
49	S2	830	A
49	S2	834	C

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Mol	Chain	Res	Type
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	842	C
49	S2	847	A
49	S2	869	A
49	S2	870	A
49	S2	872	A
49	S2	873	G
49	S2	874	G
49	S2	877	C
49	S2	878	G
49	S2	880	G
49	S2	882	U
49	S2	883	U
49	S2	887	U
49	S2	888	U
49	S2	889	U
49	S2	891	G
49	S2	893	U
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	920	A
49	S2	930	C
49	S2	933	G
49	S2	934	G
49	S2	963	A
49	S2	972	A
49	S2	990	A
49	S2	992	A
49	S2	999	G

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Mol	Chain	Res	Type
49	S2	1001	A
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	1034	A
49	S2	1047	C
49	S2	1061	U
49	S2	1062	A
49	S2	1083	A
49	S2	1085	C
49	S2	1088	U
49	S2	1094	C
49	S2	1109	C
49	S2	1115	U
49	S2	1116	C
49	S2	1118	C
49	S2	1121	G
49	S2	1133	A
49	S2	1138	C
49	S2	1150	A
49	S2	1153	C
49	S2	1154	U
49	S2	1155	U
49	S2	1170	A
49	S2	1195	A
49	S2	1203	G
49	S2	1207	G
49	S2	1208	A
49	S2	1211	G
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

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Mol	Chain	Res	Type
49	S2	1257	G
49	S2	1259	A
49	S2	1264	C
49	S2	1265	A
49	S2	1274	G
49	S2	1275	G
49	S2	1281	G
49	S2	1283	C
49	S2	1284	A
49	S2	1286	G
49	S2	1294	G
49	S2	1295	A
49	S2	1298	G
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	1318	G
49	S2	1342	U
49	S2	1343	U
49	S2	1348	G
49	S2	1371	U
49	S2	1372	U
49	S2	1373	C
49	S2	1378	A
49	S2	1402	A
49	S2	1404	U
49	S2	1406	G
49	S2	1409	A
49	S2	1412	C
49	S2	1414	A
49	S2	1415	C
49	S2	1420	G
49	S2	1421	A
49	S2	1422	G
49	S2	1423	C
49	S2	1424	G
49	S2	1428	G
49	S2	1433	C
49	S2	1435	C

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Mol	Chain	Res	Type
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	1497	G
49	S2	1498	A
49	S2	1506	A
49	S2	1508	A
49	S2	1509	U
49	S2	1520	G
49	S2	1521	C
49	S2	1531	A
49	S2	1533	A
49	S2	1537	A
49	S2	1544	C
49	S2	1553	C
49	S2	1555	U
49	S2	1556	A
49	S2	1558	C
49	S2	1570	G
49	S2	1574	C
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	1621	U
49	S2	1623	A
49	S2	1634	A
49	S2	1637	A
49	S2	1638	G
49	S2	1640	A
49	S2	1644	C

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Mol	Chain	Res	Type
49	S2	1648	G
49	S2	1654	G
49	S2	1663	A
49	S2	1665	G
49	S2	1671	G
49	S2	1680	G
49	S2	1686	G
49	S2	1699	A
49	S2	1701	C
49	S2	1715	A
49	S2	1719	A
49	S2	1721	U
49	S2	1722	G
49	S2	1735	A
49	S2	1742	C
49	S2	1743	G
49	S2	1744	G
49	S2	1745	A
49	S2	1752	C
49	S2	1753	C
49	S2	1754	G
49	S2	1757	G
49	S2	1758	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	1781	A
49	S2	1783	C
49	S2	1784	G
49	S2	1786	U
49	S2	1822	A
49	S2	1823	A
49	S2	1829	G
49	S2	1831	A
49	S2	1835	A
49	S2	1838	U
49	S2	1849	G

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Mol	Chain	Res	Type
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	11	C
84	CC	16	C
84	CC	17	G
84	CC	18	G
84	CC	19	C
84	CC	20	U
84	CC	21	A
84	CC	23	C
84	CC	28	C
84	CC	31	G
84	CC	32	C
84	CC	33	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	55	C
84	CC	57	A
84	CC	61	C
84	CC	72	G
84	CC	73	C
84	CC	75	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	406	C
1	L5	504	G
1	L5	914	U
1	L5	1082	C
1	L5	1633	G

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Mol	Chain	Res	Type
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	4548	A
1	L5	4699	U
1	L5	4910	A
1	L5	4913	G
1	L5	4914	C
49	S2	60	G
49	S2	112	U
49	S2	158	A
49	S2	291	G
49	S2	369	C
49	S2	417	C
49	S2	420	G
49	S2	563	G
49	S2	567	C
49	S2	688	U
49	S2	797	C
49	S2	1434	C
84	CC	35	U
84	CC	74	C

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 267 ligands modelled in this entry, 264 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
91	SF4	CI	601	-	0,12,12	-	-	-		
92	ADP	CI	603	-	24,29,29	0.94	1 (4%)	29,45,45	1.35	4 (13%)
91	SF4	CI	602	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	SF4	CI	601	-	-	-	0/6/5/5
92	ADP	CI	603	-	-	6/12/32/32	0/3/3/3
91	SF4	CI	602	-	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	CI	603	ADP	C5-C4	2.41	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
92	CI	603	ADP	N3-C2-N1	-3.25	123.59	128.68
92	CI	603	ADP	C4-C5-N7	-2.78	106.50	109.40
92	CI	603	ADP	C3'-C2'-C1'	2.72	105.07	100.98
92	CI	603	ADP	PA-O3A-PB	-2.49	124.29	132.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	CI	603	ADP	PB-O3A-PA-O5'
92	CI	603	ADP	C5'-O5'-PA-O1A

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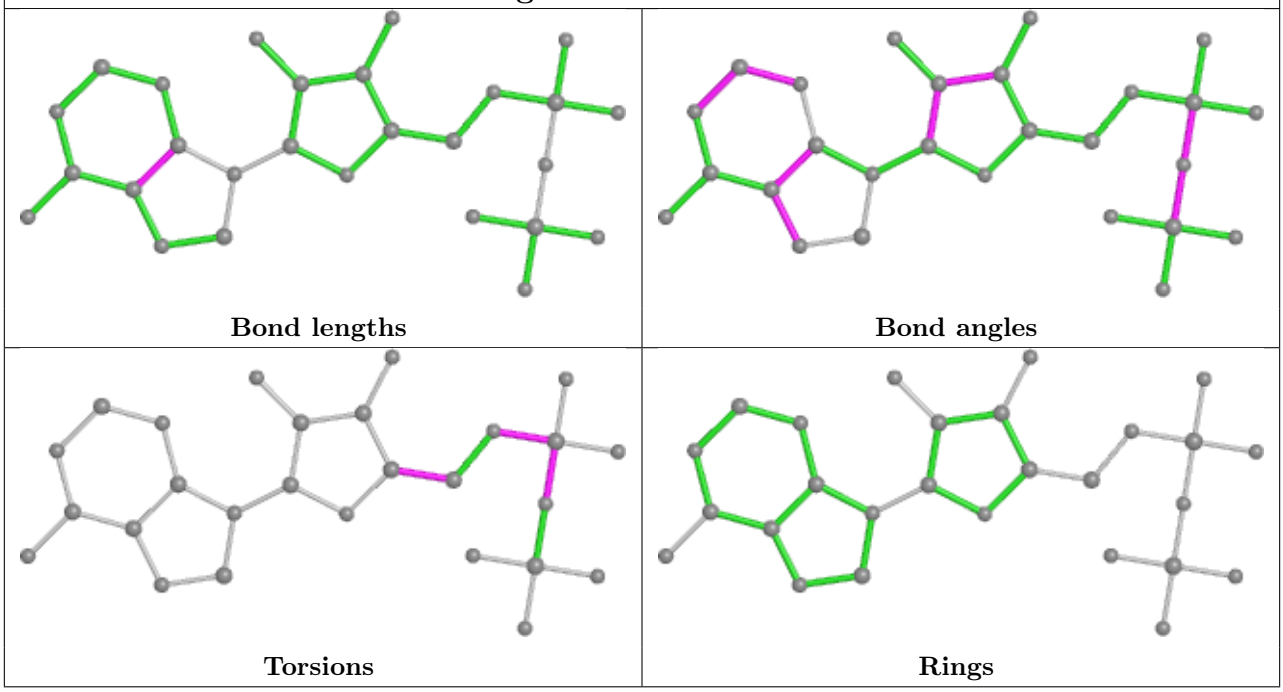
Mol	Chain	Res	Type	Atoms
92	CI	603	ADP	C5'-O5'-PA-O2A
92	CI	603	ADP	O4'-C4'-C5'-O5'
92	CI	603	ADP	C3'-C4'-C5'-O5'
92	CI	603	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP CI 603



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.

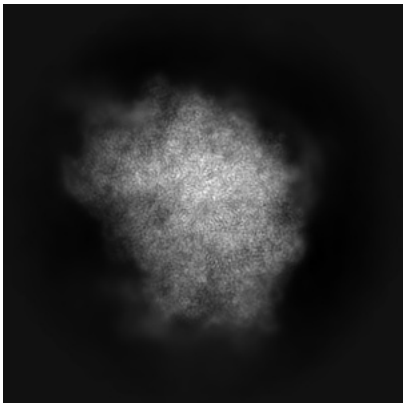
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11289. These allow visual inspection of the internal detail of the map and identification of artifacts.

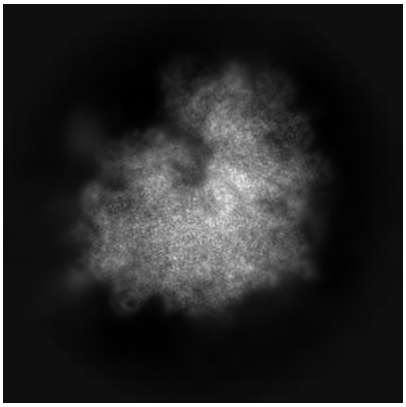
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

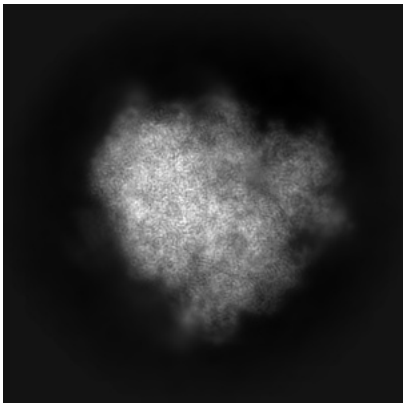
6.1.1 Primary map



X



Y

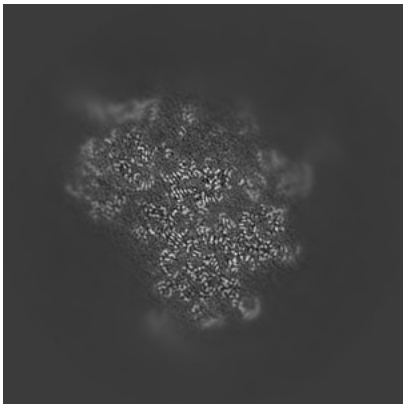


Z

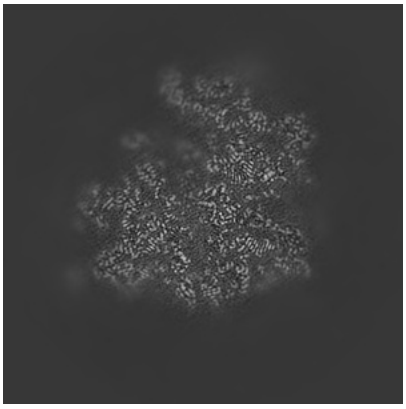
The images above show the map projected in three orthogonal directions.

6.2 Central slices

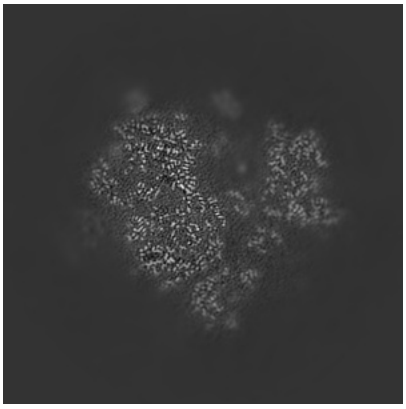
6.2.1 Primary map



X Index: 200



Y Index: 200

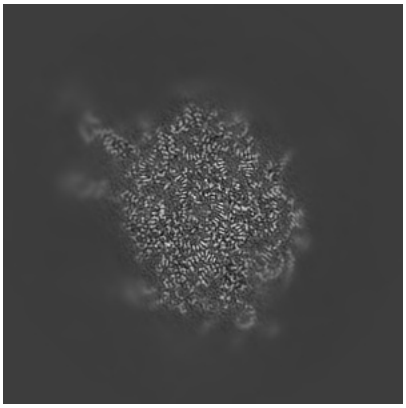


Z Index: 200

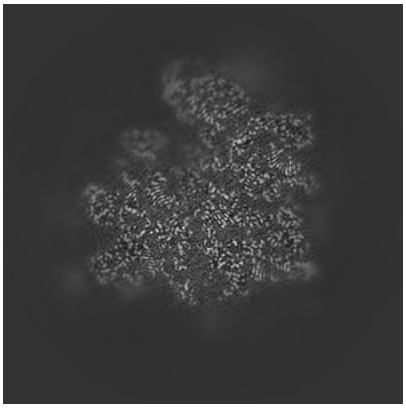
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 178



Y Index: 194

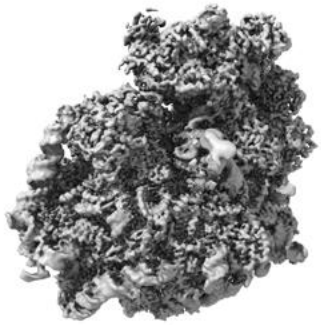
Z Index: 224

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.

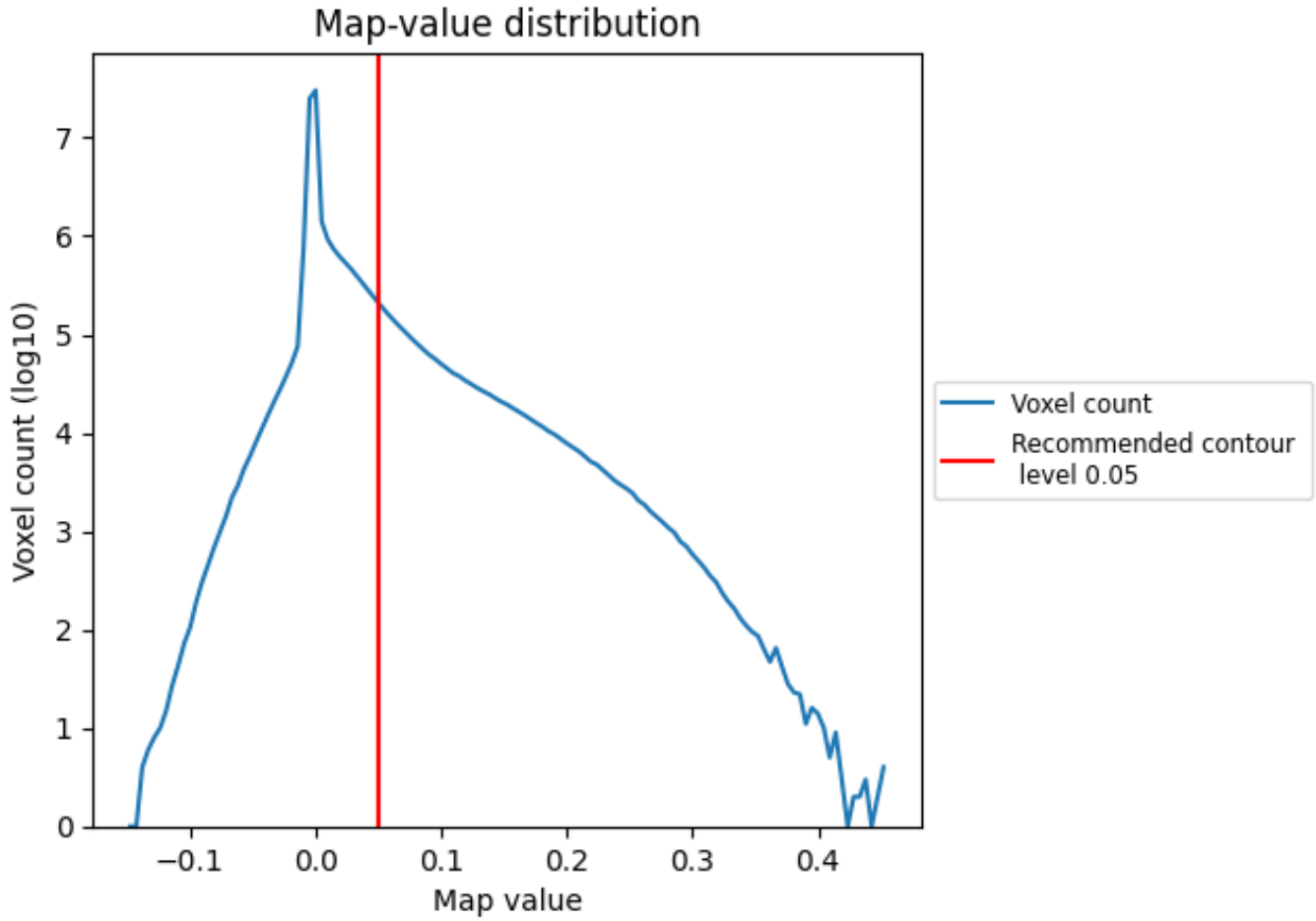
6.5 Mask visualisation (i)

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

7 Map analysis

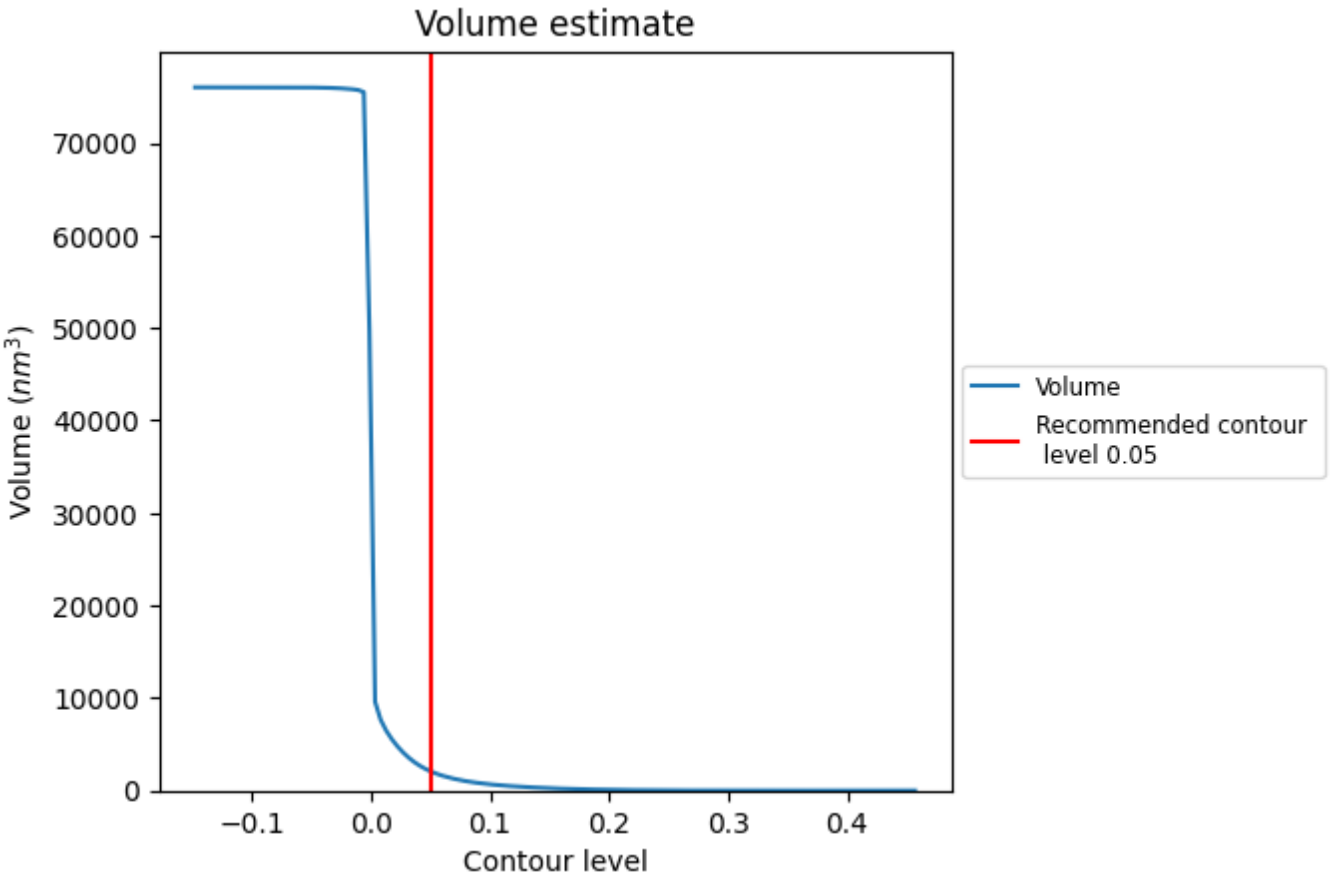
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

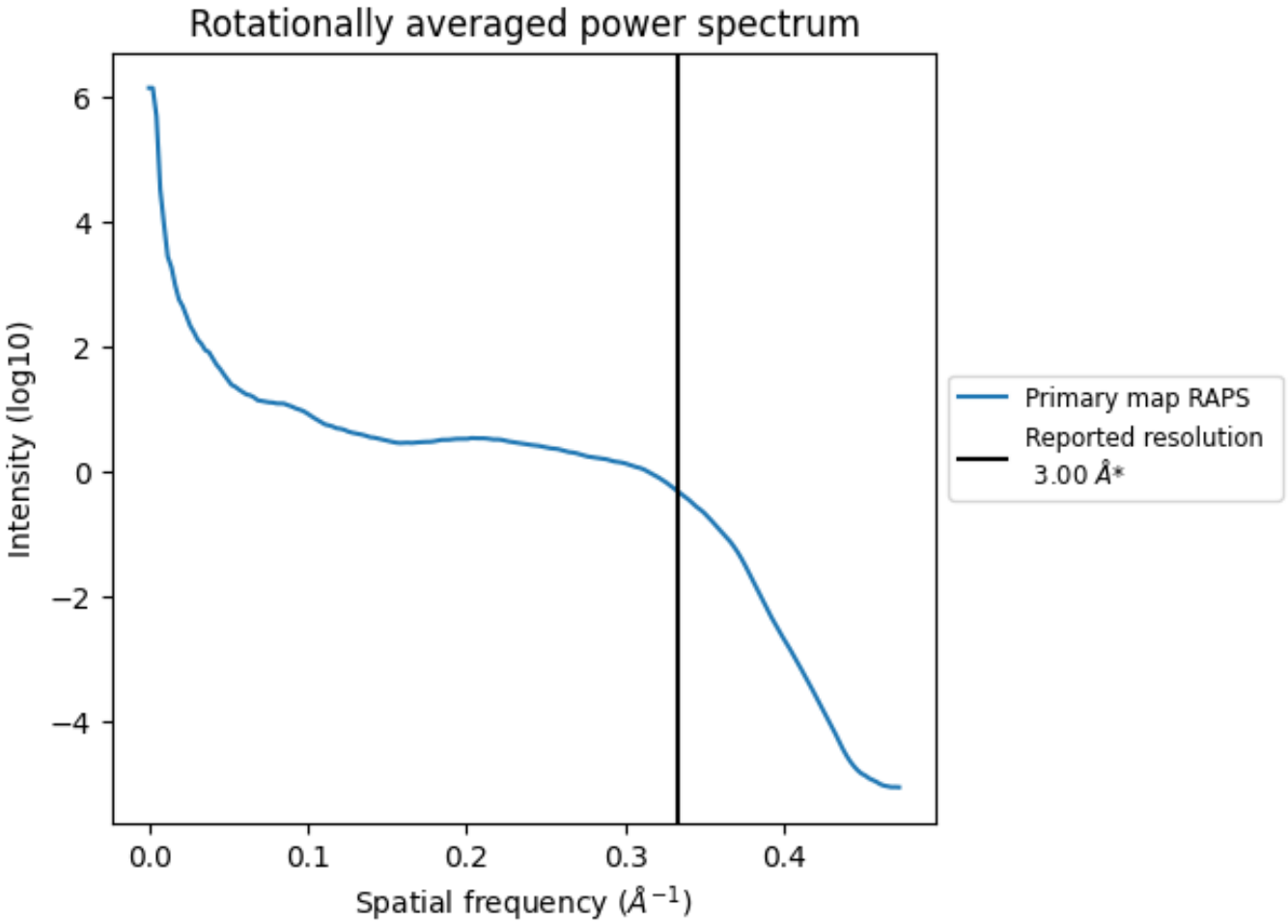
7.2 Volume estimate



The volume at the recommended contour level is 2092 nm^3; this corresponds to an approximate mass of 1890 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)

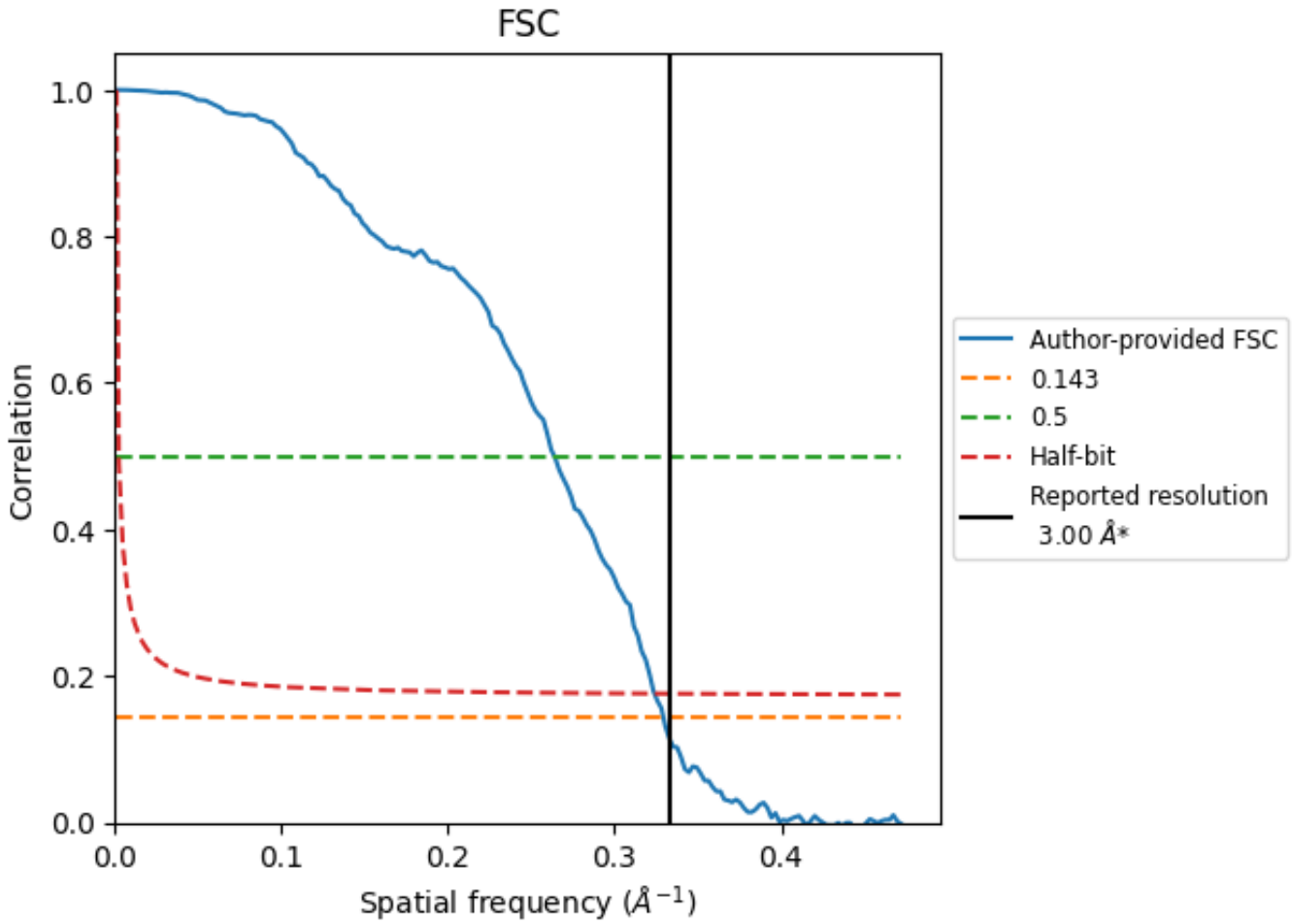


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

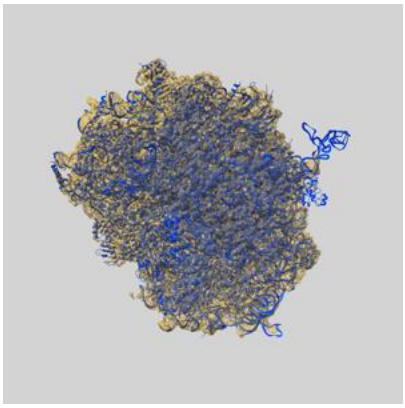
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.04	3.79	3.09
Unmasked-calculated*	-	-	-

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

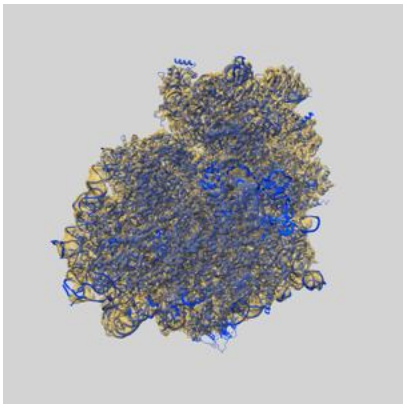
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11289 and PDB model 6ZME. Per-residue inclusion information can be found in section 3 on page 22.

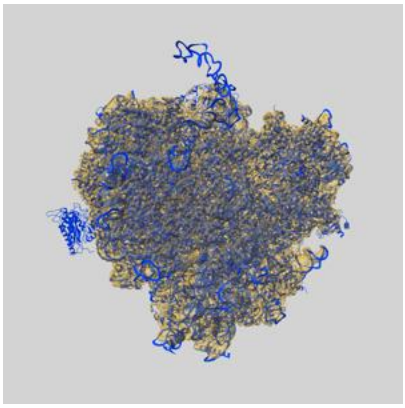
9.1 Map-model overlay



X



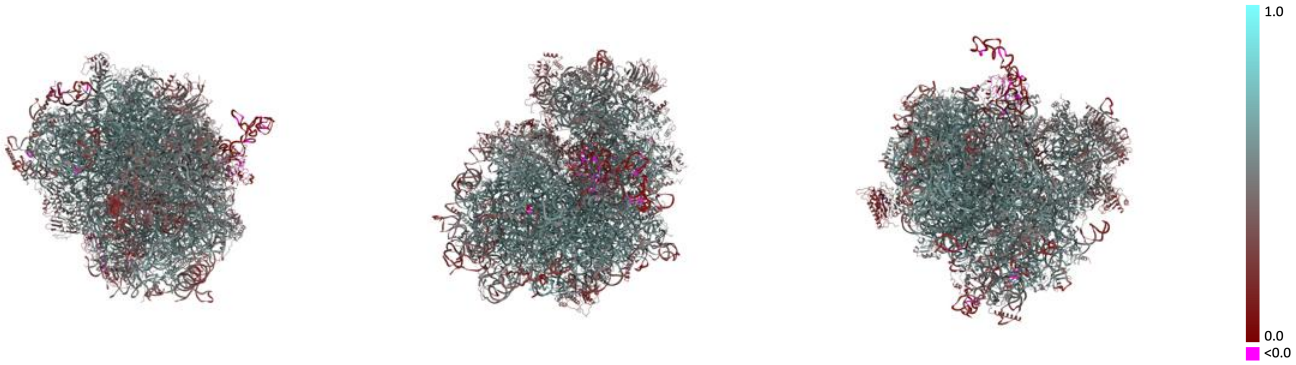
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

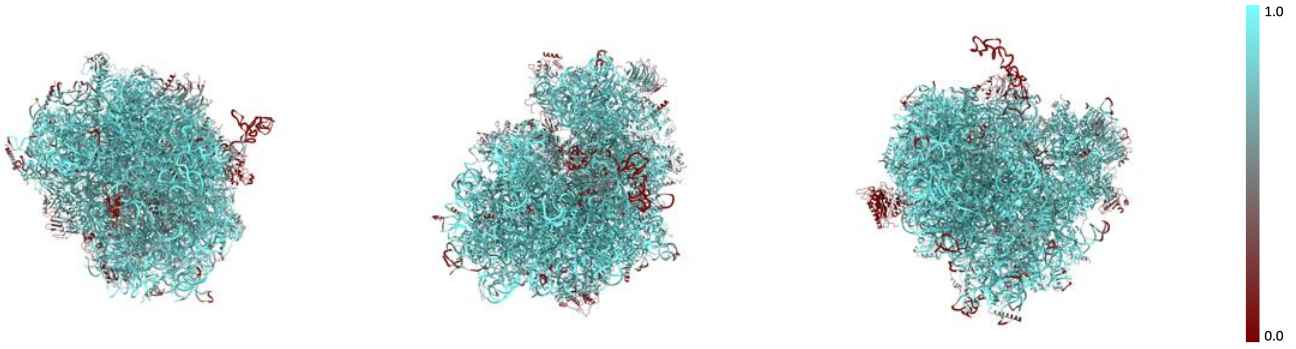
9.2 Q-score mapped to coordinate model



X Y Z

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

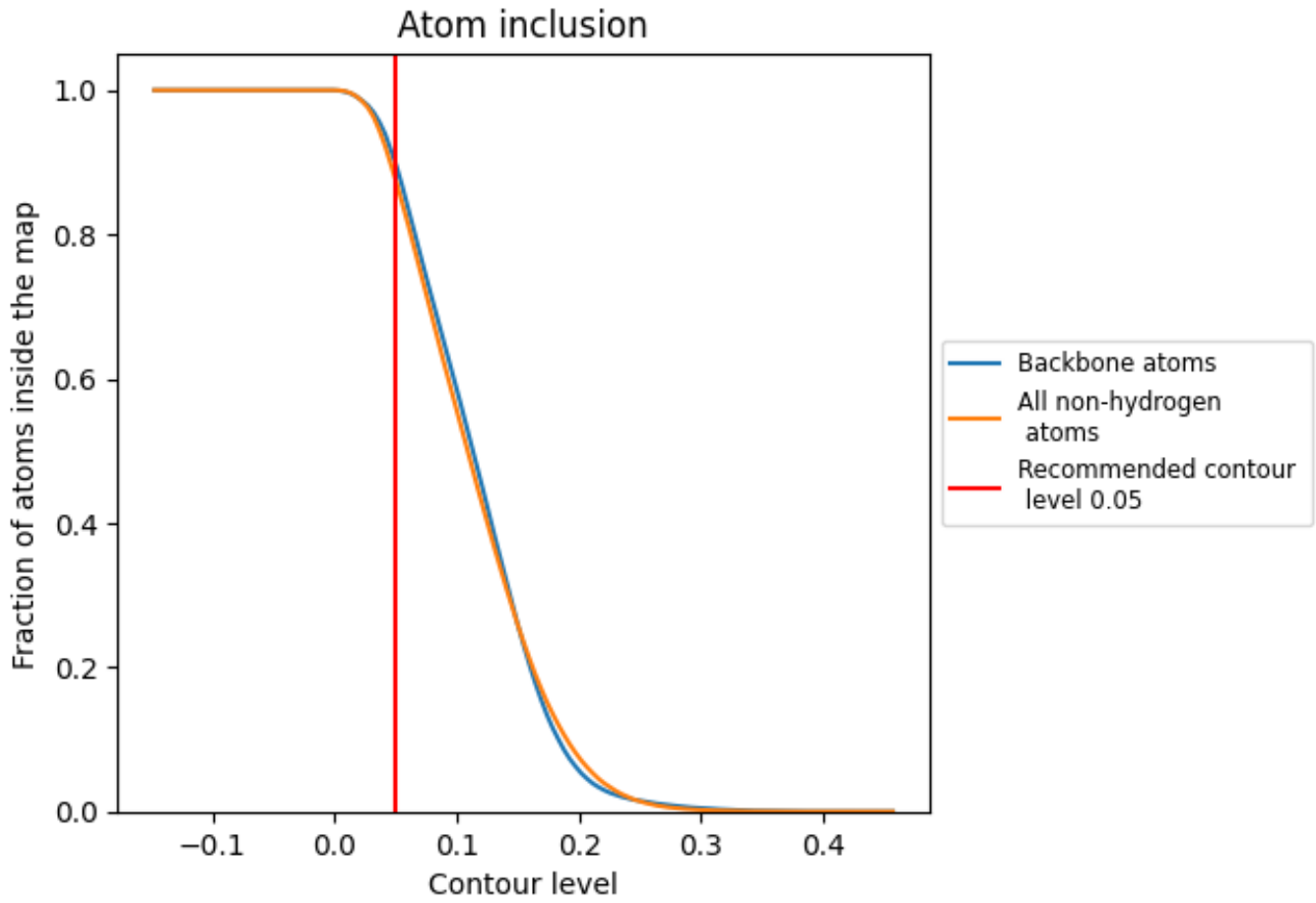
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% 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	0.8752	0.5200
CA	0.0418	0.2520
CC	0.8735	0.2970
CE	0.7321	0.4260
CF	0.9227	0.5470
CH	0.5680	0.3700
CI	0.6837	0.4610
L5	0.9331	0.5400
L7	0.9860	0.5750
L8	0.9656	0.5680
LA	0.9809	0.6180
LB	0.9339	0.5870
LC	0.9283	0.5780
LD	0.8681	0.5220
LE	0.8254	0.4970
LF	0.9629	0.5860
LG	0.8067	0.5060
LH	0.9054	0.5490
LI	0.9364	0.5660
LJ	0.7787	0.4470
LL	0.8819	0.5450
LM	0.9160	0.5440
LN	0.9870	0.6250
LO	0.9442	0.5940
LP	0.9577	0.6110
LQ	0.9675	0.6020
LR	0.8753	0.5450
LS	0.9636	0.5930
LT	0.9311	0.5590
LU	0.8154	0.4710
LV	0.9676	0.5970
LW	0.7010	0.4520
LX	0.9187	0.5670
LY	0.9026	0.5640
LZ	0.8993	0.5590

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Chain	Atom inclusion	Q-score
La	0.9540	0.6050
Lb	0.8300	0.5030
Lc	0.9116	0.5520
Ld	0.9125	0.5680
Le	0.9676	0.5970
Lf	0.9667	0.6100
Lg	0.9208	0.5790
Lh	0.9001	0.5490
Li	0.8972	0.5450
Lj	0.9807	0.6110
Lk	0.7774	0.5000
Ll	0.9811	0.5910
Lm	0.9327	0.5710
Ln	0.9856	0.6110
Lo	0.9104	0.5780
Lp	0.9463	0.6000
Lr	0.9491	0.5740
Ls	0.3313	0.2650
Lt	0.4747	0.2590
Lz	0.1144	0.1150
S2	0.9383	0.5330
SA	0.8447	0.5200
SB	0.8858	0.5350
SC	0.9143	0.5530
SD	0.7770	0.4540
SE	0.9096	0.5520
SF	0.8551	0.4850
SG	0.7753	0.4650
SH	0.7211	0.4510
SI	0.8783	0.5330
SJ	0.8805	0.5310
SK	0.7441	0.4100
SL	0.8977	0.5670
SM	0.2511	0.2210
SN	0.9300	0.5670
SO	0.8784	0.5390
SP	0.7342	0.4250
SQ	0.8092	0.4820
SR	0.7604	0.4670
SS	0.7858	0.4500
ST	0.8272	0.4790
SU	0.7338	0.4230

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Chain	Atom inclusion	Q-score
SV	0.8762	0.5390
SW	0.9455	0.5830
SX	0.9421	0.5810
SY	0.8184	0.5020
SZ	0.7101	0.4320
Sa	0.9202	0.5630
Sb	0.8388	0.5140
Sc	0.7387	0.4570
Sd	0.9525	0.5380
Se	0.8184	0.5030
Sf	0.4494	0.2880
Sg	0.6098	0.3900