Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 01:41 pm GMT

PDB ID	:	6Z6L
EMDB ID	:	EMD-11098
Title	:	Cryo-EM structure of human CCDC124 bound to 80S ribosomes
Authors	:	Wells, J.N.; Buschauer, R.; Mackens-Kiani, T.; Best, K.; Kratzat, H.; Berninghausen, O.; Becker, T.; Cheng, J.; Beckmann, R.
Deposited on	:	2020-05-28
Resolution	:	3.00 Å(reported)
Based on initial model	:	6EK0

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

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

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

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

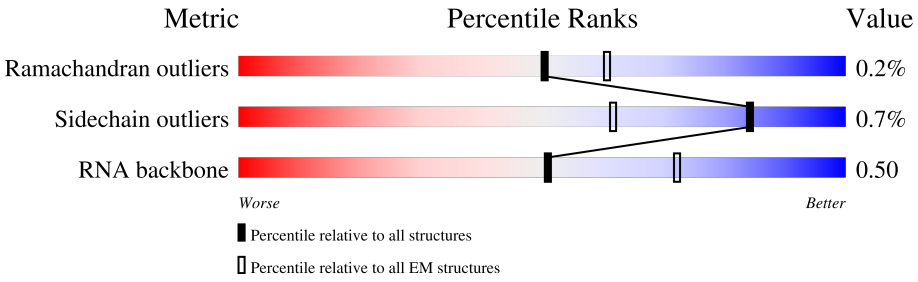
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	5070	53% 19% 26%
2	L7	121	90% 9%
3	L8	157	78% 20%
4	LA	257	94%
5	LB	403	99%
6	LC	427	85% 14%
7	LD	297	98%
8	LE	288	81% 18%

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Mol	Chain	Length	Quality of chain
9	LF	248	90% 9%
10	LG	266	90% 9%
11	LH	192	98%
12	LI	214	94% 6%
13	LJ	178	98%
14	LL	211	99%
15	LM	215	64% 35%
16	LN	204	98%
17	LO	203	98%
18	LP	184	83% 17%
19	LQ	188	99%
20	LR	196	95% 5%
21	LS	176	99%
22	LT	160	98%
23	LU	128	78% 21%
24	LV	140	93% 6%
25	LW	157	78% 21%
26	LX	156	77% 23%
27	LY	145	91% 8%
28	LZ	136	99%
29	La	148	97%
30	Lb	159	67% 31%
31	Lc	115	84% 15%
32	Ld	125	85% 14%
33	Le	135	94% 5%

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Mol	Chain	Length	Quality of chain
34	Lf	110	95% 5%
35	Lg	117	97%
36	Lh	123	98%
37	Li	105	97%
38	Lj	97	86% 11%
39	Lk	70	94%
40	Ll	51	94%
41	Lm	128	41% 59%
42	Ln	25	96%
43	Lo	104	99%
44	Lp	92	99%
45	Lr	137	91% 9%
46	Lz	217	5% 97%
47	S2	1869	68% 23% 7%
48	SA	295	75% 25%
49	SB	264	80% 19%
50	SD	243	92% 7%
51	SE	263	99%
52	SF	204	90% 10%
53	SH	194	93%
54	SI	208	99%
55	SK	165	58% 41%
56	SL	158	96%
57	SP	145	86% 12%
58	SQ	146	97%

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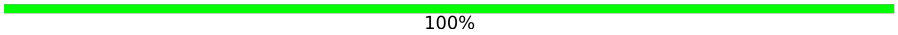
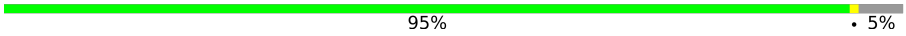
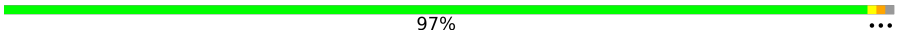
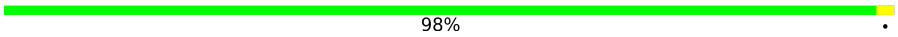
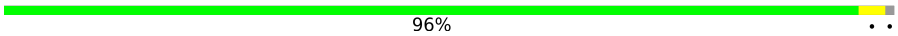
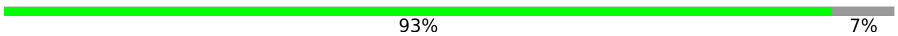
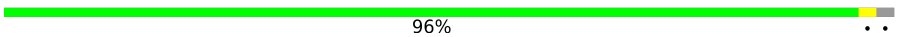
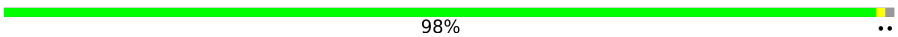
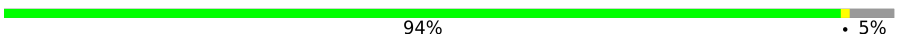
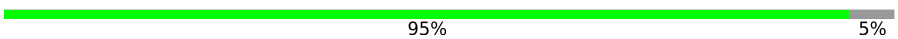
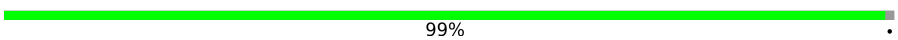
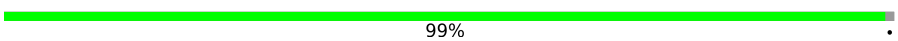
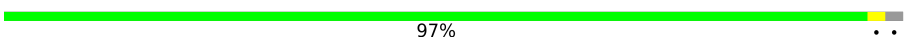
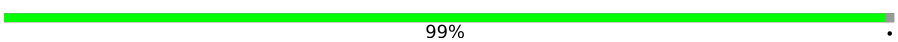
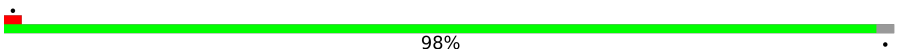
Mol	Chain	Length	Quality of chain
59	SR	135	
60	SS	152	
61	ST	145	
62	SU	119	
63	SV	83	
64	SX	143	
65	Sa	115	
66	Sc	69	
67	Sd	56	
68	Sg	317	
69	SC	293	
70	SG	249	
71	SJ	194	
72	SM	132	
73	SN	151	
74	SO	151	
75	SW	130	
76	SY	133	
77	SZ	125	
78	Sb	84	
79	Se	59	
80	Sf	156	
81	CA	394	
82	CC	75	
83	CE	223	

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 222284 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L5	3772	80116	35645	14585	26115	3771	0	0

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

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 rRNA.

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	103	Total	C	N	O	S	0	0
			842	528	172	136	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 ribosomal protein L10a.

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

- Molecule 47 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S2	1740	Total	C	N	O	P	0	0
			36898	16459	6599	12101	1739		

- Molecule 48 is a protein called 40S ribosomal protein SA.

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

- Molecule 49 is a protein called 40S ribosomal protein S3a.

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

- Molecule 50 is a protein called 40S ribosomal protein S3.

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

- Molecule 51 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 52 is a protein called 40S ribosomal protein S5.

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

- Molecule 53 is a protein called 40S ribosomal protein S7.

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

- Molecule 54 is a protein called 40S ribosomal protein S8.

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

- Molecule 55 is a protein called 40S ribosomal protein S10.

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

- Molecule 56 is a protein called 40S ribosomal protein S11.

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

- Molecule 57 is a protein called 40S ribosomal protein S15.

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

- Molecule 58 is a protein called 40S ribosomal protein S16.

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

- Molecule 59 is a protein called 40S ribosomal protein S17.

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

- Molecule 60 is a protein called 40S ribosomal protein S18.

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

- Molecule 61 is a protein called 40S ribosomal protein S19.

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

- Molecule 62 is a protein called 40S ribosomal protein S20.

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

- Molecule 63 is a protein called 40S ribosomal protein S21.

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

- Molecule 64 is a protein called 40S ribosomal protein S23.

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

- Molecule 65 is a protein called 40S ribosomal protein S26.

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

- Molecule 66 is a protein called 40S ribosomal protein S28.

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

- Molecule 67 is a protein called 40S ribosomal protein S29.

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

- Molecule 68 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 69 is a protein called 40S ribosomal protein S2.

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

- Molecule 70 is a protein called 40S ribosomal protein S6.

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

- Molecule 71 is a protein called 40S ribosomal protein S9.

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

- Molecule 72 is a protein called 40S ribosomal protein S12.

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

- Molecule 73 is a protein called 40S ribosomal protein S13.

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

- Molecule 74 is a protein called 40S ribosomal protein S14.

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

- Molecule 75 is a protein called 40S ribosomal protein S15a.

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

- Molecule 76 is a protein called 40S ribosomal protein S24.

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

- Molecule 77 is a protein called 40S ribosomal protein S25.

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

- Molecule 78 is a protein called 40S ribosomal protein S27.

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

- Molecule 79 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 81 is a protein called Proliferation-associated protein 2G4.

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

- Molecule 82 is a RNA chain called tRNA.

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

- Molecule 83 is a protein called Coiled-coil domain-containing protein 124.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	CE	73	Total	C	N	O	S	0	0
			613	369	122	121	1		

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

Mol	Chain	Residues	Atoms	AltConf
84	L5	210	Total Mg 210 210	0
84	L7	3	Total Mg 3 3	0
84	L8	5	Total Mg 5 5	0
84	LA	1	Total Mg 1 1	0
84	LI	1	Total Mg 1 1	0
84	LP	1	Total Mg 1 1	0
84	LV	1	Total Mg 1 1	0
84	Le	2	Total Mg 2 2	0
84	Lg	1	Total Mg 1 1	0
84	Lj	1	Total Mg 1 1	0
84	S2	29	Total Mg 29 29	0
84	SG	1	Total Mg 1 1	0

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

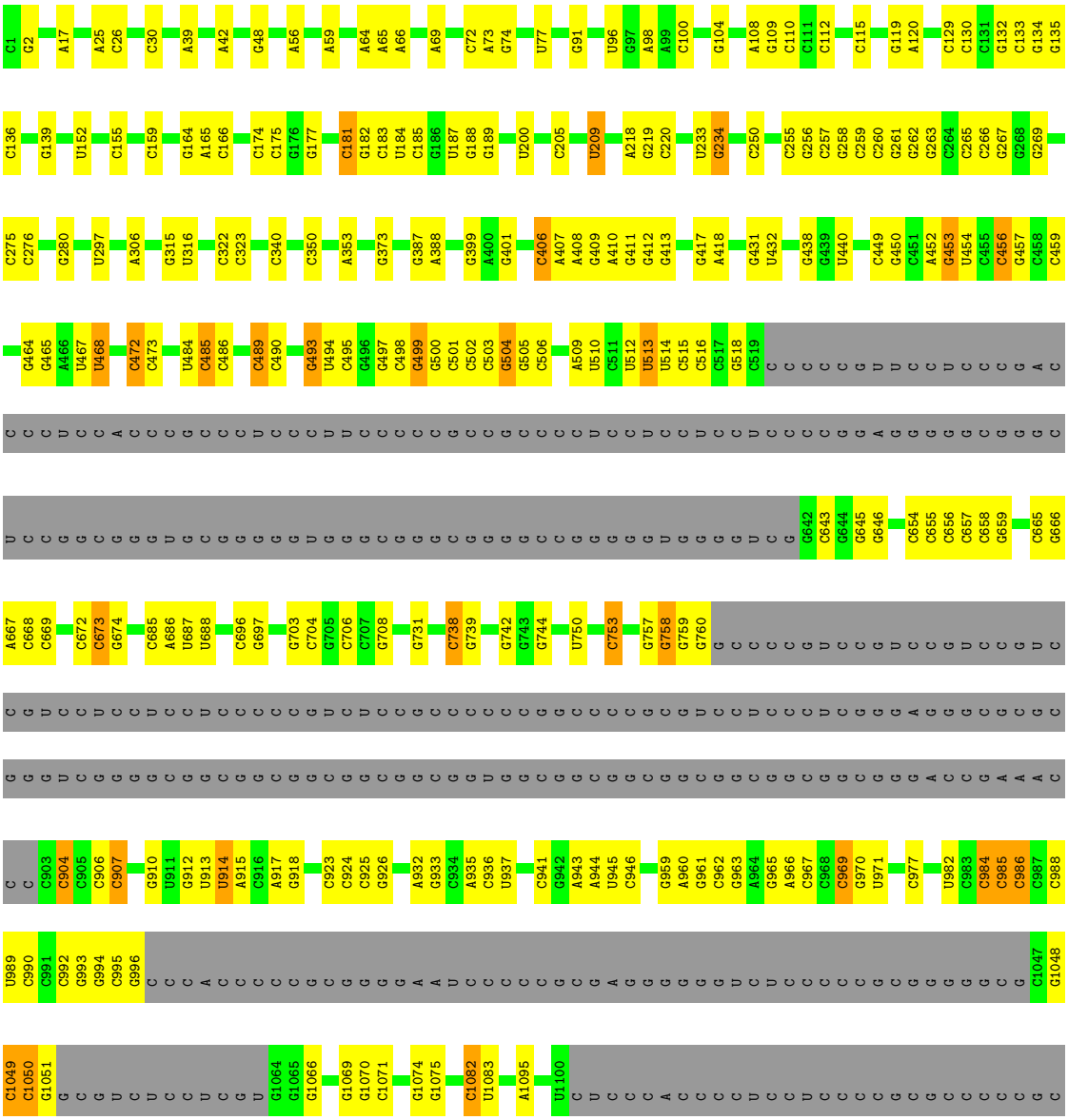
Mol	Chain	Residues	Atoms	AltConf
85	Lg	1	Total Zn 1 1	0
85	Lj	1	Total Zn 1 1	0
85	Lm	1	Total Zn 1 1	0
85	Lo	1	Total Zn 1 1	0
85	Lp	1	Total Zn 1 1	0
85	Sa	1	Total Zn 1 1	0
85	Sd	1	Total Zn 1 1	0
85	Sf	1	Total Zn 1 1	0

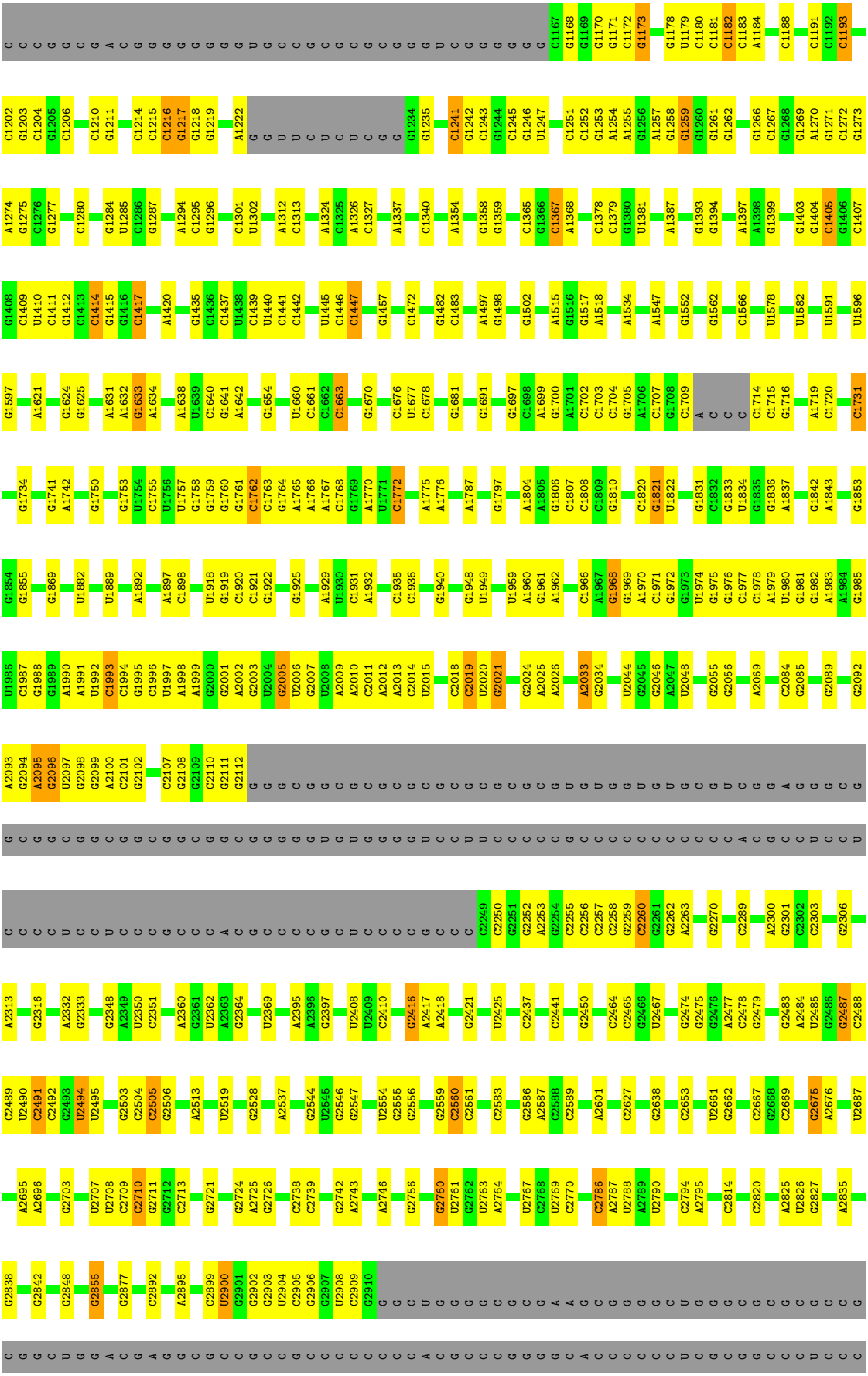
3 Residue-property plots (i)

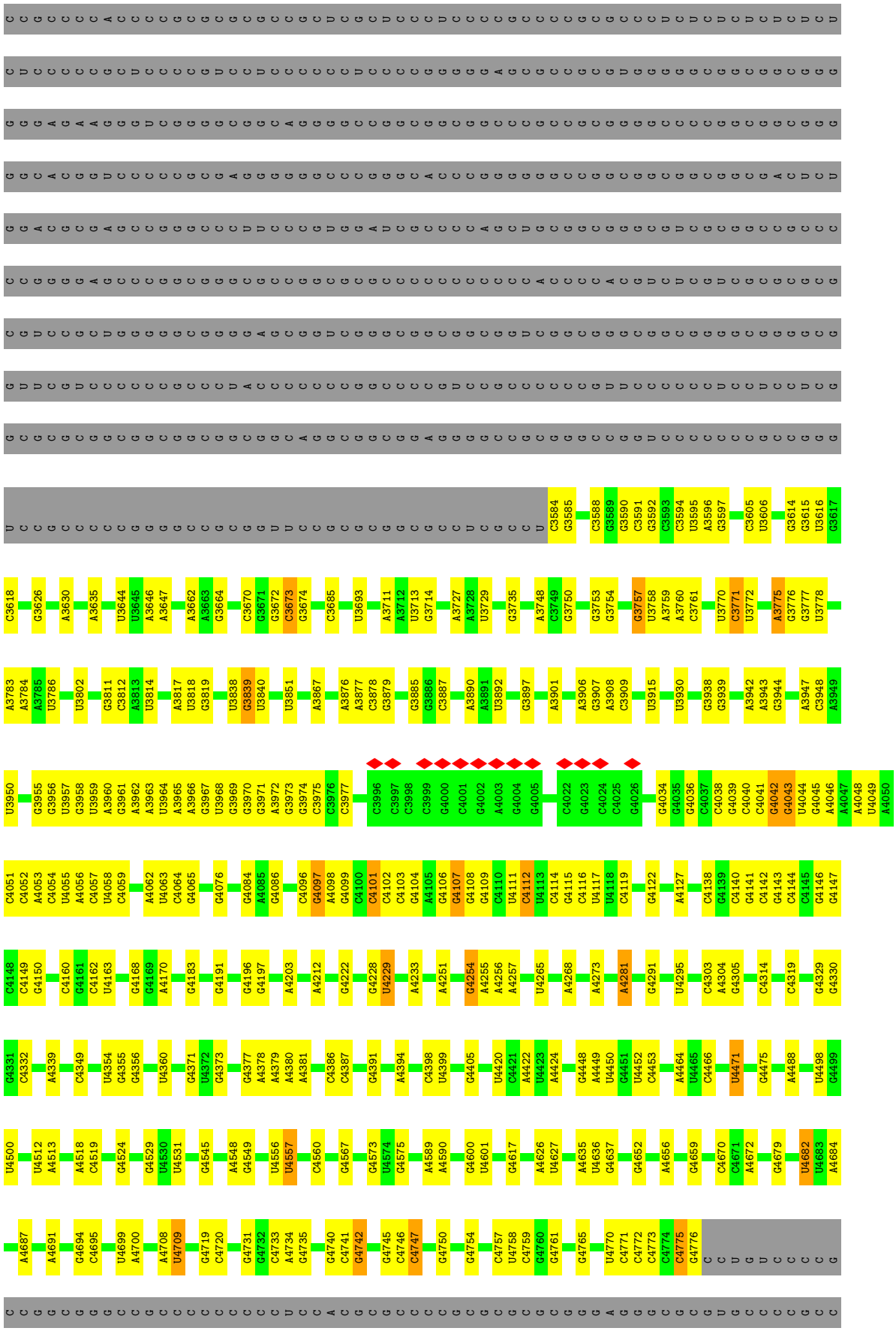
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

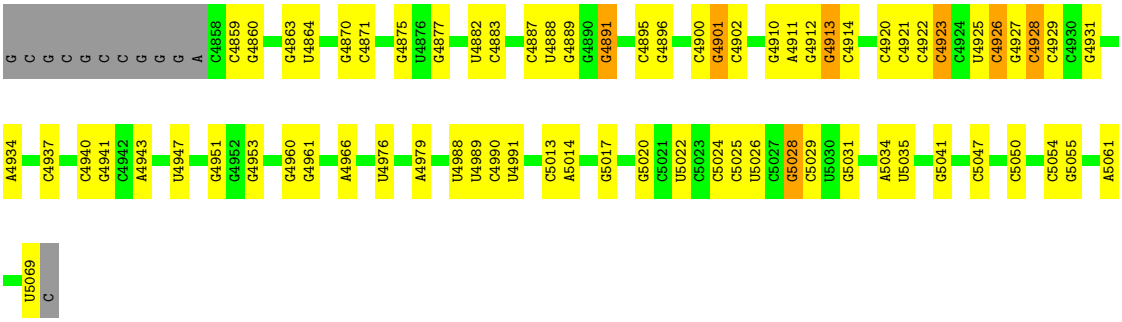
- Molecule 1: 28S rRNA

Chain L5:



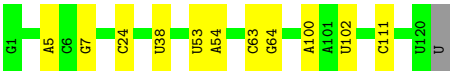






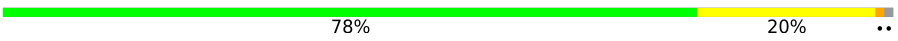
• Molecule 2: 5S rRNA

Chain L7:



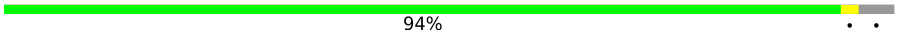
• Molecule 3: 5.8S rRNA

Chain L8:



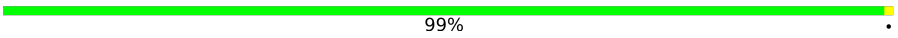
• Molecule 4: 60S ribosomal protein L8

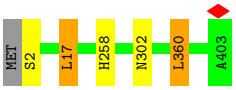
Chain LA:



• Molecule 5: 60S ribosomal protein L3

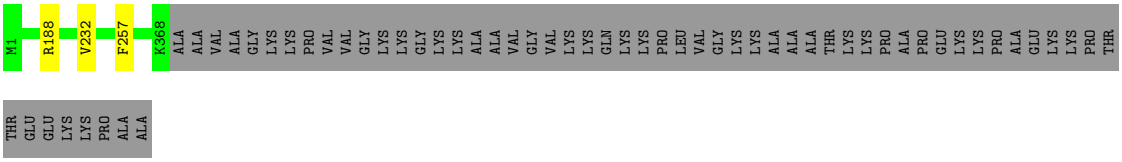
Chain LB:





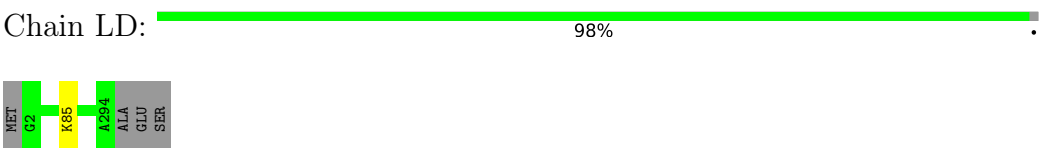
• Molecule 6: 60S ribosomal protein L4

Chain LC:



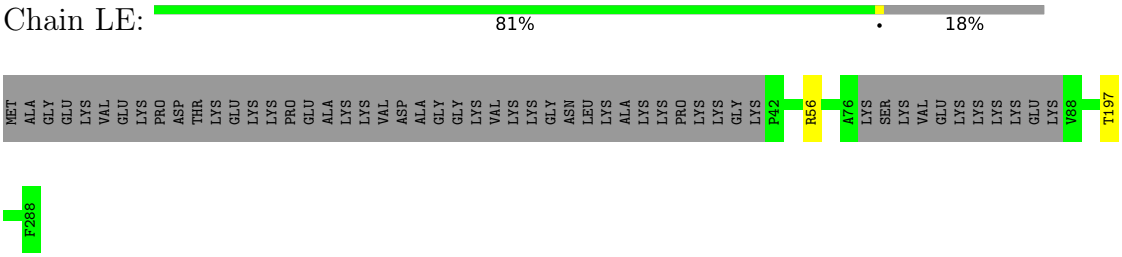
• Molecule 7: 60S ribosomal protein L5

Chain LD:



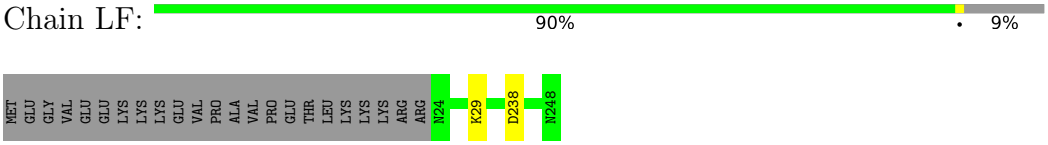
• Molecule 8: 60S ribosomal protein L6

Chain LE:



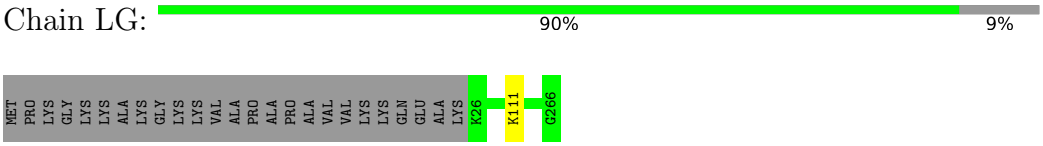
• Molecule 9: 60S ribosomal protein L7

Chain LF:



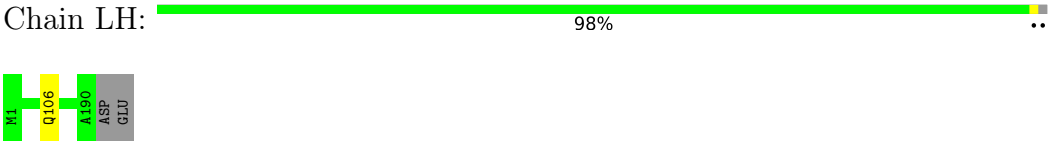
• Molecule 10: 60S ribosomal protein L7a

Chain LG:



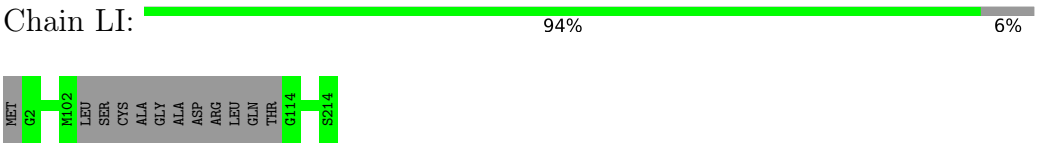
• Molecule 11: 60S ribosomal protein L9

Chain LH:



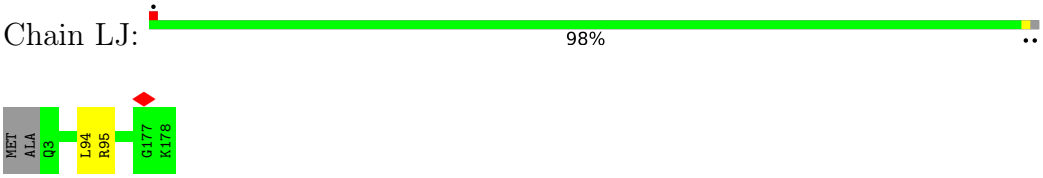
• Molecule 12: 60S ribosomal protein L10-like

Chain LI:



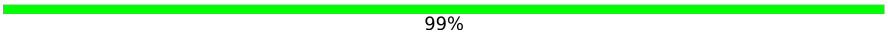
• Molecule 13: 60S ribosomal protein L11

Chain LJ:



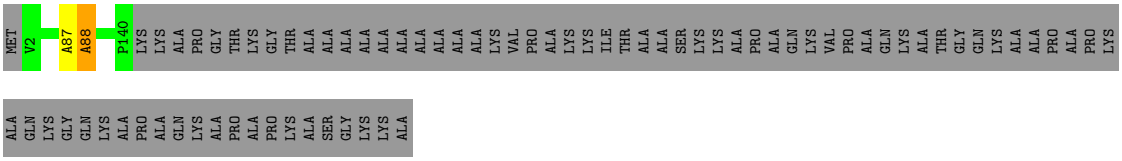
• Molecule 14: 60S ribosomal protein L13

Chain LL:



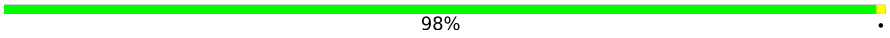
• Molecule 15: 60S ribosomal protein L14

Chain LM:



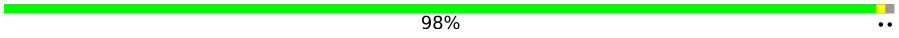
• Molecule 16: 60S ribosomal protein L15

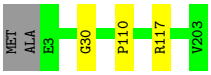
Chain LN:



• Molecule 17: 60S ribosomal protein L13a

Chain LO:



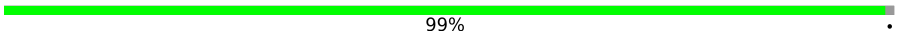


• Molecule 18: 60S ribosomal protein L17

Chain LP:

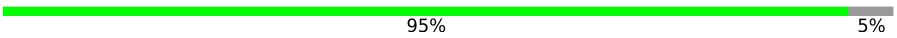
• Molecule 19: 60S ribosomal protein L18

Chain LQ:



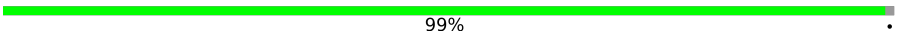
• Molecule 20: 60S ribosomal protein L19

Chain LR:



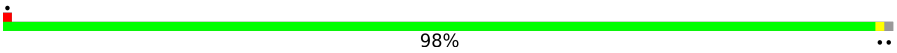
• Molecule 21: 60S ribosomal protein L18a

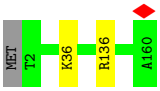
Chain LS:



• Molecule 22: 60S ribosomal protein L21

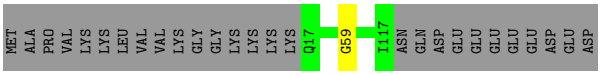
Chain LT:





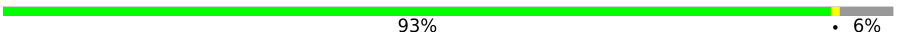
• Molecule 23: 60S ribosomal protein L22

Chain LU:



• Molecule 24: 60S ribosomal protein L23

Chain LV:

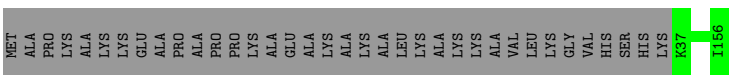


• Molecule 25: 60S ribosomal protein L24

Chain LW:

• Molecule 26: 60S ribosomal protein L23a

Chain LX:

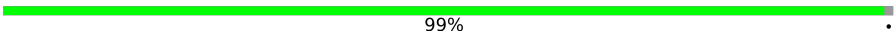


• Molecule 27: 60S ribosomal protein L26

Chain LY:

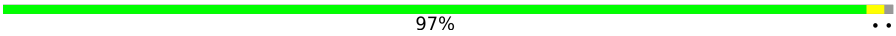
• Molecule 28: 60S ribosomal protein L27

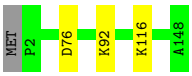
Chain LZ:



• Molecule 29: 60S ribosomal protein L27a

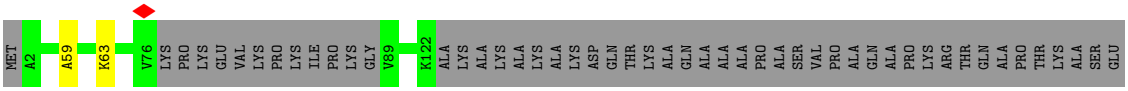
Chain La:





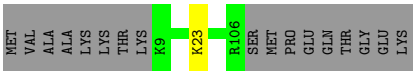
• Molecule 30: 60S ribosomal protein L29

Chain Lb:



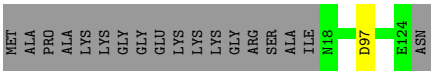
• Molecule 31: 60S ribosomal protein L30

Chain Lc:



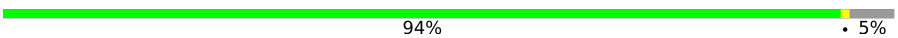
• Molecule 32: 60S ribosomal protein L31

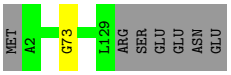
Chain Ld:



• Molecule 33: 60S ribosomal protein L32

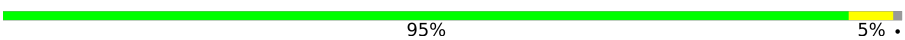
Chain Le:





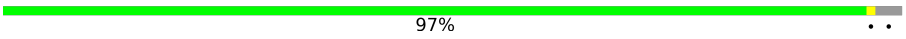
• Molecule 34: 60S ribosomal protein L35a

Chain Lf:



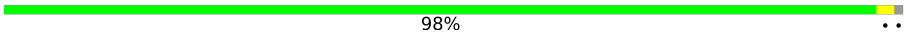
• Molecule 35: 60S ribosomal protein L34

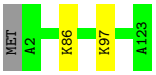
Chain Lg:



• Molecule 36: 60S ribosomal protein L35

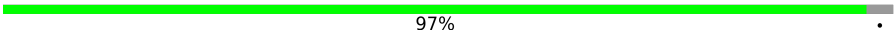
Chain Lh:

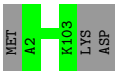




• Molecule 37: 60S ribosomal protein L36

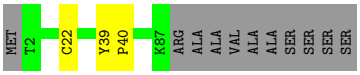
Chain Li:





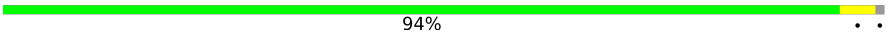
• Molecule 38: 60S ribosomal protein L37

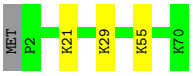
Chain Lj:



• Molecule 39: 60S ribosomal protein L38

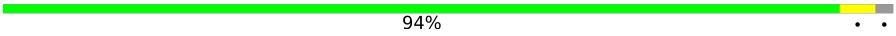
Chain Lk:





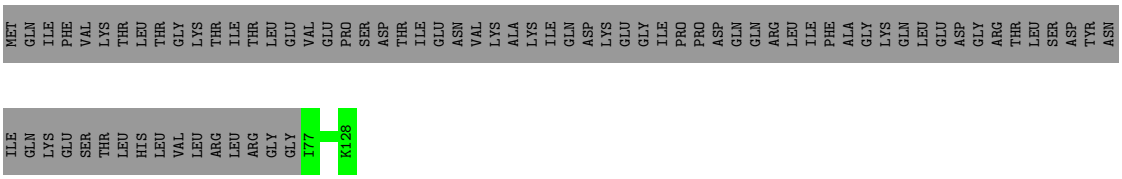
• Molecule 40: 60S ribosomal protein L39

Chain Ll:



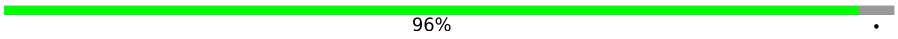
• Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:



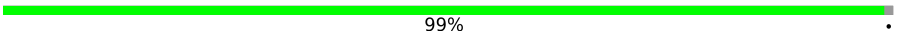
• Molecule 42: 60S ribosomal protein L41

Chain Ln:



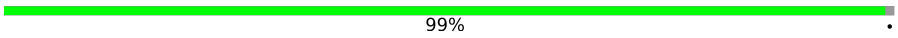
• Molecule 43: 60S ribosomal protein L36a

Chain Lo:



• Molecule 44: 60S ribosomal protein L37a

Chain Lp:

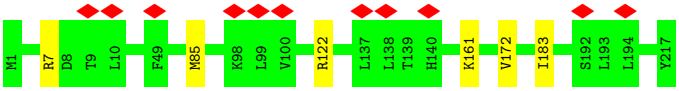


• Molecule 45: 60S ribosomal protein L28

Chain Lr:

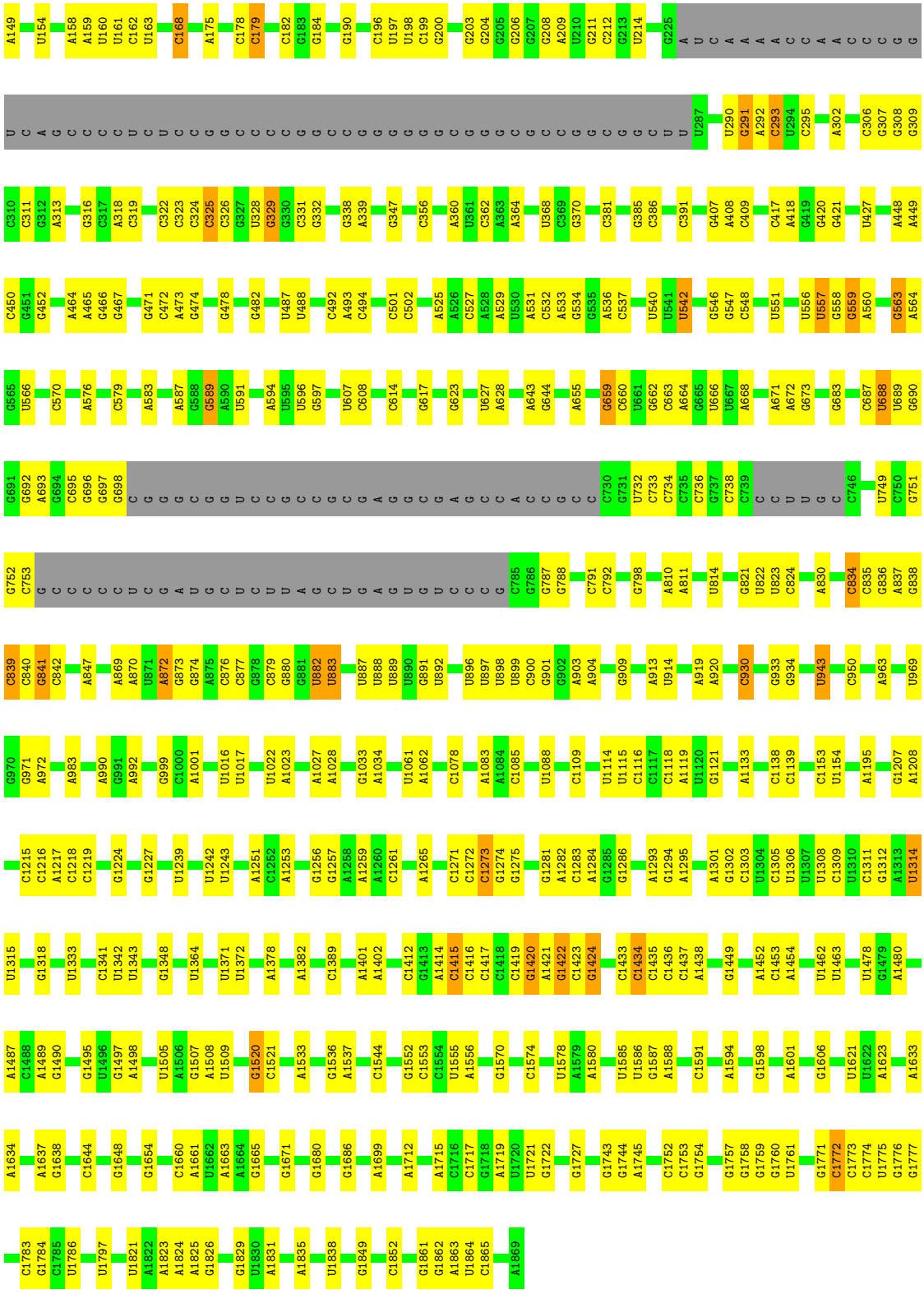
• Molecule 46: 60S ribosomal protein L10a

Chain Lz:



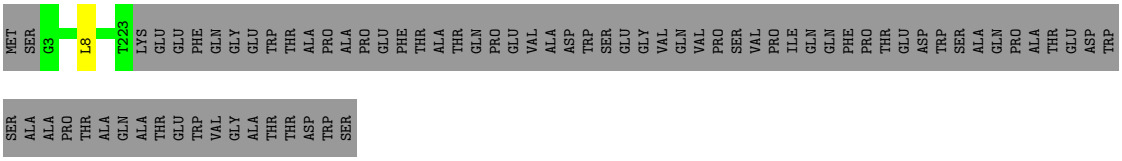
• Molecule 47: 18S rRNA

Chain S2:



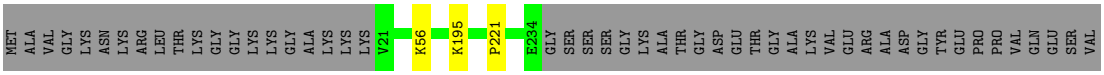
• Molecule 48: 40S ribosomal protein SA

Chain SA: 75% 25%



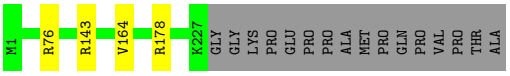
• Molecule 49: 40S ribosomal protein S3a

Chain SB:



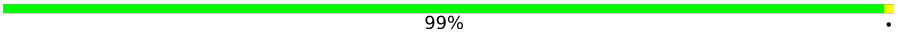
• Molecule 50: 40S ribosomal protein S3

Chain SD:



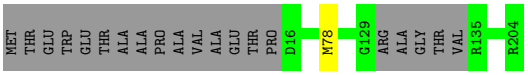
• Molecule 51: 40S ribosomal protein S4, X isoform

Chain SE:



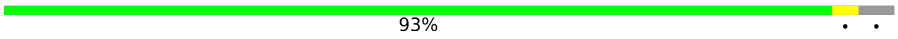
• Molecule 52: 40S ribosomal protein S5

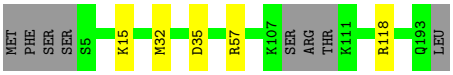
Chain SF:



• Molecule 53: 40S ribosomal protein S7

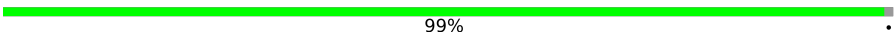
Chain SH:

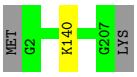




• Molecule 54: 40S ribosomal protein S8

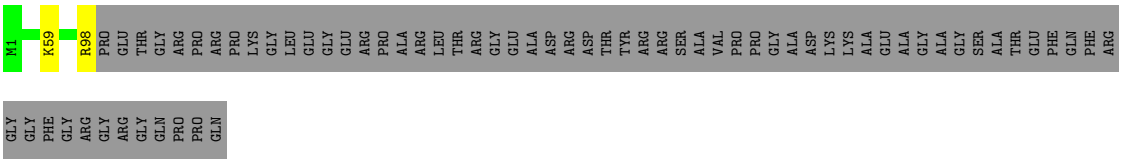
Chain SI:





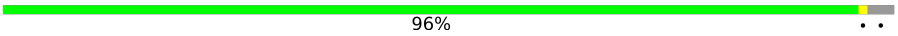
• Molecule 55: 40S ribosomal protein S10

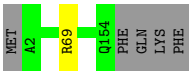
Chain SK:



• Molecule 56: 40S ribosomal protein S11

Chain SL:



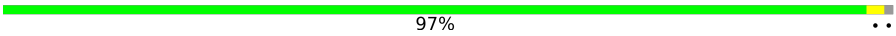


• Molecule 57: 40S ribosomal protein S15

Chain SP:

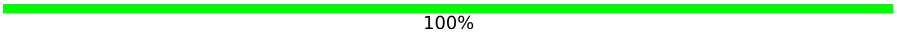
• Molecule 58: 40S ribosomal protein S16

Chain SQ:



• Molecule 59: 40S ribosomal protein S17

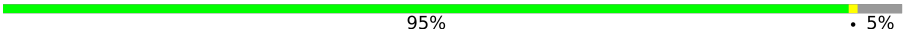
Chain SR:

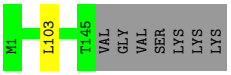


There are no outlier residues recorded for this chain.

• Molecule 60: 40S ribosomal protein S18

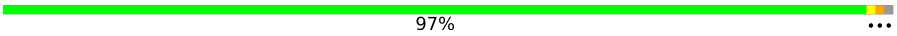
Chain SS:

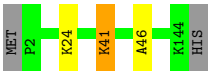




• Molecule 61: 40S ribosomal protein S19

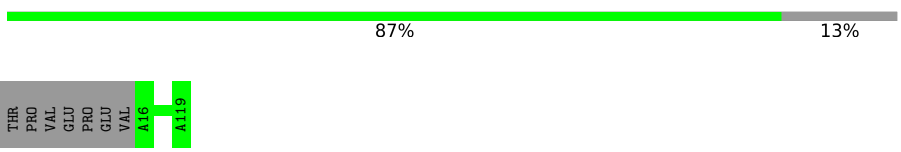
Chain ST:





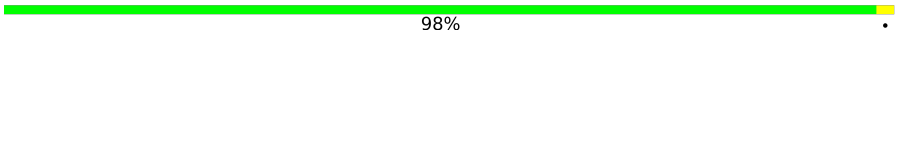
• Molecule 62: 40S ribosomal protein S20

Chain SU:



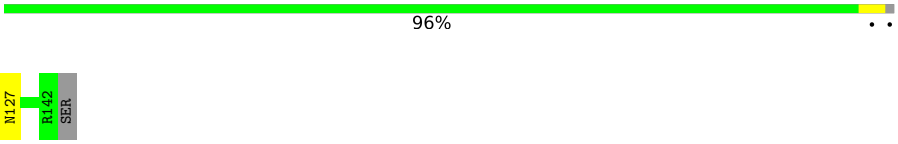
• Molecule 63: 40S ribosomal protein S21

Chain SV:



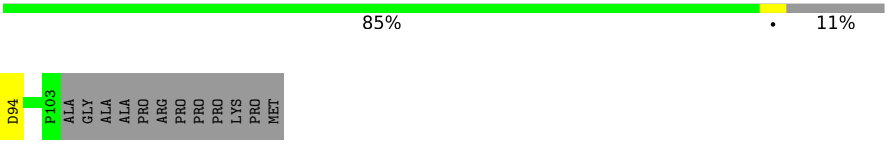
• Molecule 64: 40S ribosomal protein S23

Chain SX:



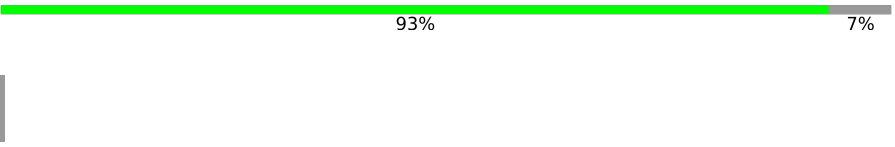
• Molecule 65: 40S ribosomal protein S26

Chain Sa:



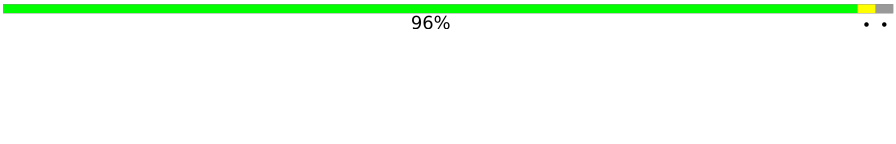
• Molecule 66: 40S ribosomal protein S28

Chain Sc:



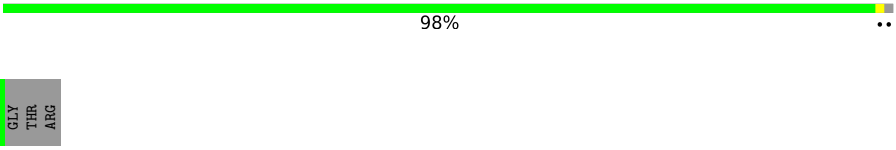
• Molecule 67: 40S ribosomal protein S29

Chain Sd:



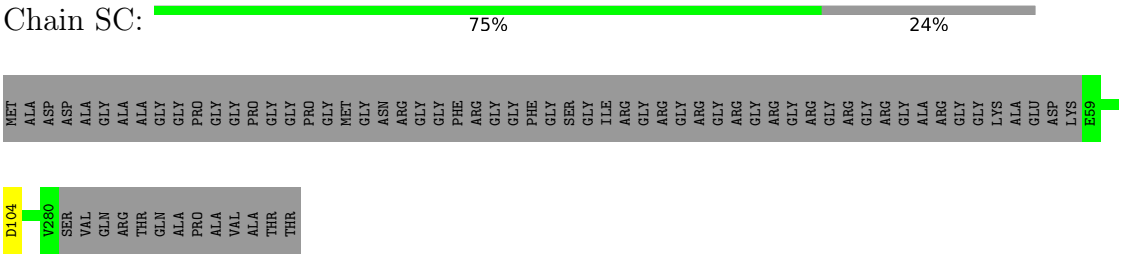
• Molecule 68: Receptor of activated protein C kinase 1

Chain Sg:



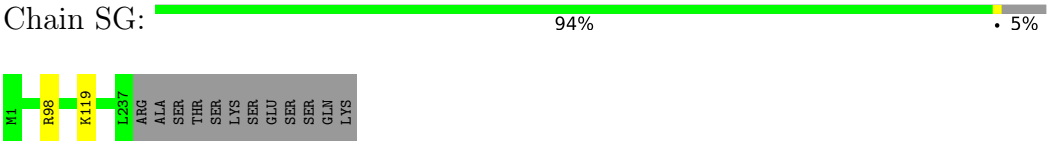
• Molecule 69: 40S ribosomal protein S2

Chain SC:



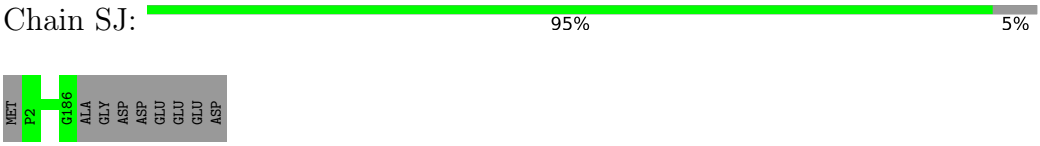
- Molecule 70: 40S ribosomal protein S6

Chain SG:



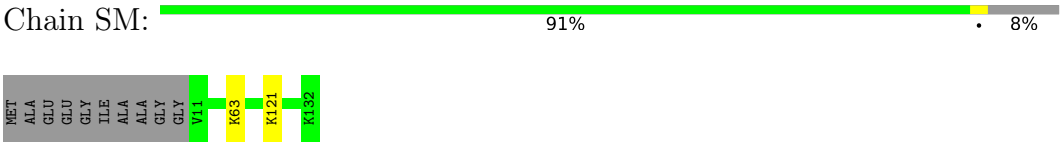
- Molecule 71: 40S ribosomal protein S9

Chain SJ:



- Molecule 72: 40S ribosomal protein S12

Chain SM:

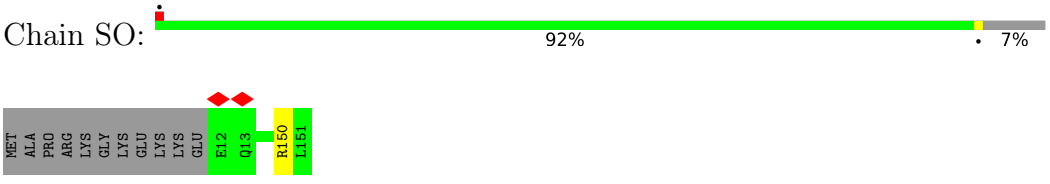


- Molecule 73: 40S ribosomal protein S13

Chain SN:

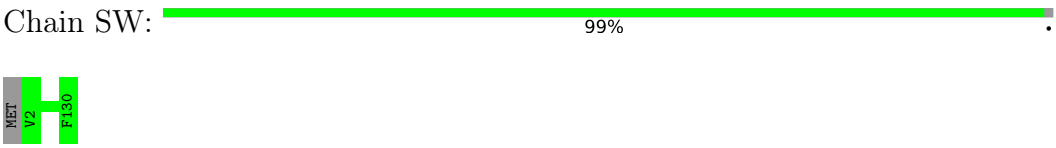
- Molecule 74: 40S ribosomal protein S14

Chain SO:



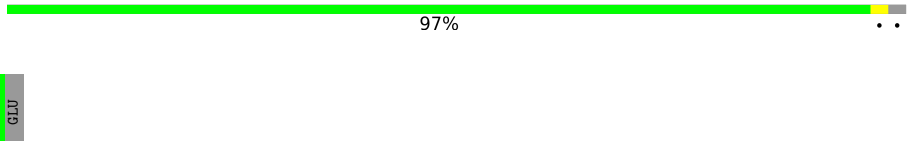
- Molecule 75: 40S ribosomal protein S15a

Chain SW:



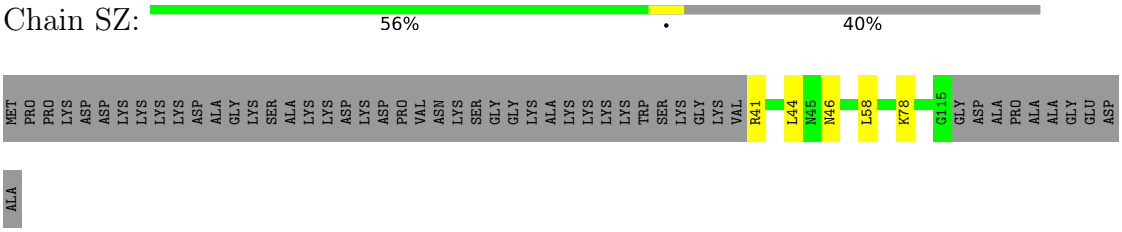
• Molecule 76: 40S ribosomal protein S24

Chain SY:



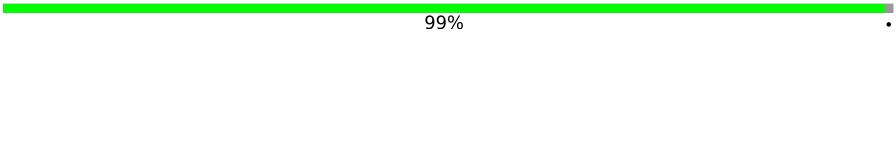
• Molecule 77: 40S ribosomal protein S25

Chain SZ:



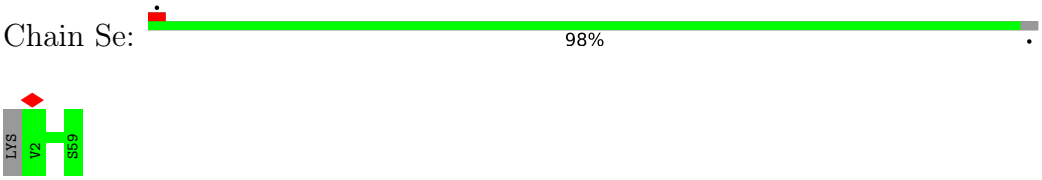
• Molecule 78: 40S ribosomal protein S27

Chain Sb:



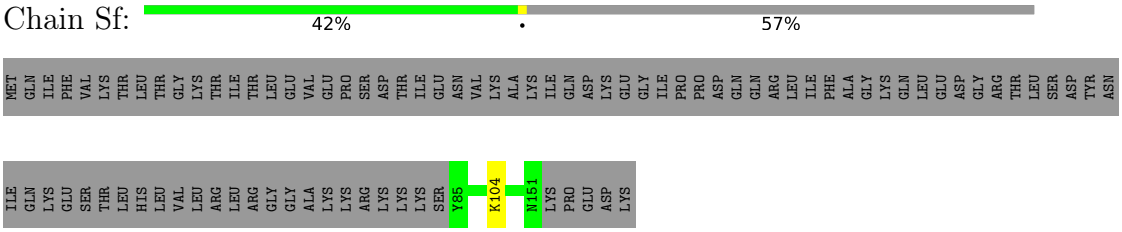
• Molecule 79: 40S ribosomal protein S30

Chain Se:



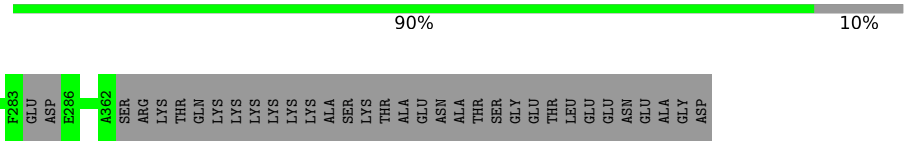
• Molecule 80: Ubiquitin-40S ribosomal protein S27a

Chain Sf:



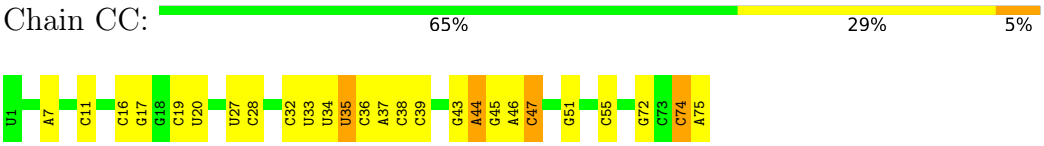
• Molecule 81: Proliferation-associated protein 2G4

Chain CA:



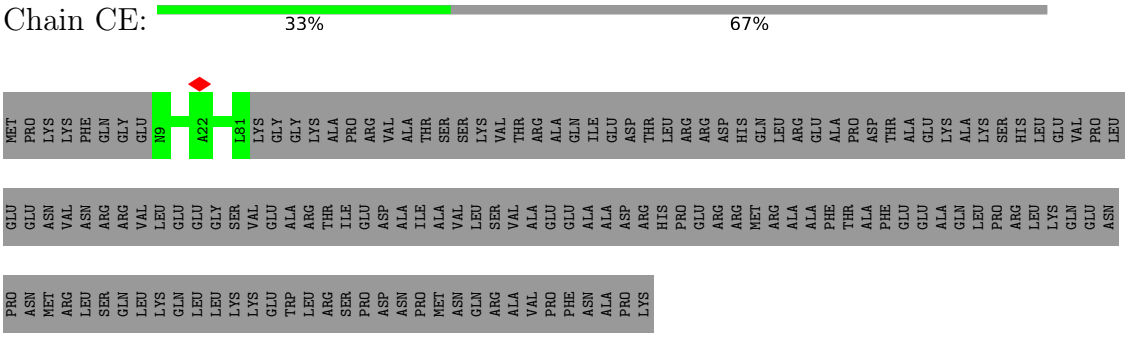
• Molecule 82: tRNA

Chain CC:



• Molecule 83: Coiled-coil domain-containing protein 124

Chain CE:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84429	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 ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.245	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	424.4, 424.4, 424.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	L5	0.75	3/89570 (0.0%)	1.06	467/139647 (0.3%)
2	L7	0.72	0/2861	0.93	2/4459 (0.0%)
3	L8	0.72	0/3701	0.91	4/5766 (0.1%)
4	LA	0.44	0/1936	0.60	1/2596 (0.0%)
5	LB	0.40	0/3306	0.57	2/4424 (0.0%)
6	LC	0.39	0/2981	0.54	0/4002
7	LD	0.36	0/2428	0.50	0/3252
8	LE	0.33	0/1942	0.55	0/2606
9	LF	0.41	0/1905	0.53	0/2539
10	LG	0.36	0/1960	0.53	0/2637
11	LH	0.37	0/1537	0.52	0/2066
12	LI	0.38	0/1673	0.51	0/2233
13	LJ	0.34	0/1433	0.61	0/1915
14	LL	0.35	0/1732	0.53	0/2315
15	LM	0.36	0/1161	0.53	0/1554
16	LN	0.43	0/1746	0.56	1/2338 (0.0%)
17	LO	0.40	0/1682	0.48	0/2250
18	LP	0.39	0/1268	0.50	0/1701
19	LQ	0.40	0/1537	0.52	0/2052
20	LR	0.34	0/1582	0.51	0/2091
21	LS	0.40	0/1493	0.48	0/2003
22	LT	0.40	0/1326	0.54	0/1770
23	LU	0.34	0/839	0.58	0/1126
24	LV	0.42	0/993	0.56	0/1332
25	LW	0.36	0/1030	0.50	0/1364
26	LX	0.36	0/1002	0.51	0/1345
27	LY	0.37	0/1132	0.50	0/1504
28	LZ	0.39	0/1130	0.51	0/1507
29	La	0.39	0/1191	0.51	0/1591
30	Lb	0.33	0/889	0.51	0/1175
31	Lc	0.38	0/774	0.53	0/1038
32	Ld	0.39	0/903	0.54	1/1216 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Le	0.41	0/1071	0.54	0/1429
34	Lf	0.41	0/895	0.56	0/1198
35	Lg	0.39	0/916	0.54	0/1220
36	Lh	0.33	0/1023	0.49	0/1351
37	Li	0.31	0/843	0.48	0/1115
38	Lj	0.42	0/720	0.53	0/952
39	Lk	0.36	0/575	0.54	0/761
40	Ll	0.37	0/454	0.49	0/599
41	Lm	0.36	0/435	0.52	0/575
42	Ln	0.37	0/231	0.46	0/294
43	Lo	0.39	0/855	0.49	0/1128
44	Lp	0.40	0/718	0.51	0/953
45	Lr	0.37	0/1017	0.52	0/1364
46	Lz	0.31	0/1769	0.62	0/2371
47	S2	0.61	0/41244	1.02	175/64263 (0.3%)
48	SA	0.35	0/1778	0.53	0/2416
49	SB	0.33	0/1765	0.53	0/2362
50	SD	0.32	0/1793	0.56	0/2414
51	SE	0.33	0/2118	0.52	0/2849
52	SF	0.31	0/1481	0.53	0/1988
53	SH	0.33	0/1519	0.59	1/2033 (0.0%)
54	SI	0.34	0/1715	0.55	0/2287
55	SK	0.29	0/851	0.55	0/1147
56	SL	0.37	0/1268	0.53	0/1696
57	SP	0.29	0/1065	0.58	1/1423 (0.1%)
58	SQ	0.31	0/1160	0.57	0/1553
59	SR	0.29	0/1105	0.57	0/1484
60	SS	0.28	0/1216	0.52	0/1628
61	ST	0.28	0/1131	0.51	0/1515
62	SU	0.28	0/831	0.54	0/1115
63	SV	0.32	0/643	0.53	0/860
64	SX	0.36	0/1116	0.57	0/1490
65	Sa	0.36	0/836	0.56	0/1121
66	Sc	0.31	0/508	0.59	0/680
67	Sd	0.32	0/470	0.53	0/623
68	Sg	0.28	0/2493	0.57	1/3394 (0.0%)
69	SC	0.37	0/1762	0.55	0/2381
70	SG	0.29	0/1946	0.51	0/2590
71	SJ	0.33	0/1550	0.51	0/2069
72	SM	0.29	0/950	0.62	0/1275
73	SN	0.35	0/1232	0.48	0/1656
74	SO	0.34	0/1062	0.55	0/1425
75	SW	0.36	0/1051	0.51	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	SY	0.32	0/1083	0.48	0/1438
77	SZ	0.31	0/604	0.65	1/810 (0.1%)
78	Sb	0.31	0/665	0.52	0/891
79	Se	0.30	0/465	0.50	0/612
80	Sf	0.28	0/560	0.59	0/745
81	CA	0.32	0/2810	0.64	0/3780
82	CC	0.43	0/1773	1.13	15/2759 (0.5%)
83	CE	0.28	0/616	0.54	0/812
All	All	0.59	3/238400 (0.0%)	0.88	672/349714 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	LA	0	2
5	LB	0	3
11	LH	0	1
13	LJ	0	1
14	LL	0	1
15	LM	0	2
17	LO	0	2
22	LT	0	1
30	Lb	0	1
34	Lf	0	2
36	Lh	0	1
38	Lj	0	1
46	Lz	0	1
49	SB	0	1
50	SD	0	1
52	SF	0	1
53	SH	0	1
57	SP	0	1
58	SQ	0	1
61	ST	0	1
63	SV	0	1
64	SX	0	2
65	Sa	0	1
77	SZ	0	1
All	All	0	31

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	1709	C	N3-C4	-6.39	1.29	1.33
1	L5	1761	G	C6-N1	-5.18	1.35	1.39
1	L5	1173	G	N9-C4	-5.07	1.33	1.38

All (672) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	S2	1417	C	N3-C4-N4	-24.05	101.17	118.00
47	S2	1422	G	N1-C6-O6	-20.08	107.85	119.90
47	S2	1417	C	C5-C4-N4	18.43	133.10	120.20
47	S2	1422	G	C5-C6-O6	17.25	138.95	128.60
1	L5	1716	G	N1-C6-O6	-15.48	110.61	119.90
47	S2	1772	C	N3-C2-O2	-14.72	111.59	121.90
47	S2	1772	C	N1-C2-O2	14.47	127.58	118.90
1	L5	1761	G	C5-C6-O6	13.35	136.61	128.60
82	CC	27	U	N3-C2-O2	-12.75	113.28	122.20
1	L5	485	C	C2-N1-C1'	12.64	132.70	118.80
47	S2	293	C	N1-C2-O2	12.39	126.33	118.90
1	L5	1761	G	N1-C6-O6	-12.34	112.50	119.90
1	L5	2710	C	C2-N1-C1'	12.22	132.24	118.80
1	L5	2710	C	N1-C2-O2	12.06	126.14	118.90
47	S2	839	C	N1-C2-O2	12.05	126.13	118.90
1	L5	1709	C	C5-C4-N4	11.95	128.57	120.20
47	S2	883	U	N3-C2-O2	-11.83	113.92	122.20
1	L5	2019	C	N3-C2-O2	-11.55	113.81	121.90
1	L5	1709	C	N3-C4-N4	-11.52	109.94	118.00
1	L5	906	C	N3-C2-O2	-11.39	113.93	121.90
1	L5	985	C	N3-C2-O2	-11.07	114.15	121.90
1	L5	3948	C	C2-N1-C1'	10.97	130.86	118.80
1	L5	1173	G	N3-C4-N9	-10.66	119.60	126.00
1	L5	1709	C	N1-C2-O2	10.61	125.27	118.90
1	L5	181	C	N1-C2-O2	10.49	125.19	118.90
1	L5	1414	C	N3-C2-O2	-10.20	114.76	121.90
47	S2	293	C	C2-N1-C1'	10.19	130.01	118.80
1	L5	1709	C	N3-C2-O2	-10.16	114.78	121.90
1	L5	2019	C	N1-C2-O2	10.16	125.00	118.90
1	L5	322	C	N3-C2-O2	-10.06	114.86	121.90
82	CC	44	A	N1-C6-N6	-10.02	112.59	118.60
47	S2	1453	C	C2-N1-C1'	9.90	129.69	118.80
1	L5	1709	C	C6-N1-C2	-9.86	116.36	120.30
47	S2	501	C	C2-N1-C1'	9.85	129.63	118.80
1	L5	969	C	N1-C2-O2	9.84	124.80	118.90
47	S2	501	C	N1-C2-O2	9.79	124.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	S2	322	C	N3-C2-O2	-9.74	115.08	121.90
47	S2	1453	C	N1-C2-O2	9.68	124.71	118.90
57	SP	107	ILE	C-N-CA	9.66	145.85	121.70
1	L5	485	C	C6-N1-C1'	-9.65	109.22	120.80
47	S2	839	C	N3-C2-O2	-9.55	115.22	121.90
1	L5	323	C	N3-C2-O2	-9.53	115.23	121.90
47	S2	1417	C	C4-C5-C6	-9.49	112.66	117.40
1	L5	1082	C	O4'-C1'-N1	9.38	115.70	108.20
1	L5	655	C	N3-C2-O2	-9.38	115.34	121.90
1	L5	2505	C	N1-C2-O2	9.37	124.52	118.90
1	L5	2710	C	N3-C2-O2	-9.32	115.37	121.90
1	L5	174	C	N3-C2-O2	-9.32	115.38	121.90
1	L5	1050	C	N3-C2-O2	-9.29	115.40	121.90
47	S2	1772	C	C6-N1-C2	-9.26	116.60	120.30
1	L5	4923	C	N3-C2-O2	-9.23	115.44	121.90
47	S2	49	C	N3-C2-O2	-9.22	115.45	121.90
47	S2	882	U	N1-C2-O2	9.15	129.20	122.80
1	L5	1414	C	N1-C2-O2	9.00	124.30	118.90
1	L5	969	C	C2-N1-C1'	8.93	128.63	118.80
47	S2	293	C	N3-C2-O2	-8.89	115.68	121.90
47	S2	882	U	C2-N1-C1'	8.88	128.36	117.70
1	L5	456	C	N3-C2-O2	-8.84	115.71	121.90
1	L5	753	C	N1-C2-O2	8.82	124.19	118.90
1	L5	2710	C	C6-N1-C1'	-8.79	110.25	120.80
1	L5	234	G	N9-C4-C5	-8.76	101.89	105.40
1	L5	181	C	N3-C2-O2	-8.76	115.77	121.90
1	L5	4149	C	N3-C2-O2	-8.72	115.80	121.90
1	L5	459	C	N3-C2-O2	-8.67	115.83	121.90
1	L5	485	C	N1-C2-O2	8.63	124.08	118.90
1	L5	986	C	C6-N1-C2	-8.63	116.85	120.30
1	L5	4138	C	N3-C2-O2	-8.60	115.88	121.90
1	L5	1762	C	C2-N1-C1'	8.59	128.25	118.80
1	L5	1762	C	N1-C2-O2	8.58	124.05	118.90
47	S2	1417	C	N3-C4-C5	8.57	125.33	121.90
1	L5	3948	C	N1-C2-O2	8.54	124.02	118.90
1	L5	260	C	N3-C2-O2	-8.53	115.93	121.90
1	L5	234	G	O4'-C1'-N9	8.53	115.02	108.20
1	L5	181	C	C2-N1-C1'	8.51	128.16	118.80
1	L5	1447	C	N3-C2-O2	-8.50	115.95	121.90
1	L5	985	C	N1-C2-O2	8.44	123.96	118.90
1	L5	100	C	C2-N1-C1'	8.39	128.03	118.80
47	S2	118	C	N1-C2-O2	8.37	123.92	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	3771	C	N3-C2-O2	-8.35	116.05	121.90
1	L5	4746	C	C2-N1-C1'	8.34	127.98	118.80
1	L5	4926	C	N1-C2-O2	8.29	123.87	118.90
47	S2	1772	C	C2-N1-C1'	8.26	127.89	118.80
1	L5	4921	C	N3-C2-O2	-8.26	116.12	121.90
47	S2	356	C	C2-N1-C1'	8.25	127.88	118.80
47	S2	1139	C	N1-C2-O2	8.25	123.85	118.90
1	L5	515	C	C2-N1-C1'	8.25	127.87	118.80
1	L5	3647	A	C6-N1-C2	-8.23	113.67	118.60
1	L5	4101	C	N3-C4-C5	8.22	125.19	121.90
47	S2	1139	C	N3-C2-O2	-8.20	116.16	121.90
1	L5	4928	C	C2-N1-C1'	8.20	127.82	118.80
1	L5	417	G	O4'-C1'-N9	8.15	114.72	108.20
1	L5	1367	C	N1-C2-O2	8.13	123.78	118.90
1	L5	516	C	N1-C2-O2	8.12	123.77	118.90
1	L5	515	C	N1-C2-O2	8.12	123.77	118.90
1	L5	3948	C	C6-N1-C1'	-8.11	111.07	120.80
47	S2	1139	C	C2-N1-C1'	8.10	127.71	118.80
1	L5	209	U	C2-N1-C1'	8.07	127.39	117.70
1	L5	234	G	C8-N9-C1'	-8.06	116.52	127.00
1	L5	969	C	N3-C2-O2	-8.06	116.26	121.90
47	S2	688	U	N3-C2-O2	-8.06	116.56	122.20
1	L5	234	G	C4-C5-N7	8.04	114.01	110.80
1	L5	1367	C	C2-N1-C1'	8.03	127.63	118.80
1	L5	1173	G	N3-C4-C5	8.02	132.61	128.60
47	S2	877	C	N3-C2-O2	-8.01	116.29	121.90
47	S2	356	C	N1-C2-O2	7.99	123.69	118.90
47	S2	501	C	N3-C2-O2	-7.98	116.31	121.90
1	L5	456	C	O4'-C1'-N1	7.98	114.58	108.20
1	L5	1709	C	C2-N1-C1'	7.97	127.56	118.80
1	L5	1716	G	C5-C6-N1	7.97	115.48	111.50
1	L5	234	G	C6-C5-N7	-7.96	125.62	130.40
1	L5	3647	A	C5-C6-N1	7.95	121.68	117.70
1	L5	4101	C	N3-C4-N4	-7.90	112.47	118.00
47	S2	1416	C	N3-C2-O2	-7.86	116.40	121.90
1	L5	1252	C	N3-C2-O2	-7.83	116.42	121.90
1	L5	4709	U	C2-N1-C1'	7.82	127.08	117.70
1	L5	4926	C	C2-N1-C1'	7.79	127.38	118.80
1	L5	1082	C	N3-C2-O2	-7.79	116.45	121.90
1	L5	100	C	N3-C2-O2	-7.79	116.45	121.90
47	S2	118	C	C2-N1-C1'	7.78	127.36	118.80
1	L5	2303	C	N1-C2-O2	7.75	123.55	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	2627	C	C2-N1-C1'	7.73	127.30	118.80
1	L5	907	C	N3-C2-O2	-7.67	116.53	121.90
1	L5	490	C	C6-N1-C2	-7.66	117.24	120.30
1	L5	1173	G	C4-N9-C1'	-7.65	116.56	126.50
1	L5	753	C	N3-C2-O2	-7.60	116.58	121.90
82	CC	44	A	C5-C6-N6	7.60	129.78	123.70
1	L5	4355	G	C5-C6-O6	7.58	133.15	128.60
1	L5	472	C	N1-C2-O2	7.58	123.45	118.90
1	L5	473	C	N3-C2-O2	-7.55	116.61	121.90
47	S2	293	C	C6-N1-C1'	-7.54	111.75	120.80
1	L5	1969	G	N1-C2-N2	-7.54	109.42	116.20
1	L5	4356	G	N3-C4-N9	-7.53	121.48	126.00
1	L5	4112	C	N3-C2-O2	-7.52	116.63	121.90
1	L5	516	C	N3-C2-O2	-7.52	116.64	121.90
1	L5	1216	C	C2-N1-C1'	7.48	127.03	118.80
47	S2	688	U	N1-C2-O2	7.45	128.01	122.80
1	L5	4928	C	N1-C2-O2	7.42	123.35	118.90
47	S2	1520	G	C4-N9-C1'	7.40	136.12	126.50
1	L5	1173	G	C8-N9-C1'	7.40	136.62	127.00
47	S2	1309	C	C2-N1-C1'	7.39	126.93	118.80
1	L5	1050	C	N1-C2-O2	7.39	123.34	118.90
1	L5	3757	G	O4'-C1'-N9	7.39	114.11	108.20
47	S2	1022	U	C2-N1-C1'	7.38	126.56	117.70
47	S2	882	U	N3-C2-O2	-7.35	117.05	122.20
1	L5	4355	G	N9-C4-C5	7.35	108.34	105.40
1	L5	489	C	C2-N1-C1'	7.31	126.84	118.80
1	L5	175	C	N3-C2-O2	-7.31	116.79	121.90
47	S2	883	U	C6-N1-C2	-7.29	116.63	121.00
1	L5	2505	C	N3-C2-O2	-7.29	116.80	121.90
47	S2	688	U	C2-N1-C1'	7.25	126.39	117.70
1	L5	4303	C	C2-N1-C1'	7.22	126.75	118.80
1	L5	1405	C	N1-C2-O2	7.21	123.23	118.90
1	L5	1968	G	N3-C4-N9	7.21	130.33	126.00
1	L5	4355	G	N1-C6-O6	-7.21	115.57	119.90
1	L5	100	C	N1-C2-O2	7.21	123.22	118.90
82	CC	27	U	N1-C2-O2	7.20	127.84	122.80
47	S2	527	C	N3-C2-O2	-7.17	116.88	121.90
1	L5	234	G	C4-N9-C1'	7.16	135.81	126.50
47	S2	1453	C	N3-C2-O2	-7.16	116.89	121.90
1	L5	4356	G	C5-C6-O6	7.15	132.89	128.60
1	L5	906	C	N1-C2-O2	7.11	123.16	118.90
1	L5	1193	C	C2-N1-C1'	7.10	126.61	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	1969	G	C2-N3-C4	-7.09	108.36	111.90
1	L5	1367	C	N3-C2-O2	-7.08	116.95	121.90
1	L5	1772	C	N3-C4-N4	-7.07	113.05	118.00
1	L5	3775	A	O4'-C1'-N9	7.07	113.86	108.20
47	S2	1453	C	C6-N1-C1'	-7.07	112.32	120.80
1	L5	673	C	C2-N1-C1'	7.05	126.56	118.80
1	L5	907	C	C6-N1-C2	-7.02	117.49	120.30
47	S2	883	U	N1-C2-O2	7.02	127.71	122.80
1	L5	1968	G	C4-N9-C1'	7.00	135.60	126.50
1	L5	4557	U	N3-C2-O2	-7.00	117.30	122.20
1	L5	2710	C	C6-N1-C2	-6.98	117.51	120.30
1	L5	986	C	N3-C2-O2	-6.96	117.03	121.90
1	L5	4775	C	N1-C2-O2	6.92	123.05	118.90
1	L5	472	C	C2-N1-C1'	6.89	126.38	118.80
1	L5	2257	C	C2-N1-C1'	6.89	126.38	118.80
1	L5	985	C	C6-N1-C2	-6.89	117.55	120.30
1	L5	2410	C	C2-N1-C1'	6.88	126.37	118.80
47	S2	570	C	N1-C2-O2	6.88	123.03	118.90
1	L5	4557	U	N1-C2-O2	6.87	127.61	122.80
1	L5	490	C	N3-C2-O2	-6.85	117.11	121.90
1	L5	77	U	N3-C2-O2	-6.84	117.41	122.20
1	L5	1173	G	C6-C5-N7	6.83	134.50	130.40
1	L5	1716	G	C5-C6-O6	6.82	132.69	128.60
1	L5	1241	C	N1-C2-O2	6.82	122.99	118.90
47	S2	883	U	C2-N1-C1'	6.82	125.88	117.70
82	CC	34	U	C2-N1-C1'	6.82	125.88	117.70
1	L5	4926	C	N3-C2-O2	-6.81	117.13	121.90
1	L5	3775	A	N7-C8-N9	6.81	117.20	113.80
1	L5	2528	G	C4-N9-C1'	6.81	135.35	126.50
47	S2	1520	G	N3-C4-N9	6.81	130.08	126.00
47	S2	501	C	C6-N1-C2	-6.79	117.58	120.30
47	S2	118	C	N3-C2-O2	-6.78	117.15	121.90
1	L5	1082	C	OP1-P-O3'	6.77	120.09	105.20
47	S2	1273	C	C6-N1-C2	-6.76	117.60	120.30
1	L5	3909	C	C6-N1-C2	-6.74	117.61	120.30
1	L5	2005	G	C4-N9-C1'	6.72	135.24	126.50
47	S2	501	C	C6-N1-C1'	-6.72	112.73	120.80
1	L5	1714	C	N1-C2-O2	6.71	122.93	118.90
1	L5	4557	U	C2-N1-C1'	6.70	125.74	117.70
47	S2	1520	G	C8-N9-C1'	-6.70	118.29	127.00
1	L5	969	C	C6-N1-C2	-6.67	117.63	120.30
47	S2	356	C	N3-C2-O2	-6.67	117.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	1217	G	N3-C4-N9	6.66	130.00	126.00
1	L5	925	C	C6-N1-C2	-6.64	117.64	120.30
1	L5	654	C	N1-C2-O2	6.64	122.88	118.90
1	L5	1082	C	P-O3'-C3'	6.63	127.66	119.70
1	L5	4356	G	N9-C4-C5	6.62	108.05	105.40
1	L5	2260	C	N1-C2-O2	6.61	122.87	118.90
1	L5	1762	C	N3-C2-O2	-6.61	117.27	121.90
1	L5	2260	C	C2-N1-C1'	6.60	126.06	118.80
1	L5	4923	C	N1-C2-O2	6.60	122.86	118.90
1	L5	1216	C	N1-C2-O2	6.58	122.85	118.90
1	L5	4355	G	N3-C4-N9	-6.58	122.05	126.00
1	L5	1968	G	C8-N9-C1'	-6.57	118.46	127.00
82	CC	27	U	N1-C2-N3	6.57	118.84	114.90
1	L5	4149	C	C6-N1-C2	-6.56	117.67	120.30
1	L5	925	C	N1-C2-O2	6.56	122.84	118.90
47	S2	570	C	C2-N1-C1'	6.56	126.02	118.80
1	L5	1241	C	C2-N1-C1'	6.56	126.01	118.80
1	L5	4356	G	N3-C2-N2	-6.55	115.31	119.90
47	S2	322	C	N1-C2-O2	6.54	122.83	118.90
47	S2	872	A	O4'-C1'-N9	6.54	113.43	108.20
1	L5	4746	C	C6-N1-C1'	-6.53	112.96	120.80
1	L5	4303	C	N1-C2-O2	6.53	122.82	118.90
1	L5	323	C	N3-C4-N4	-6.53	113.43	118.00
1	L5	3778	U	N1-C2-O2	6.52	127.36	122.80
47	S2	882	U	C5-C6-N1	6.51	125.95	122.70
47	S2	841	G	N1-C6-O6	-6.50	116.00	119.90
47	S2	943	U	C2-N1-C1'	6.50	125.50	117.70
1	L5	4303	C	N3-C2-O2	-6.49	117.36	121.90
1	L5	459	C	C6-N1-C2	-6.48	117.71	120.30
1	L5	100	C	C6-N1-C2	-6.46	117.72	120.30
1	L5	4097	G	C5-C6-O6	6.43	132.46	128.60
1	L5	2627	C	N1-C2-O2	6.43	122.76	118.90
1	L5	2303	C	N3-C2-O2	-6.43	117.40	121.90
47	S2	877	C	C6-N1-C2	-6.43	117.73	120.30
1	L5	2021	G	N3-C4-N9	6.42	129.85	126.00
1	L5	925	C	N3-C2-O2	-6.41	117.41	121.90
47	S2	1273	C	N3-C2-O2	-6.41	117.41	121.90
1	L5	4929	C	N3-C2-O2	-6.41	117.42	121.90
1	L5	753	C	C2-N1-C1'	6.39	125.83	118.80
1	L5	1251	C	N1-C2-O2	6.39	122.73	118.90
47	S2	548	C	C2-N1-C1'	6.38	125.82	118.80
1	L5	1049	C	N1-C2-O2	6.38	122.73	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	2505	C	C2-N1-C1'	6.37	125.81	118.80
47	S2	1139	C	C6-N1-C2	-6.37	117.75	120.30
1	L5	453	G	N3-C4-C5	-6.36	125.42	128.60
1	L5	1808	C	N3-C2-O2	-6.35	117.45	121.90
3	L8	64	U	N3-C2-O2	-6.35	117.76	122.20
1	L5	4138	C	C6-N1-C2	-6.34	117.76	120.30
3	L8	84	A	O5'-P-OP2	-6.34	100.00	105.70
82	CC	55	C	N1-C2-O2	6.33	122.70	118.90
1	L5	4742	G	C8-N9-C1'	6.33	135.23	127.00
1	L5	129	C	N3-C2-O2	-6.33	117.47	121.90
1	L5	130	C	N3-C2-O2	-6.32	117.48	121.90
1	L5	4147	G	C5-C6-O6	6.31	132.39	128.60
1	L5	2262	G	C4-N9-C1'	6.31	134.70	126.50
1	L5	4355	G	C4-C5-N7	-6.31	108.28	110.80
1	L5	1762	C	C6-N1-C1'	-6.31	113.23	120.80
1	L5	3778	U	N3-C2-O2	-6.30	117.79	122.20
47	S2	179	C	N1-C2-O2	6.29	122.67	118.90
47	S2	1591	C	N1-C2-O2	6.28	122.67	118.90
47	S2	1417	C	N1-C2-N3	-6.28	114.80	119.20
1	L5	3948	C	C5-C6-N1	6.28	124.14	121.00
1	L5	1447	C	C6-N1-C2	-6.28	117.79	120.30
1	L5	1772	C	N3-C4-C5	6.27	124.41	121.90
47	S2	688	U	P-O3'-C3'	6.26	127.21	119.70
47	S2	1389	C	C2-N1-C1'	6.25	125.67	118.80
1	L5	2760	G	P-O3'-C3'	6.24	127.19	119.70
1	L5	4773	C	N1-C2-O2	6.24	122.64	118.90
1	L5	4112	C	N1-C2-O2	6.23	122.64	118.90
1	L5	3772	U	C2-N1-C1'	6.21	125.15	117.70
1	L5	504	G	C4-N9-C1'	6.21	134.57	126.50
1	L5	906	C	C6-N1-C2	-6.20	117.82	120.30
1	L5	1327	C	C5-C6-N1	6.20	124.10	121.00
1	L5	2257	C	N1-C2-O2	6.20	122.62	118.90
5	LB	17	LEU	CA-CB-CG	6.20	129.55	115.30
1	L5	234	G	N3-C2-N2	6.19	124.23	119.90
47	S2	168	C	N1-C2-O2	6.18	122.61	118.90
47	S2	1453	C	C5-C6-N1	6.18	124.09	121.00
1	L5	209	U	C6-N1-C1'	-6.16	112.58	121.20
1	L5	2096	G	C4-N9-C1'	6.15	134.50	126.50
47	S2	1415	C	N1-C2-O2	6.15	122.59	118.90
1	L5	485	C	C5-C6-N1	6.15	124.07	121.00
1	L5	453	G	N3-C4-N9	6.15	129.69	126.00
1	L5	4742	G	C4-N9-C1'	-6.14	118.52	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	S2	909	G	N3-C4-N9	6.12	129.68	126.00
1	L5	738	C	N1-C2-O2	6.12	122.57	118.90
1	L5	914	U	P-O3'-C3'	6.11	127.03	119.70
1	L5	4147	G	N1-C6-O6	-6.11	116.23	119.90
1	L5	738	C	C2-N1-C1'	6.10	125.51	118.80
1	L5	1772	C	C5-C6-N1	6.09	124.05	121.00
1	L5	1417	C	C2-N1-C1'	6.09	125.50	118.80
47	S2	478	G	C5-C6-O6	6.09	132.25	128.60
47	S2	1078	C	C2-N1-C1'	6.08	125.49	118.80
47	S2	1272	C	N1-C2-O2	6.08	122.55	118.90
1	L5	2494	U	N1-C2-O2	6.08	127.06	122.80
47	S2	478	G	N3-C4-N9	-6.07	122.36	126.00
1	L5	2096	G	N3-C4-N9	6.07	129.64	126.00
1	L5	4887	C	N1-C2-O2	6.07	122.54	118.90
1	L5	515	C	C6-N1-C1'	-6.07	113.52	120.80
47	S2	1314	U	C2-N1-C1'	6.06	124.97	117.70
1	L5	2560	C	C2-N1-C1'	6.06	125.47	118.80
1	L5	1217	G	C4-N9-C1'	6.06	134.38	126.50
47	S2	1261	C	C2-N1-C1'	6.06	125.47	118.80
1	L5	2528	G	N3-C4-N9	6.06	129.63	126.00
47	S2	557	U	C2-N3-C4	-6.05	123.37	127.00
1	L5	4682	U	N3-C2-O2	-6.05	117.97	122.20
1	L5	2710	C	C5-C6-N1	6.05	124.02	121.00
1	L5	181	C	C6-N1-C2	-6.03	117.89	120.30
1	L5	262	G	N1-C6-O6	-6.02	116.29	119.90
1	L5	129	C	C6-N1-C2	-6.02	117.89	120.30
1	L5	904	C	N1-C2-O2	6.01	122.51	118.90
1	L5	234	G	N3-C4-N9	6.01	129.61	126.00
47	S2	178	C	N1-C2-O2	6.01	122.51	118.90
1	L5	2528	G	C8-N9-C1'	-6.00	119.21	127.00
1	L5	4758	U	C2-N1-C1'	5.99	124.89	117.70
1	L5	489	C	N1-C2-O2	5.98	122.49	118.90
1	L5	969	C	C6-N1-C1'	-5.98	113.62	120.80
47	S2	1022	U	N1-C2-O2	5.98	126.98	122.80
1	L5	2675	G	P-O3'-C3'	5.97	126.86	119.70
1	L5	4040	C	N1-C2-O2	5.97	122.48	118.90
1	L5	1807	C	N1-C2-O2	5.96	122.48	118.90
1	L5	1173	G	N9-C4-C5	5.96	107.78	105.40
1	L5	1217	G	C8-N9-C1'	-5.96	119.25	127.00
1	L5	4775	C	N3-C2-O2	-5.96	117.73	121.90
1	L5	2900	U	C2-N1-C1'	5.95	124.84	117.70
1	L5	1182	C	N1-C2-O2	5.95	122.47	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	1188	C	C6-N1-C2	-5.95	117.92	120.30
1	L5	4040	C	N3-C2-O2	-5.95	117.74	121.90
47	S2	1416	C	C6-N1-C2	-5.95	117.92	120.30
1	L5	3584	C	N1-C2-O2	5.94	122.47	118.90
1	L5	155	C	N3-C2-O2	-5.94	117.74	121.90
1	L5	453	G	C4-N9-C1'	5.93	134.21	126.50
1	L5	115	C	C2-N1-C1'	5.93	125.32	118.80
1	L5	4229	U	N3-C2-O2	-5.92	118.06	122.20
47	S2	427	U	C2-N1-C1'	5.92	124.80	117.70
1	L5	4928	C	N3-C2-O2	-5.91	117.76	121.90
1	L5	1216	C	N3-C2-O2	-5.91	117.76	121.90
47	S2	329	G	N1-C2-N2	-5.91	110.88	116.20
82	CC	34	U	N3-C2-O2	-5.91	118.06	122.20
47	S2	1309	C	C5-C6-N1	5.91	123.95	121.00
1	L5	654	C	C2-N1-C1'	5.91	125.30	118.80
47	S2	130	G	C4-N9-C1'	5.90	134.17	126.50
47	S2	1016	U	N1-C2-O2	5.90	126.93	122.80
1	L5	473	C	C6-N1-C2	-5.90	117.94	120.30
1	L5	4682	U	N1-C2-O2	5.89	126.93	122.80
82	CC	35	U	P-O3'-C3'	5.88	126.75	119.70
1	L5	994	G	N3-C2-N2	5.87	124.01	119.90
1	L5	234	G	N1-C2-N2	-5.86	110.93	116.20
1	L5	4926	C	C6-N1-C2	-5.86	117.96	120.30
1	L5	4913	G	P-O3'-C3'	5.85	126.72	119.70
47	S2	882	U	C6-N1-C1'	-5.85	113.01	121.20
1	L5	2262	G	N3-C4-C5	-5.84	125.68	128.60
47	S2	1271	C	C2-N1-C1'	5.84	125.22	118.80
82	CC	74	C	C6-N1-C2	-5.84	117.97	120.30
1	L5	1182	C	C2-N1-C1'	5.83	125.21	118.80
47	S2	1016	U	N3-C2-O2	-5.83	118.12	122.20
1	L5	2099	G	C5-C6-O6	5.82	132.09	128.60
1	L5	2494	U	N3-C2-O2	-5.82	118.13	122.20
47	S2	356	C	C6-N1-C1'	-5.81	113.83	120.80
47	S2	943	U	C5-C4-O4	-5.80	122.42	125.90
1	L5	323	C	C5-C4-N4	5.80	124.26	120.20
1	L5	181	C	C6-N1-C1'	-5.80	113.84	120.80
1	L5	994	G	N1-C2-N2	-5.79	110.98	116.20
47	S2	1453	C	C6-N1-C2	-5.79	117.98	120.30
47	S2	814	U	N3-C2-O2	-5.79	118.15	122.20
1	L5	259	C	N1-C2-O2	5.79	122.37	118.90
1	L5	1245	C	C2-N1-C1'	5.79	125.16	118.80
1	L5	904	C	N3-C2-O2	-5.78	117.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	489	C	C6-N1-C1'	-5.77	113.87	120.80
1	L5	4709	U	C6-N1-C1'	-5.77	113.12	121.20
47	S2	930	C	N1-C2-O2	5.76	122.36	118.90
1	L5	4742	G	N3-C4-N9	-5.76	122.54	126.00
1	L5	4758	U	N1-C2-O2	5.75	126.82	122.80
47	S2	427	U	N3-C2-O2	-5.75	118.18	122.20
1	L5	2814	C	N1-C2-O2	5.74	122.35	118.90
1	L5	2005	G	C8-N9-C1'	-5.73	119.55	127.00
1	L5	4742	G	O4'-C1'-N9	5.73	112.78	108.20
1	L5	1853	G	C4-N9-C1'	5.73	133.95	126.50
1	L5	220	C	C2-N1-C1'	5.72	125.10	118.80
1	L5	1191	C	N3-C2-O2	-5.72	117.89	121.90
1	L5	1405	C	N3-C2-O2	-5.72	117.90	121.90
1	L5	1968	G	C6-C5-N7	-5.72	126.97	130.40
1	L5	4107	G	C4-N9-C1'	5.71	133.92	126.50
47	S2	1660	C	C2-N1-C1'	5.71	125.08	118.80
1	L5	4281	A	O4'-C1'-N9	5.71	112.77	108.20
1	L5	112	C	C2-N1-C1'	5.71	125.08	118.80
1	L5	985	C	C2-N1-C1'	5.71	125.08	118.80
1	L5	925	C	C5-C6-N1	5.70	123.85	121.00
1	L5	4355	G	N1-C2-N3	5.70	127.32	123.90
47	S2	1261	C	N1-C2-O2	5.70	122.32	118.90
1	L5	4928	C	C6-N1-C1'	-5.70	113.96	120.80
47	S2	1578	U	N3-C2-O2	-5.70	118.21	122.20
1	L5	1969	G	C5-C6-O6	5.69	132.01	128.60
1	L5	2820	C	N1-C2-O2	5.69	122.31	118.90
1	L5	1821	G	N3-C4-N9	5.69	129.41	126.00
1	L5	655	C	C6-N1-C2	-5.68	118.03	120.30
1	L5	4864	U	N1-C2-O2	5.67	126.77	122.80
1	L5	260	C	C6-N1-C2	-5.67	118.03	120.30
1	L5	4040	C	C6-N1-C2	-5.66	118.04	120.30
47	S2	570	C	N3-C2-O2	-5.66	117.94	121.90
47	S2	1420	G	C4-N9-C1'	5.66	133.86	126.50
1	L5	2096	G	N3-C4-C5	-5.65	125.78	128.60
1	L5	4709	U	C5-C4-O4	-5.64	122.52	125.90
1	L5	504	G	N3-C4-N9	5.64	129.38	126.00
1	L5	1188	C	C6-N1-C1'	5.64	127.56	120.80
1	L5	3948	C	C6-N1-C2	-5.64	118.05	120.30
47	S2	659	G	C4-N9-C1'	5.64	133.83	126.50
16	LN	134	LEU	CA-CB-CG	5.63	128.26	115.30
4	LA	149	LYS	C-N-CA	5.63	135.77	121.70
47	S2	1520	G	N3-C4-C5	-5.63	125.79	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	1714	C	N3-C2-O2	-5.62	117.96	121.90
1	L5	1808	C	C6-N1-C1'	5.62	127.55	120.80
1	L5	3772	U	N3-C2-O2	-5.62	118.27	122.20
47	S2	130	G	N3-C4-N9	5.62	129.37	126.00
1	L5	513	U	N1-C2-O2	5.62	126.73	122.80
1	L5	3948	C	N3-C2-O2	-5.61	117.97	121.90
47	S2	4	C	C2-N1-C1'	5.61	124.97	118.80
47	S2	579	C	N1-C2-O2	5.60	122.26	118.90
47	S2	527	C	N1-C2-O2	5.59	122.25	118.90
1	L5	139	G	N9-C4-C5	5.59	107.64	105.40
1	L5	984	C	N1-C2-O2	5.58	122.25	118.90
1	L5	2033	A	P-O3'-C3'	5.58	126.40	119.70
1	L5	485	C	C6-N1-C2	-5.58	118.07	120.30
47	S2	1315	U	N1-C2-O2	5.57	126.70	122.80
82	CC	55	C	N3-C2-O2	-5.57	118.00	121.90
47	S2	834	C	N3-C2-O2	-5.56	118.01	121.90
1	L5	2491	C	N3-C2-O2	-5.56	118.01	121.90
1	L5	2820	C	N3-C2-O2	-5.55	118.01	121.90
5	LB	360	LEU	CA-CB-CG	5.55	128.06	115.30
47	S2	478	G	N9-C4-C5	5.55	107.62	105.40
1	L5	1367	C	C6-N1-C2	-5.54	118.08	120.30
1	L5	4040	C	C2-N1-C1'	5.54	124.90	118.80
1	L5	2262	G	N3-C4-N9	5.54	129.32	126.00
1	L5	4398	C	N1-C2-O2	5.53	122.22	118.90
1	L5	1969	G	N3-C2-N2	5.53	123.77	119.90
2	L7	102	U	N1-C2-O2	5.53	126.67	122.80
47	S2	814	U	N1-C2-O2	5.53	126.67	122.80
47	S2	1016	U	C2-N1-C1'	5.52	124.33	117.70
47	S2	112	U	P-O3'-C3'	5.52	126.33	119.70
47	S2	529	A	C5-C6-N6	-5.51	119.29	123.70
47	S2	1022	U	N3-C2-O2	-5.51	118.34	122.20
1	L5	130	C	C6-N1-C2	-5.51	118.09	120.30
1	L5	2362	U	N3-C2-O2	-5.51	118.34	122.20
47	S2	559	G	O4'-C1'-N9	5.51	112.61	108.20
47	S2	883	U	N1-C2-N3	5.51	118.20	114.90
47	S2	478	G	N1-C6-O6	-5.50	116.60	119.90
1	L5	1472	C	C2-N1-C1'	5.49	124.84	118.80
47	S2	118	C	C6-N1-C1'	-5.49	114.21	120.80
1	L5	2627	C	C6-N1-C1'	-5.49	114.22	120.80
3	L8	51	U	N3-C2-O2	-5.49	118.36	122.20
1	L5	4498	U	C2-N3-C4	-5.48	123.71	127.00
1	L5	504	G	C8-N9-C1'	-5.48	119.88	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L8	51	U	N1-C2-O2	5.48	126.63	122.80
1	L5	2492	C	C6-N1-C2	-5.47	118.11	120.30
1	L5	2005	G	N3-C4-N9	5.47	129.28	126.00
47	S2	1364	U	N1-C2-O2	5.46	126.62	122.80
1	L5	100	C	C6-N1-C1'	-5.46	114.25	120.80
1	L5	468	U	N3-C4-O4	5.45	123.22	119.40
47	S2	1420	G	N3-C4-N9	5.45	129.27	126.00
1	L5	323	C	C6-N1-C2	-5.45	118.12	120.30
1	L5	1633	G	P-O3'-C3'	5.45	126.24	119.70
47	S2	1417	C	C2-N3-C4	5.45	122.62	119.90
1	L5	257	C	C6-N1-C2	-5.45	118.12	120.30
1	L5	1367	C	C6-N1-C1'	-5.45	114.27	120.80
47	S2	983	A	N3-C4-N9	5.44	131.75	127.40
1	L5	1831	G	C5-C6-O6	5.44	131.86	128.60
1	L5	234	G	N9-C1'-C2'	5.44	121.07	114.00
1	L5	205	C	N3-C2-O2	-5.43	118.10	121.90
47	S2	1424	G	N3-C4-N9	5.43	129.26	126.00
1	L5	2528	G	N3-C4-C5	-5.43	125.89	128.60
1	L5	468	U	C5-C4-O4	-5.42	122.65	125.90
1	L5	516	C	C2-N1-C1'	5.42	124.77	118.80
1	L5	4356	G	N1-C6-O6	-5.42	116.64	119.90
1	L5	115	C	N1-C2-O2	5.42	122.15	118.90
47	S2	876	C	N1-C2-O2	5.42	122.15	118.90
1	L5	3909	C	C2-N1-C1'	5.41	124.75	118.80
47	S2	322	C	C6-N1-C2	-5.41	118.14	120.30
47	S2	325	C	C2-N1-C1'	5.41	124.75	118.80
1	L5	3775	A	C8-N9-C4	-5.41	103.64	105.80
1	L5	5028	G	N3-C4-N9	5.41	129.25	126.00
1	L5	1821	G	N3-C4-C5	-5.40	125.90	128.60
1	L5	3778	U	C2-N1-C1'	5.40	124.18	117.70
1	L5	738	C	C6-N1-C2	-5.40	118.14	120.30
47	S2	130	G	N3-C4-C5	-5.40	125.90	128.60
1	L5	4773	C	N3-C2-O2	-5.40	118.12	121.90
1	L5	4420	U	C2-N1-C1'	5.39	124.17	117.70
1	L5	758	G	C5-C6-O6	5.39	131.83	128.60
47	S2	1219	C	N1-C2-O2	5.38	122.13	118.90
1	L5	323	C	N1-C2-N3	5.38	122.97	119.20
1	L5	5035	U	N3-C2-O2	-5.37	118.44	122.20
77	SZ	58	LEU	CA-CB-CG	5.37	127.66	115.30
1	L5	4887	C	C2-N1-C1'	5.37	124.71	118.80
1	L5	1731	C	C2-N1-C1'	5.37	124.70	118.80
47	S2	563	G	P-O3'-C3'	5.37	126.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	S2	1434	C	P-O3'-C3'	5.37	126.14	119.70
1	L5	4901	G	N1-C6-O6	-5.36	116.68	119.90
1	L5	1173	G	C5-C6-O6	5.36	131.82	128.60
1	L5	3693	U	N1-C2-O2	5.35	126.55	122.80
1	L5	1405	C	C6-N1-C2	-5.35	118.16	120.30
1	L5	2786	C	P-O3'-C3'	5.35	126.12	119.70
1	L5	4864	U	N3-C2-O2	-5.35	118.45	122.20
47	S2	494	C	N1-C2-O2	5.35	122.11	118.90
47	S2	501	C	C5-C6-N1	5.35	123.68	121.00
1	L5	499	G	C4-N9-C1'	5.35	133.46	126.50
47	S2	542	U	N1-C2-O2	5.35	126.55	122.80
1	L5	4928	C	C6-N1-C2	-5.35	118.16	120.30
1	L5	175	C	C6-N1-C1'	5.34	127.21	120.80
47	S2	293	C	C5-C6-N1	5.34	123.67	121.00
1	L5	2260	C	N3-C2-O2	-5.34	118.16	121.90
1	L5	1216	C	C6-N1-C2	-5.33	118.17	120.30
1	L5	456	C	N1-C2-O2	5.33	122.10	118.90
1	L5	4758	U	N3-C2-O2	-5.33	118.47	122.20
1	L5	77	U	N1-C2-O2	5.33	126.53	122.80
1	L5	1582	U	N1-C2-O2	5.32	126.53	122.80
1	L5	1808	C	N1-C2-N3	5.32	122.93	119.20
1	L5	4747	C	C2-N1-C1'	5.32	124.65	118.80
1	L5	1241	C	N3-C2-O2	-5.32	118.18	121.90
1	L5	2855	G	N1-C2-N2	-5.31	111.42	116.20
1	L5	4891	G	C5-C6-O6	5.31	131.79	128.60
1	L5	2096	G	C8-N9-C1'	-5.31	120.10	127.00
1	L5	3839	G	O4'-C1'-N9	-5.31	103.95	108.20
1	L5	4901	G	C5-C6-O6	5.31	131.78	128.60
82	CC	44	A	N1-C2-N3	-5.31	126.65	129.30
47	S2	1578	U	N1-C2-O2	5.31	126.52	122.80
1	L5	259	C	N3-C2-O2	-5.31	118.19	121.90
1	L5	4360	U	N3-C2-O2	-5.30	118.49	122.20
1	L5	2255	C	C2-N1-C1'	5.30	124.63	118.80
47	S2	1218	C	C5-C6-N1	5.30	123.65	121.00
47	S2	1660	C	N1-C2-O2	5.30	122.08	118.90
1	L5	485	C	N3-C2-O2	-5.29	118.19	121.90
1	L5	1327	C	C6-N1-C2	-5.29	118.18	120.30
1	L5	456	C	C6-N1-C2	-5.29	118.18	120.30
1	L5	1702	C	C2-N1-C1'	5.29	124.62	118.80
1	L5	4112	C	C6-N1-C2	-5.28	118.19	120.30
1	L5	472	C	N3-C2-O2	-5.27	118.21	121.90
82	CC	34	U	N1-C2-O2	5.27	126.49	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	2767	U	N3-C2-O2	-5.27	118.51	122.20
47	S2	589	G	O4'-C1'-N9	-5.27	103.99	108.20
1	L5	129	C	N1-C2-N3	5.27	122.89	119.20
1	L5	209	U	N1-C2-O2	5.27	126.49	122.80
82	CC	47	C	C2-N1-C1'	-5.26	113.01	118.80
47	S2	1139	C	C6-N1-C1'	-5.26	114.49	120.80
1	L5	1714	C	C2-N1-C1'	5.25	124.58	118.80
1	L5	2560	C	N1-C2-O2	5.25	122.05	118.90
1	L5	4097	G	N1-C6-O6	-5.25	116.75	119.90
1	L5	4107	G	N1-C6-O6	-5.25	116.75	119.90
1	L5	4042	G	N3-C4-N9	5.25	129.15	126.00
1	L5	969	C	C5-C6-N1	5.24	123.62	121.00
47	S2	1591	C	N3-C2-O2	-5.24	118.24	121.90
1	L5	1853	G	C8-N9-C1'	-5.23	120.20	127.00
47	S2	1415	C	N3-C2-O2	-5.23	118.24	121.90
1	L5	977	C	C2-N1-C1'	5.23	124.55	118.80
1	L5	3673	C	P-O3'-C3'	5.22	125.97	119.70
47	S2	1219	C	C2-N1-C1'	5.22	124.55	118.80
47	S2	1309	C	N1-C2-O2	5.22	122.03	118.90
1	L5	406	C	P-O3'-C3'	5.21	125.96	119.70
1	L5	4775	C	C2-N1-C1'	5.21	124.54	118.80
1	L5	1378	C	N1-C2-O2	5.21	122.03	118.90
1	L5	1552	G	O4'-C1'-N9	5.21	112.37	108.20
1	L5	2410	C	C5-C6-N1	5.21	123.60	121.00
1	L5	4356	G	C4-C5-N7	-5.21	108.72	110.80
47	S2	841	G	N1-C2-N2	-5.21	111.51	116.20
1	L5	472	C	C6-N1-C1'	-5.19	114.57	120.80
47	S2	1271	C	N1-C2-O2	5.18	122.01	118.90
47	S2	1261	C	N3-C2-O2	-5.18	118.27	121.90
1	L5	490	C	C6-N1-C1'	5.18	127.02	120.80
1	L5	2021	G	C4-N9-C1'	5.18	133.23	126.50
1	L5	493	G	P-O3'-C3'	5.18	125.91	119.70
1	L5	963	G	N3-C4-C5	-5.18	126.01	128.60
1	L5	3909	C	N3-C2-O2	-5.18	118.28	121.90
1	L5	3930	U	C2-N1-C1'	5.17	123.91	117.70
1	L5	4682	U	C2-N1-C1'	5.17	123.90	117.70
1	L5	1403	G	N3-C4-N9	5.17	129.10	126.00
1	L5	4773	C	C2-N1-C1'	5.17	124.49	118.80
47	S2	427	U	N1-C2-O2	5.17	126.42	122.80
1	L5	1049	C	C5-C6-N1	5.17	123.58	121.00
1	L5	2094	G	C4-N9-C1'	5.17	133.22	126.50
1	L5	4043	G	N3-C4-N9	5.17	129.10	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	S2	1422	G	C6-C5-N7	5.16	133.50	130.40
1	L5	1259	G	N1-C2-N2	-5.16	111.56	116.20
47	S2	1389	C	N1-C2-O2	5.15	121.99	118.90
1	L5	963	G	C4-N9-C1'	5.15	133.19	126.50
47	S2	293	C	C6-N1-C2	-5.15	118.24	120.30
47	S2	391	C	C2-N1-C1'	5.15	124.46	118.80
1	L5	963	G	N3-C4-N9	5.14	129.09	126.00
47	S2	1417	C	N1-C2-O2	5.14	121.99	118.90
47	S2	291	G	P-O3'-C3'	5.14	125.87	119.70
1	L5	757	G	N1-C2-N2	-5.14	111.58	116.20
1	L5	1582	U	N3-C2-O2	-5.13	118.61	122.20
1	L5	2899	C	C2-N1-C1'	5.13	124.44	118.80
1	L5	2667	C	N1-C2-O2	5.13	121.98	118.90
1	L5	1663	C	C2-N1-C1'	5.13	124.44	118.80
1	L5	1340	C	C6-N1-C2	-5.12	118.25	120.30
1	L5	2900	U	N1-C2-O2	5.11	126.38	122.80
1	L5	4926	C	C6-N1-C1'	-5.11	114.67	120.80
1	L5	1808	C	C5-C4-N4	5.11	123.78	120.20
1	L5	2627	C	C5-C6-N1	5.11	123.56	121.00
1	L5	4398	C	N3-C2-O2	-5.11	118.32	121.90
47	S2	331	C	N1-C2-O2	5.11	121.96	118.90
1	L5	3770	U	N1-C2-O2	5.10	126.37	122.80
1	L5	4471	U	N3-C2-O2	-5.10	118.63	122.20
1	L5	516	C	C6-N1-C2	-5.10	118.26	120.30
1	L5	177	G	N1-C2-N2	-5.09	111.61	116.20
1	L5	1716	G	C6-N1-C2	-5.09	122.04	125.10
1	L5	2416	G	P-O3'-C3'	5.09	125.81	119.70
82	CC	74	C	P-O3'-C3'	5.09	125.81	119.70
1	L5	504	G	N3-C4-C5	-5.09	126.06	128.60
1	L5	2262	G	C8-N9-C1'	-5.09	120.39	127.00
32	Ld	97	ASP	C-N-CA	5.08	134.40	121.70
1	L5	139	G	N3-C2-N2	-5.08	116.34	119.90
1	L5	4303	C	C6-N1-C1'	-5.08	114.71	120.80
47	S2	1437	C	N1-C2-O2	5.08	121.95	118.90
1	L5	1050	C	C6-N1-C2	-5.07	118.27	120.30
47	S2	1364	U	N3-C2-O2	-5.07	118.65	122.20
1	L5	655	C	N1-C2-N3	5.07	122.75	119.20
1	L5	220	C	C6-N1-C2	-5.07	118.27	120.30
1	L5	2257	C	C6-N1-C1'	-5.07	114.72	120.80
1	L5	2487	G	N1-C6-O6	-5.07	116.86	119.90
1	L5	4742	G	C6-C5-N7	5.07	133.44	130.40
1	L5	2021	G	C8-N9-C1'	-5.06	120.42	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	S2	1309	C	C6-N1-C2	-5.06	118.27	120.30
2	L7	102	U	N3-C2-O2	-5.06	118.66	122.20
1	L5	1968	G	N3-C4-C5	-5.06	126.07	128.60
1	L5	175	C	C6-N1-C2	-5.06	118.28	120.30
1	L5	1808	C	C6-N1-C2	-5.06	118.28	120.30
47	S2	1315	U	N3-C2-O2	-5.05	118.66	122.20
1	L5	738	C	C5-C6-N1	5.05	123.53	121.00
47	S2	1309	C	C6-N1-C1'	-5.05	114.74	120.80
1	L5	1993	C	N1-C2-O2	5.05	121.93	118.90
1	L5	96	U	N3-C2-O2	-5.05	118.67	122.20
1	L5	1251	C	N3-C2-O2	-5.05	118.37	121.90
47	S2	659	G	C8-N9-C1'	-5.05	120.44	127.00
1	L5	3771	C	C6-N1-C2	-5.04	118.28	120.30
47	S2	1424	G	C4-N9-C1'	5.04	133.06	126.50
1	L5	1447	C	N1-C2-O2	5.04	121.92	118.90
1	L5	2005	G	N7-C8-N9	5.04	115.62	113.10
47	S2	329	G	N3-C2-N2	5.04	123.43	119.90
68	Sg	7	LEU	CA-CB-CG	5.04	126.90	115.30
1	L5	5028	G	C4-N9-C1'	5.04	133.05	126.50
47	S2	1417	C	C5-C6-N1	5.04	123.52	121.00
1	L5	654	C	C5-C6-N1	5.03	123.52	121.00
1	L5	1929	A	C4-N9-C1'	5.03	135.36	126.30
53	SH	35	ASP	CB-CG-OD2	5.03	122.83	118.30
1	L5	753	C	C6-N1-C2	-5.03	118.29	120.30
1	L5	3772	U	N1-C2-O2	5.03	126.32	122.80
1	L5	4399	U	N3-C2-O2	-5.03	118.68	122.20
47	S2	356	C	C6-N1-C2	-5.03	118.29	120.30
1	L5	2560	C	C5-C6-N1	5.03	123.51	121.00
1	L5	3771	C	N1-C2-O2	5.03	121.92	118.90
1	L5	260	C	N1-C2-O2	5.03	121.92	118.90
1	L5	3930	U	N3-C2-O2	-5.02	118.68	122.20
47	S2	559	G	C5-C6-O6	5.02	131.61	128.60
1	L5	2095	A	O4'-C1'-N9	5.02	112.22	108.20
1	L5	499	G	N3-C4-N9	5.02	129.01	126.00
1	L5	1069	G	N3-C4-N9	-5.02	122.99	126.00
1	L5	4920	C	N1-C2-O2	5.02	121.91	118.90
47	S2	119	U	N3-C2-O2	-5.02	118.69	122.20
1	L5	1252	C	C6-N1-C2	-5.02	118.29	120.30
1	L5	2410	C	C6-N1-C2	-5.02	118.29	120.30
47	S2	1660	C	N3-C2-O2	-5.02	118.39	121.90
47	S2	130	G	C8-N9-C1'	-5.02	120.48	127.00
47	S2	666	U	C2-N1-C1'	5.01	123.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	1720	C	C6-N1-C2	-5.01	118.30	120.30
1	L5	4746	C	N1-C2-O2	5.01	121.90	118.90
1	L5	504	G	OP1-P-O3'	5.00	116.21	105.20
1	L5	4254	G	N3-C4-N9	5.00	129.00	126.00
47	S2	179	C	N3-C2-O2	-5.00	118.40	121.90
47	S2	1420	G	C8-N9-C1'	-5.00	120.50	127.00

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	LA	110	GLY	Peptide
4	LA	54	ARG	Peptide
5	LB	17	LEU	Peptide
5	LB	2	SER	Peptide
5	LB	258	HIS	Peptide
11	LH	106	GLN	Peptide
13	LJ	94	LEU	Peptide
14	LL	154	VAL	Peptide
15	LM	87	ALA	Peptide
15	LM	88	ALA	Peptide
17	LO	110	PRO	Peptide
17	LO	30	GLY	Peptide
22	LT	136	ARG	Peptide
30	Lb	59	ALA	Peptide
34	Lf	103	VAL	Peptide
34	Lf	106	TYR	Peptide
36	Lh	86	LYS	Peptide
38	Lj	39	TYR	Peptide
46	Lz	183	ILE	Peptide
49	SB	221	PRO	Peptide
50	SD	164	VAL	Peptide
52	SF	78	MET	Peptide
53	SH	15	LYS	Peptide
57	SP	127	LYS	Peptide
58	SQ	43	GLU	Peptide
61	ST	46	ALA	Peptide
63	SV	78	ILE	Peptide
64	SX	126	ALA	Peptide
64	SX	86	PRO	Peptide
77	SZ	46	ASN	Peptide
65	Sa	93	LYS	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%)	224 (91%)	21 (8%)	1 (0%)	34	72
5	LB	400/403 (99%)	370 (92%)	28 (7%)	2 (0%)	29	68
6	LC	366/427 (86%)	331 (90%)	34 (9%)	1 (0%)	41	76
7	LD	291/297 (98%)	271 (93%)	20 (7%)	0	100	100
8	LE	232/288 (81%)	216 (93%)	16 (7%)	0	100	100
9	LF	223/248 (90%)	213 (96%)	10 (4%)	0	100	100
10	LG	239/266 (90%)	223 (93%)	16 (7%)	0	100	100
11	LH	188/192 (98%)	168 (89%)	20 (11%)	0	100	100
12	LI	198/214 (92%)	183 (92%)	15 (8%)	0	100	100
13	LJ	174/178 (98%)	158 (91%)	16 (9%)	0	100	100
14	LL	208/211 (99%)	191 (92%)	17 (8%)	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%)	190 (96%)	9 (4%)	0	100	100
18	LP	151/184 (82%)	140 (93%)	11 (7%)	0	100	100
19	LQ	185/188 (98%)	176 (95%)	9 (5%)	0	100	100
20	LR	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
21	LS	173/176 (98%)	162 (94%)	11 (6%)	0	100	100
22	LT	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
23	LU	99/128 (77%)	85 (86%)	13 (13%)	1 (1%)	15	53
24	LV	129/140 (92%)	120 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	LW	122/157 (78%)	115 (94%)	7 (6%)	0	100	100
26	LX	118/156 (76%)	112 (95%)	6 (5%)	0	100	100
27	LY	132/145 (91%)	120 (91%)	12 (9%)	0	100	100
28	LZ	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
29	La	145/148 (98%)	136 (94%)	9 (6%)	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%)	100 (95%)	5 (5%)	0	100	100
33	Le	126/135 (93%)	120 (95%)	5 (4%)	1 (1%)	19	57
34	Lf	107/110 (97%)	98 (92%)	7 (6%)	2 (2%)	8	36
35	Lg	112/117 (96%)	108 (96%)	4 (4%)	0	100	100
36	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
37	Li	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
38	Lj	84/97 (87%)	76 (90%)	7 (8%)	1 (1%)	13	48
39	Lk	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
40	Ll	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
41	Lm	50/128 (39%)	50 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	101/104 (97%)	95 (94%)	6 (6%)	0	100	100
44	Lp	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
45	Lr	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
46	Lz	215/217 (99%)	171 (80%)	44 (20%)	0	100	100
48	SA	219/295 (74%)	196 (90%)	23 (10%)	0	100	100
49	SB	212/264 (80%)	197 (93%)	15 (7%)	0	100	100
50	SD	225/243 (93%)	202 (90%)	23 (10%)	0	100	100
51	SE	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
52	SF	180/204 (88%)	165 (92%)	15 (8%)	0	100	100
53	SH	182/194 (94%)	161 (88%)	21 (12%)	0	100	100
54	SI	204/208 (98%)	193 (95%)	11 (5%)	0	100	100
55	SK	96/165 (58%)	85 (88%)	11 (12%)	0	100	100
56	SL	151/158 (96%)	139 (92%)	12 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	SP	125/145 (86%)	115 (92%)	10 (8%)	0	100	100
58	SQ	142/146 (97%)	128 (90%)	13 (9%)	1 (1%)	22	60
59	SR	133/135 (98%)	121 (91%)	12 (9%)	0	100	100
60	SS	143/152 (94%)	131 (92%)	12 (8%)	0	100	100
61	ST	141/145 (97%)	129 (92%)	11 (8%)	1 (1%)	22	60
62	SU	102/119 (86%)	91 (89%)	11 (11%)	0	100	100
63	SV	81/83 (98%)	73 (90%)	7 (9%)	1 (1%)	13	48
64	SX	139/143 (97%)	124 (89%)	14 (10%)	1 (1%)	22	60
65	Sa	100/115 (87%)	90 (90%)	9 (9%)	1 (1%)	15	53
66	Sc	62/69 (90%)	50 (81%)	12 (19%)	0	100	100
67	Sd	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
68	Sg	311/317 (98%)	267 (86%)	44 (14%)	0	100	100
69	SC	220/293 (75%)	206 (94%)	14 (6%)	0	100	100
70	SG	235/249 (94%)	218 (93%)	17 (7%)	0	100	100
71	SJ	183/194 (94%)	170 (93%)	13 (7%)	0	100	100
72	SM	120/132 (91%)	109 (91%)	11 (9%)	0	100	100
73	SN	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
74	SO	138/151 (91%)	126 (91%)	12 (9%)	0	100	100
75	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
76	SY	129/133 (97%)	121 (94%)	8 (6%)	0	100	100
77	SZ	73/125 (58%)	59 (81%)	13 (18%)	1 (1%)	11	43
78	Sb	81/84 (96%)	70 (86%)	11 (14%)	0	100	100
79	Se	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
80	Sf	65/156 (42%)	54 (83%)	11 (17%)	0	100	100
81	CA	350/394 (89%)	332 (95%)	18 (5%)	0	100	100
83	CE	71/223 (32%)	70 (99%)	1 (1%)	0	100	100
All	All	11958/13520 (88%)	11007 (92%)	933 (8%)	18 (0%)	50	82

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	LN	124	ASP
64	SX	127	ASN

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Mol	Chain	Res	Type
15	LM	88	ALA
61	ST	41	LYS
5	LB	302	ASN
5	LB	360	LEU
34	Lf	80	ASN
65	Sa	47	ALA
77	SZ	78	LYS
4	LA	55	GLY
58	SQ	44	PRO
38	Lj	40	PRO
16	LN	83	LYS
6	LC	232	VAL
23	LU	59	GLY
33	Le	73	GLY
34	Lf	107	PRO
63	SV	79	VAL

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%)	348 (100%)	0	100 100
6	LC	306/348 (88%)	304 (99%)	2 (1%)	84 94
7	LD	246/250 (98%)	245 (100%)	1 (0%)	91 97
8	LE	209/252 (83%)	207 (99%)	2 (1%)	76 91
9	LF	194/215 (90%)	192 (99%)	2 (1%)	76 91
10	LG	203/223 (91%)	202 (100%)	1 (0%)	88 96
11	LH	169/171 (99%)	169 (100%)	0	100 100
12	LI	172/181 (95%)	172 (100%)	0	100 100
13	LJ	148/149 (99%)	147 (99%)	1 (1%)	84 94
14	LL	176/177 (99%)	176 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	LM	118/161 (73%)	118 (100%)	0	100	100
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%)	91 (100%)	0	100	100
24	LV	101/107 (94%)	100 (99%)	1 (1%)	76	91
25	LW	103/126 (82%)	102 (99%)	1 (1%)	76	91
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%)	117 (98%)	3 (2%)	47	79
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%)	98 (100%)	0	100	100
33	Le	114/121 (94%)	114 (100%)	0	100	100
34	Lf	88/89 (99%)	87 (99%)	1 (1%)	73	90
35	Lg	98/100 (98%)	97 (99%)	1 (1%)	76	91
36	Lh	109/110 (99%)	108 (99%)	1 (1%)	78	92
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%)	61 (95%)	3 (5%)	26	63
40	Ll	47/48 (98%)	45 (96%)	2 (4%)	29	66
41	Lm	48/116 (41%)	48 (100%)	0	100	100
42	Ln	23/24 (96%)	23 (100%)	0	100	100
43	Lo	91/92 (99%)	91 (100%)	0	100	100
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/121 (90%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	Lz	195/196 (100%)	190 (97%)	5 (3%)	46 78
48	SA	183/243 (75%)	182 (100%)	1 (0%)	88 96
49	SB	195/231 (84%)	193 (99%)	2 (1%)	76 91
50	SD	190/202 (94%)	187 (98%)	3 (2%)	62 86
51	SE	224/225 (100%)	222 (99%)	2 (1%)	78 92
52	SF	156/170 (92%)	156 (100%)	0	100 100
53	SH	166/174 (95%)	163 (98%)	3 (2%)	59 85
54	SI	178/180 (99%)	177 (99%)	1 (1%)	86 95
55	SK	89/136 (65%)	87 (98%)	2 (2%)	52 81
56	SL	137/142 (96%)	136 (99%)	1 (1%)	84 94
57	SP	113/130 (87%)	113 (100%)	0	100 100
58	SQ	119/121 (98%)	118 (99%)	1 (1%)	81 93
59	SR	122/122 (100%)	122 (100%)	0	100 100
60	SS	126/132 (96%)	125 (99%)	1 (1%)	81 93
61	ST	113/115 (98%)	111 (98%)	2 (2%)	59 85
62	SU	94/107 (88%)	94 (100%)	0	100 100
63	SV	67/67 (100%)	67 (100%)	0	100 100
64	SX	113/115 (98%)	112 (99%)	1 (1%)	78 92
65	Sa	89/98 (91%)	87 (98%)	2 (2%)	52 81
66	Sc	57/62 (92%)	57 (100%)	0	100 100
67	Sd	48/49 (98%)	47 (98%)	1 (2%)	53 82
68	Sg	272/275 (99%)	271 (100%)	1 (0%)	91 97
69	SC	188/225 (84%)	187 (100%)	1 (0%)	88 96
70	SG	207/218 (95%)	205 (99%)	2 (1%)	76 91
71	SJ	161/168 (96%)	161 (100%)	0	100 100
72	SM	102/108 (94%)	100 (98%)	2 (2%)	55 83
73	SN	130/131 (99%)	130 (100%)	0	100 100
74	SO	110/119 (92%)	109 (99%)	1 (1%)	78 92
75	SW	112/113 (99%)	112 (100%)	0	100 100
76	SY	113/115 (98%)	111 (98%)	2 (2%)	59 85
77	SZ	66/103 (64%)	64 (97%)	2 (3%)	41 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
78	Sb	75/76 (99%)	75 (100%)	0	100 100
79	Se	47/48 (98%)	47 (100%)	0	100 100
80	Sf	60/140 (43%)	59 (98%)	1 (2%)	60 85
81	CA	303/336 (90%)	303 (100%)	0	100 100
83	CE	62/190 (33%)	62 (100%)	0	100 100
All	All	10421/11521 (90%)	10350 (99%)	71 (1%)	84 94

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	207	VAL
4	LA	247	ARG
6	LC	188	ARG
6	LC	257	PHE
7	LD	85	LYS
8	LE	56	ARG
8	LE	197	THR
9	LF	29	LYS
9	LF	238	ASP
10	LG	111	LYS
13	LJ	95	ARG
17	LO	117	ARG
22	LT	36	LYS
24	LV	48	ARG
25	LW	116	LYS
27	LY	79	VAL
27	LY	84	ARG
29	La	76	ASP
29	La	92	LYS
29	La	116	LYS
30	Lb	63	LYS
31	Lc	23	LYS
34	Lf	37	ASP
35	Lg	54	ARG
36	Lh	97	LYS
38	Lj	22	CYS
39	Lk	21	LYS
39	Lk	29	LYS
39	Lk	55	LYS
40	Ll	36	ARG

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Mol	Chain	Res	Type
40	Ll	46	ARG
46	Lz	7	ARG
46	Lz	85	MET
46	Lz	122	ARG
46	Lz	161	LYS
46	Lz	172	VAL
48	SA	8	LEU
49	SB	56	LYS
49	SB	195	LYS
50	SD	76	ARG
50	SD	143	ARG
50	SD	178	ARG
51	SE	69	PHE
51	SE	254	LYS
53	SH	32	MET
53	SH	57	ARG
53	SH	118	ARG
54	SI	140	LYS
55	SK	59	LYS
55	SK	98	ARG
56	SL	69	ARG
58	SQ	25	CYS
60	SS	103	LEU
61	ST	24	LYS
61	ST	41	LYS
64	SX	105	PHE
65	Sa	52	ASP
65	Sa	94	ASP
67	Sd	49	ASP
68	Sg	47	ARG
69	SC	104	ASP
70	SG	98	ARG
70	SG	119	LYS
72	SM	63	LYS
72	SM	121	LYS
74	SO	150	ARG
76	SY	16	ARG
76	SY	118	ARG
77	SZ	41	ARG
77	SZ	44	LEU
80	Sf	104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106)

such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	97	ASN
4	LA	132	ASN
4	LA	162	ASN
4	LA	216	HIS
5	LB	204	GLN
5	LB	208	ASN
6	LC	21	ASN
6	LC	38	ASN
6	LC	48	ASN
6	LC	50	GLN
6	LC	299	GLN
7	LD	191	ASN
7	LD	198	HIS
7	LD	225	GLN
7	LD	282	GLN
8	LE	190	HIS
9	LF	39	GLN
13	LJ	3	GLN
13	LJ	98	ASN
16	LN	196	ASN
17	LO	184	ASN
18	LP	21	ASN
18	LP	80	GLN
18	LP	97	ASN
18	LP	116	HIS
18	LP	137	ASN
19	LQ	21	GLN
19	LQ	44	ASN
20	LR	40	GLN
20	LR	130	ASN
20	LR	143	HIS
21	LS	77	ASN
22	LT	144	ASN
23	LU	50	ASN
24	LV	77	HIS
27	LY	14	ASN
29	La	34	ASN
29	La	66	ASN
30	Lb	50	ASN
30	Lb	60	ASN
31	Lc	15	ASN
33	Le	107	ASN

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Mol	Chain	Res	Type
34	Lf	56	ASN
34	Lf	80	ASN
38	Lj	13	ASN
38	Lj	66	HIS
38	Lj	76	HIS
41	Lm	87	GLN
43	Lo	45	GLN
44	Lp	56	HIS
45	Lr	6	GLN
45	Lr	100	ASN
46	Lz	19	HIS
46	Lz	35	GLN
46	Lz	72	GLN
48	SA	131	HIS
48	SA	141	ASN
49	SB	53	GLN
49	SB	149	GLN
49	SB	177	GLN
49	SB	186	ASN
50	SD	57	ASN
50	SD	145	GLN
51	SE	98	ASN
51	SE	138	HIS
51	SE	157	ASN
52	SF	31	ASN
52	SF	148	ASN
54	SI	9	HIS
54	SI	35	ASN
55	SK	44	HIS
55	SK	50	GLN
56	SL	11	GLN
56	SL	19	ASN
56	SL	65	ASN
57	SP	24	GLN
57	SP	98	ASN
57	SP	104	GLN
58	SQ	29	ASN
58	SQ	80	GLN
59	SR	31	ASN
59	SR	62	GLN
59	SR	93	GLN
60	SS	10	GLN

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Mol	Chain	Res	Type
61	ST	128	GLN
62	SU	92	HIS
64	SX	127	ASN
67	Sd	26	ASN
68	Sg	14	HIS
68	Sg	15	ASN
68	Sg	117	ASN
68	Sg	237	ASN
68	Sg	296	GLN
73	SN	5	HIS
73	SN	49	GLN
74	SO	13	GLN
78	Sb	26	GLN
81	CA	10	GLN
81	CA	29	ASN
81	CA	113	HIS
81	CA	134	GLN
81	CA	161	ASN
81	CA	162	GLN
81	CA	165	GLN
81	CA	178	ASN
81	CA	203	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3705/5070 (73%)	962 (25%)	19 (0%)
2	L7	119/121 (98%)	10 (8%)	0
3	L8	155/157 (98%)	31 (20%)	2 (1%)
47	S2	1717/1869 (91%)	426 (24%)	8 (0%)
82	CC	74/75 (98%)	22 (29%)	3 (4%)
All	All	5770/7292 (79%)	1451 (25%)	32 (0%)

All (1451) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	2	G
1	L5	17	A
1	L5	25	A
1	L5	26	C
1	L5	30	C

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Mol	Chain	Res	Type
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	152	U
1	L5	159	C
1	L5	164	G
1	L5	165	A
1	L5	166	C
1	L5	181	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	218	A
1	L5	219	G

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Mol	Chain	Res	Type
1	L5	233	U
1	L5	234	G
1	L5	250	C
1	L5	255	C
1	L5	256	G
1	L5	258	G
1	L5	261	G
1	L5	263	G
1	L5	265	C
1	L5	266	C
1	L5	267	G
1	L5	269	G
1	L5	275	C
1	L5	276	C
1	L5	280	G
1	L5	297	U
1	L5	306	A
1	L5	315	G
1	L5	316	U
1	L5	340	C
1	L5	350	C
1	L5	353	A
1	L5	373	G
1	L5	387	G
1	L5	388	A
1	L5	399	G
1	L5	401	G
1	L5	407	A
1	L5	408	A
1	L5	409	G
1	L5	410	A
1	L5	411	G
1	L5	412	G
1	L5	413	G
1	L5	418	A
1	L5	431	G
1	L5	432	U
1	L5	438	G
1	L5	440	U
1	L5	449	C
1	L5	450	G
1	L5	452	A

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Mol	Chain	Res	Type
1	L5	453	G
1	L5	454	U
1	L5	456	C
1	L5	457	G
1	L5	464	G
1	L5	465	G
1	L5	467	U
1	L5	468	U
1	L5	472	C
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	495	C
1	L5	497	G
1	L5	498	C
1	L5	499	G
1	L5	500	G
1	L5	501	C
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	518	G
1	L5	643	C
1	L5	645	G
1	L5	646	G
1	L5	656	C
1	L5	657	C
1	L5	658	C
1	L5	659	G
1	L5	665	C
1	L5	666	G
1	L5	667	A

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Mol	Chain	Res	Type
1	L5	668	C
1	L5	669	C
1	L5	672	C
1	L5	673	C
1	L5	674	G
1	L5	685	C
1	L5	686	A
1	L5	687	U
1	L5	688	U
1	L5	696	C
1	L5	697	G
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	744	G
1	L5	750	U
1	L5	753	C
1	L5	758	G
1	L5	759	G
1	L5	760	G
1	L5	904	C
1	L5	907	C
1	L5	910	G
1	L5	912	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	937	U

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Mol	Chain	Res	Type
1	L5	941	C
1	L5	943	A
1	L5	944	A
1	L5	945	U
1	L5	946	C
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	969	C
1	L5	970	G
1	L5	971	U
1	L5	982	U
1	L5	984	C
1	L5	985	C
1	L5	986	C
1	L5	988	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	1066	G
1	L5	1070	G
1	L5	1071	C
1	L5	1074	G
1	L5	1075	G
1	L5	1082	C
1	L5	1083	U
1	L5	1095	A
1	L5	1168	G
1	L5	1170	G
1	L5	1171	G
1	L5	1172	C

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Mol	Chain	Res	Type
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
1	L5	1184	A
1	L5	1193	C
1	L5	1202	C
1	L5	1203	G
1	L5	1204	C
1	L5	1206	C
1	L5	1210	C
1	L5	1211	G
1	L5	1214	C
1	L5	1215	C
1	L5	1216	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	1243	C
1	L5	1246	G
1	L5	1247	U
1	L5	1253	G
1	L5	1254	A
1	L5	1255	A
1	L5	1257	A
1	L5	1258	G
1	L5	1259	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

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Mol	Chain	Res	Type
1	L5	1273	G
1	L5	1274	A
1	L5	1275	G
1	L5	1277	G
1	L5	1280	C
1	L5	1284	G
1	L5	1285	U
1	L5	1287	G
1	L5	1294	A
1	L5	1295	C
1	L5	1296	G
1	L5	1301	C
1	L5	1302	U
1	L5	1312	A
1	L5	1313	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	1368	A
1	L5	1379	C
1	L5	1381	U
1	L5	1387	A
1	L5	1393	G
1	L5	1394	G
1	L5	1397	A
1	L5	1399	G
1	L5	1404	G
1	L5	1405	C
1	L5	1407	C
1	L5	1409	C
1	L5	1410	U
1	L5	1411	C
1	L5	1412	G
1	L5	1414	C
1	L5	1415	G
1	L5	1417	C
1	L5	1420	A

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Mol	Chain	Res	Type
1	L5	1435	G
1	L5	1437	C
1	L5	1439	C
1	L5	1440	U
1	L5	1441	C
1	L5	1442	C
1	L5	1445	U
1	L5	1446	C
1	L5	1447	C
1	L5	1457	G
1	L5	1482	G
1	L5	1483	C
1	L5	1497	A
1	L5	1498	G
1	L5	1502	G
1	L5	1515	A
1	L5	1517	G
1	L5	1518	A
1	L5	1534	A
1	L5	1547	A
1	L5	1562	G
1	L5	1566	C
1	L5	1578	U
1	L5	1591	U
1	L5	1596	U
1	L5	1597	G
1	L5	1621	A
1	L5	1624	G
1	L5	1625	G
1	L5	1631	A
1	L5	1632	A
1	L5	1633	G
1	L5	1634	A
1	L5	1638	A
1	L5	1640	C
1	L5	1641	G
1	L5	1642	A
1	L5	1654	G
1	L5	1660	U
1	L5	1661	C
1	L5	1663	C
1	L5	1670	G

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Mol	Chain	Res	Type
1	L5	1676	C
1	L5	1677	U
1	L5	1678	C
1	L5	1681	G
1	L5	1691	G
1	L5	1697	G
1	L5	1699	A
1	L5	1700	G
1	L5	1703	C
1	L5	1704	C
1	L5	1705	G
1	L5	1707	C
1	L5	1715	C
1	L5	1719	A
1	L5	1731	C
1	L5	1734	G
1	L5	1741	G
1	L5	1742	A
1	L5	1750	G
1	L5	1753	G
1	L5	1755	C
1	L5	1757	U
1	L5	1758	G
1	L5	1759	G
1	L5	1760	G
1	L5	1762	C
1	L5	1763	C
1	L5	1764	G
1	L5	1765	A
1	L5	1766	A
1	L5	1767	A
1	L5	1768	C
1	L5	1770	A
1	L5	1772	C
1	L5	1775	A
1	L5	1776	A
1	L5	1787	A
1	L5	1797	G
1	L5	1804	A
1	L5	1806	G
1	L5	1810	G
1	L5	1820	C

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Mol	Chain	Res	Type
1	L5	1821	G
1	L5	1822	U
1	L5	1833	G
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	1889	U
1	L5	1892	A
1	L5	1897	A
1	L5	1898	C
1	L5	1918	U
1	L5	1919	G
1	L5	1920	C
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G
1	L5	1931	C
1	L5	1932	A
1	L5	1935	C
1	L5	1936	C
1	L5	1940	G
1	L5	1948	G
1	L5	1949	U
1	L5	1959	U
1	L5	1960	A
1	L5	1961	G
1	L5	1962	A
1	L5	1966	C
1	L5	1968	G
1	L5	1970	A
1	L5	1971	C
1	L5	1972	G
1	L5	1974	U
1	L5	1975	G
1	L5	1976	G
1	L5	1977	C
1	L5	1978	C

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Mol	Chain	Res	Type
1	L5	1979	A
1	L5	1980	U
1	L5	1981	G
1	L5	1982	G
1	L5	1983	A
1	L5	1985	G
1	L5	1987	C
1	L5	1988	G
1	L5	1990	A
1	L5	1991	A
1	L5	1992	U
1	L5	1993	C
1	L5	1994	C
1	L5	1995	G
1	L5	1996	C
1	L5	1997	U
1	L5	1998	A
1	L5	1999	A
1	L5	2001	G
1	L5	2002	A
1	L5	2003	G
1	L5	2005	G
1	L5	2006	U
1	L5	2007	G
1	L5	2009	A
1	L5	2010	A
1	L5	2011	C
1	L5	2012	A
1	L5	2013	A
1	L5	2014	C
1	L5	2015	U
1	L5	2018	C
1	L5	2019	C
1	L5	2020	U
1	L5	2021	G
1	L5	2024	G
1	L5	2025	A
1	L5	2026	A
1	L5	2034	G
1	L5	2044	U
1	L5	2046	G
1	L5	2048	U

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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	2092	G
1	L5	2093	A
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	2107	C
1	L5	2108	G
1	L5	2110	C
1	L5	2111	G
1	L5	2112	G
1	L5	2250	C
1	L5	2252	G
1	L5	2253	A
1	L5	2256	C
1	L5	2258	C
1	L5	2259	G
1	L5	2260	C
1	L5	2263	A
1	L5	2270	G
1	L5	2289	C
1	L5	2300	A
1	L5	2301	G
1	L5	2306	G
1	L5	2313	A
1	L5	2316	G
1	L5	2332	A
1	L5	2333	G
1	L5	2348	G
1	L5	2350	U
1	L5	2351	C
1	L5	2360	A
1	L5	2364	G

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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	2437	C
1	L5	2441	C
1	L5	2450	G
1	L5	2464	C
1	L5	2465	C
1	L5	2467	U
1	L5	2474	G
1	L5	2475	G
1	L5	2477	A
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	2495	U
1	L5	2503	G
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G
1	L5	2513	A
1	L5	2519	U
1	L5	2537	A
1	L5	2544	G
1	L5	2546	G
1	L5	2547	G
1	L5	2554	U
1	L5	2555	G
1	L5	2556	G

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Mol	Chain	Res	Type
1	L5	2559	G
1	L5	2560	C
1	L5	2561	C
1	L5	2583	C
1	L5	2586	G
1	L5	2587	A
1	L5	2589	C
1	L5	2601	A
1	L5	2638	G
1	L5	2653	C
1	L5	2661	U
1	L5	2662	G
1	L5	2669	C
1	L5	2675	G
1	L5	2676	A
1	L5	2687	U
1	L5	2695	A
1	L5	2696	A
1	L5	2703	G
1	L5	2707	U
1	L5	2708	U
1	L5	2709	C
1	L5	2710	C
1	L5	2711	G
1	L5	2713	C
1	L5	2721	G
1	L5	2724	G
1	L5	2725	A
1	L5	2726	G
1	L5	2738	C
1	L5	2739	C
1	L5	2742	G
1	L5	2743	A
1	L5	2746	A
1	L5	2756	G
1	L5	2761	U
1	L5	2763	U
1	L5	2764	A
1	L5	2769	U
1	L5	2770	C
1	L5	2787	A
1	L5	2788	U

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Mol	Chain	Res	Type
1	L5	2790	U
1	L5	2794	C
1	L5	2795	A
1	L5	2825	A
1	L5	2826	U
1	L5	2827	G
1	L5	2835	A
1	L5	2838	G
1	L5	2842	G
1	L5	2848	G
1	L5	2855	G
1	L5	2877	G
1	L5	2892	C
1	L5	2895	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	2908	U
1	L5	2909	C
1	L5	3585	G
1	L5	3588	C
1	L5	3590	G
1	L5	3591	C
1	L5	3592	G
1	L5	3594	C
1	L5	3595	U
1	L5	3596	A
1	L5	3597	G
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
1	L5	3662	A

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Mol	Chain	Res	Type
1	L5	3664	G
1	L5	3670	C
1	L5	3672	G
1	L5	3673	C
1	L5	3674	G
1	L5	3685	C
1	L5	3711	A
1	L5	3713	U
1	L5	3714	G
1	L5	3727	A
1	L5	3729	U
1	L5	3735	G
1	L5	3748	A
1	L5	3750	G
1	L5	3753	G
1	L5	3754	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	3802	U
1	L5	3811	G
1	L5	3812	C
1	L5	3814	U
1	L5	3817	A
1	L5	3818	U
1	L5	3819	G
1	L5	3838	U
1	L5	3839	G
1	L5	3840	U
1	L5	3851	U
1	L5	3867	A
1	L5	3876	A
1	L5	3877	A

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Mol	Chain	Res	Type
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	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	3944	G
1	L5	3947	A
1	L5	3950	U
1	L5	3955	G
1	L5	3956	G
1	L5	3957	U
1	L5	3958	G
1	L5	3959	U
1	L5	3960	A
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	3968	U
1	L5	3969	G
1	L5	3970	G
1	L5	3971	G
1	L5	3972	A
1	L5	3973	G
1	L5	3974	G
1	L5	3975	C
1	L5	3977	C
1	L5	4034	G

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Mol	Chain	Res	Type
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	4044	U
1	L5	4045	G
1	L5	4046	A
1	L5	4048	A
1	L5	4049	U
1	L5	4051	C
1	L5	4052	C
1	L5	4053	A
1	L5	4054	C
1	L5	4055	U
1	L5	4056	A
1	L5	4057	C
1	L5	4058	U
1	L5	4059	C
1	L5	4062	A
1	L5	4063	U
1	L5	4064	C
1	L5	4065	G
1	L5	4076	G
1	L5	4084	G
1	L5	4086	G
1	L5	4096	C
1	L5	4097	G
1	L5	4098	A
1	L5	4099	G
1	L5	4101	C
1	L5	4102	C
1	L5	4103	C
1	L5	4104	G
1	L5	4106	G
1	L5	4107	G
1	L5	4108	G
1	L5	4109	G
1	L5	4111	U
1	L5	4112	C
1	L5	4114	C

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Mol	Chain	Res	Type
1	L5	4115	G
1	L5	4116	C
1	L5	4117	U
1	L5	4119	C
1	L5	4122	G
1	L5	4127	A
1	L5	4140	C
1	L5	4141	G
1	L5	4142	C
1	L5	4143	G
1	L5	4144	C
1	L5	4146	G
1	L5	4150	G
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	4191	G
1	L5	4196	G
1	L5	4197	G
1	L5	4203	A
1	L5	4212	A
1	L5	4222	G
1	L5	4228	G
1	L5	4229	U
1	L5	4233	A
1	L5	4251	A
1	L5	4254	G
1	L5	4255	A
1	L5	4256	A
1	L5	4257	A
1	L5	4265	U
1	L5	4268	A
1	L5	4273	A
1	L5	4281	A
1	L5	4291	G
1	L5	4295	U
1	L5	4304	A
1	L5	4305	G
1	L5	4314	C

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Mol	Chain	Res	Type
1	L5	4319	C
1	L5	4329	G
1	L5	4330	G
1	L5	4332	C
1	L5	4339	A
1	L5	4349	C
1	L5	4354	U
1	L5	4371	G
1	L5	4373	G
1	L5	4377	G
1	L5	4378	A
1	L5	4379	A
1	L5	4380	A
1	L5	4381	A
1	L5	4386	C
1	L5	4387	C
1	L5	4391	G
1	L5	4394	A
1	L5	4405	G
1	L5	4422	A
1	L5	4424	A
1	L5	4448	G
1	L5	4449	A
1	L5	4450	U
1	L5	4452	U
1	L5	4453	C
1	L5	4464	A
1	L5	4466	C
1	L5	4471	U
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	4529	G
1	L5	4531	U
1	L5	4545	G
1	L5	4548	A
1	L5	4549	G

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Mol	Chain	Res	Type
1	L5	4556	U
1	L5	4557	U
1	L5	4560	C
1	L5	4567	G
1	L5	4573	G
1	L5	4575	G
1	L5	4589	A
1	L5	4590	A
1	L5	4600	G
1	L5	4601	U
1	L5	4617	G
1	L5	4626	A
1	L5	4627	U
1	L5	4635	A
1	L5	4636	U
1	L5	4637	G
1	L5	4652	G
1	L5	4656	A
1	L5	4659	G
1	L5	4670	C
1	L5	4672	A
1	L5	4679	G
1	L5	4682	U
1	L5	4684	A
1	L5	4687	A
1	L5	4691	A
1	L5	4694	G
1	L5	4695	C
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4719	G
1	L5	4720	C
1	L5	4731	G
1	L5	4733	C
1	L5	4734	A
1	L5	4735	G
1	L5	4740	G
1	L5	4741	C
1	L5	4742	G
1	L5	4745	G
1	L5	4747	C

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Mol	Chain	Res	Type
1	L5	4750	G
1	L5	4754	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G
1	L5	4765	G
1	L5	4770	U
1	L5	4771	C
1	L5	4772	C
1	L5	4775	C
1	L5	4776	G
1	L5	4859	C
1	L5	4860	G
1	L5	4863	G
1	L5	4870	G
1	L5	4871	C
1	L5	4875	G
1	L5	4877	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	4900	C
1	L5	4901	G
1	L5	4902	C
1	L5	4910	G
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	4931	G
1	L5	4934	A
1	L5	4937	C
1	L5	4940	C

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Mol	Chain	Res	Type
1	L5	4941	G
1	L5	4943	A
1	L5	4947	U
1	L5	4951	G
1	L5	4953	G
1	L5	4960	G
1	L5	4961	G
1	L5	4966	A
1	L5	4976	U
1	L5	4979	A
1	L5	4988	U
1	L5	4989	U
1	L5	4990	C
1	L5	4991	U
1	L5	5013	C
1	L5	5014	A
1	L5	5017	G
1	L5	5020	G
1	L5	5022	U
1	L5	5024	C
1	L5	5025	C
1	L5	5026	U
1	L5	5028	G
1	L5	5029	C
1	L5	5031	G
1	L5	5034	A
1	L5	5041	G
1	L5	5047	C
1	L5	5050	C
1	L5	5054	C
1	L5	5055	G
1	L5	5061	A
1	L5	5069	U
2	L7	5	A
2	L7	7	G
2	L7	24	C
2	L7	38	U
2	L7	53	U
2	L7	54	A
2	L7	63	C
2	L7	64	G
2	L7	100	A

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Mol	Chain	Res	Type
2	L7	111	C
3	L8	2	G
3	L8	25	G
3	L8	34	U
3	L8	35	C
3	L8	48	A
3	L8	59	A
3	L8	60	G
3	L8	61	A
3	L8	62	A
3	L8	63	U
3	L8	68	G
3	L8	82	A
3	L8	83	C
3	L8	84	A
3	L8	85	U
3	L8	86	U
3	L8	87	G
3	L8	94	G
3	L8	103	A
3	L8	105	C
3	L8	110	U
3	L8	111	U
3	L8	114	G
3	L8	123	U
3	L8	124	U
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	150	C
3	L8	151	G
3	L8	156	U
47	S2	2	A
47	S2	13	C
47	S2	14	C
47	S2	25	A
47	S2	33	G
47	S2	39	A
47	S2	41	G
47	S2	46	A
47	S2	49	C
47	S2	56	G

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Mol	Chain	Res	Type
47	S2	58	C
47	S2	59	U
47	S2	62	G
47	S2	64	A
47	S2	67	C
47	S2	68	A
47	S2	72	C
47	S2	73	C
47	S2	74	G
47	S2	76	U
47	S2	92	A
47	S2	103	A
47	S2	113	G
47	S2	115	U
47	S2	116	U
47	S2	126	G
47	S2	130	G
47	S2	139	C
47	S2	142	C
47	S2	143	U
47	S2	149	A
47	S2	154	U
47	S2	158	A
47	S2	159	A
47	S2	160	U
47	S2	161	U
47	S2	162	C
47	S2	163	U
47	S2	168	C
47	S2	175	A
47	S2	179	C
47	S2	182	C
47	S2	184	G
47	S2	190	G
47	S2	196	C
47	S2	197	U
47	S2	198	U
47	S2	199	C
47	S2	200	G
47	S2	203	G
47	S2	204	G
47	S2	206	G

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Mol	Chain	Res	Type
47	S2	208	G
47	S2	209	A
47	S2	211	G
47	S2	212	C
47	S2	214	U
47	S2	290	U
47	S2	291	G
47	S2	292	A
47	S2	293	C
47	S2	295	C
47	S2	302	A
47	S2	306	C
47	S2	307	G
47	S2	308	G
47	S2	309	G
47	S2	311	C
47	S2	313	A
47	S2	316	G
47	S2	318	A
47	S2	319	C
47	S2	323	C
47	S2	324	C
47	S2	325	C
47	S2	326	C
47	S2	328	U
47	S2	329	G
47	S2	332	G
47	S2	338	G
47	S2	339	A
47	S2	347	G
47	S2	360	A
47	S2	362	C
47	S2	364	A
47	S2	368	U
47	S2	370	G
47	S2	381	C
47	S2	385	G
47	S2	386	C
47	S2	407	G
47	S2	408	A
47	S2	409	C
47	S2	417	C

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Mol	Chain	Res	Type
47	S2	418	A
47	S2	421	G
47	S2	448	A
47	S2	449	A
47	S2	450	C
47	S2	452	G
47	S2	464	A
47	S2	465	A
47	S2	466	G
47	S2	467	G
47	S2	471	G
47	S2	472	C
47	S2	473	A
47	S2	474	G
47	S2	482	G
47	S2	487	U
47	S2	488	U
47	S2	492	C
47	S2	493	A
47	S2	502	C
47	S2	525	A
47	S2	531	A
47	S2	532	C
47	S2	533	A
47	S2	534	G
47	S2	536	A
47	S2	537	C
47	S2	540	U
47	S2	542	U
47	S2	546	G
47	S2	547	G
47	S2	551	U
47	S2	556	U
47	S2	557	U
47	S2	558	G
47	S2	559	G
47	S2	560	A
47	S2	563	G
47	S2	564	A
47	S2	566	U
47	S2	576	A
47	S2	583	A

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Mol	Chain	Res	Type
47	S2	587	A
47	S2	589	G
47	S2	591	U
47	S2	594	A
47	S2	596	U
47	S2	597	G
47	S2	607	U
47	S2	608	C
47	S2	614	C
47	S2	617	G
47	S2	623	G
47	S2	627	U
47	S2	628	A
47	S2	643	A
47	S2	644	G
47	S2	655	A
47	S2	659	G
47	S2	660	C
47	S2	662	G
47	S2	663	C
47	S2	664	A
47	S2	668	A
47	S2	671	A
47	S2	672	A
47	S2	673	G
47	S2	683	G
47	S2	687	C
47	S2	688	U
47	S2	689	U
47	S2	690	G
47	S2	692	G
47	S2	693	A
47	S2	695	C
47	S2	696	G
47	S2	697	G
47	S2	698	G
47	S2	732	U
47	S2	733	C
47	S2	734	C
47	S2	736	C
47	S2	738	C
47	S2	749	U

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Mol	Chain	Res	Type
47	S2	751	G
47	S2	752	G
47	S2	753	C
47	S2	787	G
47	S2	788	G
47	S2	791	C
47	S2	792	C
47	S2	798	G
47	S2	810	A
47	S2	811	A
47	S2	821	G
47	S2	822	U
47	S2	823	U
47	S2	824	C
47	S2	830	A
47	S2	834	C
47	S2	835	C
47	S2	836	G
47	S2	837	A
47	S2	838	G
47	S2	839	C
47	S2	840	C
47	S2	841	G
47	S2	842	C
47	S2	847	A
47	S2	869	A
47	S2	870	A
47	S2	872	A
47	S2	873	G
47	S2	874	G
47	S2	879	C
47	S2	880	G
47	S2	882	U
47	S2	883	U
47	S2	887	U
47	S2	888	U
47	S2	889	U
47	S2	891	G
47	S2	892	U
47	S2	896	U
47	S2	897	U
47	S2	898	U

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Mol	Chain	Res	Type
47	S2	899	U
47	S2	900	C
47	S2	901	G
47	S2	903	A
47	S2	904	A
47	S2	913	A
47	S2	914	U
47	S2	919	A
47	S2	920	A
47	S2	930	C
47	S2	933	G
47	S2	934	G
47	S2	943	U
47	S2	950	C
47	S2	963	A
47	S2	969	U
47	S2	971	G
47	S2	972	A
47	S2	990	A
47	S2	992	A
47	S2	999	G
47	S2	1001	A
47	S2	1017	U
47	S2	1023	A
47	S2	1027	A
47	S2	1028	A
47	S2	1033	G
47	S2	1034	A
47	S2	1061	U
47	S2	1062	A
47	S2	1083	A
47	S2	1085	C
47	S2	1088	U
47	S2	1109	C
47	S2	1114	U
47	S2	1115	U
47	S2	1116	C
47	S2	1118	C
47	S2	1119	A
47	S2	1121	G
47	S2	1133	A
47	S2	1138	C

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Mol	Chain	Res	Type
47	S2	1153	C
47	S2	1154	U
47	S2	1195	A
47	S2	1207	G
47	S2	1208	A
47	S2	1215	C
47	S2	1216	C
47	S2	1217	A
47	S2	1224	G
47	S2	1227	G
47	S2	1239	U
47	S2	1242	U
47	S2	1243	U
47	S2	1251	A
47	S2	1253	A
47	S2	1256	G
47	S2	1257	G
47	S2	1259	A
47	S2	1265	A
47	S2	1273	C
47	S2	1274	G
47	S2	1275	G
47	S2	1281	G
47	S2	1282	A
47	S2	1283	C
47	S2	1284	A
47	S2	1286	G
47	S2	1293	A
47	S2	1294	G
47	S2	1295	A
47	S2	1301	A
47	S2	1302	G
47	S2	1303	C
47	S2	1305	C
47	S2	1306	U
47	S2	1308	U
47	S2	1311	C
47	S2	1312	G
47	S2	1314	U
47	S2	1318	G
47	S2	1333	U
47	S2	1341	C

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Mol	Chain	Res	Type
47	S2	1342	U
47	S2	1343	U
47	S2	1348	G
47	S2	1371	U
47	S2	1372	U
47	S2	1378	A
47	S2	1382	A
47	S2	1401	A
47	S2	1402	A
47	S2	1412	C
47	S2	1414	A
47	S2	1415	C
47	S2	1419	C
47	S2	1420	G
47	S2	1421	A
47	S2	1422	G
47	S2	1423	C
47	S2	1424	G
47	S2	1433	C
47	S2	1434	C
47	S2	1435	C
47	S2	1436	C
47	S2	1438	A
47	S2	1449	G
47	S2	1452	A
47	S2	1454	A
47	S2	1462	U
47	S2	1463	U
47	S2	1478	U
47	S2	1480	A
47	S2	1487	A
47	S2	1489	A
47	S2	1490	G
47	S2	1495	G
47	S2	1497	G
47	S2	1498	A
47	S2	1505	U
47	S2	1507	G
47	S2	1508	A
47	S2	1509	U
47	S2	1520	G
47	S2	1521	C

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Mol	Chain	Res	Type
47	S2	1533	A
47	S2	1536	G
47	S2	1537	A
47	S2	1544	C
47	S2	1552	G
47	S2	1553	C
47	S2	1555	U
47	S2	1556	A
47	S2	1570	G
47	S2	1574	C
47	S2	1580	A
47	S2	1585	U
47	S2	1586	U
47	S2	1587	G
47	S2	1588	A
47	S2	1594	A
47	S2	1598	G
47	S2	1601	A
47	S2	1606	G
47	S2	1621	U
47	S2	1623	A
47	S2	1633	A
47	S2	1634	A
47	S2	1637	A
47	S2	1638	G
47	S2	1644	C
47	S2	1648	G
47	S2	1654	G
47	S2	1661	A
47	S2	1663	A
47	S2	1665	G
47	S2	1671	G
47	S2	1680	G
47	S2	1686	G
47	S2	1699	A
47	S2	1712	A
47	S2	1715	A
47	S2	1717	C
47	S2	1719	A
47	S2	1721	U
47	S2	1722	G
47	S2	1727	G

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Mol	Chain	Res	Type
47	S2	1743	G
47	S2	1744	G
47	S2	1745	A
47	S2	1752	C
47	S2	1753	C
47	S2	1754	G
47	S2	1757	G
47	S2	1758	G
47	S2	1759	G
47	S2	1760	G
47	S2	1761	U
47	S2	1771	G
47	S2	1772	C
47	S2	1773	C
47	S2	1774	C
47	S2	1775	U
47	S2	1776	G
47	S2	1777	G
47	S2	1783	C
47	S2	1784	G
47	S2	1786	U
47	S2	1797	U
47	S2	1821	U
47	S2	1823	A
47	S2	1824	A
47	S2	1825	A
47	S2	1826	G
47	S2	1829	G
47	S2	1831	A
47	S2	1835	A
47	S2	1838	U
47	S2	1849	G
47	S2	1852	C
47	S2	1861	G
47	S2	1862	G
47	S2	1863	A
47	S2	1864	U
47	S2	1865	C
82	CC	7	A
82	CC	11	C
82	CC	16	C
82	CC	17	G

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Mol	Chain	Res	Type
82	CC	19	C
82	CC	20	U
82	CC	28	C
82	CC	32	C
82	CC	33	U
82	CC	35	U
82	CC	36	C
82	CC	37	A
82	CC	38	C
82	CC	39	C
82	CC	43	G
82	CC	44	A
82	CC	45	G
82	CC	46	A
82	CC	47	C
82	CC	51	G
82	CC	72	G
82	CC	75	A

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	183	C
1	L5	406	C
1	L5	493	G
1	L5	504	G
1	L5	914	U
1	L5	1082	C
1	L5	1633	G
1	L5	2019	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	4045	G
1	L5	4378	A
1	L5	4699	U
1	L5	4913	G
3	L8	83	C

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Mol	Chain	Res	Type
3	L8	86	U
47	S2	112	U
47	S2	291	G
47	S2	417	C
47	S2	420	G
47	S2	563	G
47	S2	668	A
47	S2	688	U
47	S2	1434	C
82	CC	35	U
82	CC	37	A
82	CC	74	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

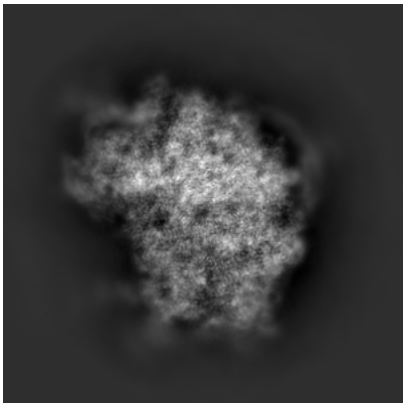
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11098. These allow visual inspection of the internal detail of the map and identification of artifacts.

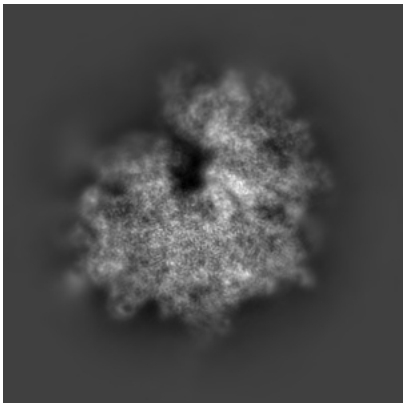
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

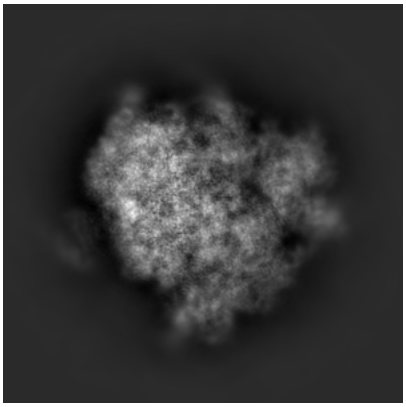
6.1.1 Primary map



X



Y

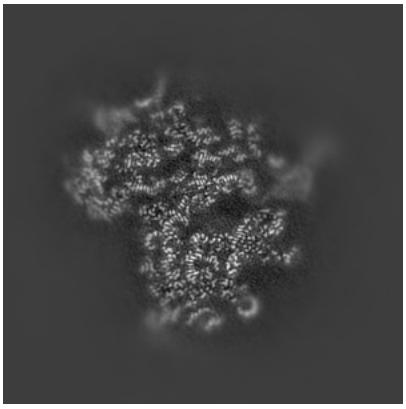


Z

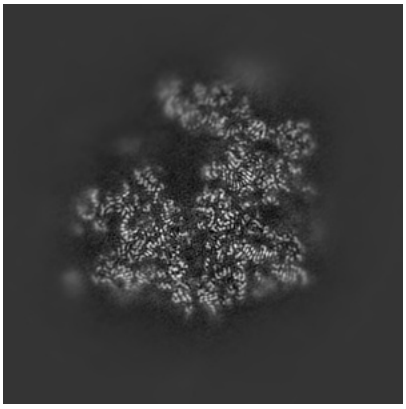
The images above show the map projected in three orthogonal directions.

6.2 Central slices

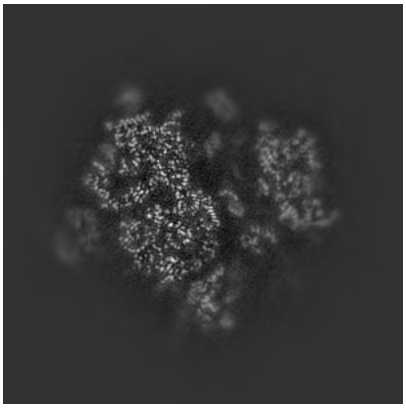
6.2.1 Primary map



X Index: 200



Y Index: 200

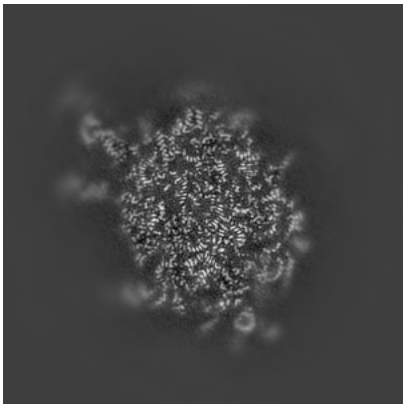


Z Index: 200

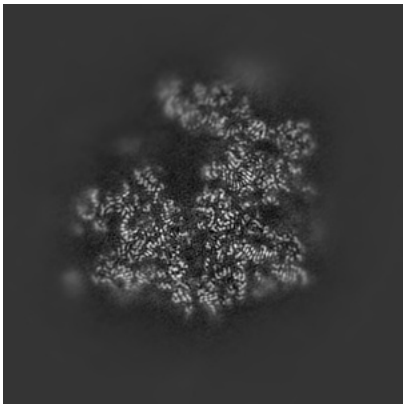
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

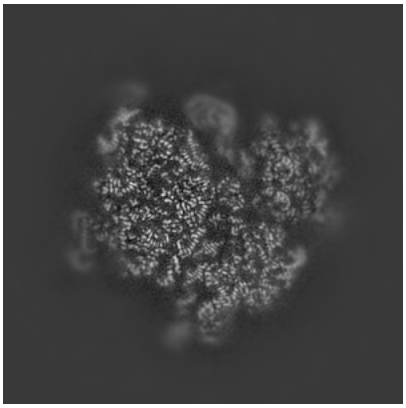
6.3.1 Primary map



X Index: 172



Y Index: 200

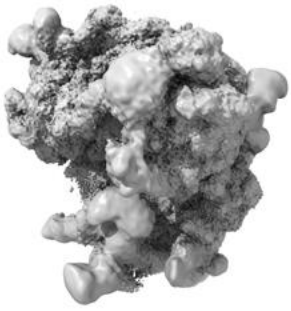


Z Index: 222

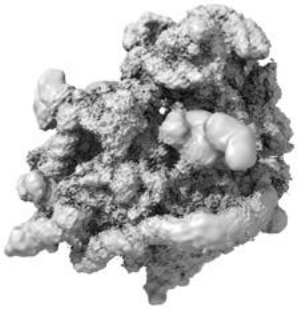
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

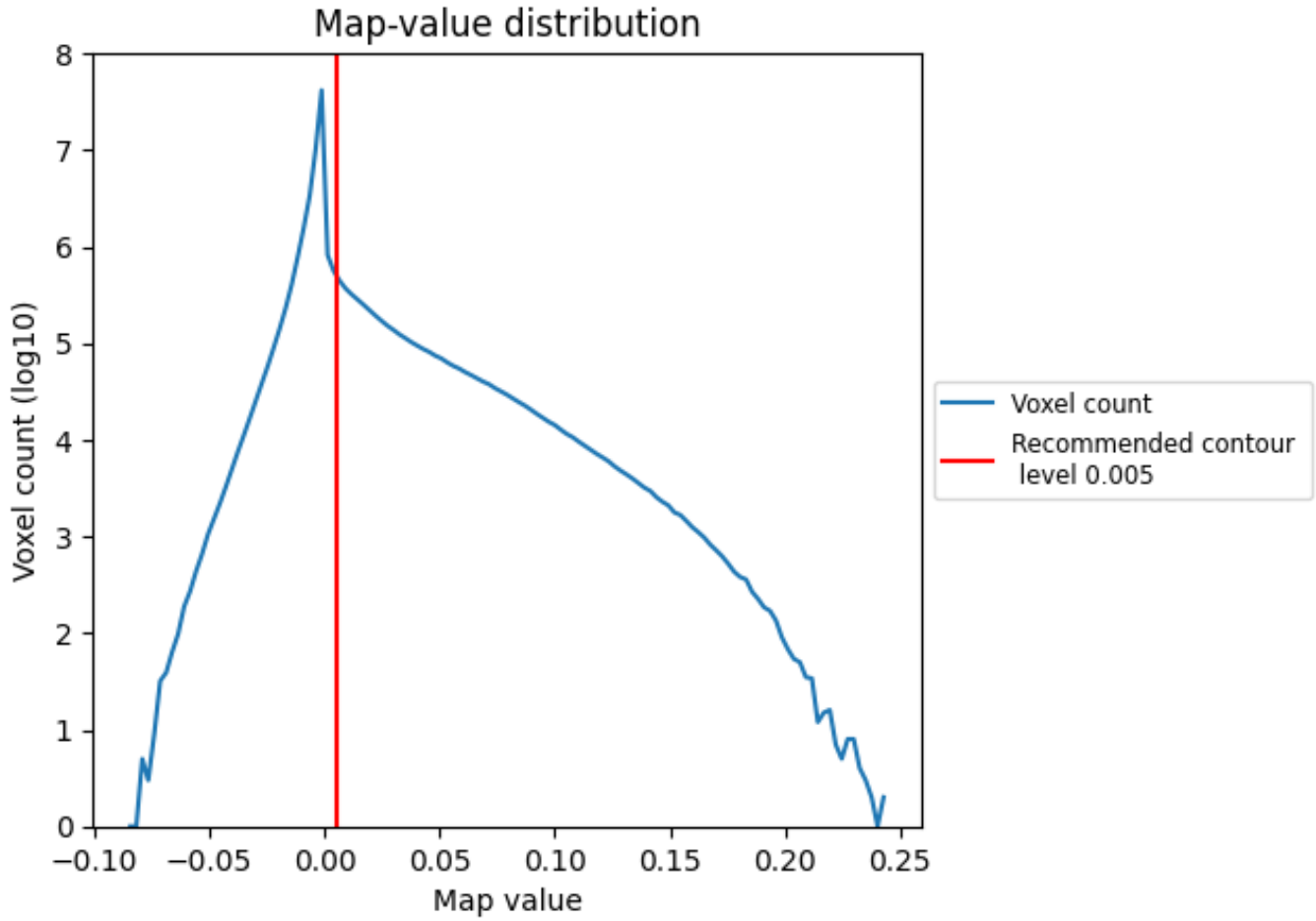
6.5 Mask visualisation (i)

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

7 Map analysis

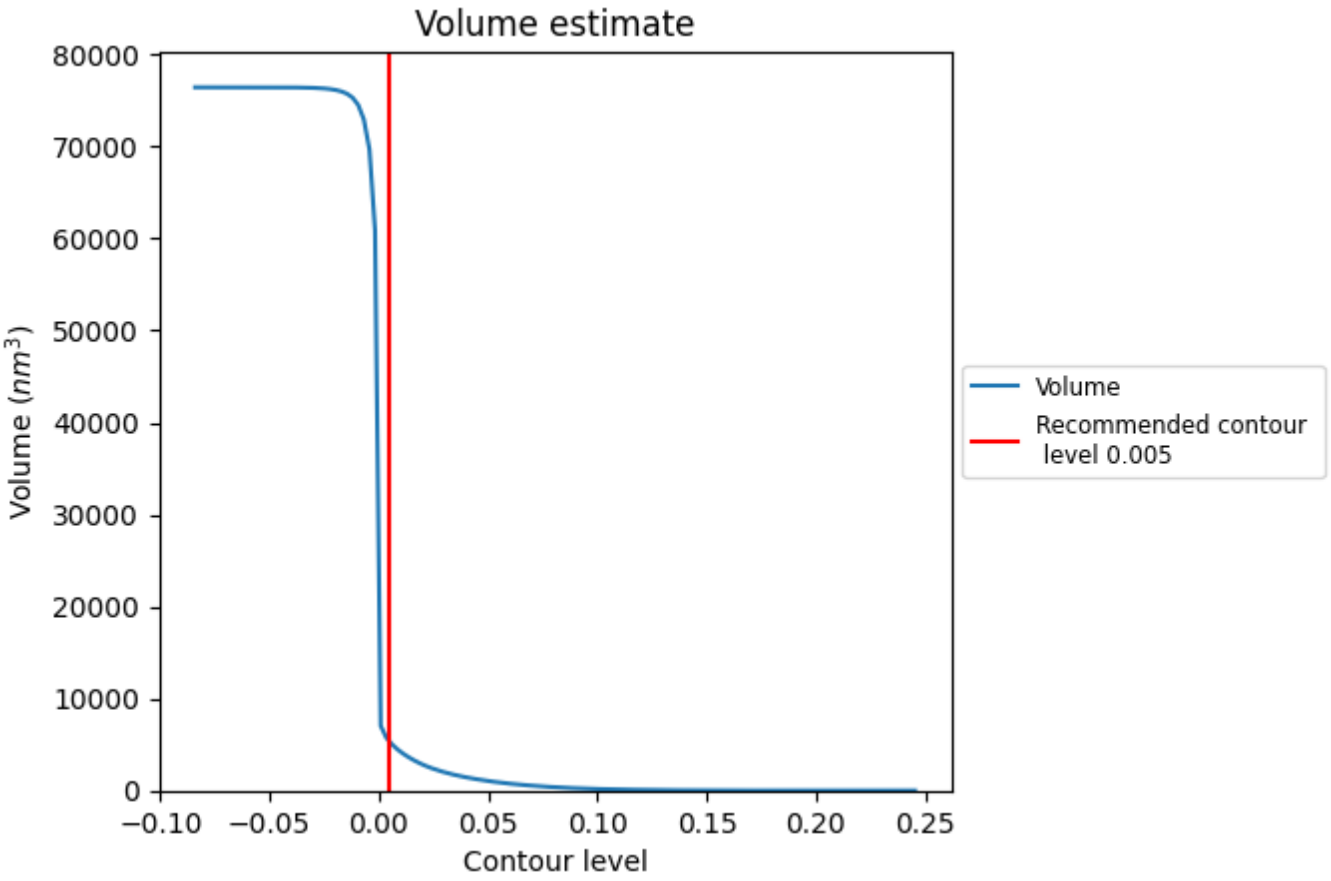
This section contains the results of statistical analysis of the map.

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.

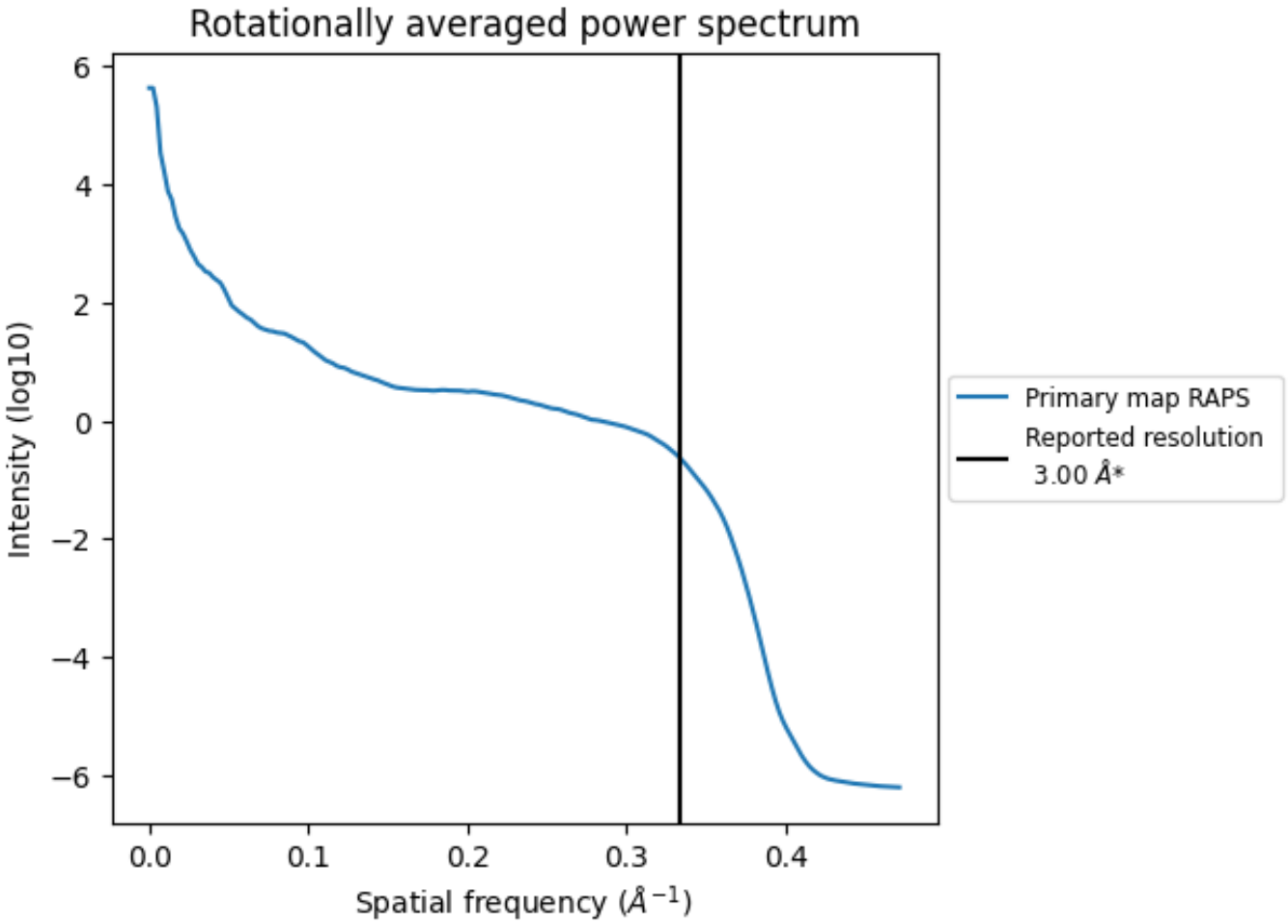
7.2 Volume estimate



The volume at the recommended contour level is 5303 nm^3; this corresponds to an approximate mass of 4790 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)

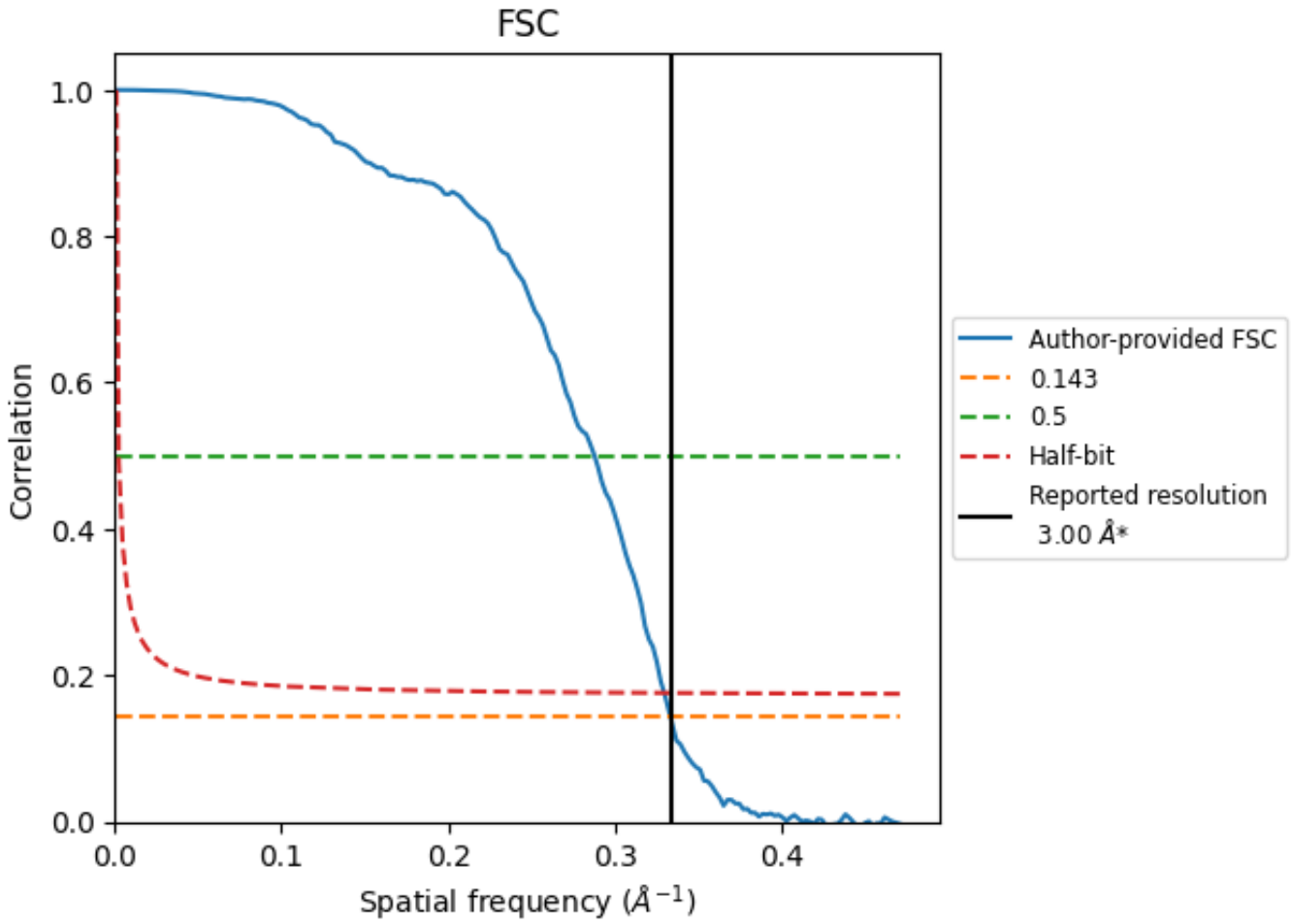


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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)

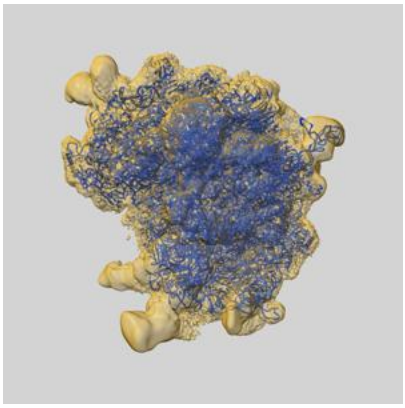
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.48	3.03
Unmasked-calculated*	-	-	-

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

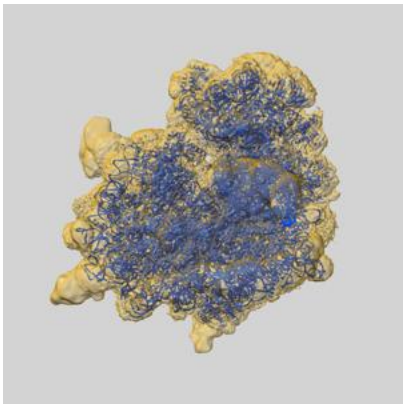
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11098 and PDB model 6Z6L. Per-residue inclusion information can be found in section 3 on page 19.

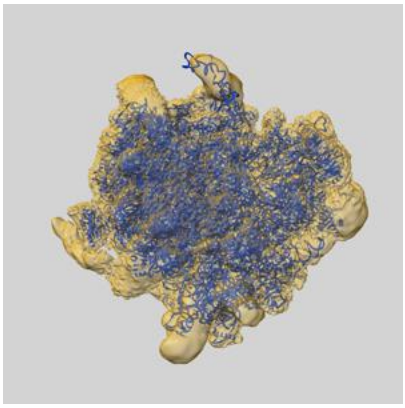
9.1 Map-model overlay



X



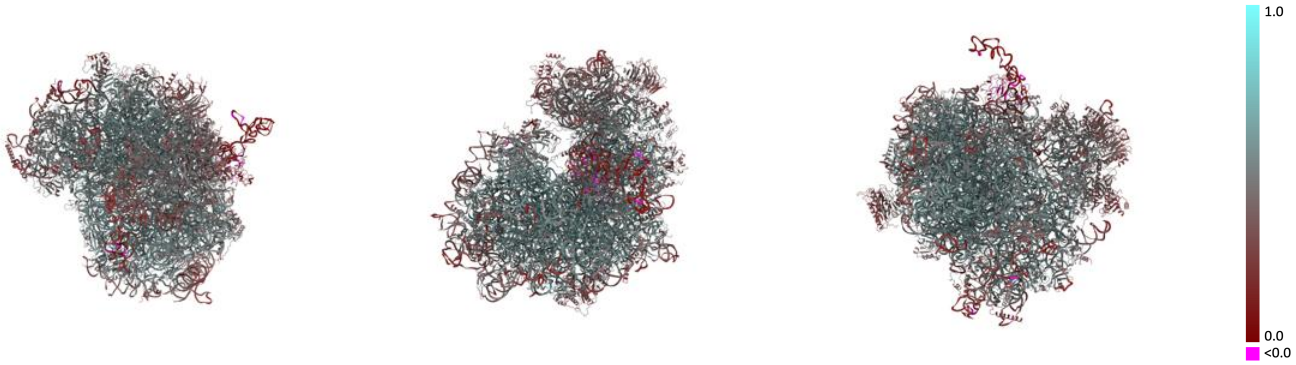
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

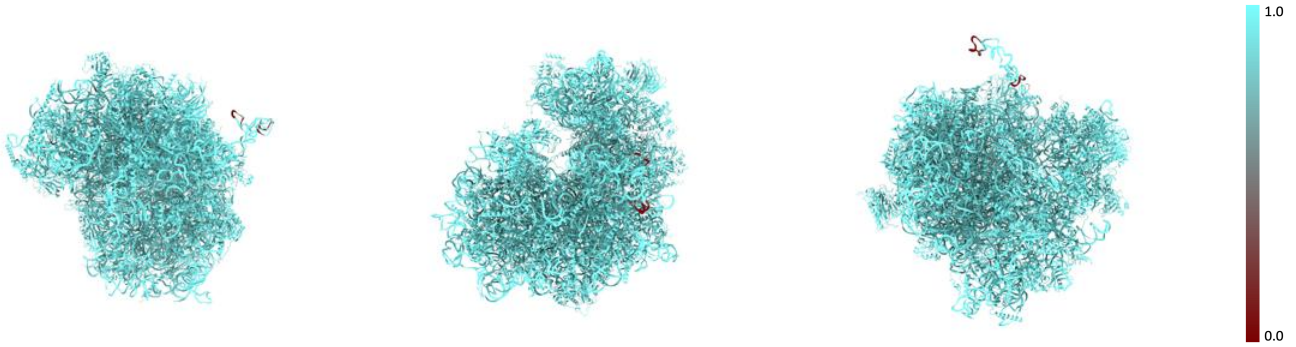
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

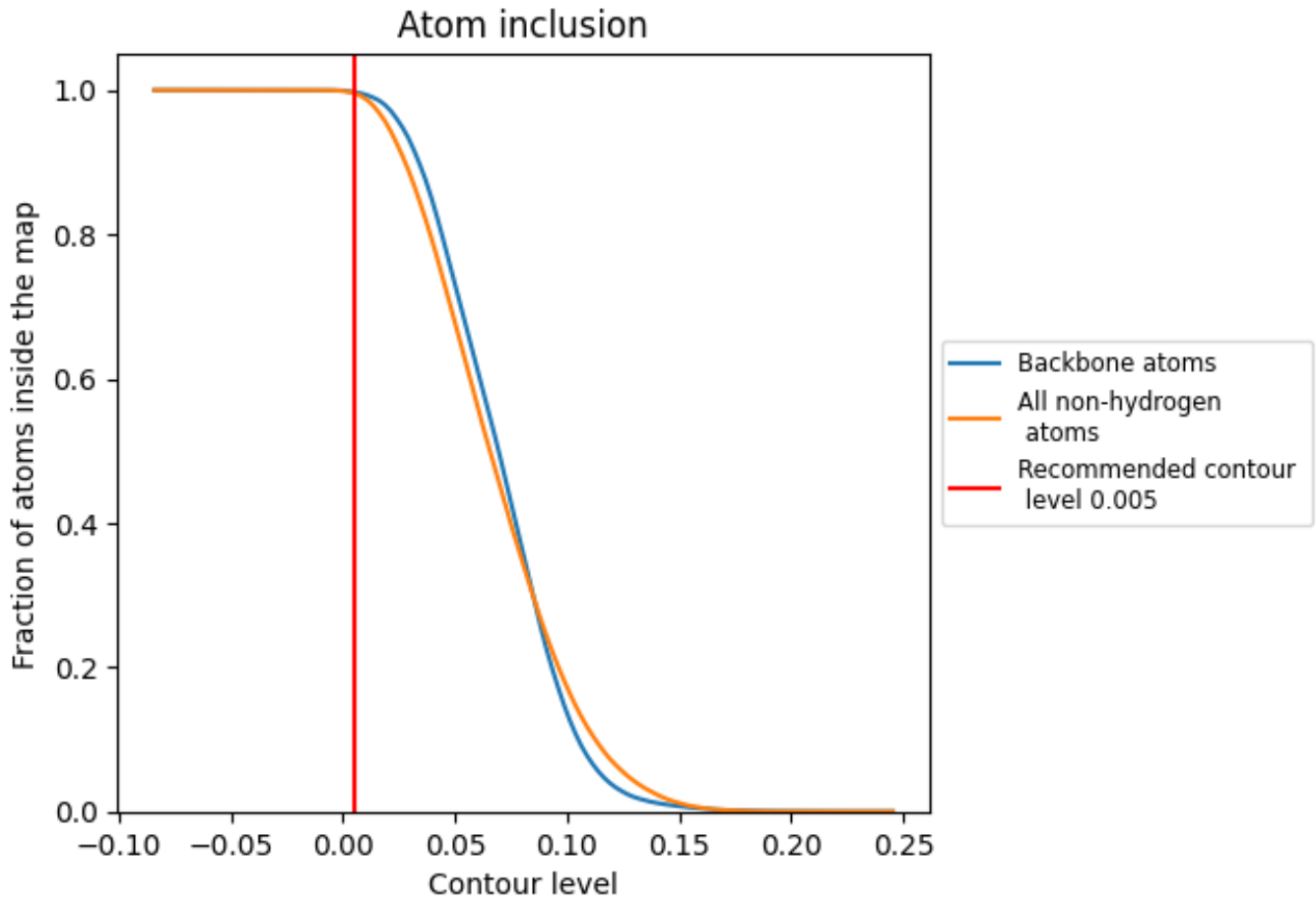
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9958	0.4990
CA	0.9806	0.3130
CC	0.9899	0.3030
CE	0.8550	0.3980
L5	0.9980	0.5190
L7	1.0000	0.5610
L8	0.9991	0.5420
LA	0.9940	0.5970
LB	0.9953	0.5600
LC	0.9958	0.5540
LD	0.9996	0.4970
LE	0.9973	0.4710
LF	0.9956	0.5580
LG	0.9941	0.4750
LH	0.9966	0.5240
LI	0.9918	0.5480
LJ	0.9890	0.4430
LL	0.9933	0.5130
LM	0.9946	0.5090
LN	0.9957	0.5940
LO	0.9925	0.5690
LP	0.9959	0.5780
LQ	0.9938	0.5800
LR	0.9980	0.5240
LS	0.9993	0.5750
LT	0.9913	0.5470
LU	0.9988	0.4450
LV	0.9916	0.5750
LW	0.9918	0.4110
LX	0.9916	0.5400
LY	0.9981	0.5300
LZ	1.0000	0.5180
La	0.9956	0.5790
Lb	0.9882	0.4870
Lc	0.9880	0.5300

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Chain	Atom inclusion	Q-score
Ld	0.9965	0.5370
Le	0.9951	0.5880
Lf	0.9905	0.5860
Lg	0.9954	0.5650
Lh	0.9908	0.5190
Li	0.9975	0.5100
Lj	0.9941	0.5850
Lk	0.9946	0.4860
Ll	0.9882	0.5700
Lm	0.9904	0.5420
Ln	0.9952	0.5990
Lo	0.9902	0.5580
Lp	0.9869	0.5760
Lr	0.9979	0.5470
Lz	0.9358	0.1350
S2	0.9998	0.4920
SA	0.9982	0.4750
SB	0.9959	0.5010
SC	0.9947	0.5190
SD	0.9954	0.4220
SE	0.9985	0.5130
SF	0.9937	0.4390
SG	0.9984	0.4140
SH	0.9946	0.4040
SI	0.9939	0.4970
SJ	0.9911	0.4820
SK	1.0000	0.3350
SL	0.9868	0.5410
SM	0.9968	0.2010
SN	0.9898	0.5370
SO	0.9716	0.5010
SP	0.9960	0.3540
SQ	0.9955	0.4320
SR	0.9953	0.4330
SS	0.9957	0.3880
ST	1.0000	0.4070
SU	0.9962	0.3900
SV	1.0000	0.4810
SW	0.9911	0.5500
SX	0.9925	0.5450
SY	0.9981	0.4420
SZ	1.0000	0.3380

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Chain	Atom inclusion	Q-score
Sa	0.9911	0.5280
Sb	1.0000	0.4920
Sc	0.9938	0.4410
Sd	0.9955	0.4590
Se	0.9595	0.4460
Sf	1.0000	0.2130
Sg	0.9996	0.3530