



Full wwPDB EM Validation Report ⓘ

May 12, 2024 – 06:29 am BST

PDB ID : 8RXX
EMDB ID : EMD-19582
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME
WITH A/P/E-site tRNA AND mRNA : LM32Cs3H1 sKO STRAIN
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2024-02-08
Resolution : 2.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

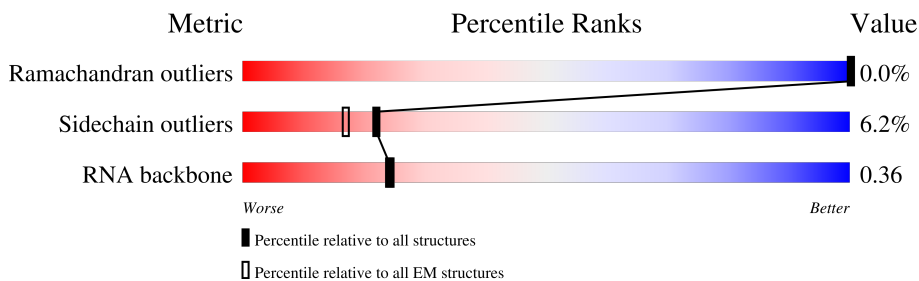
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.97 Å.

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



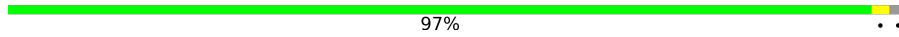
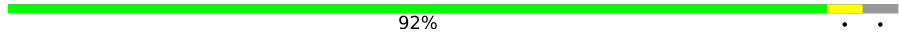
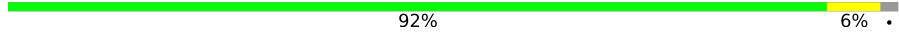




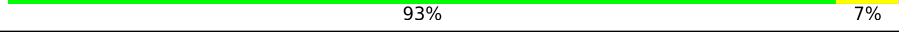
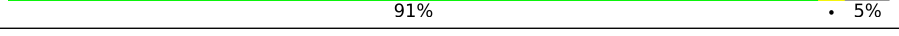
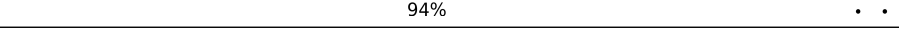
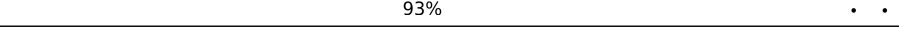
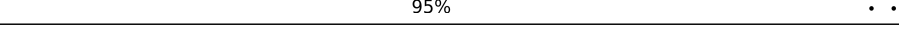
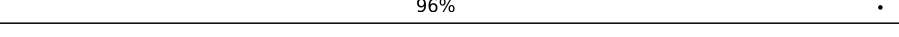
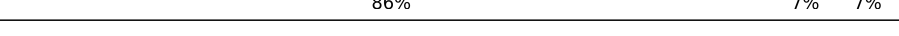
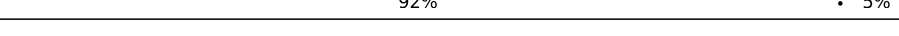
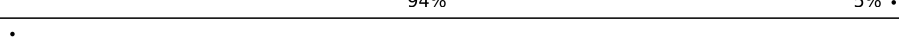
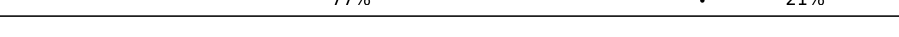
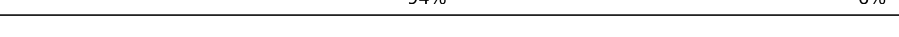
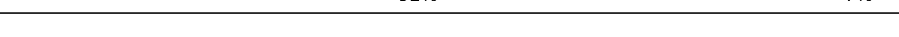






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	L1	1782	58% 33% 7%
2	L2	1526	48% 26% 25%
3	L3	216	53% 31% 15%
4	L4	184	64% 35%
5	L5	135	59% 30% 10%
6	L6	73	42% 51%
7	L7	171	59% 36%
8	L8	123	72% 24%

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Mol	Chain	Length	Quality of chain
9	LA	260	 97%
10	LB	419	 92%
11	LC	373	 92% 6%
12	LD	188	 86% 7% 7%
13	LE	190	 91% 7%
14	LF	195	 71% 5% 24%
15	LG	264	 87% 9%
16	LH	222	 93% 7%
17	LI	220	 91% 5%
18	LJ	139	 94%
19	LK	175	 93%
20	LL	145	 95%
21	LM	204	 96%
22	LN	213	 86% 7% 7%
23	LO	305	 92% 5%
24	LP	198	 94% 5%
25	LQ	254	 77% 21%
26	LR	179	 94% 6%
27	LS	159	 92% 7%
28	LT	166	 88% 8%
29	LU	129	 88% 6% 5%
30	LV	145	 80% 18%
31	LW	143	 80% 5% 15%
32	LX	124	 68% 31%
33	LY	134	 95%

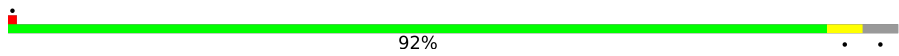
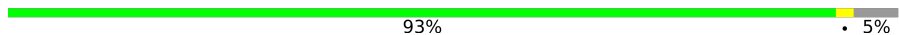
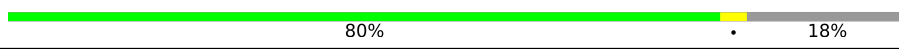

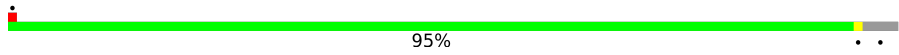

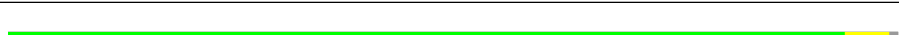
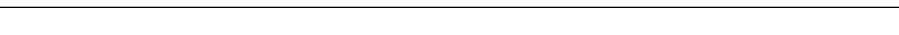
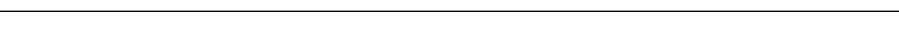
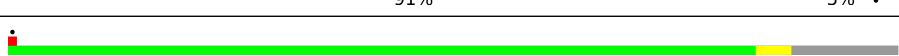


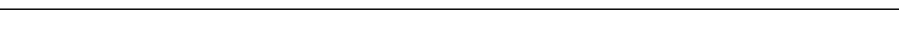
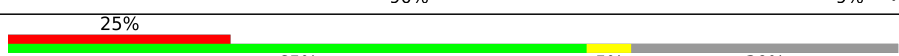
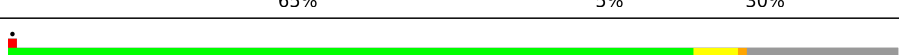

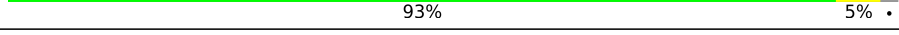






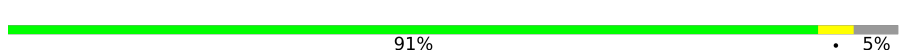

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Mol	Chain	Length	Quality of chain
34	LZ	147	92% 7%
35	La	127	94%
36	Lb	70	90% 7%
37	Lc	252	89% 9%
38	Ld	104	87% 7% 7%
39	Le	188	94% 5%
40	Lf	133	93%
41	Lg	144	97%
42	Lh	168	73% 24%
43	Li	105	94%
44	Lj	83	94%
45	Lk	83	93% 6%
46	Ll	51	96%
47	Lm	128	37% 60%
48	Ln	34	88% 9%
49	Lo	92	89% 8%
50	Lp	106	83% 8% 8%
51	S1	2204	52% 30% 17%
52	S2	76	8% 8% 84%
53	S3	77	56% 35% 8%
54	S4	76	37% 50% 13%
55	S5	13	54% 31% 15%
56	SA	264	86% 10%
57	SB	246	82% 14%
58	SC	219	91% 5%

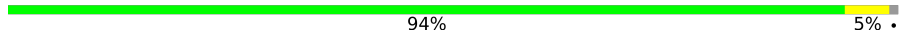





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Mol	Chain	Length	Quality of chain
59	SD	190	 92% . .
60	SE	273	 93% . 5%
61	SF	265	 80% . 18%
62	SG	249	 92% 6% .
63	SH	190	 95% . .
64	SI	200	 96% .
65	SJ	130	 94% 5% .
66	SK	220	 85% 5% 10%
67	SL	149	 91% 5% .
68	SM	116	 84% . 12%
69	SN	168	 55% . 41%
70	SO	144	 88% 6% 6%
71	SP	143	 90% 9% .
72	SQ	141	 25% 65% 5% 30%
73	SR	153	 77% 5% . 17%
74	SS	57	 93% 5% .
75	ST	151	 88% 6% 6%
76	SU	173	 82% 7% 12%
77	SV	143	 83% . 15%
78	SW	152	 72% . 24%
79	SX	161	 91% . 6%
80	SY	164	 51% . 46%
81	SZ	137	 91% . 5%
82	Sa	120	 51% 9% 40%
83	Sb	112	 87% 6% 7%

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Mol	Chain	Length	Quality of chain
84	Sc	86	 94% 5%
85	Sd	87	 69% 7% 24%
86	Se	66	 83% 5% 12%
87	Sf	152	 29% 70%
88	Sg	312	 87% 10%
89	Sh	235	 37% 6% 56%

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 213449 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 LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L1	1657	35568	15899	6506	11505	1658	1	0

- Molecule 2 is a RNA chain called LSUb_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L2	1149	24609	11017	4437	8005	1150	1	0

- Molecule 3 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L3	183	3877	1735	669	1290	183	0	0

- Molecule 4 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L4	184	3937	1756	712	1285	184	0	0

- Molecule 5 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	L5	122	2600	1160	466	852	122	0	0

- Molecule 6 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	L6	71	1506	675	271	489	71	0	0

- Molecule 7 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	L7	166	3532	1583	626	1158	165	0	0

- Molecule 8 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	L8	119	2531	1132	452	828	119	0	0

- Molecule 9 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LA	255	1931	1201	394	326	10	0	0

- Molecule 10 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LB	401	3169	1997	629	530	13	0	0

- Molecule 11 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LC	366	2815	1759	561	480	15	0	0

- Molecule 12 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LD	175	1340	849	258	225	8	0	0

- Molecule 13 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LE	186	1472	934	273	259	6	0	0

- Molecule 14 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LF	149	1151	731	216	202	2	0	0

- Molecule 15 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LG	241	1905	1200	380	318	7	1	0

- Molecule 16 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	LH	221	1764	1122	353	282	7	0	0

- Molecule 17 is a protein called Putative 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LI	208	1635	1022	331	274	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	203	ARG	ASN	conflict	UNP E9AEA8

- Molecule 18 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LJ	135	1008	636	190	176	6	0	0

- Molecule 19 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LK	169	1327	829	261	229	8	0	0

- Molecule 20 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	144	Total	C	N	O	S	0	0
			1124	707	226	185	6		

- Molecule 21 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	203	Total	C	N	O	S	0	0
			1711	1079	362	262	8		

- Molecule 22 is a protein called Putative 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LN	199	Total	C	N	O	S	0	0
			1615	1018	321	262	14		

- Molecule 23 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	290	Total	C	N	O	S	0	0
			2212	1405	416	385	6		

- Molecule 24 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LP	197	Total	C	N	O	S	0	0
			1535	965	306	258	6		

- Molecule 25 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LQ	201	Total	C	N	O	S	0	0
			1679	1034	367	272	6		

- Molecule 26 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LR	178	Total	C	N	O	S	0	0
			1455	925	279	246	5		

- Molecule 27 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LS	158	Total	C	N	O	S	0	0
			1247	793	243	207	4		

- Molecule 28 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LT	152	Total	C	N	O	S	0	0
			1218	761	241	205	11		

- Molecule 29 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LU	122	Total	C	N	O	S	0	0
			957	623	176	155	3		

- Molecule 30 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LV	119	Total	C	N	O	S	0	0
			945	599	180	164	2		

- Molecule 31 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LW	121	Total	C	N	O	S	0	0
			956	598	200	154	4		

- Molecule 32 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LX	85	Total	C	N	O	S	0	0
			714	461	140	109	4		

- Molecule 33 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LY	133	Total	C	N	O	S	0	0
			1067	684	215	165	3		

- Molecule 34 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LZ	145	1113	682	237	189	5	0	0

- Molecule 35 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	La	125	1043	650	217	172	4	0	0

- Molecule 36 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Lb	68	546	335	125	86		0	0

- Molecule 37 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Lc	229	1862	1185	358	308	11	0	0

- Molecule 38 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Ld	97	744	464	136	139	5	0	0

- Molecule 39 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Le	186	1469	922	296	247	4	0	0

- Molecule 40 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Lf	128	1046	658	210	174	4	0	0

- Molecule 41 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lg	143	Total	C	N	O	S	0	0
			1149	714	240	190	5		

- Molecule 42 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lh	127	Total	C	N	O	S	0	0
			1029	633	224	166	6		

- Molecule 43 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Li	102	Total	C	N	O	S	0	0
			807	508	163	133	3		

- Molecule 44 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lj	81	Total	C	N	O	S	0	0
			672	409	154	103	6		

- Molecule 45 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lk	78	Total	C	N	O	S	0	0
			581	365	115	98	3		

- Molecule 46 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ll	50	Total	C	N	O	S	0	0
			450	291	95	63	1		

- Molecule 47 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lm	51	Total	C	N	O	S	0	0
			402	254	80	63	5		

- Molecule 48 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Ln	33	290	178	73	37	2	0	0

- Molecule 49 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Lo	89	693	431	143	113	6	0	0

- Molecule 50 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Lp	97	780	494	158	123	5	0	0

- Molecule 51 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	S1	1836	39285	17572	7085	12791	1837	1	0

- Molecule 52 is a RNA chain called A-site_tRNA_chain_S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
52	S2	12	263	121	47	82	12	1	0	0

- Molecule 53 is a RNA chain called P-site_tRNA_chain_S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	S3	71	1513	676	277	490	70	0	0

- Molecule 54 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	S4	66	1406	628	253	460	65	0	0

- Molecule 55 is a RNA chain called mRNA_chain_S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	S5	11	229	103	38	77	11	0	0

- Molecule 56 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	SA	238	1909	1194	366	338	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	SB	211	1649	1047	301	290	11	0	0

- Molecule 58 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	SC	212	1627	1030	297	287	13	0	0

- Molecule 59 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	SD	183	1504	947	305	244	8	0	0

- Molecule 60 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	SE	260	2054	1301	393	351	9	0	0

- Molecule 61 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	SF	218	1662	1063	297	293	9	0	0

- Molecule 62 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SG	245	Total	C	N	O	S	0	0
			1948	1213	401	331	3		

- Molecule 63 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SH	182	Total	C	N	O	S	0	0
			1430	889	275	259	7		

- Molecule 64 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SI	200	Total	C	N	O	S	0	0
			1639	1044	316	271	8		

- Molecule 65 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SJ	129	Total	C	N	O	S	0	0
			1021	646	188	179	8		

- Molecule 66 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SK	198	Total	C	N	O	S	0	0
			1600	998	330	270	2		

- Molecule 67 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SL	144	Total	C	N	O	S	0	0
			1140	731	210	196	3		

- Molecule 68 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SM	102	Total	C	N	O	S	0	0
			796	498	145	151	2		

- Molecule 69 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	SN	99	808	518	141	142	7	0	0

- Molecule 70 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	SO	136	1010	624	197	182	7	0	0

- Molecule 71 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	SP	141	1096	691	216	186	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	SQ	98	655	400	119	131	5	0	0

- Molecule 73 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	SR	127	1011	641	195	171	4	0	0

- Molecule 74 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	SS	56	451	279	94	73	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	ST	142	1159	731	230	190	8	0	0

- Molecule 76 is a protein called Ribosomal protein S17 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SU	153	Total	C	N	O	S	0	0
			1251	792	248	206	5		

- Molecule 77 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SV	122	Total	C	N	O	S	0	0
			936	588	180	164	4		

- Molecule 78 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SW	115	Total	C	N	O	S	0	0
			925	590	176	155	4		

- Molecule 79 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SX	152	Total	C	N	O	S	0	0
			1206	766	237	199	4		

- Molecule 80 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SY	88	Total	C	N	O	S	0	0
			659	407	121	127	4		

- Molecule 81 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	SZ	130	Total	C	N	O	S	0	0
			1051	675	204	169	3		

- Molecule 82 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sa	72	Total	C	N	O	S	0	0
			567	361	100	103	3		

- Molecule 83 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sb	104	Total	C	N	O	S	0	0
			827	513	177	130	7		

- Molecule 84 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Sc	85	Total	C	N	O	S	0	0
			674	416	131	119	8		

- Molecule 85 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Sd	66	Total	C	N	O	S	0	0
			479	293	96	86	4		

- Molecule 86 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Se	58	Total	C	N	O	S	0	0
			465	293	97	74	1		

- Molecule 87 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms				AltConf	Trace
87	Sf	46	Total	C	N	O	0	0
			300	187	63	50		

- Molecule 88 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Sg	301	Total	C	N	O	S	0	0
			2341	1468	418	442	13		

- Molecule 89 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Sh	103	Total	C	N	O	S	0	0
			826	520	158	145	3		

- Molecule 90 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
90	L1	34	Total 34	K 34	0
90	L2	22	Total 22	K 22	0
90	L3	3	Total 3	K 3	0
90	L4	6	Total 6	K 6	0
90	L5	1	Total 1	K 1	0
90	L7	2	Total 2	K 2	0
90	LA	1	Total 1	K 1	0
90	LM	1	Total 1	K 1	0
90	S1	19	Total 19	K 19	0

- Molecule 91 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
91	L1	16	Total 16	Na 16	0
91	L2	14	Total 14	Na 14	0
91	L8	1	Total 1	Na 1	0
91	LA	1	Total 1	Na 1	0
91	Lh	1	Total 1	Na 1	0
91	S1	7	Total 7	Na 7	0
91	SK	1	Total 1	Na 1	0

- Molecule 92 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
92	L1	73	Total 73	Mg 73	0
92	L2	42	Total 42	Mg 42	0

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Mol	Chain	Residues	Atoms		AltConf
92	L3	3	Total 3	Mg 3	0
92	L4	2	Total 2	Mg 2	0
92	L5	2	Total 2	Mg 2	0
92	L6	1	Total 1	Mg 1	0
92	L7	3	Total 3	Mg 3	0
92	L8	2	Total 2	Mg 2	0
92	LB	1	Total 1	Mg 1	0
92	LJ	1	Total 1	Mg 1	0
92	LT	1	Total 1	Mg 1	0
92	Lf	1	Total 1	Mg 1	0
92	Lj	1	Total 1	Mg 1	0
92	S1	31	Total 31	Mg 31	0
92	S5	1	Total 1	Mg 1	0
92	SK	1	Total 1	Mg 1	0

- Molecule 93 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
93	Lm	1	Total 1	Zn 1	0
93	SS	1	Total 1	Zn 1	0
93	Sb	1	Total 1	Zn 1	0

- Molecule 94 is water.

Mol	Chain	Residues	Atoms		AltConf
94	L1	337	Total 337	O 337	0
94	L2	235	Total 235	O 235	0
94	L3	21	Total 21	O 21	0
94	L4	39	Total 39	O 39	0
94	L5	30	Total 30	O 30	0
94	L6	6	Total 6	O 6	0
94	L7	38	Total 38	O 38	0
94	L8	2	Total 2	O 2	0
94	LA	14	Total 14	O 14	0
94	LB	20	Total 20	O 20	0
94	LC	18	Total 18	O 18	0
94	LF	3	Total 3	O 3	0
94	LG	2	Total 2	O 2	0
94	LH	6	Total 6	O 6	0
94	LI	5	Total 5	O 5	0
94	LJ	6	Total 6	O 6	0
94	LK	1	Total 1	O 1	0
94	LL	8	Total 8	O 8	0
94	LM	12	Total 12	O 12	0
94	LP	6	Total 6	O 6	0
94	LQ	8	Total 8	O 8	0
94	LR	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
94	LT	11	Total 11	O 11	0
94	LV	4	Total 4	O 4	0
94	LW	2	Total 2	O 2	0
94	LX	3	Total 3	O 3	0
94	LZ	1	Total 1	O 1	0
94	La	3	Total 3	O 3	0
94	Lb	1	Total 1	O 1	0
94	Lc	5	Total 5	O 5	0
94	Ld	1	Total 1	O 1	0
94	Le	3	Total 3	O 3	0
94	Lf	8	Total 8	O 8	0
94	Lg	7	Total 7	O 7	0
94	Lh	7	Total 7	O 7	0
94	Lj	11	Total 11	O 11	0
94	Lk	1	Total 1	O 1	0
94	Ll	4	Total 4	O 4	0
94	Lm	1	Total 1	O 1	0
94	Ln	1	Total 1	O 1	0
94	Lo	6	Total 6	O 6	0
94	Lp	1	Total 1	O 1	0
94	S1	78	Total 78	O 78	0

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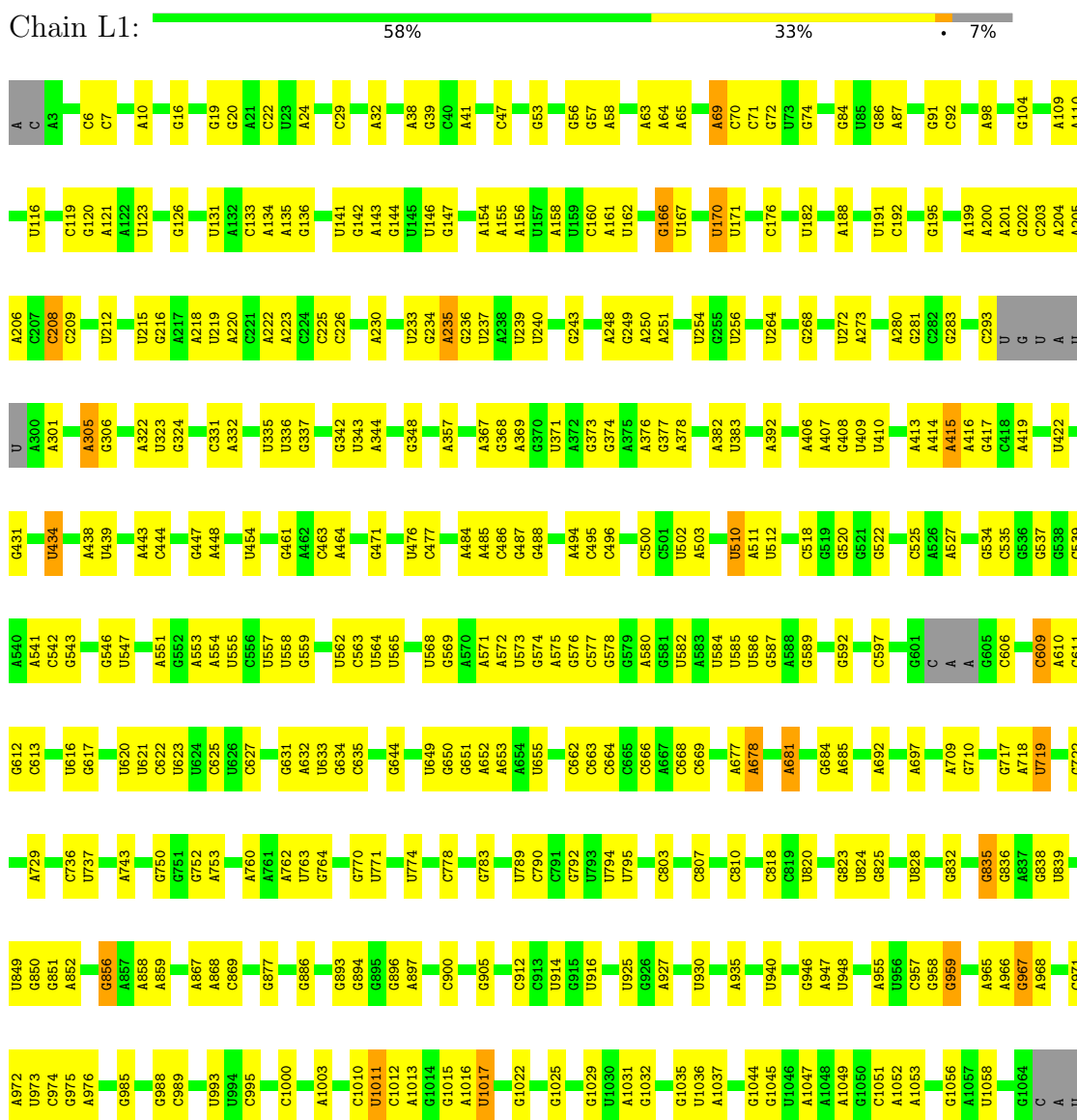
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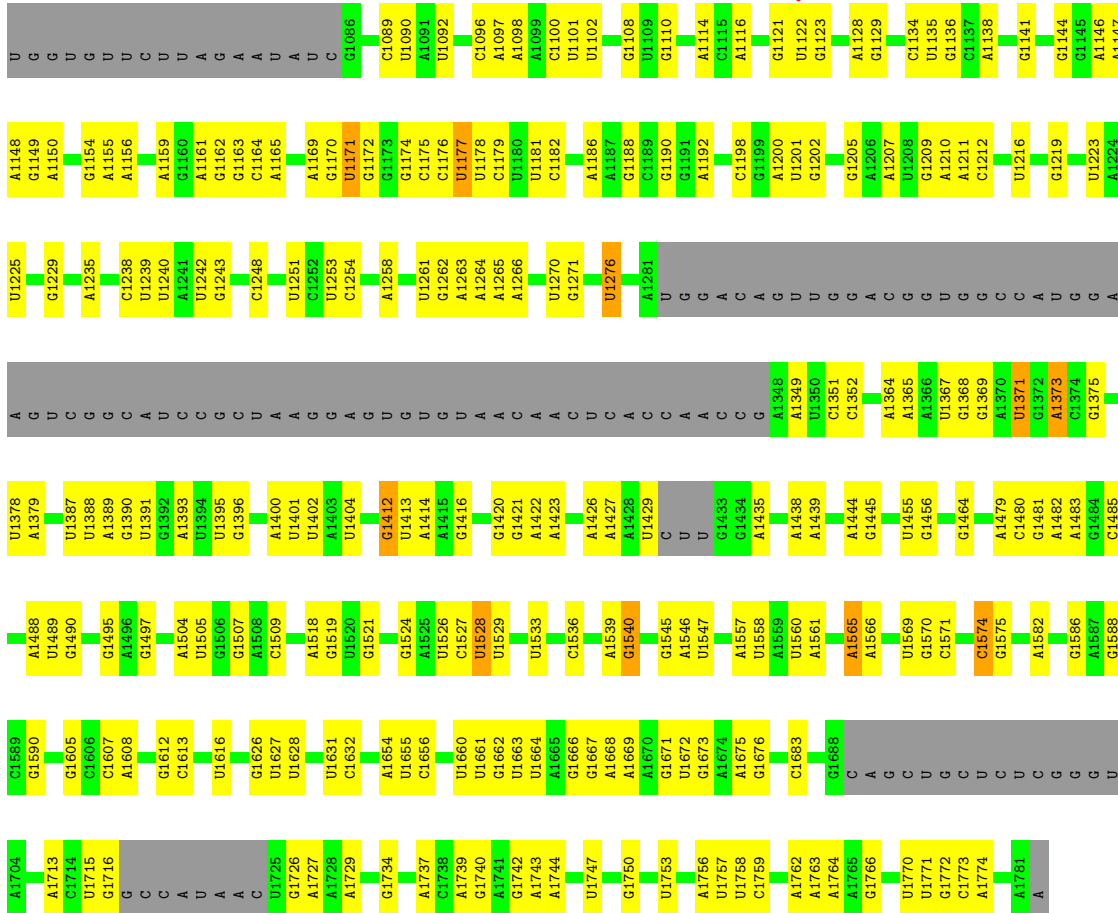
Mol	Chain	Residues	Atoms		AltConf
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94	S4	1	Total 1	O 1	0
94	S5	3	Total 3	O 3	0
94	SK	2	Total 2	O 2	0
94	SO	1	Total 1	O 1	0
94	SP	1	Total 1	O 1	0
94	ST	3	Total 3	O 3	0
94	Sb	1	Total 1	O 1	0

3 Residue-property plots

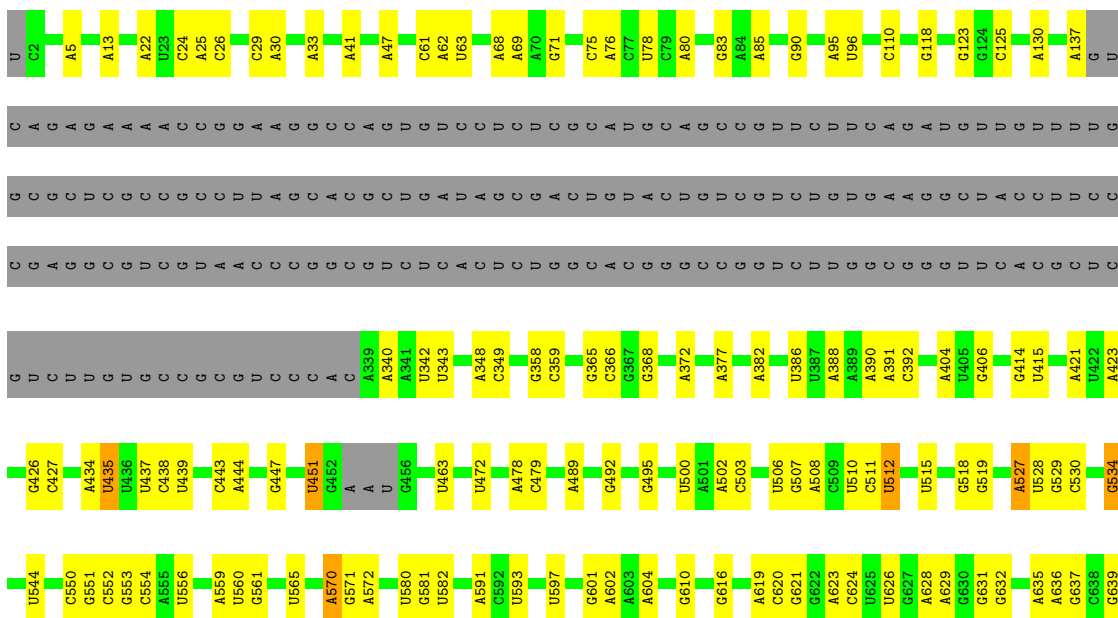
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

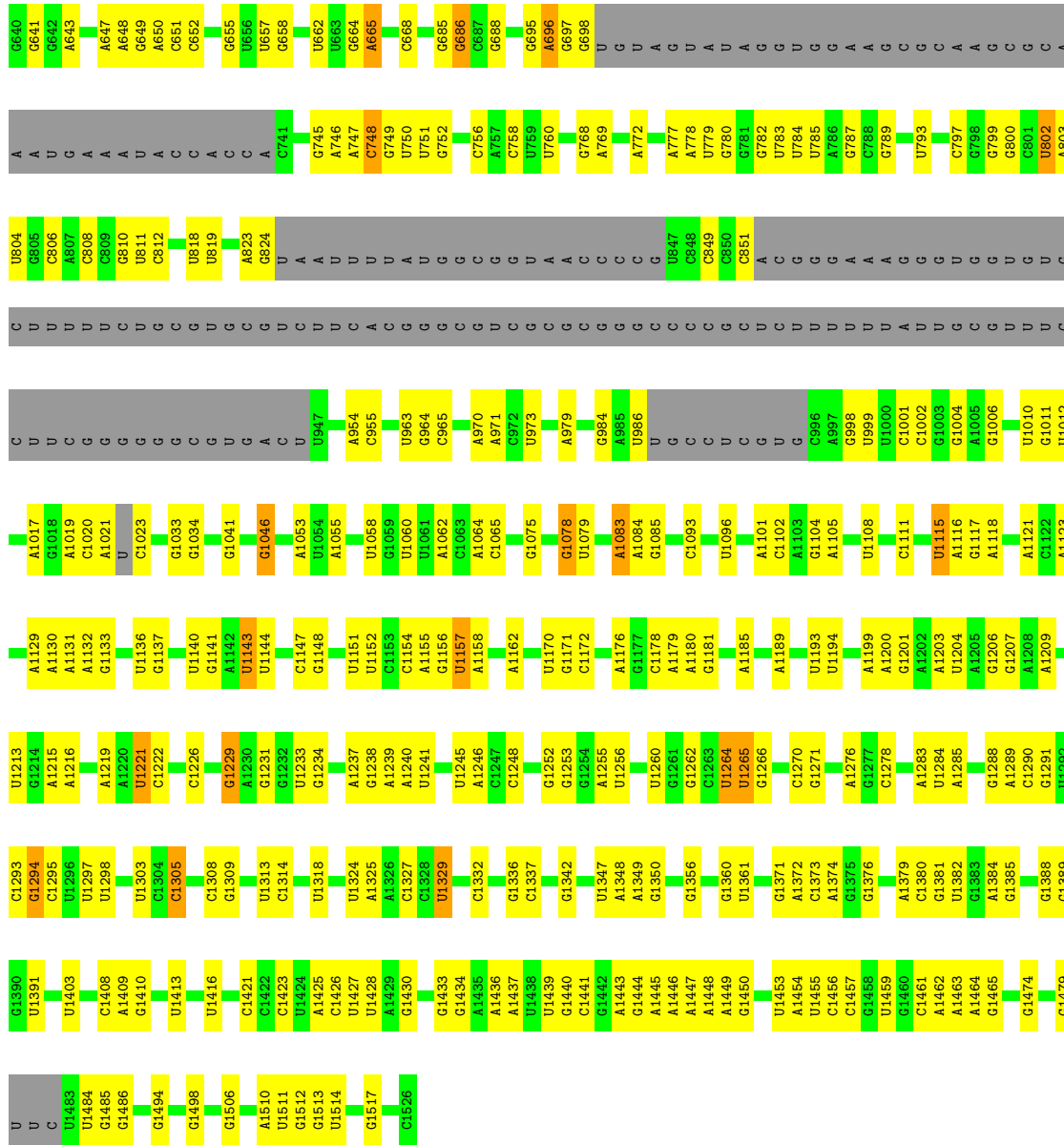
- Molecule 1: LSUa_rRNA_chain_1



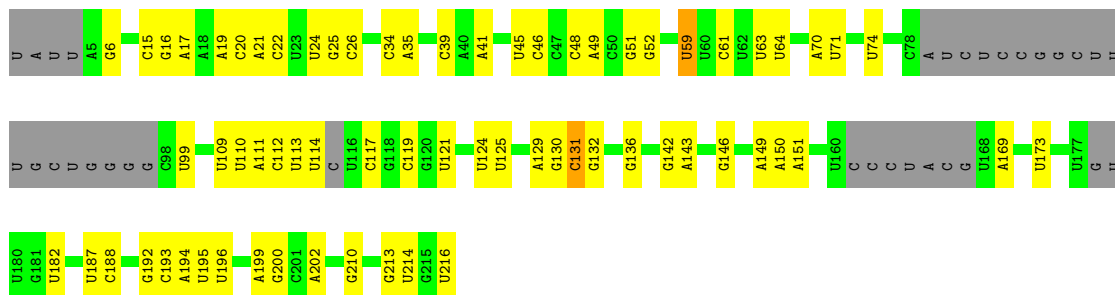


● Molecule 2: LSub_rRNA_chain_2




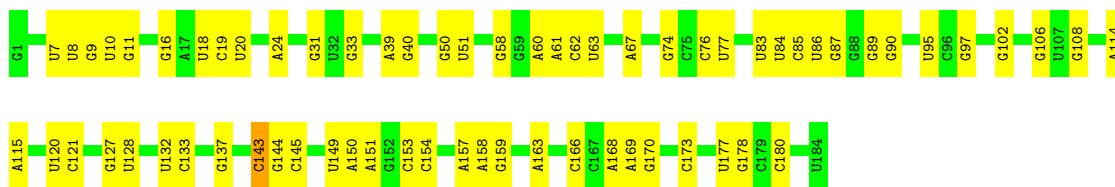


• Molecule 3: SR1_chain_3



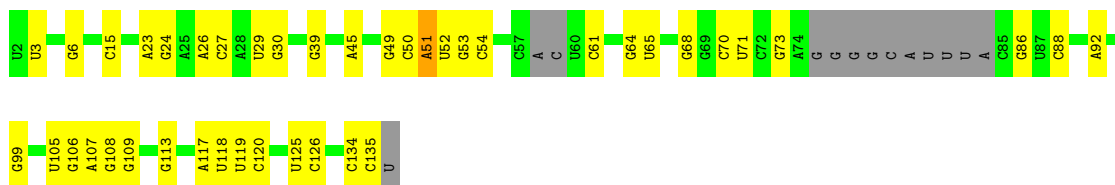
• Molecule 4: SR2_chain_4

Chain L4:  64% 35%



• Molecule 5: SR4_chain_5

Chain L5:  59% 30% 10%



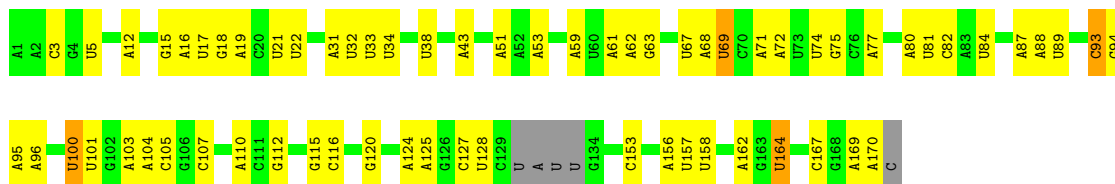
• Molecule 6: SR6_chain_6

Chain L6:  42% 51%



• Molecule 7: 5.8S_rRNA_chain_7

Chain L7:  59% 36%



• Molecule 8: 5S_rRNA_chain_8

Chain L8:  72% 24%



• Molecule 9: Putative 60S ribosomal protein L2

Chain LA:  97%



- Molecule 10: Putative ribosomal protein L3

Chain LB:  92%




- Molecule 11: Putative ribosomal protein L1a

Chain LC:  92%



- Molecule 12: 60S ribosomal protein L11

Chain LD:  86%



- Molecule 13: Putative 60S ribosomal protein L9

Chain LE:  91%



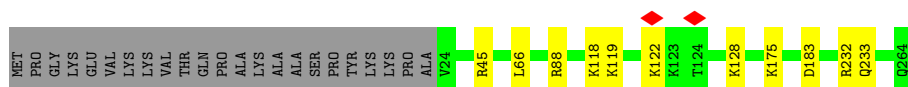
- Molecule 14: Putative 60S ribosomal protein L6

Chain LF:  71%



- Molecule 15: 60S ribosomal protein L7a

Chain LG:  87%



- Molecule 16: Putative 60S ribosomal protein L13a

Chain LH:  93%



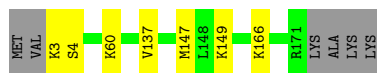
• Molecule 17: Putative 60S ribosomal protein L13



• Molecule 18: Putative 60S ribosomal protein L23



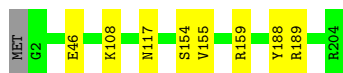
• Molecule 19: Putative 40S ribosomal protein L14



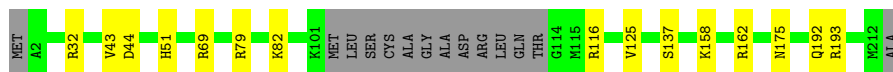
• Molecule 20: Putative 60S ribosomal protein L27A/L29



• Molecule 21: Ribosomal protein L15



• Molecule 22: Putative 60S ribosomal protein L10



• Molecule 23: Putative 60S ribosomal protein L5

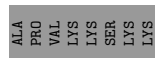
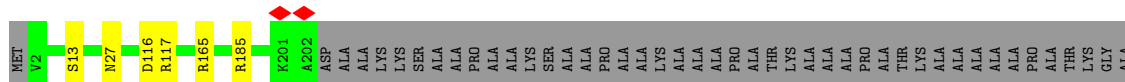
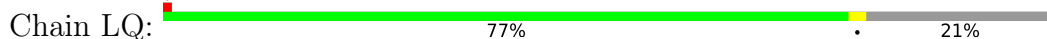




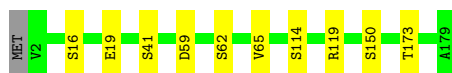
- Molecule 24: 60S ribosomal protein L18



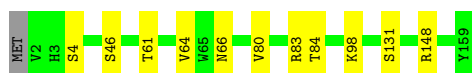
- Molecule 25: Putative 60S ribosomal protein L19



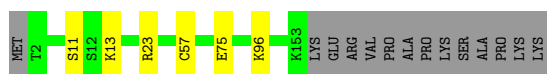
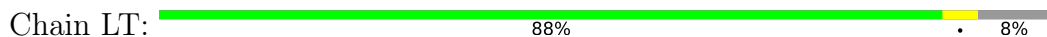
- Molecule 26: 60S ribosomal protein L18a



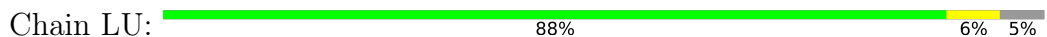
- Molecule 27: Putative 60S ribosomal protein L21



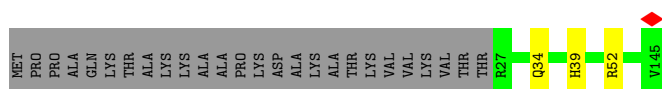
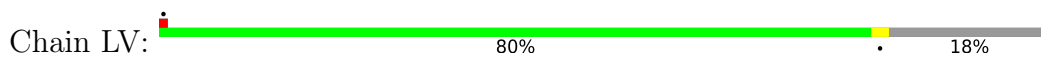
- Molecule 28: Putative 60S ribosomal protein L17



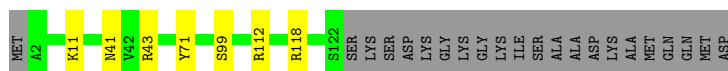
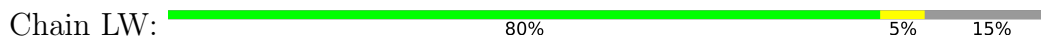
- Molecule 29: Putative 60S ribosomal protein L22



- Molecule 30: Putative 60S ribosomal protein L23a



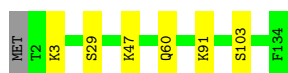
- Molecule 31: Putative 60S ribosomal protein L26



- Molecule 32: Putative ribosomal protein L24



- Molecule 33: 60S ribosomal protein L27



- Molecule 34: Putative 60S ribosomal protein L28




- Molecule 35: Putative 60S ribosomal protein L35

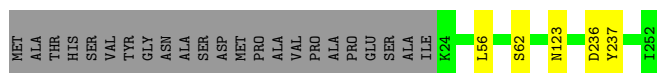


- Molecule 36: 60S ribosomal protein L29




- Molecule 37: Putative 60S ribosomal protein L7

Chain Lc:  89% 9%



- Molecule 38: 60S ribosomal protein L30

Chain Ld:  87% 7% 7%



- Molecule 39: Putative 60S ribosomal subunit protein L31

Chain Le:  94% 5%



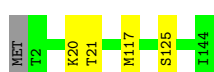
- Molecule 40: 60S ribosomal protein L32

Chain Lf:  93%




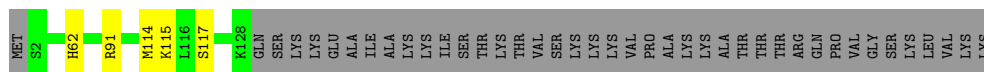
- Molecule 41: Putative ribosomal protein l35a

Chain Lg:  97%



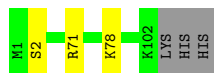
- Molecule 42: Putative 60S ribosomal protein L34

Chain Lh:  73% 24%



- Molecule 43: Putative 60S Ribosomal protein L36

Chain Li:  94%



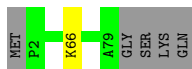
- Molecule 44: Ribosomal protein L37

Chain Lj:  94% . .



- Molecule 45: Putative ribosomal protein L38

Chain Lk:  93% • 6%



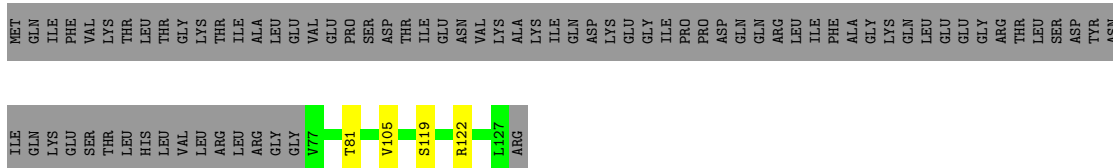
- Molecule 46: Putative 60S ribosomal protein L39

Chain Ll:  96% . .




- Molecule 47: Ubiquitin-60S ribosomal protein L40

Chain Lm:  37% • 60%



- Molecule 48: 60S ribosomal protein L41

Chain Ln:  88% 9% •




- Molecule 49: 60S ribosomal protein L37a

Chain Lo:  89% 8% •

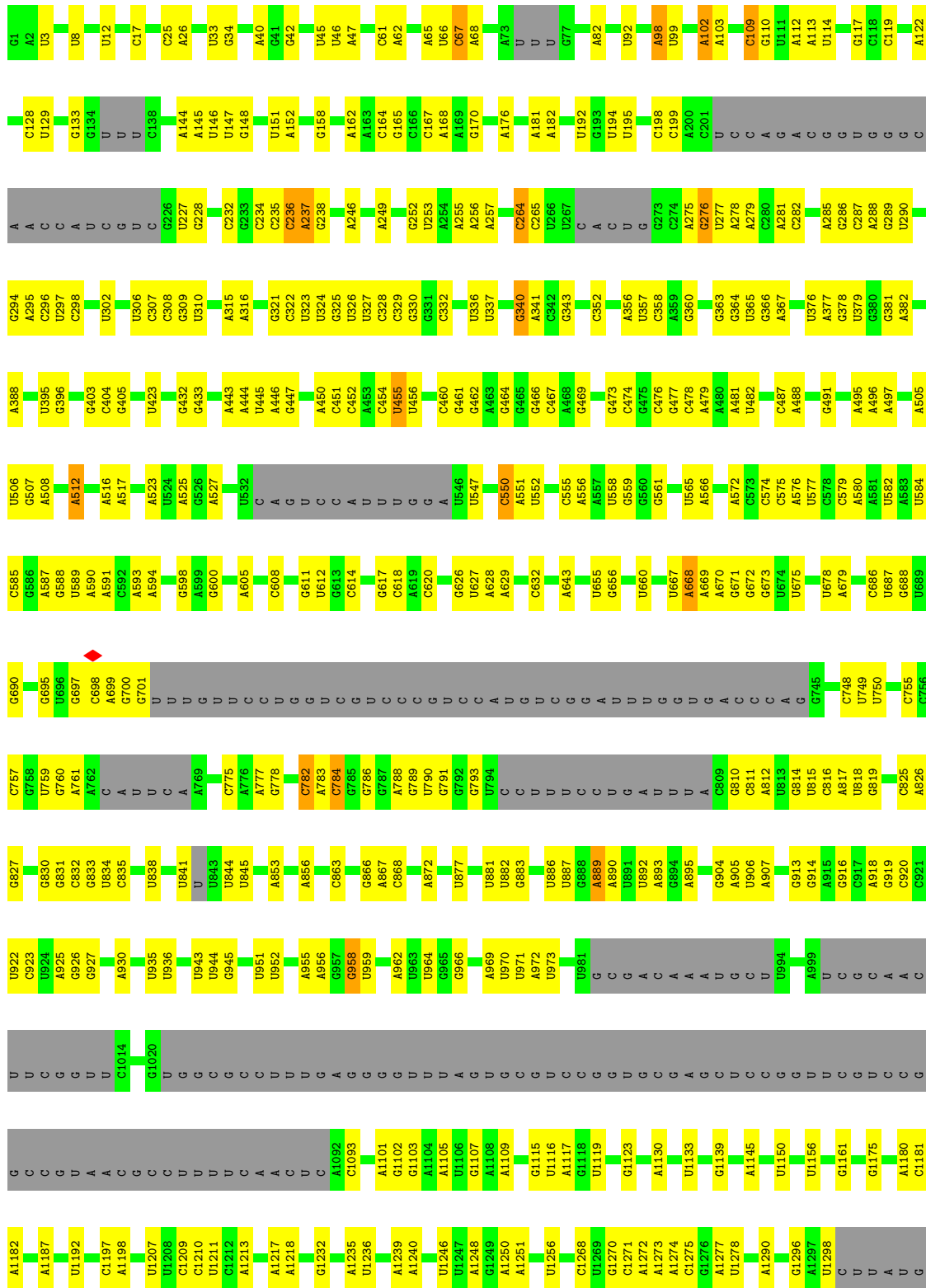


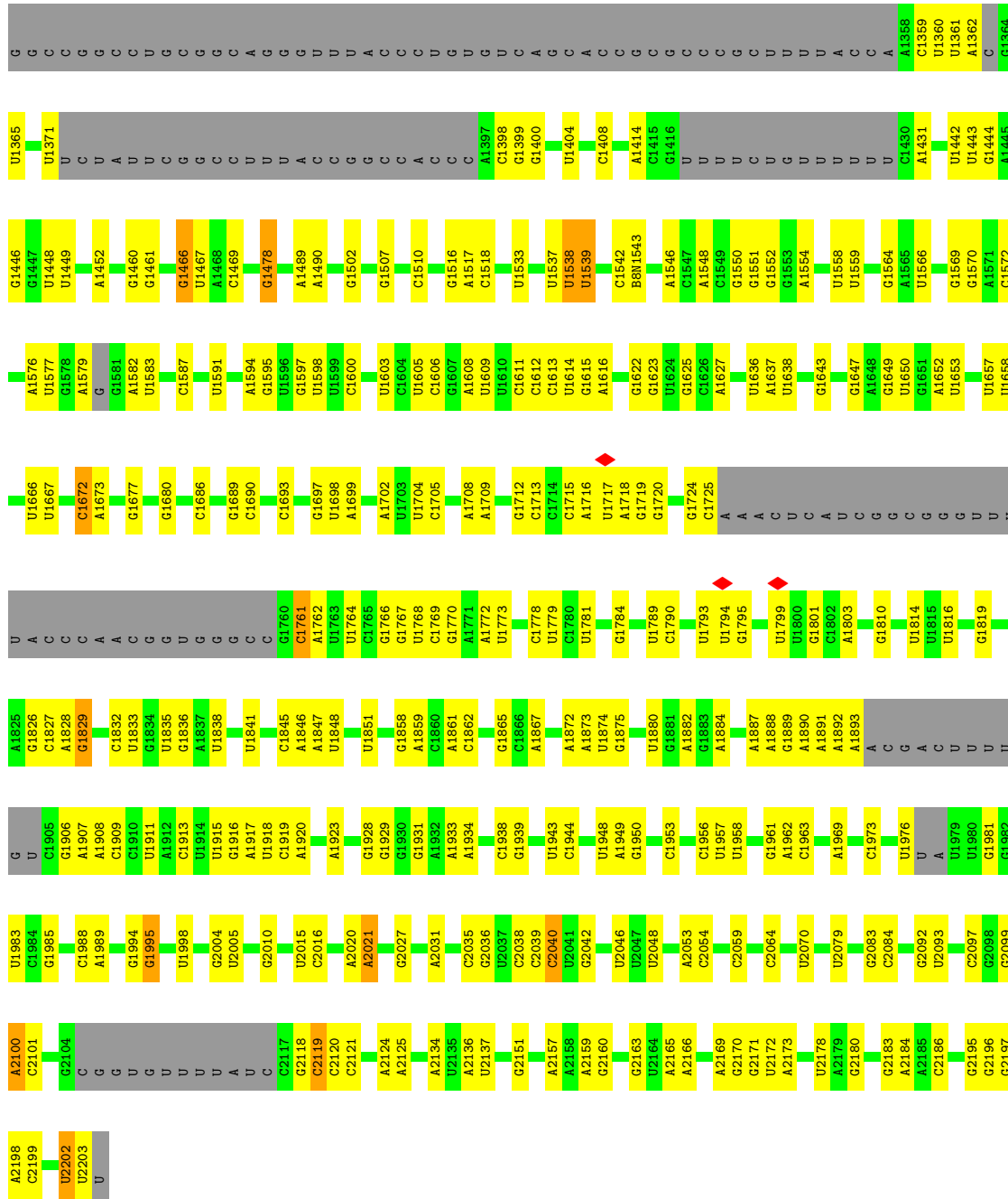
- Molecule 50: Putative 60S ribosomal protein L44

Chain Lp:  83% 8% 8%

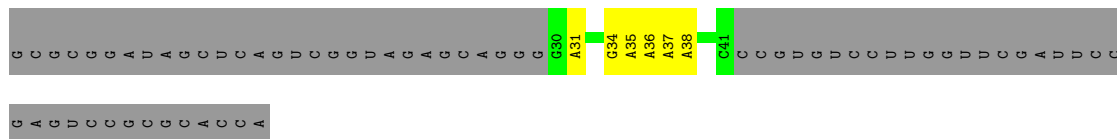


• Molecule 51: SSU_rRNA_chain_S1



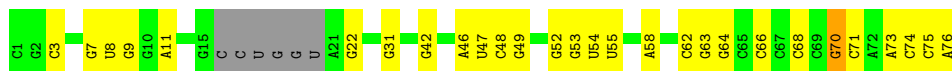


● Molecule 52: A-site_tRNA_chain_S2

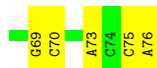
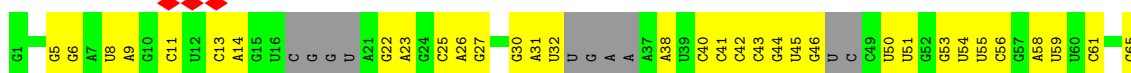


● Molecule 53: P-site_tRNA_chain_S3





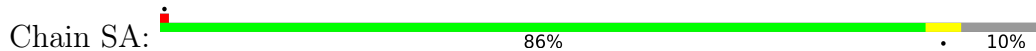
- Molecule 54: E-site_tRNA_chain_S4



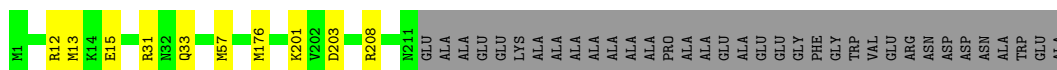
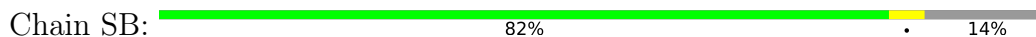
- Molecule 55: mRNA_chain_S5



- Molecule 56: 40S ribosomal protein S3a



- Molecule 57: 40S ribosomal protein SA



- Molecule 58: Putative 40S ribosomal protein S3

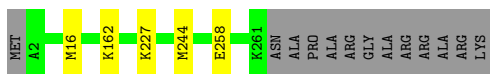


- Molecule 59: Putative 40S ribosomal protein S9




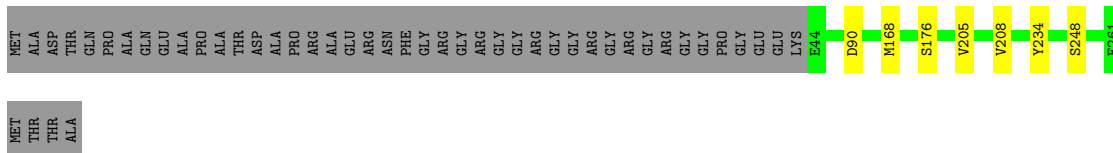
- Molecule 60: 40S ribosomal protein S4

Chain SE:  93% • 5%



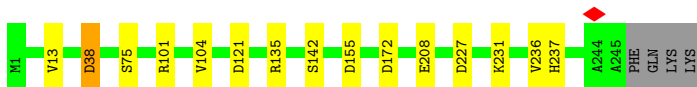
- Molecule 61: 40S ribosomal protein S2

Chain SF:  80% • 18%



- Molecule 62: 40S ribosomal protein S6

Chain SG:  92% • 6%



- Molecule 63: 40S ribosomal protein S5

Chain SH:  95% • •



- Molecule 64: 40S ribosomal protein S7

Chain SI:  96% •




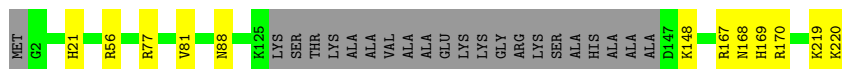
- Molecule 65: Putative 40S ribosomal protein S15A

Chain SJ:  94% •



- Molecule 66: 40S ribosomal protein S8

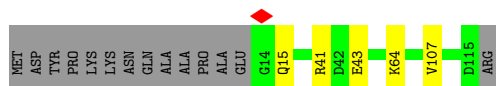
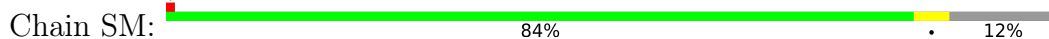
Chain SK:  85% 5% 10%



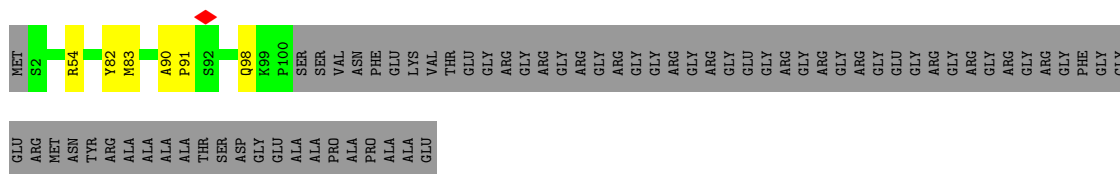
• Molecule 67: Putative 40S ribosomal protein S16



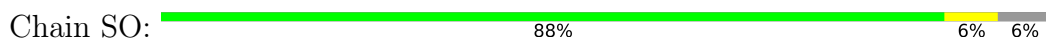
• Molecule 68: Putative ribosomal protein S20



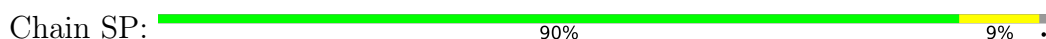
• Molecule 69: Putative 40S ribosomal protein S10



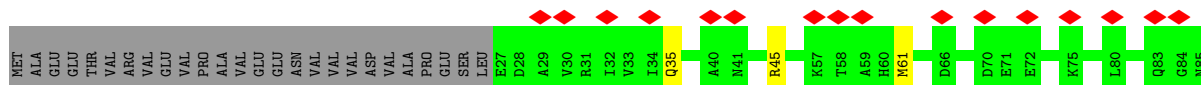
• Molecule 70: 40S ribosomal protein S14



• Molecule 71: Putative 40S ribosomal protein S23

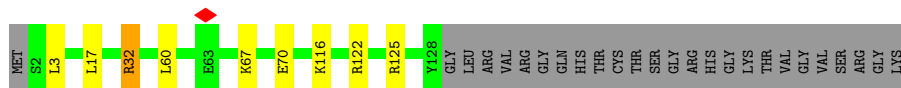
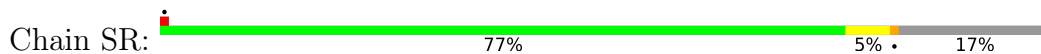


• Molecule 72: 40S ribosomal protein S12





- Molecule 73: Putative 40S ribosomal protein S18



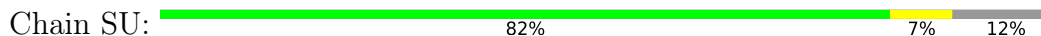
- Molecule 74: Putative ribosomal protein S29



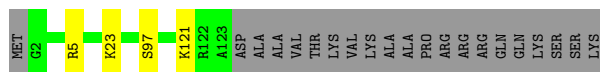
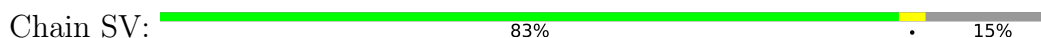
- Molecule 75: Putative 40S ribosomal protein S13



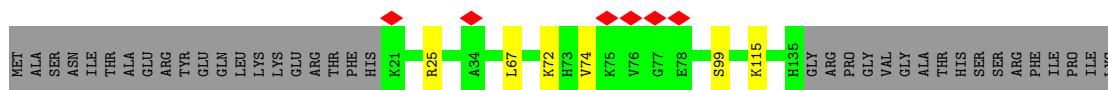
- Molecule 76: Ribosomal protein S17 family protein



- Molecule 77: Putative 40S ribosomal protein S17

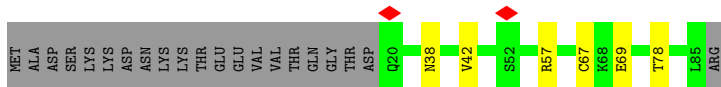


- Molecule 78: Putative 40S ribosomal protein S15

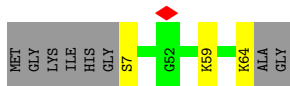
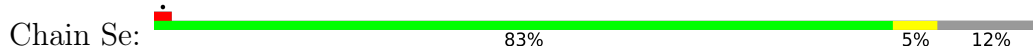


- Molecule 79: 40S ribosomal protein S19-like protein

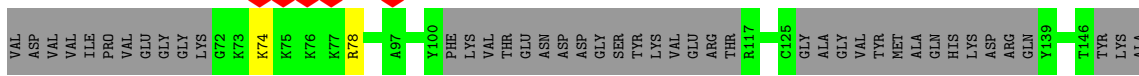
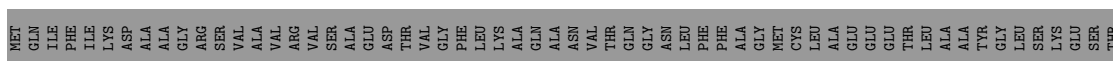




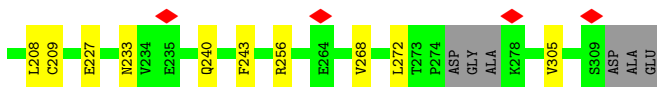
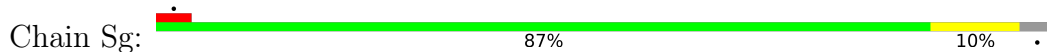
• Molecule 86: 40S ribosomal protein S30



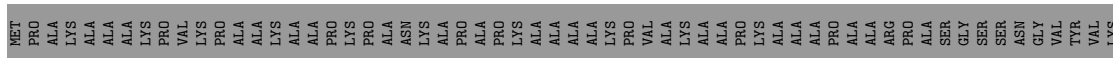
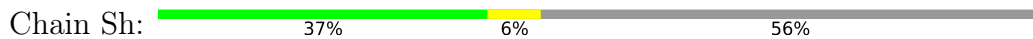
• Molecule 87: Ubiquitin-60S ribosomal protein L40



• Molecule 88: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 89: Putative RNA binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	490938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.273	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, OMG, NA, K, MA6, ZN, B8N, PSU, MG, OMC, OMU, A2M, MIA, 7MG, 5MC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L1	0.66	0/38810	1.11	28/60514 (0.0%)
2	L2	0.67	0/25898	1.11	25/40361 (0.1%)
3	L3	0.67	0/4302	1.13	5/6687 (0.1%)
4	L4	0.66	0/4376	1.10	4/6822 (0.1%)
5	L5	0.68	0/2903	1.14	3/4518 (0.1%)
6	L6	0.70	0/1683	1.14	3/2618 (0.1%)
7	L7	0.65	0/3802	1.11	3/5917 (0.1%)
8	L8	0.68	0/2829	1.08	4/4405 (0.1%)
9	LA	0.28	0/1972	0.58	0/2646
10	LB	0.27	0/3236	0.55	0/4354
11	LC	0.27	0/2865	0.54	0/3854
12	LD	0.30	0/1363	0.53	0/1825
13	LE	0.27	0/1492	0.53	0/2011
14	LF	0.27	0/1173	0.52	0/1586
15	LG	0.26	0/1932	0.54	0/2599
16	LH	0.26	0/1800	0.53	0/2418
17	LI	0.31	0/1668	0.54	0/2236
18	LJ	0.27	0/1025	0.52	0/1383
19	LK	0.27	0/1346	0.49	0/1805
20	LL	0.29	0/1151	0.53	0/1538
21	LM	0.27	0/1751	0.57	0/2338
22	LN	0.25	0/1647	0.54	0/2203
23	LO	0.29	0/2252	0.50	0/3024
24	LP	0.27	0/1560	0.55	0/2088
25	LQ	0.26	0/1698	0.55	0/2246
26	LR	0.28	0/1489	0.53	0/2008
27	LS	0.27	0/1276	0.53	0/1720
28	LT	0.28	0/1242	0.53	0/1666
29	LU	0.26	0/973	0.51	0/1299
30	LV	0.26	0/960	0.52	0/1293
31	LW	0.27	0/970	0.56	0/1296
32	LX	0.27	0/735	0.55	0/989

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LY	0.26	0/1088	0.53	0/1455
34	LZ	0.29	0/1129	0.55	0/1512
35	La	0.26	0/1054	0.55	0/1399
36	Lb	0.25	0/557	0.53	0/743
37	Lc	0.28	0/1896	0.53	0/2540
38	Ld	0.28	0/754	0.52	0/1019
39	Le	0.26	0/1488	0.54	0/1979
40	Lf	0.27	0/1066	0.55	0/1424
41	Lg	0.32	0/1172	0.59	0/1573
42	Lh	0.33	0/1045	0.59	0/1390
43	Li	0.28	0/822	0.53	0/1099
44	Lj	0.27	0/686	0.62	0/915
45	Lk	0.26	0/590	0.52	0/798
46	Ll	0.26	0/463	0.52	0/617
47	Lm	0.24	0/408	0.52	0/545
48	Ln	0.25	0/294	0.67	0/383
49	Lo	0.32	0/705	0.61	0/940
50	Lp	0.27	0/793	0.50	0/1048
51	S1	0.69	0/42900	1.10	49/66828 (0.1%)
52	S2	0.73	0/260	1.07	0/400
53	S3	0.73	0/1690	1.06	1/2631 (0.0%)
54	S4	0.73	0/1568	1.11	0/2436
55	S5	0.69	0/254	1.12	0/392
56	SA	0.24	0/1933	0.56	0/2596
57	SB	0.25	0/1683	0.50	0/2279
58	SC	0.31	0/1650	0.54	0/2209
59	SD	0.26	0/1532	0.55	0/2054
60	SE	0.25	0/2092	0.52	0/2819
61	SF	0.26	0/1698	0.50	0/2301
62	SG	0.27	0/1972	0.58	1/2635 (0.0%)
63	SH	0.24	0/1452	0.50	0/1948
64	SI	0.25	0/1669	0.52	0/2244
65	SJ	0.26	0/1038	0.52	0/1391
66	SK	0.25	0/1623	0.57	0/2169
67	SL	0.33	0/1161	0.53	0/1559
68	SM	0.24	0/806	0.54	0/1093
69	SN	3.35	1/831 (0.1%)	1.21	3/1127 (0.3%)
70	SO	0.26	0/1025	0.59	0/1379
71	SP	0.25	0/1116	0.51	0/1496
72	SQ	0.26	0/655	0.57	0/890
73	SR	0.28	0/1029	0.56	0/1384
74	SS	0.23	0/457	0.52	0/606
75	ST	0.26	0/1182	0.54	0/1584

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SU	0.27	0/1280	0.53	0/1720
77	SV	0.24	0/945	0.50	0/1265
78	SW	0.25	0/945	0.53	0/1271
79	SX	0.24	0/1237	0.51	0/1661
80	SY	0.24	0/669	0.50	0/908
81	SZ	0.25	0/1071	0.51	0/1425
82	Sa	0.24	0/572	0.55	0/769
83	Sb	0.25	0/844	0.58	0/1129
84	Sc	0.26	0/688	0.57	0/921
85	Sd	0.24	0/481	0.55	0/647
86	Se	0.25	0/473	0.51	0/627
87	Sf	0.73	0/303	0.63	0/408
88	Sg	0.24	0/2398	0.51	0/3256
89	Sh	0.26	0/843	0.54	0/1134
All	All	0.58	1/224214 (0.0%)	0.94	129/329237 (0.0%)

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
13	LE	0	1
17	LI	0	1
25	LQ	0	1
34	LZ	0	2
49	Lo	0	1
58	SC	0	1
73	SR	0	1
87	Sf	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	SN	91	PRO	N-CD	95.85	2.82	1.47

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	SN	91	PRO	N-CD-CG	-33.16	53.46	103.20
69	SN	91	PRO	CA-N-CD	-14.57	91.11	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	99	U	O4'-C1'-N1	6.82	113.65	108.20
51	S1	92	U	O4'-C1'-N1	6.81	113.65	108.20
51	S1	337	U	O4'-C1'-N1	6.77	113.61	108.20
51	S1	1538	U	O4'-C1'-N1	6.74	113.59	108.20
4	L4	95	U	O4'-C1'-N1	6.63	113.51	108.20
2	L2	1221	U	O4'-C1'-N1	6.60	113.48	108.20
1	L1	1058	U	O4'-C1'-N1	6.54	113.43	108.20
2	L2	1115	U	O4'-C1'-N1	6.50	113.40	108.20
4	L4	63	U	O4'-C1'-N1	6.44	113.35	108.20
51	S1	1773	U	O4'-C1'-N1	6.42	113.34	108.20
2	L2	1143	U	O4'-C1'-N1	6.41	113.33	108.20
5	L5	71	U	O4'-C1'-N1	6.41	113.33	108.20
1	L1	208	C	O4'-C1'-N1	6.41	113.32	108.20
2	L2	1157	U	O4'-C1'-N1	6.40	113.32	108.20
1	L1	916	U	O4'-C1'-N1	6.39	113.31	108.20
1	L1	914	U	O4'-C1'-N1	6.38	113.31	108.20
2	L2	435	U	O4'-C1'-N1	6.35	113.28	108.20
51	S1	558	U	O4'-C1'-N1	6.33	113.27	108.20
51	S1	2059	C	O4'-C1'-N1	6.33	113.27	108.20
7	L7	164	U	O4'-C1'-N1	6.32	113.26	108.20
4	L4	177	U	O4'-C1'-N1	6.32	113.26	108.20
6	L6	57	U	O4'-C1'-N1	6.30	113.24	108.20
2	L2	1151	U	O4'-C1'-N1	6.26	113.21	108.20
51	S1	2119	C	OP1-P-O3'	6.22	118.88	105.20
1	L1	993	U	O4'-C1'-N1	6.21	113.17	108.20
3	L3	59	U	O4'-C1'-N1	6.18	113.14	108.20
1	L1	166	G	O4'-C1'-N9	6.15	113.12	108.20
2	L2	696	A	OP1-P-O3'	6.14	118.72	105.20
8	L8	39	C	O4'-C1'-N1	6.10	113.08	108.20
51	S1	1404	U	O4'-C1'-N1	6.08	113.07	108.20
2	L2	479	C	O4'-C1'-N1	6.05	113.04	108.20
1	L1	476	U	O4'-C1'-N1	6.04	113.04	108.20
1	L1	331	C	O4'-C1'-N1	6.04	113.03	108.20
3	L3	188	C	O4'-C1'-N1	6.03	113.03	108.20
2	L2	1222	C	O4'-C1'-N1	6.02	113.02	108.20
2	L2	1065	C	O4'-C1'-N1	6.01	113.01	108.20
1	L1	1276	U	O4'-C1'-N1	5.96	112.97	108.20
51	S1	1764	U	O4'-C1'-N1	5.95	112.96	108.20
1	L1	22	C	O4'-C1'-N1	5.93	112.94	108.20
1	L1	967	G	OP1-P-O3'	5.92	118.22	105.20
51	S1	109	C	O4'-C1'-N1	5.91	112.92	108.20
51	S1	336	U	O4'-C1'-N1	5.90	112.92	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	506	U	O4'-C1'-N1	5.88	112.91	108.20
6	L6	11	G	C3'-C2'-C1'	-5.87	96.81	101.50
51	S1	1600	C	O4'-C1'-N1	5.87	112.89	108.20
7	L7	93	C	C4'-C3'-C2'	-5.86	96.74	102.60
2	L2	1010	U	O4'-C1'-N1	5.86	112.89	108.20
51	S1	236	C	OP1-P-O3'	5.85	118.08	105.20
2	L2	1083	A	OP1-P-O3'	5.84	118.05	105.20
51	S1	784	C	O4'-C1'-N1	5.84	112.87	108.20
5	L5	70	C	O4'-C1'-N1	5.84	112.87	108.20
51	S1	1973	C	O4'-C1'-N1	5.80	112.84	108.20
2	L2	1329	U	O4'-C1'-N1	5.79	112.83	108.20
51	S1	264	C	O4'-C1'-N1	5.79	112.83	108.20
2	L2	1305	C	O4'-C1'-N1	5.76	112.81	108.20
2	L2	748	C	OP1-P-O3'	5.75	117.86	105.20
51	S1	1466	G	C3'-C2'-C1'	-5.75	96.90	101.50
8	L8	92	U	O4'-C1'-N1	5.75	112.80	108.20
51	S1	1779	U	O4'-C1'-N1	5.75	112.80	108.20
3	L3	131	C	O4'-C1'-N1	5.75	112.80	108.20
51	S1	302	U	O4'-C1'-N1	5.72	112.77	108.20
51	S1	1572	C	O4'-C1'-N1	5.71	112.77	108.20
6	L6	40	C	O4'-C1'-N1	5.70	112.76	108.20
51	S1	1983	U	O4'-C1'-N1	5.69	112.75	108.20
51	S1	782	C	O4'-C1'-N1	5.66	112.73	108.20
1	L1	820	U	O4'-C1'-N1	5.65	112.72	108.20
5	L5	51	A	OP1-P-O3'	5.62	117.57	105.20
51	S1	1558	U	O4'-C1'-N1	5.59	112.67	108.20
1	L1	719	U	O4'-C1'-N1	5.59	112.67	108.20
51	S1	102	A	OP2-P-O3'	5.59	117.50	105.20
1	L1	1574	C	OP1-P-O3'	5.55	117.41	105.20
1	L1	562	U	O4'-C1'-N1	5.55	112.64	108.20
7	L7	100	U	O4'-C1'-N1	5.47	112.58	108.20
2	L2	479	C	C2-N1-C1'	5.46	124.80	118.80
51	S1	1761	C	OP1-P-O3'	5.45	117.19	105.20
1	L1	434	U	O4'-C1'-N1	5.40	112.52	108.20
1	L1	208	C	C4'-C3'-C2'	-5.39	97.21	102.60
1	L1	415	A	OP1-P-O3'	5.38	117.03	105.20
51	S1	340	G	C3'-C2'-C1'	-5.38	97.20	101.50
51	S1	1911	U	O4'-C1'-N1	5.38	112.50	108.20
1	L1	254	U	O4'-C1'-N1	5.37	112.50	108.20
8	L8	123	C	O4'-C1'-N1	5.37	112.49	108.20
51	S1	906	U	O4'-C1'-N1	5.36	112.49	108.20
51	S1	943	U	O4'-C1'-N1	5.35	112.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1565	A	OP1-P-O3'	5.35	116.97	105.20
2	L2	756	C	O4'-C1'-N1	5.35	112.48	108.20
51	S1	2100	A	OP1-P-O3'	5.34	116.95	105.20
2	L2	1294	G	OP1-P-OP2	-5.31	111.63	119.60
51	S1	1600	C	C2-N1-C1'	5.30	124.63	118.80
1	L1	1571	C	O4'-C1'-N1	5.29	112.43	108.20
51	S1	2040	C	O4'-C1'-N1	5.29	112.43	108.20
1	L1	1588	G	C3'-C2'-C1'	-5.28	97.28	101.50
2	L2	1305	C	C2-N1-C1'	5.26	124.59	118.80
69	SN	90	ALA	C-N-CD	5.25	139.43	128.40
51	S1	264	C	C2-N1-C1'	5.24	124.57	118.80
51	S1	958	G	C3'-C2'-C1'	-5.24	97.31	101.50
2	L2	502[A]	A2M	OP2-P-O3'	5.24	116.72	105.20
2	L2	502[B]	A2M	OP2-P-O3'	5.24	116.72	105.20
2	L2	451	U	O4'-C1'-N1	5.23	112.39	108.20
51	S1	2059	C	C2-N1-C1'	5.23	124.55	118.80
1	L1	170	U	OP2-P-O3'	5.22	116.69	105.20
4	L4	143	C	OP2-P-O3'	5.20	116.65	105.20
1	L1	835	G	OP2-P-O3'	5.18	116.59	105.20
51	S1	237	A	OP1-P-OP2	-5.17	111.85	119.60
2	L2	631	G	O4'-C1'-N9	5.16	112.32	108.20
1	L1	1412	G	OP1-P-O3'	5.15	116.53	105.20
51	S1	889	A	OP2-P-O3'	5.15	116.52	105.20
51	S1	748	C	O4'-C1'-N1	5.13	112.31	108.20
51	S1	582	U	O4'-C1'-N1	5.12	112.30	108.20
62	SG	38	ASP	CB-CG-OD1	5.12	122.91	118.30
51	S1	550	C	OP1-P-O3'	5.12	116.46	105.20
2	L2	1065	C	C2-N1-C1'	5.11	124.42	118.80
53	S3	70	G	OP2-P-O3'	5.11	116.44	105.20
3	L3	119	C	O4'-C1'-N1	5.11	112.29	108.20
1	L1	609	C	O4'-C1'-N1	5.10	112.28	108.20
51	S1	276	G	OP1-P-O3'	5.09	116.40	105.20
1	L1	719	U	C1'-O4'-C4'	-5.08	105.83	109.90
1	L1	331	C	C2-N1-C1'	5.06	124.37	118.80
51	S1	109	C	C2-N1-C1'	5.06	124.36	118.80
51	S1	958	G	OP1-P-O3'	5.05	116.32	105.20
51	S1	67	C	O4'-C1'-N1	5.05	112.24	108.20
2	L2	1023	C	O4'-C1'-N1	5.05	112.24	108.20
51	S1	784	C	C2-N1-C1'	5.04	124.34	118.80
51	S1	1672	C	OP1-P-O3'	5.04	116.28	105.20
8	L8	39	C	C2-N1-C1'	5.03	124.34	118.80
3	L3	188	C	C2-N1-C1'	5.03	124.33	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	832	C	O4'-C1'-N1	5.02	112.22	108.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	LE	155	ARG	Sidechain
17	LI	157	ARG	Sidechain
25	LQ	117	ARG	Sidechain
34	LZ	13	ARG	Sidechain
34	LZ	22	ARG	Sidechain
49	Lo	4	ARG	Sidechain
58	SC	172	ARG	Sidechain
73	SR	32	ARG	Sidechain
87	Sf	78	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	LA	253/260 (97%)	246 (97%)	7 (3%)	0	100	100
10	LB	399/419 (95%)	391 (98%)	8 (2%)	0	100	100
11	LC	364/373 (98%)	352 (97%)	12 (3%)	0	100	100
12	LD	173/188 (92%)	169 (98%)	4 (2%)	0	100	100
13	LE	184/190 (97%)	177 (96%)	7 (4%)	0	100	100
14	LF	145/195 (74%)	138 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	LG	240/264 (91%)	238 (99%)	2 (1%)	0	100	100
16	LH	219/222 (99%)	215 (98%)	4 (2%)	0	100	100
17	LI	206/220 (94%)	202 (98%)	3 (2%)	1 (0%)	29	66
18	LJ	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
19	LK	167/175 (95%)	163 (98%)	4 (2%)	0	100	100
20	LL	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
21	LM	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
22	LN	195/213 (92%)	191 (98%)	4 (2%)	0	100	100
23	LO	284/305 (93%)	279 (98%)	5 (2%)	0	100	100
24	LP	195/198 (98%)	191 (98%)	4 (2%)	0	100	100
25	LQ	199/254 (78%)	199 (100%)	0	0	100	100
26	LR	176/179 (98%)	176 (100%)	0	0	100	100
27	LS	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
28	LT	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
29	LU	120/129 (93%)	117 (98%)	3 (2%)	0	100	100
30	LV	117/145 (81%)	116 (99%)	1 (1%)	0	100	100
31	LW	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
32	LX	81/124 (65%)	78 (96%)	3 (4%)	0	100	100
33	LY	131/134 (98%)	129 (98%)	2 (2%)	0	100	100
34	LZ	143/147 (97%)	140 (98%)	3 (2%)	0	100	100
35	La	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
36	Lb	66/70 (94%)	62 (94%)	4 (6%)	0	100	100
37	Lc	227/252 (90%)	222 (98%)	5 (2%)	0	100	100
38	Ld	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
39	Le	184/188 (98%)	182 (99%)	2 (1%)	0	100	100
40	Lf	126/133 (95%)	123 (98%)	3 (2%)	0	100	100
41	Lg	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
42	Lh	125/168 (74%)	123 (98%)	2 (2%)	0	100	100
43	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
44	Lj	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
45	Lk	76/83 (92%)	76 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	Ll	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
47	Lm	49/128 (38%)	49 (100%)	0	0	100	100
48	Ln	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
49	Lo	87/92 (95%)	80 (92%)	5 (6%)	2 (2%)	6	28
50	Lp	95/106 (90%)	93 (98%)	2 (2%)	0	100	100
56	SA	234/264 (89%)	225 (96%)	9 (4%)	0	100	100
57	SB	209/246 (85%)	203 (97%)	6 (3%)	0	100	100
58	SC	210/219 (96%)	208 (99%)	2 (1%)	0	100	100
59	SD	181/190 (95%)	180 (99%)	1 (1%)	0	100	100
60	SE	258/273 (94%)	251 (97%)	7 (3%)	0	100	100
61	SF	216/265 (82%)	214 (99%)	2 (1%)	0	100	100
62	SG	243/249 (98%)	239 (98%)	4 (2%)	0	100	100
63	SH	178/190 (94%)	176 (99%)	2 (1%)	0	100	100
64	SI	198/200 (99%)	196 (99%)	2 (1%)	0	100	100
65	SJ	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
66	SK	194/220 (88%)	194 (100%)	0	0	100	100
67	SL	142/149 (95%)	138 (97%)	4 (3%)	0	100	100
68	SM	100/116 (86%)	95 (95%)	5 (5%)	0	100	100
69	SN	97/168 (58%)	94 (97%)	3 (3%)	0	100	100
70	SO	134/144 (93%)	129 (96%)	5 (4%)	0	100	100
71	SP	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
72	SQ	94/141 (67%)	89 (95%)	5 (5%)	0	100	100
73	SR	125/153 (82%)	123 (98%)	2 (2%)	0	100	100
74	SS	54/57 (95%)	54 (100%)	0	0	100	100
75	ST	140/151 (93%)	138 (99%)	2 (1%)	0	100	100
76	SU	151/173 (87%)	147 (97%)	4 (3%)	0	100	100
77	SV	120/143 (84%)	118 (98%)	2 (2%)	0	100	100
78	SW	113/152 (74%)	111 (98%)	2 (2%)	0	100	100
79	SX	150/161 (93%)	147 (98%)	3 (2%)	0	100	100
80	SY	86/164 (52%)	85 (99%)	1 (1%)	0	100	100
81	SZ	128/137 (93%)	126 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
82	Sa	70/120 (58%)	68 (97%)	2 (3%)	0	100	100
83	Sb	102/112 (91%)	102 (100%)	0	0	100	100
84	Sc	83/86 (96%)	79 (95%)	4 (5%)	0	100	100
85	Sd	64/87 (74%)	63 (98%)	1 (2%)	0	100	100
86	Se	56/66 (85%)	55 (98%)	1 (2%)	0	100	100
87	Sf	40/152 (26%)	38 (95%)	2 (5%)	0	100	100
88	Sg	293/312 (94%)	289 (99%)	4 (1%)	0	100	100
89	Sh	101/235 (43%)	100 (99%)	1 (1%)	0	100	100
All	All	11374/12926 (88%)	11132 (98%)	239 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	Lo	51	ALA
17	LI	66	PRO
49	Lo	52	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	
9	LA	197/204 (97%)	193 (98%)	4 (2%)	55	81
10	LB	329/351 (94%)	313 (95%)	16 (5%)	25	59
11	LC	289/301 (96%)	265 (92%)	24 (8%)	11	37
12	LD	131/162 (81%)	118 (90%)	13 (10%)	8	28
13	LE	164/172 (95%)	151 (92%)	13 (8%)	12	39
14	LF	122/153 (80%)	112 (92%)	10 (8%)	11	37
15	LG	196/221 (89%)	185 (94%)	11 (6%)	21	54
16	LH	181/188 (96%)	166 (92%)	15 (8%)	11	37
17	LI	170/183 (93%)	165 (97%)	5 (3%)	42	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	LJ	105/111 (95%)	101 (96%)	4 (4%)	33	67
19	LK	136/145 (94%)	129 (95%)	7 (5%)	24	57
20	LL	113/114 (99%)	107 (95%)	6 (5%)	22	56
21	LM	178/180 (99%)	170 (96%)	8 (4%)	27	62
22	LN	168/179 (94%)	153 (91%)	15 (9%)	9	33
23	LO	210/242 (87%)	201 (96%)	9 (4%)	29	64
24	LP	162/164 (99%)	152 (94%)	10 (6%)	18	50
25	LQ	169/198 (85%)	164 (97%)	5 (3%)	41	73
26	LR	157/159 (99%)	147 (94%)	10 (6%)	17	49
27	LS	128/134 (96%)	117 (91%)	11 (9%)	10	35
28	LT	128/143 (90%)	122 (95%)	6 (5%)	26	61
29	LU	92/114 (81%)	84 (91%)	8 (9%)	10	35
30	LV	100/124 (81%)	97 (97%)	3 (3%)	41	73
31	LW	101/122 (83%)	94 (93%)	7 (7%)	15	46
32	LX	74/104 (71%)	73 (99%)	1 (1%)	67	86
33	LY	111/116 (96%)	105 (95%)	6 (5%)	22	55
34	LZ	113/118 (96%)	105 (93%)	8 (7%)	14	44
35	La	114/118 (97%)	109 (96%)	5 (4%)	28	63
36	Lb	56/58 (97%)	51 (91%)	5 (9%)	9	33
37	Lc	191/209 (91%)	186 (97%)	5 (3%)	46	76
38	Ld	85/89 (96%)	78 (92%)	7 (8%)	11	37
39	Le	154/158 (98%)	144 (94%)	10 (6%)	17	48
40	Lf	111/115 (96%)	107 (96%)	4 (4%)	35	68
41	Lg	120/121 (99%)	116 (97%)	4 (3%)	38	71
42	Lh	107/146 (73%)	102 (95%)	5 (5%)	26	61
43	Li	84/88 (96%)	81 (96%)	3 (4%)	35	68
44	Lj	68/70 (97%)	65 (96%)	3 (4%)	28	63
45	Lk	57/74 (77%)	56 (98%)	1 (2%)	59	83
46	Ll	46/47 (98%)	45 (98%)	1 (2%)	52	80
47	Lm	41/113 (36%)	37 (90%)	4 (10%)	8	29
48	Ln	30/32 (94%)	27 (90%)	3 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	Lo	69/74 (93%)	65 (94%)	4 (6%)	20	53
50	Lp	82/92 (89%)	73 (89%)	9 (11%)	6	23
56	SA	205/222 (92%)	194 (95%)	11 (5%)	22	55
57	SB	175/202 (87%)	165 (94%)	10 (6%)	20	54
58	SC	170/184 (92%)	158 (93%)	12 (7%)	14	44
59	SD	158/164 (96%)	150 (95%)	8 (5%)	24	57
60	SE	216/225 (96%)	211 (98%)	5 (2%)	50	79
61	SF	174/208 (84%)	167 (96%)	7 (4%)	31	66
62	SG	201/208 (97%)	186 (92%)	15 (8%)	13	41
63	SH	150/159 (94%)	148 (99%)	2 (1%)	69	88
64	SI	179/186 (96%)	170 (95%)	9 (5%)	24	58
65	SJ	110/111 (99%)	103 (94%)	7 (6%)	17	49
66	SK	162/176 (92%)	150 (93%)	12 (7%)	13	42
67	SL	116/120 (97%)	108 (93%)	8 (7%)	15	46
68	SM	92/104 (88%)	87 (95%)	5 (5%)	22	55
69	SN	86/128 (67%)	82 (95%)	4 (5%)	26	61
70	SO	101/113 (89%)	92 (91%)	9 (9%)	9	33
71	SP	113/117 (97%)	100 (88%)	13 (12%)	5	22
72	SQ	56/120 (47%)	49 (88%)	7 (12%)	4	18
73	SR	105/130 (81%)	96 (91%)	9 (9%)	10	35
74	SS	46/49 (94%)	43 (94%)	3 (6%)	17	48
75	ST	125/132 (95%)	116 (93%)	9 (7%)	14	43
76	SU	134/152 (88%)	122 (91%)	12 (9%)	9	33
77	SV	96/126 (76%)	92 (96%)	4 (4%)	30	64
78	SW	97/130 (75%)	91 (94%)	6 (6%)	18	50
79	SX	122/131 (93%)	117 (96%)	5 (4%)	30	65
80	SY	71/116 (61%)	66 (93%)	5 (7%)	15	45
81	SZ	111/118 (94%)	105 (95%)	6 (5%)	22	55
82	Sa	64/95 (67%)	53 (83%)	11 (17%)	2	9
83	Sb	85/93 (91%)	78 (92%)	7 (8%)	11	37
84	Sc	75/76 (99%)	71 (95%)	4 (5%)	22	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
85	Sd	48/75 (64%)	42 (88%)	6 (12%)	4	18
86	Se	50/54 (93%)	47 (94%)	3 (6%)	19	51
87	Sf	19/126 (15%)	18 (95%)	1 (5%)	22	56
88	Sg	258/265 (97%)	227 (88%)	31 (12%)	5	20
89	Sh	85/177 (48%)	70 (82%)	15 (18%)	2	9
All	All	9494/10798 (88%)	8905 (94%)	589 (6%)	22	50

All (589) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	LA	18	VAL
9	LA	157	SER
9	LA	161	THR
9	LA	185	SER
10	LB	5	LYS
10	LB	26	ARG
10	LB	40	LYS
10	LB	44	THR
10	LB	79	LEU
10	LB	87	VAL
10	LB	148	ARG
10	LB	171	LEU
10	LB	211	ASP
10	LB	282	GLN
10	LB	305	TYR
10	LB	307	LEU
10	LB	323	THR
10	LB	341	ARG
10	LB	360	LYS
10	LB	380	LYS
11	LC	4	ARG
11	LC	6	SER
11	LC	11	SER
11	LC	55	ARG
11	LC	56	LEU
11	LC	70	ARG
11	LC	84	SER
11	LC	94	MET
11	LC	107	PHE
11	LC	121	PHE

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Mol	Chain	Res	Type
11	LC	124	VAL
11	LC	138	SER
11	LC	169	PHE
11	LC	182	VAL
11	LC	192	ARG
11	LC	217	ARG
11	LC	259	ASP
11	LC	271	VAL
11	LC	309	LYS
11	LC	333	VAL
11	LC	343	MET
11	LC	344	ARG
11	LC	354	LYS
11	LC	365	LYS
12	LD	13	GLU
12	LD	19	LEU
12	LD	20	CYS
12	LD	53	ARG
12	LD	58	THR
12	LD	63	ARG
12	LD	71	CYS
12	LD	77	LYS
12	LD	89	LYS
12	LD	94	LYS
12	LD	157	THR
12	LD	159	GLU
12	LD	178	LYS
13	LE	6	SER
13	LE	16	VAL
13	LE	17	THR
13	LE	46	ARG
13	LE	50	LYS
13	LE	56	VAL
13	LE	85	LYS
13	LE	137	SER
13	LE	140	LYS
13	LE	141	ASP
13	LE	172	ARG
13	LE	176	ASP
13	LE	182	THR
14	LF	22	LYS
14	LF	80	ASP

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Mol	Chain	Res	Type
14	LF	81	SER
14	LF	84	VAL
14	LF	98	THR
14	LF	108	ARG
14	LF	148	ASP
14	LF	152	GLN
14	LF	154	GLN
14	LF	172	LYS
15	LG	45	ARG
15	LG	66	LEU
15	LG	88	ARG
15	LG	118	LYS
15	LG	119	LYS
15	LG	122	LYS
15	LG	128	LYS
15	LG	175	LYS
15	LG	183	ASP
15	LG	232	ARG
15	LG	233	GLN
16	LH	19	LYS
16	LH	30	LYS
16	LH	64	THR
16	LH	67	ARG
16	LH	83	ASN
16	LH	85	THR
16	LH	86	LYS
16	LH	136	ARG
16	LH	149	ARG
16	LH	155	THR
16	LH	160	MET
16	LH	162	LYS
16	LH	169	SER
16	LH	177	LYS
16	LH	184	SER
17	LI	68	VAL
17	LI	137	LYS
17	LI	169	PRO
17	LI	202	THR
17	LI	206	ARG
18	LJ	29	ASP
18	LJ	53	SER
18	LJ	65	LYS

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Mol	Chain	Res	Type
18	LJ	114	SER
19	LK	3	LYS
19	LK	4	SER
19	LK	60	LYS
19	LK	137	VAL
19	LK	147	MET
19	LK	149	LYS
19	LK	166	LYS
20	LL	8	CYS
20	LL	39	HIS
20	LL	60	HIS
20	LL	79	SER
20	LL	128	LYS
20	LL	144	GLN
21	LM	46	GLU
21	LM	108	LYS
21	LM	117	ASN
21	LM	154	SER
21	LM	155	VAL
21	LM	159	ARG
21	LM	188	TYR
21	LM	189	ARG
22	LN	32	ARG
22	LN	43	VAL
22	LN	44	ASP
22	LN	51	HIS
22	LN	69	ARG
22	LN	79	ARG
22	LN	82	LYS
22	LN	116	ARG
22	LN	125	VAL
22	LN	137	SER
22	LN	158	LYS
22	LN	162	ARG
22	LN	175	ASN
22	LN	192	GLN
22	LN	193	ARG
23	LO	3	PHE
23	LO	15	ARG
23	LO	33	ARG
23	LO	59	ASP
23	LO	108	ARG

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Mol	Chain	Res	Type
23	LO	195	SER
23	LO	204	ARG
23	LO	226	ASP
23	LO	261	SER
24	LP	14	VAL
24	LP	56	ARG
24	LP	57	SER
24	LP	115	SER
24	LP	128	LEU
24	LP	135	MET
24	LP	144	TYR
24	LP	162	SER
24	LP	178	LYS
24	LP	190	TYR
25	LQ	13	SER
25	LQ	27	ASN
25	LQ	116	ASP
25	LQ	165	ARG
25	LQ	185	ARG
26	LR	16	SER
26	LR	19	GLU
26	LR	41	SER
26	LR	59	ASP
26	LR	62	SER
26	LR	65	VAL
26	LR	114	SER
26	LR	119	ARG
26	LR	150	SER
26	LR	173	THR
27	LS	4	SER
27	LS	46	SER
27	LS	61	THR
27	LS	64	VAL
27	LS	66	ASN
27	LS	80	VAL
27	LS	83	ARG
27	LS	84	THR
27	LS	98	LYS
27	LS	131	SER
27	LS	148	ARG
28	LT	11	SER
28	LT	13	LYS

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Mol	Chain	Res	Type
28	LT	23	ARG
28	LT	57	CYS
28	LT	75	GLU
28	LT	96	LYS
29	LU	5	ARG
29	LU	23	LYS
29	LU	70	LEU
29	LU	73	ASN
29	LU	75	ASN
29	LU	76	VAL
29	LU	99	LYS
29	LU	118	GLN
30	LV	34	GLN
30	LV	39	HIS
30	LV	52	ARG
31	LW	11	LYS
31	LW	41	ASN
31	LW	43	ARG
31	LW	71	TYR
31	LW	99	SER
31	LW	112	ARG
31	LW	118	ARG
32	LX	30	LYS
33	LY	3	LYS
33	LY	29	SER
33	LY	47	LYS
33	LY	60	GLN
33	LY	91	LYS
33	LY	103	SER
34	LZ	14	GLN
34	LZ	17	ARG
34	LZ	62	CYS
34	LZ	67	ASP
34	LZ	75	ARG
34	LZ	81	THR
34	LZ	93	SER
34	LZ	146	ARG
35	La	5	MET
35	La	9	ASP
35	La	14	SER
35	La	15	LYS
35	La	30	SER

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Mol	Chain	Res	Type
36	Lb	5	LYS
36	Lb	7	HIS
36	Lb	34	ARG
36	Lb	53	LYS
36	Lb	69	LYS
37	Lc	56	LEU
37	Lc	62	SER
37	Lc	123	ASN
37	Lc	236	ASP
37	Lc	237	TYR
38	Ld	7	SER
38	Ld	24	LYS
38	Ld	26	VAL
38	Ld	41	SER
38	Ld	90	CYS
38	Ld	92	LEU
38	Ld	101	ASP
39	Le	3	ARG
39	Le	6	MET
39	Le	23	ARG
39	Le	30	ARG
39	Le	32	ASN
39	Le	39	LYS
39	Le	51	LYS
39	Le	168	THR
39	Le	171	SER
39	Le	177	SER
40	Lf	31	SER
40	Lf	56	LYS
40	Lf	79	ASN
40	Lf	85	MET
41	Lg	20	LYS
41	Lg	21	THR
41	Lg	117	MET
41	Lg	125	SER
42	Lh	62	HIS
42	Lh	91	ARG
42	Lh	114	MET
42	Lh	115	LYS
42	Lh	117	SER
43	Li	2	SER
43	Li	71	ARG

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Mol	Chain	Res	Type
43	Li	78	LYS
44	Lj	3	LYS
44	Lj	24	ARG
44	Lj	43	SER
45	Lk	66	LYS
46	Ll	5	LYS
47	Lm	81	THR
47	Lm	105	VAL
47	Lm	119	SER
47	Lm	122	ARG
48	Ln	29	MET
48	Ln	33	SER
48	Ln	34	LYS
49	Lo	40	SER
49	Lo	41	PHE
49	Lo	42	CYS
49	Lo	80	ARG
50	Lp	2	VAL
50	Lp	20	HIS
50	Lp	24	LYS
50	Lp	29	LYS
50	Lp	32	LYS
50	Lp	78	LYS
50	Lp	88	THR
50	Lp	95	ASP
50	Lp	98	LYS
56	SA	22	GLU
56	SA	37	ASN
56	SA	46	THR
56	SA	64	ARG
56	SA	84	ARG
56	SA	109	THR
56	SA	110	ASP
56	SA	139	LEU
56	SA	215	ARG
56	SA	221	ARG
56	SA	232	SER
57	SB	12	ARG
57	SB	13	MET
57	SB	15	GLU
57	SB	31	ARG
57	SB	33	GLN

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Mol	Chain	Res	Type
57	SB	57	MET
57	SB	176	MET
57	SB	201	LYS
57	SB	203	ASP
57	SB	208	ARG
58	SC	19	GLU
58	SC	33	PHE
58	SC	37	SER
58	SC	55	ARG
58	SC	82	LYS
58	SC	98	MET
58	SC	115	ARG
58	SC	155	TYR
58	SC	159	SER
58	SC	172	ARG
58	SC	174	CYS
58	SC	200	SER
59	SD	15	ARG
59	SD	28	LYS
59	SD	49	SER
59	SD	70	LEU
59	SD	91	LYS
59	SD	93	ASP
59	SD	107	ARG
59	SD	121	VAL
60	SE	16	MET
60	SE	162	LYS
60	SE	227	LYS
60	SE	244	MET
60	SE	258	GLU
61	SF	90	ASP
61	SF	168	MET
61	SF	176	SER
61	SF	205	VAL
61	SF	208	VAL
61	SF	234	TYR
61	SF	248	SER
62	SG	13	VAL
62	SG	38	ASP
62	SG	75	SER
62	SG	101	ARG
62	SG	104	VAL

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Mol	Chain	Res	Type
62	SG	121	ASP
62	SG	135	ARG
62	SG	142	SER
62	SG	155	ASP
62	SG	172	ASP
62	SG	208	GLU
62	SG	227	ASP
62	SG	231	LYS
62	SG	236	VAL
62	SG	237	HIS
63	SH	67	ARG
63	SH	153	LYS
64	SI	9	ARG
64	SI	17	SER
64	SI	31	GLU
64	SI	53	LYS
64	SI	57	SER
64	SI	75	ARG
64	SI	79	ARG
64	SI	146	ARG
64	SI	147	THR
65	SJ	18	GLU
65	SJ	30	SER
65	SJ	36	LYS
65	SJ	55	ASP
65	SJ	81	CYS
65	SJ	118	SER
65	SJ	124	LYS
66	SK	21	HIS
66	SK	56	ARG
66	SK	77	ARG
66	SK	81	VAL
66	SK	88	ASN
66	SK	148	LYS
66	SK	167	ARG
66	SK	168	ASN
66	SK	169	HIS
66	SK	170	ARG
66	SK	219	LYS
66	SK	220	LYS
67	SL	9	LEU
67	SL	11	GLN

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Mol	Chain	Res	Type
67	SL	17	LYS
67	SL	33	CYS
67	SL	133	LYS
67	SL	134	LYS
67	SL	142	THR
67	SL	143	ARG
68	SM	15	GLN
68	SM	41	ARG
68	SM	43	GLU
68	SM	64	LYS
68	SM	107	VAL
69	SN	54	ARG
69	SN	82	TYR
69	SN	83	MET
69	SN	98	GLN
70	SO	15	LYS
70	SO	29	SER
70	SO	40	MET
70	SO	45	THR
70	SO	58	ASP
70	SO	77	ARG
70	SO	93	VAL
70	SO	133	THR
70	SO	135	ARG
71	SP	2	THR
71	SP	7	GLN
71	SP	15	ARG
71	SP	21	ARG
71	SP	29	ARG
71	SP	36	ARG
71	SP	67	ARG
71	SP	72	VAL
71	SP	77	ASN
71	SP	88	ASP
71	SP	100	VAL
71	SP	102	VAL
71	SP	105	PHE
72	SQ	35	GLN
72	SQ	45	ARG
72	SQ	61	MET
72	SQ	87	ASP
72	SQ	95	GLU

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Mol	Chain	Res	Type
72	SQ	107	ASP
72	SQ	112	VAL
73	SR	3	LEU
73	SR	17	LEU
73	SR	32	ARG
73	SR	60	LEU
73	SR	67	LYS
73	SR	70	GLU
73	SR	116	LYS
73	SR	122	ARG
73	SR	125	ARG
74	SS	9	SER
74	SS	15	MET
74	SS	57	ARG
75	ST	3	ARG
75	ST	30	SER
75	ST	48	SER
75	ST	53	GLU
75	ST	73	ARG
75	ST	87	ASP
75	ST	100	LYS
75	ST	104	ARG
75	ST	107	THR
76	SU	13	VAL
76	SU	16	THR
76	SU	21	LYS
76	SU	25	ARG
76	SU	44	SER
76	SU	51	LYS
76	SU	58	LYS
76	SU	92	SER
76	SU	101	ILE
76	SU	127	SER
76	SU	133	LYS
76	SU	153	ASN
77	SV	5	ARG
77	SV	23	LYS
77	SV	97	SER
77	SV	121	LYS
78	SW	25	ARG
78	SW	67	LEU
78	SW	72	LYS

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Mol	Chain	Res	Type
78	SW	74	VAL
78	SW	99	SER
78	SW	115	LYS
79	SX	13	LYS
79	SX	20	LYS
79	SX	21	ASP
79	SX	127	GLU
79	SX	138	ARG
80	SY	4	ILE
80	SY	15	ASP
80	SY	55	THR
80	SY	86	LYS
80	SY	89	LYS
81	SZ	27	GLN
81	SZ	76	THR
81	SZ	85	ASP
81	SZ	91	ARG
81	SZ	107	ARG
81	SZ	131	LYS
82	Sa	36	LEU
82	Sa	40	VAL
82	Sa	43	ASP
82	Sa	50	LEU
82	Sa	51	ARG
82	Sa	53	GLU
82	Sa	56	LYS
82	Sa	84	CYS
82	Sa	92	VAL
82	Sa	97	LYS
82	Sa	98	THR
83	Sb	21	LYS
83	Sb	32	THR
83	Sb	35	ASP
83	Sb	53	ARG
83	Sb	75	GLN
83	Sb	87	THR
83	Sb	88	VAL
84	Sc	35	ASP
84	Sc	60	CYS
84	Sc	63	LYS
84	Sc	65	CYS
85	Sd	38	ASN

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Mol	Chain	Res	Type
85	Sd	42	VAL
85	Sd	57	ARG
85	Sd	67	CYS
85	Sd	69	GLU
85	Sd	78	THR
86	Se	7	SER
86	Se	59	LYS
86	Se	64	LYS
87	Sf	74	LYS
88	Sg	8	LYS
88	Sg	13	TRP
88	Sg	34	ARG
88	Sg	46	ASP
88	Sg	60	ARG
88	Sg	64	HIS
88	Sg	95	ARG
88	Sg	103	PHE
88	Sg	104	LEU
88	Sg	115	PHE
88	Sg	123	VAL
88	Sg	146	ARG
88	Sg	147	ASP
88	Sg	151	ASP
88	Sg	155	SER
88	Sg	158	PHE
88	Sg	178	VAL
88	Sg	188	ARG
88	Sg	193	HIS
88	Sg	198	SER
88	Sg	200	VAL
88	Sg	208	LEU
88	Sg	209	CYS
88	Sg	227	GLU
88	Sg	233	ASN
88	Sg	240	GLN
88	Sg	243	PHE
88	Sg	256	ARG
88	Sg	268	VAL
88	Sg	272	LEU
88	Sg	305	VAL
89	Sh	133	GLU
89	Sh	147	SER

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Mol	Chain	Res	Type
89	Sh	156	LEU
89	Sh	157	PHE
89	Sh	166	ARG
89	Sh	169	ARG
89	Sh	185	LYS
89	Sh	189	GLU
89	Sh	201	ARG
89	Sh	207	ARG
89	Sh	215	ARG
89	Sh	216	GLN
89	Sh	227	ARG
89	Sh	228	HIS
89	Sh	229	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
14	LF	154	GLN
21	LM	171	HIS
22	LN	210	ASN
23	LO	94	ASN
26	LR	75	ASN
26	LR	145	HIS
28	LT	9	GLN
58	SC	74	GLN
66	SK	169	HIS
66	SK	194	GLN
68	SM	94	GLN
69	SN	98	GLN
77	SV	48	ASN
83	Sb	7	ASN
86	Se	60	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1648/1782 (92%)	571 (34%)	54 (3%)
2	L2	1139/1526 (74%)	369 (32%)	38 (3%)
3	L3	178/216 (82%)	66 (37%)	7 (3%)
4	L4	183/184 (99%)	60 (32%)	5 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L5	119/135 (88%)	37 (31%)	6 (5%)
51	S1	1809/2204 (82%)	632 (34%)	50 (2%)
52	S2	10/76 (13%)	5 (50%)	1 (10%)
53	S3	69/77 (89%)	27 (39%)	2 (2%)
54	S4	62/76 (81%)	37 (59%)	2 (3%)
55	S5	10/13 (76%)	4 (40%)	1 (10%)
6	L6	70/73 (95%)	40 (57%)	5 (7%)
7	L7	162/171 (94%)	58 (35%)	5 (3%)
8	L8	118/123 (95%)	27 (22%)	2 (1%)
All	All	5577/6656 (83%)	1933 (34%)	178 (3%)

All (1933) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	6	C
1	L1	7	C
1	L1	10	A
1	L1	16	G
1	L1	19	G
1	L1	20	G
1	L1	24	A
1	L1	29	C
1	L1	32	A
1	L1	38	A
1	L1	39	G
1	L1	41	A
1	L1	47	C
1	L1	53	G
1	L1	56	G
1	L1	57	G
1	L1	58	A
1	L1	63	A
1	L1	64	A
1	L1	65	A
1	L1	69	A2M
1	L1	70	C
1	L1	71	C
1	L1	72	G
1	L1	74	G
1	L1	84	G
1	L1	86	G
1	L1	87	A

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Mol	Chain	Res	Type
1	L1	91	G
1	L1	98	A
1	L1	104	G
1	L1	109	A
1	L1	110	A
1	L1	116	U
1	L1	119	C
1	L1	120	G
1	L1	121	A
1	L1	123	U
1	L1	126	G
1	L1	131	U
1	L1	133	C
1	L1	134	A
1	L1	135	A
1	L1	136	G
1	L1	141	U
1	L1	142	G
1	L1	143	A
1	L1	144	G
1	L1	146	U
1	L1	147	G
1	L1	154	A
1	L1	155	A
1	L1	156	A
1	L1	158	A
1	L1	160	C
1	L1	161	A
1	L1	162	U
1	L1	166	G
1	L1	167	U
1	L1	170	U
1	L1	171	U
1	L1	176	C
1	L1	182	U
1	L1	188	A
1	L1	191	U
1	L1	192	C
1	L1	195	G
1	L1	199	A
1	L1	200	A
1	L1	201	A

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Mol	Chain	Res	Type
1	L1	202	G
1	L1	203	C
1	L1	204	A
1	L1	205	A
1	L1	206	A
1	L1	209	C
1	L1	212	U
1	L1	215	U
1	L1	216	G
1	L1	218	A
1	L1	219	U
1	L1	220	A
1	L1	222	A
1	L1	223	A
1	L1	225	C
1	L1	226	C
1	L1	230	A
1	L1	233	U
1	L1	234	G
1	L1	235	A2M
1	L1	236	G
1	L1	237	U
1	L1	240	U
1	L1	243	G
1	L1	248	A
1	L1	249	G
1	L1	250	A
1	L1	251	A
1	L1	256	U
1	L1	264	U
1	L1	268	G
1	L1	272	U
1	L1	273	A
1	L1	280	A
1	L1	281	G
1	L1	283	G
1	L1	293	C
1	L1	301	A
1	L1	305	A2M
1	L1	306	G
1	L1	322	A
1	L1	323	U

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Mol	Chain	Res	Type
1	L1	324	G
1	L1	332	A
1	L1	335	U
1	L1	336	U
1	L1	337	G
1	L1	342	G
1	L1	343	U
1	L1	344	A
1	L1	348	G
1	L1	357	A
1	L1	367	A
1	L1	368	G
1	L1	369	A
1	L1	371	U
1	L1	373	G
1	L1	374	G
1	L1	376	A
1	L1	377	G
1	L1	378	A
1	L1	382	A
1	L1	383	U
1	L1	392	A
1	L1	406	A
1	L1	408	G
1	L1	409	U
1	L1	410	U
1	L1	413	A
1	L1	414	A
1	L1	416	A
1	L1	417	G
1	L1	419	A
1	L1	431	G
1	L1	434	U
1	L1	438	A
1	L1	439	U
1	L1	443	A
1	L1	444	C
1	L1	447	G
1	L1	448	A
1	L1	454	U
1	L1	461	G
1	L1	463	C

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Mol	Chain	Res	Type
1	L1	464	A
1	L1	471	G
1	L1	477	C
1	L1	484	A
1	L1	485	A
1	L1	486	C
1	L1	487	G
1	L1	488	G
1	L1	494	A
1	L1	495	C
1	L1	496	C
1	L1	500	C
1	L1	502	U
1	L1	503	A
1	L1	510	PSU
1	L1	511	A
1	L1	512	U
1	L1	518	C
1	L1	520	G
1	L1	522	G
1	L1	525	C
1	L1	527	A
1	L1	534	G
1	L1	535	C
1	L1	537	G
1	L1	539	C
1	L1	541	A
1	L1	542	C
1	L1	546	G
1	L1	547	U
1	L1	551	A
1	L1	553	A
1	L1	554	A
1	L1	555	U
1	L1	557	U
1	L1	558	U
1	L1	559	G
1	L1	563	C
1	L1	564	U
1	L1	565	U
1	L1	568	U
1	L1	569	G

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Mol	Chain	Res	Type
1	L1	571	A
1	L1	572	A
1	L1	573	U
1	L1	575	A
1	L1	576	G
1	L1	577	C
1	L1	578	G
1	L1	580	A
1	L1	584	U
1	L1	585	U
1	L1	586	U
1	L1	587	G
1	L1	589	G
1	L1	592	G
1	L1	597	C
1	L1	606	C
1	L1	609	C
1	L1	610	A
1	L1	611	C
1	L1	612	G
1	L1	613	C
1	L1	616	U
1	L1	617	G
1	L1	620	U
1	L1	621	U
1	L1	622	C
1	L1	623	U
1	L1	625	C
1	L1	627	C
1	L1	631	G
1	L1	632	A
1	L1	633	U
1	L1	634	G
1	L1	635	C
1	L1	644	G
1	L1	649	U
1	L1	650	G
1	L1	651	G
1	L1	652	A
1	L1	653	A
1	L1	655	U
1	L1	662	C

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Mol	Chain	Res	Type
1	L1	663	C
1	L1	664	C
1	L1	666	C
1	L1	668	C
1	L1	669	C
1	L1	678	A2M
1	L1	681	A2M
1	L1	684	G
1	L1	685	A
1	L1	692	A
1	L1	709	A
1	L1	710	G
1	L1	717	G
1	L1	718	A
1	L1	719	U
1	L1	722	G
1	L1	729	A
1	L1	736	C
1	L1	737	U
1	L1	743	A
1	L1	750	G
1	L1	752	G
1	L1	753	A
1	L1	760	A
1	L1	762	A
1	L1	763	U
1	L1	764	G
1	L1	770	G
1	L1	771	U
1	L1	778	C
1	L1	783	G
1	L1	789	U
1	L1	790	C
1	L1	792	G
1	L1	794	U
1	L1	795	U
1	L1	803	C
1	L1	807	C
1	L1	810	C
1	L1	818	C
1	L1	823	G
1	L1	824	U

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Mol	Chain	Res	Type
1	L1	825	G
1	L1	828	U
1	L1	832	G
1	L1	835	G
1	L1	836	G
1	L1	838	G
1	L1	839	U
1	L1	849	U
1	L1	850	G
1	L1	851	G
1	L1	852	A
1	L1	856	OMG
1	L1	859	A
1	L1	867	A
1	L1	868	A
1	L1	869	C
1	L1	877	G
1	L1	886	G
1	L1	893	G
1	L1	894	G
1	L1	896	G
1	L1	897	A
1	L1	900	C
1	L1	905	G
1	L1	912	C
1	L1	925	U
1	L1	930	U
1	L1	935	A
1	L1	946	G
1	L1	947	A
1	L1	948	U
1	L1	957	C
1	L1	958	G
1	L1	959	OMG
1	L1	965	A
1	L1	966	A
1	L1	967	G
1	L1	968	A
1	L1	971	C
1	L1	972	A
1	L1	973	U
1	L1	974	C

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Mol	Chain	Res	Type
1	L1	975	G
1	L1	976	A
1	L1	985	G
1	L1	988	G
1	L1	989	C
1	L1	995	C
1	L1	1000	C
1	L1	1003	A
1	L1	1010	OMC
1	L1	1011	PSU
1	L1	1013	A
1	L1	1015	G
1	L1	1016	A
1	L1	1017	PSU
1	L1	1022	G
1	L1	1025	G
1	L1	1029	G
1	L1	1031	A
1	L1	1032	G
1	L1	1035	G
1	L1	1036	U
1	L1	1037	A
1	L1	1044	G
1	L1	1045	G
1	L1	1047	A
1	L1	1049	A
1	L1	1052	A
1	L1	1053	A
1	L1	1056	G
1	L1	1089	C
1	L1	1090	U
1	L1	1092	U
1	L1	1097	A
1	L1	1098	A
1	L1	1100	C
1	L1	1101	U
1	L1	1102	U
1	L1	1108	G
1	L1	1110	G
1	L1	1116	A
1	L1	1121	G
1	L1	1122	U

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Mol	Chain	Res	Type
1	L1	1123	G
1	L1	1128	A
1	L1	1129	G
1	L1	1134	C
1	L1	1135	U
1	L1	1136	G
1	L1	1138	A
1	L1	1141	G
1	L1	1144	G
1	L1	1146	A
1	L1	1147	A
1	L1	1148	A
1	L1	1149	G
1	L1	1150	A
1	L1	1154	G
1	L1	1155	A
1	L1	1156	A
1	L1	1159	A
1	L1	1161	A
1	L1	1162	G
1	L1	1163	G
1	L1	1164	C
1	L1	1165	A
1	L1	1169	A
1	L1	1170	G
1	L1	1171	PSU
1	L1	1172	G
1	L1	1174	G
1	L1	1175	C
1	L1	1176	C
1	L1	1177	PSU
1	L1	1178	U
1	L1	1179	C
1	L1	1182	C
1	L1	1186	A
1	L1	1188	G
1	L1	1192	A
1	L1	1198	C
1	L1	1201	U
1	L1	1202	G
1	L1	1205	G
1	L1	1207	A

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Mol	Chain	Res	Type
1	L1	1210	A
1	L1	1211	A
1	L1	1212	C
1	L1	1216	U
1	L1	1219	G
1	L1	1223	U
1	L1	1225	U
1	L1	1229	G
1	L1	1235	A
1	L1	1238	C
1	L1	1239	U
1	L1	1240	U
1	L1	1242	U
1	L1	1243	G
1	L1	1248	C
1	L1	1251	U
1	L1	1253	U
1	L1	1254	C
1	L1	1258	A
1	L1	1261	U
1	L1	1262	G
1	L1	1263	A
1	L1	1264	A
1	L1	1265	A
1	L1	1266	A
1	L1	1270	U
1	L1	1271	G
1	L1	1276	U
1	L1	1349	A
1	L1	1351	C
1	L1	1352	C
1	L1	1364	A
1	L1	1365	A
1	L1	1367	U
1	L1	1368	G
1	L1	1369	G
1	L1	1371	OMU
1	L1	1373	A2M
1	L1	1375	G
1	L1	1378	U
1	L1	1379	A
1	L1	1387	U

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Mol	Chain	Res	Type
1	L1	1388	U
1	L1	1389	A
1	L1	1390	G
1	L1	1391	U
1	L1	1393	A
1	L1	1395	U
1	L1	1396	G
1	L1	1400	A
1	L1	1401	U
1	L1	1402	U
1	L1	1404	U
1	L1	1412	G
1	L1	1413	U
1	L1	1414	A
1	L1	1416	G
1	L1	1420	G
1	L1	1421	G
1	L1	1422	A
1	L1	1423	A
1	L1	1426	A
1	L1	1427	A
1	L1	1429	U
1	L1	1435	A
1	L1	1438	A
1	L1	1439	A
1	L1	1444	A
1	L1	1445	G
1	L1	1455	U
1	L1	1456	G
1	L1	1464	G
1	L1	1479	A
1	L1	1480	C
1	L1	1481	G
1	L1	1482	A
1	L1	1483	A
1	L1	1485	C
1	L1	1488	A
1	L1	1489	U
1	L1	1490	G
1	L1	1495	G
1	L1	1497	G
1	L1	1504	A

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Mol	Chain	Res	Type
1	L1	1505	U
1	L1	1507	G
1	L1	1509	C
1	L1	1518	A
1	L1	1519	G
1	L1	1521	G
1	L1	1526	U
1	L1	1527	OMC
1	L1	1528	PSU
1	L1	1536	C
1	L1	1540	OMG
1	L1	1545	G
1	L1	1546	A
1	L1	1547	U
1	L1	1557	A
1	L1	1558	U
1	L1	1560	U
1	L1	1561	A
1	L1	1565	A
1	L1	1566	A
1	L1	1569	U
1	L1	1570	G
1	L1	1574	C
1	L1	1575	G
1	L1	1582	A
1	L1	1586	G
1	L1	1590	G
1	L1	1605	G
1	L1	1607	C
1	L1	1608	A
1	L1	1612	G
1	L1	1613	C
1	L1	1616	U
1	L1	1627	U
1	L1	1628	U
1	L1	1631	U
1	L1	1632	C
1	L1	1654	A
1	L1	1655	U
1	L1	1656	C
1	L1	1660	U
1	L1	1661	U

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Mol	Chain	Res	Type
1	L1	1662	G
1	L1	1663	U
1	L1	1666	G
1	L1	1667	G
1	L1	1668	A
1	L1	1671	G
1	L1	1672	U
1	L1	1675	A
1	L1	1676	G
1	L1	1683	C
1	L1	1713	A
1	L1	1715	U
1	L1	1716	G
1	L1	1726	G
1	L1	1727	A
1	L1	1729	A
1	L1	1734	G
1	L1	1737	A
1	L1	1739	A
1	L1	1740	G
1	L1	1742	G
1	L1	1743	A
1	L1	1744	A
1	L1	1747	U
1	L1	1750	G
1	L1	1753	U
1	L1	1756	A
1	L1	1757	U
1	L1	1758	U
1	L1	1759	C
1	L1	1762	A
1	L1	1763	A
1	L1	1764	A
1	L1	1766	G
1	L1	1770	U
1	L1	1771	U
1	L1	1772	G
1	L1	1773	C
1	L1	1774	A
2	L2	5	A
2	L2	13	A
2	L2	22	A

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Mol	Chain	Res	Type
2	L2	24	C
2	L2	25	A
2	L2	26	C
2	L2	29	C
2	L2	30	A
2	L2	33	A
2	L2	41	A
2	L2	47	A
2	L2	61	C
2	L2	62	A
2	L2	63	U
2	L2	68	A
2	L2	69	A
2	L2	75	C
2	L2	76	A
2	L2	80	A
2	L2	83	G
2	L2	85	A
2	L2	90	G
2	L2	96	U
2	L2	110	C
2	L2	118	G
2	L2	123	G
2	L2	125	C
2	L2	130	A
2	L2	137	A
2	L2	340	A
2	L2	342	U
2	L2	343	U
2	L2	348	A
2	L2	349	C
2	L2	358	G
2	L2	359	OMC
2	L2	365	G
2	L2	366	C
2	L2	368	G
2	L2	372	A
2	L2	377	A
2	L2	386	U
2	L2	388	A
2	L2	390	A
2	L2	391	A

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Mol	Chain	Res	Type
2	L2	392	C
2	L2	404	A
2	L2	406	G
2	L2	414	G
2	L2	415	U
2	L2	421	A
2	L2	423	A
2	L2	426	G
2	L2	427	C
2	L2	434	A
2	L2	435	U
2	L2	438	C
2	L2	439	U
2	L2	443	OMC
2	L2	444	A
2	L2	447	G
2	L2	451	U
2	L2	463	U
2	L2	478	A
2	L2	489	A
2	L2	492	G
2	L2	495	G
2	L2	503	C
2	L2	506	U
2	L2	507	G
2	L2	508	A
2	L2	511	C
2	L2	512	PSU
2	L2	515	U
2	L2	518	G
2	L2	519	G
2	L2	527	A2M
2	L2	528	U
2	L2	529	G
2	L2	530	C
2	L2	534	OMG
2	L2	544	U
2	L2	550	C
2	L2	552	C
2	L2	553	G
2	L2	554	C
2	L2	556	U

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Mol	Chain	Res	Type
2	L2	559	A
2	L2	561	G
2	L2	570	A2M
2	L2	571	G
2	L2	580	U
2	L2	581	G
2	L2	582	U
2	L2	601	G
2	L2	602	A
2	L2	610	G
2	L2	616	G
2	L2	619	A
2	L2	620	C
2	L2	621	G
2	L2	623	A
2	L2	624	C
2	L2	629	A
2	L2	632	G
2	L2	635	A
2	L2	636	A
2	L2	637	G
2	L2	639	G
2	L2	643	A
2	L2	647	A
2	L2	648	A
2	L2	649	G
2	L2	650	A
2	L2	651	C
2	L2	652	C
2	L2	657	U
2	L2	658	G
2	L2	664	G
2	L2	665	A2M
2	L2	668	C
2	L2	685	G
2	L2	686	OMG
2	L2	688	G
2	L2	695	G
2	L2	696	A
2	L2	697	G
2	L2	698	G
2	L2	745	G

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Mol	Chain	Res	Type
2	L2	746	A
2	L2	747	A
2	L2	749	G
2	L2	750	U
2	L2	751	U
2	L2	752	G
2	L2	758	C
2	L2	760	U
2	L2	768	G
2	L2	769	A
2	L2	772	A
2	L2	778	A
2	L2	779	U
2	L2	780	G
2	L2	782	G
2	L2	783	U
2	L2	784	U
2	L2	785	U
2	L2	787	G
2	L2	789	G
2	L2	793	U
2	L2	797	C
2	L2	799	G
2	L2	800	G
2	L2	802	PSU
2	L2	803	A
2	L2	804	U
2	L2	806	C
2	L2	808	C
2	L2	810	G
2	L2	811	U
2	L2	812	C
2	L2	818	U
2	L2	819	U
2	L2	823	A
2	L2	824	G
2	L2	849	C
2	L2	851	C
2	L2	954	A
2	L2	955	C
2	L2	963	U
2	L2	964	G

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Mol	Chain	Res	Type
2	L2	965	C
2	L2	970	A
2	L2	971	A
2	L2	973	U
2	L2	979	A
2	L2	984	G
2	L2	986	U
2	L2	998	G
2	L2	999	U
2	L2	1001	C
2	L2	1002	C
2	L2	1004	G
2	L2	1006	G
2	L2	1011	G
2	L2	1012	U
2	L2	1017	A
2	L2	1019	A
2	L2	1020	C
2	L2	1021	A
2	L2	1033	G
2	L2	1034	G
2	L2	1041	G
2	L2	1046	OMG
2	L2	1053	A
2	L2	1055	A
2	L2	1062	A
2	L2	1064	A
2	L2	1075	G
2	L2	1078	OMG
2	L2	1079	U
2	L2	1083	A
2	L2	1084	A
2	L2	1085	G
2	L2	1093	C
2	L2	1096	U
2	L2	1101	A
2	L2	1102	C
2	L2	1104	G
2	L2	1105	A
2	L2	1108	U
2	L2	1111	C
2	L2	1115	U

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Mol	Chain	Res	Type
2	L2	1116	A
2	L2	1117	G
2	L2	1118	A
2	L2	1121	A
2	L2	1123	A
2	L2	1129	A
2	L2	1130	A
2	L2	1131	A
2	L2	1132	A
2	L2	1133	G
2	L2	1137	G
2	L2	1140	U
2	L2	1141	G
2	L2	1143	U
2	L2	1147	C
2	L2	1148	G
2	L2	1154	C
2	L2	1155	A
2	L2	1156	G
2	L2	1157	U
2	L2	1158	A
2	L2	1162	A
2	L2	1171	G
2	L2	1172	C
2	L2	1176	A
2	L2	1178	C
2	L2	1179	A
2	L2	1180	A
2	L2	1181	G
2	L2	1189	A
2	L2	1193	U
2	L2	1199	A
2	L2	1200	A
2	L2	1201	G
2	L2	1203	A
2	L2	1204	U
2	L2	1206	G
2	L2	1207	G
2	L2	1209	A
2	L2	1215	A
2	L2	1216	A
2	L2	1219	A

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Mol	Chain	Res	Type
2	L2	1221	U
2	L2	1226	C
2	L2	1229	OMG
2	L2	1233	U
2	L2	1234	G
2	L2	1237	A
2	L2	1238	G
2	L2	1239	A
2	L2	1240	A
2	L2	1241	U
2	L2	1245	U
2	L2	1246	A
2	L2	1248	OMC
2	L2	1252	G
2	L2	1255	A
2	L2	1256	U
2	L2	1260	U
2	L2	1262	G
2	L2	1264	PSU
2	L2	1265	PSU
2	L2	1266	G
2	L2	1270	C
2	L2	1271	G
2	L2	1276	A
2	L2	1278	C
2	L2	1283	A
2	L2	1285	A
2	L2	1288	G
2	L2	1289	A
2	L2	1290	C
2	L2	1291	G
2	L2	1294	G
2	L2	1295	C
2	L2	1297	U
2	L2	1298	U
2	L2	1305	C
2	L2	1309	G
2	L2	1313	U
2	L2	1314	C
2	L2	1324	U
2	L2	1325	A
2	L2	1327	C

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Mol	Chain	Res	Type
2	L2	1329	U
2	L2	1332	C
2	L2	1336	G
2	L2	1337	C
2	L2	1342	G
2	L2	1347	U
2	L2	1348	A
2	L2	1349	A
2	L2	1350	G
2	L2	1356	G
2	L2	1361	U
2	L2	1371	G
2	L2	1373	C
2	L2	1374	A
2	L2	1376	G
2	L2	1379	A
2	L2	1380	C
2	L2	1381	G
2	L2	1385	G
2	L2	1388	G
2	L2	1389	G
2	L2	1391	U
2	L2	1408	C
2	L2	1409	A
2	L2	1410	G
2	L2	1416	U
2	L2	1421	C
2	L2	1423	C
2	L2	1425	A
2	L2	1426	C
2	L2	1427	U
2	L2	1428	U
2	L2	1430	G
2	L2	1433	G
2	L2	1434	G
2	L2	1436	A
2	L2	1437	A
2	L2	1439	U
2	L2	1440	G
2	L2	1441	C
2	L2	1443	A
2	L2	1444	G

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Mol	Chain	Res	Type
2	L2	1445	A
2	L2	1446	A
2	L2	1447	A
2	L2	1448	A
2	L2	1449	A
2	L2	1450	G
2	L2	1453	U
2	L2	1454	A
2	L2	1455	U
2	L2	1456	C
2	L2	1457	C
2	L2	1459	U
2	L2	1461	C
2	L2	1462	A
2	L2	1463	A
2	L2	1464	A
2	L2	1465	G
2	L2	1474	G
2	L2	1479	G
2	L2	1484	U
2	L2	1485	G
2	L2	1486	G
2	L2	1494	G
2	L2	1498	G
2	L2	1506	G
2	L2	1510	A
2	L2	1511	U
2	L2	1512	G
2	L2	1513	G
2	L2	1514	U
3	L3	6	G
3	L3	15	C
3	L3	16	G
3	L3	17	A
3	L3	19	A
3	L3	20	C
3	L3	21	A
3	L3	22	C
3	L3	24	U
3	L3	25	G
3	L3	26	C
3	L3	34	C

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Mol	Chain	Res	Type
3	L3	35	A
3	L3	39	C
3	L3	41	A
3	L3	45	U
3	L3	46	C
3	L3	48	C
3	L3	49	A
3	L3	51	G
3	L3	52	G
3	L3	59	U
3	L3	61	C
3	L3	63	U
3	L3	64	U
3	L3	70	A
3	L3	71	U
3	L3	74	U
3	L3	99	U
3	L3	109	U
3	L3	110	U
3	L3	111	A
3	L3	112	C
3	L3	113	U
3	L3	114	U
3	L3	117	C
3	L3	121	U
3	L3	124	U
3	L3	125	U
3	L3	129	A
3	L3	130	G
3	L3	131	C
3	L3	132	G
3	L3	136	G
3	L3	142	G
3	L3	143	A
3	L3	146	G
3	L3	149	A
3	L3	150	A
3	L3	151	A
3	L3	169	A
3	L3	173	U
3	L3	182	U
3	L3	187	U

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Mol	Chain	Res	Type
3	L3	192	G
3	L3	193	C
3	L3	194	A
3	L3	195	U
3	L3	196	U
3	L3	199	A
3	L3	200	G
3	L3	202	A
3	L3	210	G
3	L3	213	G
3	L3	214	U
3	L3	216	U
4	L4	7	U
4	L4	8	U
4	L4	9	G
4	L4	10	U
4	L4	11	G
4	L4	16	G
4	L4	18	U
4	L4	19	C
4	L4	20	U
4	L4	24	A
4	L4	31	G
4	L4	39	A
4	L4	40	G
4	L4	50	G
4	L4	51	U
4	L4	58	G
4	L4	60	A
4	L4	61	A
4	L4	62	C
4	L4	67	A
4	L4	76	C
4	L4	77	U
4	L4	83	U
4	L4	84	U
4	L4	85	C
4	L4	86	U
4	L4	87	G
4	L4	89	G
4	L4	90	G
4	L4	97	G

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Mol	Chain	Res	Type
4	L4	102	G
4	L4	106	G
4	L4	108	G
4	L4	114	A
4	L4	115	A
4	L4	120	U
4	L4	121	C
4	L4	128	U
4	L4	132	U
4	L4	133	C
4	L4	137	G
4	L4	143	C
4	L4	144	G
4	L4	145	C
4	L4	149	U
4	L4	150	A
4	L4	151	A
4	L4	153	C
4	L4	154	C
4	L4	157	A
4	L4	158	A
4	L4	159	G
4	L4	163	A
4	L4	166	C
4	L4	168	A
4	L4	169	A
4	L4	170	G
4	L4	173	C
4	L4	178	G
4	L4	180	C
5	L5	3	U
5	L5	6	G
5	L5	15	C
5	L5	23	A
5	L5	24	G
5	L5	26	A
5	L5	27	C
5	L5	29	U
5	L5	30	G
5	L5	39	G
5	L5	45	A
5	L5	50	C

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Mol	Chain	Res	Type
5	L5	51	A
5	L5	52	U
5	L5	53	G
5	L5	54	C
5	L5	61	C
5	L5	64	G
5	L5	65	U
5	L5	68	G
5	L5	73	G
5	L5	86	G
5	L5	88	C
5	L5	92	A
5	L5	99	G
5	L5	105	U
5	L5	106	G
5	L5	107	A
5	L5	108	G
5	L5	109	G
5	L5	113	G
5	L5	117	A
5	L5	118	U
5	L5	119	U
5	L5	120	C
5	L5	126	C
5	L5	135	C
6	L6	7	A
6	L6	10	C
6	L6	11	G
6	L6	14	A
6	L6	15	C
6	L6	22	G
6	L6	23	A
6	L6	24	C
6	L6	25	U
6	L6	26	G
6	L6	29	G
6	L6	31	U
6	L6	32	U
6	L6	33	G
6	L6	39	U
6	L6	40	C
6	L6	41	G

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Mol	Chain	Res	Type
6	L6	42	A
6	L6	43	A
6	L6	44	G
6	L6	48	C
6	L6	49	C
6	L6	50	A
6	L6	51	A
6	L6	52	G
6	L6	53	U
6	L6	54	A
6	L6	56	A
6	L6	57	U
6	L6	58	U
6	L6	62	G
6	L6	64	U
6	L6	65	C
6	L6	67	C
6	L6	68	A
6	L6	69	A
6	L6	70	G
6	L6	71	A
6	L6	72	C
6	L6	73	A
7	L7	3	C
7	L7	5	U
7	L7	12	A
7	L7	15	G
7	L7	16	A
7	L7	17	U
7	L7	18	G
7	L7	19	A
7	L7	22	U
7	L7	31	A
7	L7	32	U
7	L7	33	U
7	L7	34	U
7	L7	38	U
7	L7	51	A
7	L7	53	A
7	L7	59	A
7	L7	61	A
7	L7	62	A

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Mol	Chain	Res	Type
7	L7	63	G
7	L7	67	U
7	L7	68	A
7	L7	69	PSU
7	L7	71	A
7	L7	72	A
7	L7	77	A
7	L7	80	A
7	L7	81	U
7	L7	82	C
7	L7	84	U
7	L7	87	A
7	L7	88	A
7	L7	89	U
7	L7	94	G
7	L7	95	A
7	L7	96	A
7	L7	100	U
7	L7	103	A
7	L7	104	A
7	L7	105	C
7	L7	107	C
7	L7	110	A
7	L7	112	G
7	L7	115	G
7	L7	116	C
7	L7	120	G
7	L7	124	A
7	L7	125	A
7	L7	127	C
7	L7	128	U
7	L7	153	C
7	L7	156	A
7	L7	157	U
7	L7	158	U
7	L7	164	U
7	L7	167	C
7	L7	169	A
7	L7	170	A
8	L8	6	A
8	L8	11	G
8	L8	14	C

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Mol	Chain	Res	Type
8	L8	21	G
8	L8	22	A
8	L8	25	G
8	L8	26	A
8	L8	30	C
8	L8	37	U
8	L8	39	C
8	L8	42	U
8	L8	45	G
8	L8	46	A
8	L8	52	G
8	L8	57	U
8	L8	58	A
8	L8	59	A
8	L8	67	C
8	L8	68	A
8	L8	76	U
8	L8	80	U
8	L8	93	G
8	L8	94	A
8	L8	101	G
8	L8	104	A
8	L8	114	G
8	L8	117	G
51	S1	3	U
51	S1	8	OMU
51	S1	17	C
51	S1	25	C
51	S1	26	A
51	S1	34	G
51	S1	40	A
51	S1	42	G
51	S1	45	U
51	S1	46	U
51	S1	47	A
51	S1	61	C
51	S1	62	A
51	S1	65	A
51	S1	66	U
51	S1	67	C
51	S1	68	A
51	S1	82	A

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Mol	Chain	Res	Type
51	S1	98	A2M
51	S1	102	A
51	S1	103	A
51	S1	109	C
51	S1	110	G
51	S1	112	A
51	S1	113	A
51	S1	114	U
51	S1	117	G
51	S1	119	C
51	S1	122	A
51	S1	128	C
51	S1	129	U
51	S1	133	G
51	S1	144	A
51	S1	145	A
51	S1	146	U
51	S1	147	U
51	S1	148	G
51	S1	151	U
51	S1	152	A
51	S1	158	G
51	S1	162	A
51	S1	164	C
51	S1	165	G
51	S1	167	C
51	S1	168	A
51	S1	170	G
51	S1	176	A
51	S1	181	A
51	S1	182	A
51	S1	192	U
51	S1	194	U
51	S1	195	U
51	S1	198	C
51	S1	199	C
51	S1	227	U
51	S1	228	G
51	S1	232	C
51	S1	234	C
51	S1	235	C
51	S1	237	A

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Mol	Chain	Res	Type
51	S1	238	G
51	S1	246	A
51	S1	249	A
51	S1	252	G
51	S1	253	U
51	S1	255	A
51	S1	256	A
51	S1	257	A
51	S1	264	C
51	S1	265	C
51	S1	275	A
51	S1	276	G
51	S1	277	U
51	S1	278	A
51	S1	279	A
51	S1	281	A
51	S1	282	C
51	S1	285	A
51	S1	286	G
51	S1	287	C
51	S1	288	A
51	S1	289	G
51	S1	290	U
51	S1	295	A
51	S1	296	C
51	S1	297	U
51	S1	298	C
51	S1	306	U
51	S1	308	C
51	S1	309	G
51	S1	310	U
51	S1	315	A
51	S1	316	A
51	S1	321	G
51	S1	322	C
51	S1	323	U
51	S1	324	U
51	S1	325	G
51	S1	326	U
51	S1	327	U
51	S1	328	C
51	S1	329	C

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Mol	Chain	Res	Type
51	S1	330	G
51	S1	332	C
51	S1	340	G
51	S1	341	A
51	S1	343	G
51	S1	352	C
51	S1	356	A
51	S1	357	U
51	S1	358	C
51	S1	360	G
51	S1	363	G
51	S1	364	G
51	S1	365	U
51	S1	367	A
51	S1	376	U
51	S1	377	A
51	S1	378	G
51	S1	379	U
51	S1	381	G
51	S1	382	A
51	S1	388	A
51	S1	395	U
51	S1	396	G
51	S1	403	G
51	S1	404	C
51	S1	405	G
51	S1	423	U
51	S1	432	G
51	S1	433	G
51	S1	443	A
51	S1	444	A
51	S1	445	U
51	S1	446	A
51	S1	447	G
51	S1	450	A
51	S1	451	C
51	S1	452	C
51	S1	454	C
51	S1	455	PSU
51	S1	456	U
51	S1	460	C
51	S1	461	G

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Mol	Chain	Res	Type
51	S1	462	G
51	S1	464	G
51	S1	466	G
51	S1	467	C
51	S1	469	G
51	S1	473	G
51	S1	474	C
51	S1	476	C
51	S1	477	G
51	S1	478	C
51	S1	481	A
51	S1	482	U
51	S1	487	C
51	S1	488	A
51	S1	491	G
51	S1	495	A
51	S1	496	A
51	S1	497	A
51	S1	505	A
51	S1	507	G
51	S1	508	A
51	S1	512	A2M
51	S1	516	A
51	S1	517	A
51	S1	523	A
51	S1	525	A
51	S1	527	A
51	S1	547	U
51	S1	551	A
51	S1	552	U
51	S1	555	C
51	S1	556	A
51	S1	559	G
51	S1	561	G
51	S1	565	U
51	S1	566	A
51	S1	572	A
51	S1	574	C
51	S1	575	C
51	S1	576	A
51	S1	577	U
51	S1	579	C

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Mol	Chain	Res	Type
51	S1	580	A
51	S1	584	U
51	S1	585	C
51	S1	587	A
51	S1	588	G
51	S1	589	U
51	S1	590	A
51	S1	591	A
51	S1	593	A
51	S1	594	A
51	S1	598	G
51	S1	605	A
51	S1	608	C
51	S1	611	G
51	S1	612	U
51	S1	614	C
51	S1	617	G
51	S1	618	C
51	S1	620	C
51	S1	626	G
51	S1	627	U
51	S1	628	A
51	S1	629	A
51	S1	632	C
51	S1	643	A
51	S1	655	U
51	S1	660	U
51	S1	667	U
51	S1	668	A2M
51	S1	669	A
51	S1	670	A
51	S1	671	G
51	S1	672	G
51	S1	673	G
51	S1	675	U
51	S1	678	U
51	S1	679	A
51	S1	686	C
51	S1	687	U
51	S1	688	G
51	S1	690	G
51	S1	695	G

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Mol	Chain	Res	Type
51	S1	697	G
51	S1	698	C
51	S1	699	A
51	S1	700	G
51	S1	701	G
51	S1	749	U
51	S1	750	U
51	S1	755	C
51	S1	757	C
51	S1	759	U
51	S1	760	G
51	S1	761	A
51	S1	775	C
51	S1	778	G
51	S1	782	C
51	S1	783	A
51	S1	784	C
51	S1	786	G
51	S1	788	A
51	S1	789	G
51	S1	790	U
51	S1	791	G
51	S1	793	G
51	S1	810	G
51	S1	811	C
51	S1	812	A
51	S1	814	G
51	S1	815	U
51	S1	816	C
51	S1	817	A
51	S1	818	U
51	S1	819	G
51	S1	825	C
51	S1	826	A
51	S1	827	G
51	S1	830	G
51	S1	831	G
51	S1	833	G
51	S1	834	U
51	S1	835	C
51	S1	838	U
51	S1	841	U

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Mol	Chain	Res	Type
51	S1	844	U
51	S1	845	U
51	S1	853	A
51	S1	856	A
51	S1	863	C
51	S1	866	G
51	S1	867	A
51	S1	868	C
51	S1	872	A
51	S1	877	U
51	S1	881	U
51	S1	882	U
51	S1	883	G
51	S1	886	U
51	S1	887	U
51	S1	890	A
51	S1	892	U
51	S1	893	A
51	S1	895	A
51	S1	904	G
51	S1	905	A
51	S1	907	A
51	S1	913	G
51	S1	914	G
51	S1	916	G
51	S1	918	A
51	S1	919	G
51	S1	920	C
51	S1	922	U
51	S1	923	C
51	S1	925	A
51	S1	926	G
51	S1	927	G
51	S1	930	A
51	S1	935	U
51	S1	936	U
51	S1	944	U
51	S1	945	G
51	S1	951	U
51	S1	952	U
51	S1	955	A
51	S1	956	A

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Mol	Chain	Res	Type
51	S1	958	G
51	S1	959	U
51	S1	962	A
51	S1	964	U
51	S1	966	G
51	S1	969	A
51	S1	970	U
51	S1	971	U
51	S1	972	A
51	S1	973	U
51	S1	1093	C
51	S1	1101	A
51	S1	1102	G
51	S1	1103	G
51	S1	1105	A
51	S1	1107	G
51	S1	1109	A
51	S1	1115	G
51	S1	1116	U
51	S1	1117	A
51	S1	1119	U
51	S1	1123	G
51	S1	1130	A
51	S1	1133	U
51	S1	1139	G
51	S1	1145	A
51	S1	1150	U
51	S1	1161	G
51	S1	1175	G
51	S1	1180	A
51	S1	1181	C
51	S1	1182	A
51	S1	1187	A
51	S1	1197	C
51	S1	1198	A
51	S1	1207	U
51	S1	1210	C
51	S1	1211	U
51	S1	1213	A
51	S1	1217	A
51	S1	1218	A
51	S1	1232	G

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Mol	Chain	Res	Type
51	S1	1235	A
51	S1	1236	U
51	S1	1239	A
51	S1	1240	A
51	S1	1248	A
51	S1	1250	A
51	S1	1251	A
51	S1	1256	U
51	S1	1268	C
51	S1	1270	G
51	S1	1271	C
51	S1	1272	A
51	S1	1273	A
51	S1	1274	A
51	S1	1275	C
51	S1	1277	A
51	S1	1278	U
51	S1	1290	A
51	S1	1296	G
51	S1	1298	U
51	S1	1359	C
51	S1	1360	U
51	S1	1361	U
51	S1	1362	A
51	S1	1365	U
51	S1	1371	U
51	S1	1398	C
51	S1	1399	G
51	S1	1400	G
51	S1	1408	C
51	S1	1414	A
51	S1	1431	A
51	S1	1442	U
51	S1	1443	U
51	S1	1444	G
51	S1	1446	G
51	S1	1448	U
51	S1	1449	U
51	S1	1452	A
51	S1	1460	G
51	S1	1461	G
51	S1	1466	G

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Mol	Chain	Res	Type
51	S1	1467	U
51	S1	1469	C
51	S1	1478	OMG
51	S1	1489	A
51	S1	1490	A
51	S1	1502	G
51	S1	1507	G
51	S1	1510	C
51	S1	1516	G
51	S1	1517	A
51	S1	1518	C
51	S1	1537	U
51	S1	1538	U
51	S1	1539	PSU
51	S1	1542	C
51	S1	1546	A
51	S1	1548	A
51	S1	1551	G
51	S1	1552	G
51	S1	1554	A
51	S1	1559	U
51	S1	1564	G
51	S1	1569	G
51	S1	1570	G
51	S1	1576	A
51	S1	1577	U
51	S1	1579	A
51	S1	1582	A
51	S1	1583	U
51	S1	1587	C
51	S1	1591	U
51	S1	1594	A
51	S1	1595	G
51	S1	1597	G
51	S1	1598	U
51	S1	1603	U
51	S1	1605	U
51	S1	1606	C
51	S1	1608	A
51	S1	1609	U
51	S1	1611	C
51	S1	1612	C

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Mol	Chain	Res	Type
51	S1	1613	C
51	S1	1614	U
51	S1	1615	G
51	S1	1616	A
51	S1	1622	G
51	S1	1625	G
51	S1	1627	A
51	S1	1636	U
51	S1	1637	A
51	S1	1638	U
51	S1	1643	G
51	S1	1649	G
51	S1	1650	U
51	S1	1652	A
51	S1	1653	U
51	S1	1658	U
51	S1	1666	U
51	S1	1667	U
51	S1	1673	A
51	S1	1677	G
51	S1	1680	G
51	S1	1686	C
51	S1	1689	G
51	S1	1690	C
51	S1	1693	C
51	S1	1697	G
51	S1	1698	U
51	S1	1699	A
51	S1	1702	A
51	S1	1704	U
51	S1	1705	C
51	S1	1708	A
51	S1	1709	A
51	S1	1712	G
51	S1	1713	C
51	S1	1715	C
51	S1	1716	A
51	S1	1717	U
51	S1	1718	A
51	S1	1719	G
51	S1	1720	G
51	S1	1724	G

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Mol	Chain	Res	Type
51	S1	1725	C
51	S1	1761	C
51	S1	1762	A
51	S1	1766	G
51	S1	1767	G
51	S1	1768	U
51	S1	1769	C
51	S1	1770	G
51	S1	1772	A
51	S1	1778	C
51	S1	1781	U
51	S1	1784	G
51	S1	1789	U
51	S1	1790	C
51	S1	1793	U
51	S1	1794	U
51	S1	1795	G
51	S1	1799	U
51	S1	1801	G
51	S1	1803	A
51	S1	1810	G
51	S1	1814	U
51	S1	1816	U
51	S1	1819	G
51	S1	1824	C
51	S1	1826	G
51	S1	1827	C
51	S1	1828	A
51	S1	1829	OMG
51	S1	1832	C
51	S1	1833	OMU
51	S1	1835	U
51	S1	1836	G
51	S1	1838	U
51	S1	1845	C
51	S1	1846	A
51	S1	1847	A
51	S1	1848	U
51	S1	1851	U
51	S1	1858	G
51	S1	1859	A
51	S1	1861	A

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Mol	Chain	Res	Type
51	S1	1862	C
51	S1	1867	A
51	S1	1872	A
51	S1	1873	A
51	S1	1874	U
51	S1	1875	G
51	S1	1880	U
51	S1	1882	A
51	S1	1884	A
51	S1	1887	A
51	S1	1888	A
51	S1	1889	G
51	S1	1890	A
51	S1	1891	A
51	S1	1892	A
51	S1	1893	A
51	S1	1906	G
51	S1	1907	A
51	S1	1908	A
51	S1	1909	C
51	S1	1913	C
51	S1	1916	G
51	S1	1917	A
51	S1	1918	U
51	S1	1919	C
51	S1	1920	A
51	S1	1923	A
51	S1	1928	G
51	S1	1929	G
51	S1	1931	G
51	S1	1933	A
51	S1	1934	A
51	S1	1938	C
51	S1	1939	G
51	S1	1943	U
51	S1	1944	C
51	S1	1948	U
51	S1	1949	A
51	S1	1950	G
51	S1	1953	C
51	S1	1956	C
51	S1	1957	U

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Mol	Chain	Res	Type
51	S1	1958	U
51	S1	1961	G
51	S1	1962	A
51	S1	1963	C
51	S1	1969	A
51	S1	1976	U
51	S1	1981	G
51	S1	1985	G
51	S1	1988	C
51	S1	1989	A
51	S1	1995	7MG
51	S1	1998	U
51	S1	2004	G
51	S1	2005	U
51	S1	2010	G
51	S1	2015	U
51	S1	2016	C
51	S1	2020	A
51	S1	2021	A2M
51	S1	2027	G
51	S1	2031	A
51	S1	2036	G
51	S1	2038	C
51	S1	2039	C
51	S1	2040	C
51	S1	2042	G
51	S1	2054	C
51	S1	2064	C
51	S1	2070	U
51	S1	2079	U
51	S1	2083	G
51	S1	2084	C
51	S1	2092	G
51	S1	2093	U
51	S1	2097	C
51	S1	2099	G
51	S1	2100	A
51	S1	2101	C
51	S1	2118	G
51	S1	2119	C
51	S1	2120	C
51	S1	2121	C

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Mol	Chain	Res	Type
51	S1	2124	A
51	S1	2125	A
51	S1	2134	A
51	S1	2136	A
51	S1	2137	U
51	S1	2157	A
51	S1	2159	A
51	S1	2160	G
51	S1	2163	G
51	S1	2165	A
51	S1	2166	A
51	S1	2169	A
51	S1	2170	G
51	S1	2172	U
51	S1	2173	A
51	S1	2178	U
51	S1	2180	G
51	S1	2183	G
51	S1	2186	C
51	S1	2195	G
51	S1	2196	G
51	S1	2197	G
51	S1	2198	A
51	S1	2199	C
51	S1	2202	PSU
51	S1	2203	U
52	S2	31	A
52	S2	34	G
52	S2	35	A
52	S2	36	A
52	S2	38	A
53	S3	3	C
53	S3	7	G
53	S3	8	U
53	S3	9	G
53	S3	11	A
53	S3	22	G
53	S3	31	G
53	S3	42	G
53	S3	46	A
53	S3	47	U
53	S3	48	C

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Mol	Chain	Res	Type
53	S3	49	G
53	S3	52	G
53	S3	53	G
53	S3	54	U
53	S3	55	U
53	S3	58	A
53	S3	62	C
53	S3	63	G
53	S3	64	G
53	S3	66	C
53	S3	68	C
53	S3	70	G
53	S3	71	C
53	S3	73	A
53	S3	75	C
53	S3	76	A
54	S4	5	G
54	S4	6	G
54	S4	8	U
54	S4	9	A
54	S4	11	C
54	S4	14	A
54	S4	22	G
54	S4	23	A
54	S4	25	C
54	S4	26	A
54	S4	27	G
54	S4	30	G
54	S4	31	A
54	S4	32	U
54	S4	38	A
54	S4	40	C
54	S4	41	C
54	S4	42	C
54	S4	43	C
54	S4	44	G
54	S4	45	U
54	S4	46	G
54	S4	50	U
54	S4	51	U
54	S4	53	G
54	S4	54	U

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Mol	Chain	Res	Type
54	S4	55	U
54	S4	56	C
54	S4	58	A
54	S4	59	U
54	S4	61	C
54	S4	65	G
54	S4	69	G
54	S4	70	C
54	S4	73	A
54	S4	75	C
54	S4	76	A
55	S5	2	A
55	S5	5	A
55	S5	7	G
55	S5	8	U

All (178) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	38	A
1	L1	63	A
1	L1	92	C
1	L1	120	G
1	L1	141	U
1	L1	161	A
1	L1	170	U
1	L1	191	U
1	L1	200	A
1	L1	208	C
1	L1	233	U
1	L1	415	A
1	L1	543	G
1	L1	563	C
1	L1	574	G
1	L1	575	A
1	L1	576	G
1	L1	582	U
1	L1	584	U
1	L1	610	A
1	L1	760	A
1	L1	823	G
1	L1	824	U

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Mol	Chain	Res	Type
1	L1	835	G
1	L1	836	G
1	L1	851	G
1	L1	947	A
1	L1	967	G
1	L1	1012	C
1	L1	1031	A
1	L1	1044	G
1	L1	1051	C
1	L1	1096	C
1	L1	1114	A
1	L1	1121	G
1	L1	1200	A
1	L1	1209	G
1	L1	1211	A
1	L1	1261	U
1	L1	1387	U
1	L1	1390	G
1	L1	1412	G
1	L1	1413	U
1	L1	1439	A
1	L1	1479	A
1	L1	1519	G
1	L1	1565	A
1	L1	1574	C
1	L1	1612	G
1	L1	1662	G
1	L1	1669	A
1	L1	1673	G
1	L1	1726	G
1	L1	1742	G
2	L2	25	A
2	L2	29	C
2	L2	41	A
2	L2	62	A
2	L2	68	A
2	L2	414	G
2	L2	443	OMC
2	L2	507	G
2	L2	551	G
2	L2	623	A
2	L2	695	G

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Mol	Chain	Res	Type
2	L2	696	A
2	L2	748	C
2	L2	777	A
2	L2	998	G
2	L2	1083	A
2	L2	1101	A
2	L2	1116	A
2	L2	1131	A
2	L2	1136	U
2	L2	1141	G
2	L2	1156	G
2	L2	1170	U
2	L2	1203	A
2	L2	1246	A
2	L2	1293	C
2	L2	1297	U
2	L2	1313	U
2	L2	1324	U
2	L2	1349	A
2	L2	1388	G
2	L2	1437	A
2	L2	1439	U
2	L2	1454	A
2	L2	1461	C
2	L2	1484	U
2	L2	1485	G
2	L2	1512	G
3	L3	19	A
3	L3	34	C
3	L3	35	A
3	L3	112	C
3	L3	113	U
3	L3	149	A
3	L3	193	C
4	L4	33	G
4	L4	76	C
4	L4	83	U
4	L4	127	G
4	L4	149	U
5	L5	26	A
5	L5	49	G
5	L5	51	A

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Mol	Chain	Res	Type
5	L5	106	G
5	L5	125	U
5	L5	134	C
6	L6	41	G
6	L6	50	A
6	L6	51	A
6	L6	64	U
6	L6	71	A
7	L7	21	U
7	L7	71	A
7	L7	93	C
7	L7	95	A
7	L7	104	A
8	L8	45	G
8	L8	113	U
51	S1	102	A
51	S1	128	C
51	S1	145	A
51	S1	234	C
51	S1	236	C
51	S1	237	A
51	S1	276	G
51	S1	281	A
51	S1	294	G
51	S1	307	C
51	S1	328	C
51	S1	366	G
51	S1	443	A
51	S1	516	A
51	S1	550	C
51	S1	579	C
51	S1	588	G
51	S1	589	U
51	S1	620	C
51	S1	628	A
51	S1	656	G
51	S1	687	U
51	S1	777	A
51	S1	789	G
51	S1	814	G
51	S1	889	A
51	S1	904	G

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Mol	Chain	Res	Type
51	S1	913	G
51	S1	958	G
51	S1	1209	C
51	S1	1360	U
51	S1	1460	G
51	S1	1608	A
51	S1	1672	C
51	S1	1724	G
51	S1	1761	C
51	S1	1767	G
51	S1	1827	C
51	S1	1873	A
51	S1	1889	G
51	S1	1908	A
51	S1	1915	U
51	S1	1919	C
51	S1	1994	G
51	S1	2035	C
51	S1	2053	A
51	S1	2099	G
51	S1	2119	C
51	S1	2157	A
51	S1	2171	G
52	S2	34	G
53	S3	47	U
53	S3	74	C
54	S4	13	C
54	S4	58	A
55	S5	7	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	L2	583	2	19,22,23	0.28	0	26,31,34	0.42	0
4	OMG	L4	74	4	18,26,27	1.00	2 (11%)	19,38,41	0.64	0
2	OMG	L2	1231	2	18,26,27	1.02	3 (16%)	19,38,41	0.71	0
2	PSU	L2	500	2	18,21,22	0.86	1 (5%)	22,30,33	0.60	0
51	PSU	S1	2048	51	18,21,22	0.89	1 (5%)	22,30,33	0.66	0
1	A2M	L1	305	1	18,25,26	0.61	0	18,36,39	1.05	3 (16%)
51	PSU	S1	12	51	18,21,22	0.87	1 (5%)	22,30,33	0.68	0
1	OMC	L1	695	1	19,22,23	0.29	0	26,31,34	0.44	0
51	OMU	S1	1833	51	19,22,23	0.21	0	26,31,34	0.37	0
2	OMG	L2	686	2	18,26,27	1.01	2 (11%)	19,38,41	0.77	0
1	OMU	L1	1039	1	19,22,23	0.20	0	26,31,34	0.53	0
2	PSU	L2	472	2	18,21,22	0.85	1 (5%)	22,30,33	0.65	0
2	PSU	L2	1194	2	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
51	OMG	S1	1478	51	18,26,27	1.01	2 (11%)	19,38,41	0.69	1 (5%)
1	PSU	L1	940	1	18,21,22	0.87	1 (5%)	22,30,33	0.74	1 (4%)
1	OMC	L1	1010	92,1	19,22,23	0.30	0	26,31,34	0.39	0
51	OMC	S1	18	51	19,22,23	0.29	0	26,31,34	0.42	0
2	PSU	L2	510	2	18,21,22	0.86	1 (5%)	22,30,33	0.62	0
51	OMG	S1	1829	51,92	18,26,27	1.01	2 (11%)	19,38,41	0.66	0
1	A2M	L1	678	2,1	18,25,26	0.61	0	18,36,39	0.75	1 (5%)
2	A2M	L2	572	2	18,25,26	0.60	0	18,36,39	0.89	1 (5%)
2	OMG	L2	1229	2	18,26,27	1.02	3 (16%)	19,38,41	0.70	1 (5%)
51	OMU	S1	8	51	19,22,23	0.24	0	26,31,34	0.56	0
1	OMG	L1	856	1	18,26,27	1.02	3 (16%)	19,38,41	0.73	0
2	OMU	L2	560	2,91	19,22,23	0.21	0	26,31,34	1.00	1 (3%)
1	PSU	L1	1171	1	18,21,22	0.89	1 (5%)	22,30,33	0.66	0
51	7MG	S1	1995	51,53	22,26,27	1.05	1 (4%)	29,39,42	0.70	0
1	PSU	L1	1529	1	18,21,22	0.88	1 (5%)	22,30,33	0.70	0
51	PSU	S1	455	51	18,21,22	0.88	1 (5%)	22,30,33	0.66	0
2	PSU	L2	1264	2	18,21,22	0.86	1 (5%)	22,30,33	0.76	1 (4%)
1	OMU	L1	845	1	19,22,23	0.30	0	26,31,34	0.86	0
2	OMG	L2	641	2	18,26,27	1.00	3 (16%)	19,38,41	0.84	0
2	A2M	L2	1372	2	18,25,26	0.61	0	18,36,39	0.83	1 (5%)
1	PSU	L1	1177	1	18,21,22	0.87	1 (5%)	22,30,33	0.52	0
1	PSU	L1	1664	1	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
2	OMG	L2	71	2	18,26,27	0.99	2 (11%)	19,38,41	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	L1	235	1	18,25,26	0.61	0	18,36,39	0.81	1 (5%)
2	5MC	L2	1308	2	18,22,23	0.32	0	26,32,35	0.63	1 (3%)
1	PSU	L1	239	1	18,21,22	0.89	1 (5%)	22,30,33	0.60	0
1	PSU	L1	510	1	18,21,22	0.89	1 (5%)	22,30,33	0.59	0
2	A2M	L2	527	2	18,25,26	0.63	0	18,36,39	0.77	1 (5%)
3	OMU	L3	13	3	19,22,23	0.23	0	26,31,34	0.51	0
2	PSU	L2	1284	2	18,21,22	0.85	1 (5%)	22,30,33	0.55	0
7	PSU	L7	69	7,92	18,21,22	0.86	1 (5%)	22,30,33	0.75	0
1	A2M	L1	69	1	18,25,26	0.61	0	18,36,39	0.82	1 (5%)
1	OMG	L1	959	1	18,26,27	1.02	2 (11%)	19,38,41	0.97	1 (5%)
2	A2M	L2	570	2,1	18,25,26	0.61	0	18,36,39	0.83	1 (5%)
1	A2M	L1	681	1	18,25,26	0.59	0	18,36,39	0.73	1 (5%)
2	PSU	L2	1303	2	18,21,22	0.84	1 (5%)	22,30,33	0.73	0
2	OMC	L2	1159	2	19,22,23	0.28	0	26,31,34	0.45	0
51	PSU	S1	1841	51	18,21,22	0.87	1 (5%)	22,30,33	0.64	0
1	1MA	L1	677	1	16,25,26	0.78	1 (6%)	18,37,40	0.71	0
51	OMC	S1	2140	51	19,22,23	0.29	0	26,31,34	0.52	0
2	PSU	L2	802	2,92	18,21,22	0.87	1 (5%)	22,30,33	0.59	0
2	A2M	L2	1185	2	18,25,26	0.61	0	18,36,39	0.76	1 (5%)
51	PSU	S1	1657	51	18,21,22	0.85	1 (5%)	22,30,33	0.58	0
51	OMC	S1	1866	51	19,22,23	0.28	0	26,31,34	0.46	0
2	A2M	L2	502[B]	2	18,25,26	0.64	0	18,36,39	1.03	2 (11%)
51	PSU	S1	1246	51	18,21,22	0.87	1 (5%)	22,30,33	0.58	0
1	OMC	L1	1527	1	19,22,23	0.29	0	26,31,34	0.35	0
51	5MC	S1	1544	51	18,22,23	0.31	0	26,32,35	0.50	0
51	PSU	S1	1156	51	18,21,22	0.87	1 (5%)	22,30,33	0.62	0
2	OMC	L2	1397	2	19,22,23	0.27	0	26,31,34	0.56	0
51	OMG	S1	1550	51	18,26,27	1.00	2 (11%)	19,38,41	0.70	0
2	PSU	L2	1152	2	18,21,22	0.87	1 (5%)	22,30,33	0.63	0
51	PSU	S1	2046	51	18,21,22	0.88	1 (5%)	22,30,33	0.74	0
1	A2M	L1	927	1	18,25,26	0.60	0	18,36,39	0.72	1 (5%)
2	PSU	L2	593	2	18,21,22	0.87	1 (5%)	22,30,33	0.56	0
51	A2M	S1	98	51,92	18,25,26	0.62	0	18,36,39	0.79	1 (5%)
1	A2M	L1	1373	1	18,25,26	0.61	0	18,36,39	0.79	1 (5%)
51	PSU	S1	33	51	18,21,22	0.88	1 (5%)	22,30,33	0.66	0
2	OMC	L2	443	2,91,90	19,22,23	0.34	0	26,31,34	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	OMC	S1	38	51	19,22,23	0.28	0	26,31,34	0.52	0
2	PSU	L2	1382	2,92	18,21,22	0.87	1 (5%)	22,30,33	0.69	0
51	A2M	S1	2021	51	18,25,26	0.62	0	18,36,39	0.80	1 (5%)
51	OMG	S1	1623	51	18,26,27	1.00	3 (16%)	19,38,41	0.66	0
2	A2M	L2	382	2	18,25,26	0.60	0	18,36,39	0.73	1 (5%)
2	PSU	L2	1403	2	18,21,22	0.87	1 (5%)	22,30,33	0.71	0
1	OMG	L1	1190	1	18,26,27	1.01	2 (11%)	19,38,41	0.86	0
51	OMG	S1	2151	51	18,26,27	1.01	2 (11%)	19,38,41	0.76	0
2	A2M	L2	604	2,1	18,25,26	0.62	1 (5%)	18,36,39	0.78	1 (5%)
2	OMG	L2	1046	2,53	18,26,27	1.01	2 (11%)	19,38,41	0.65	0
1	PSU	L1	1528	1	18,21,22	0.87	1 (5%)	22,30,33	0.52	0
2	OMC	L2	1248	2	19,22,23	0.28	0	26,31,34	0.49	0
2	PSU	L2	1058	2	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
1	PSU	L1	1533	2,1	18,21,22	0.86	1 (5%)	22,30,33	0.63	0
2	OMG	L2	1517	2	18,26,27	1.01	2 (11%)	19,38,41	0.71	0
51	5MC	S1	2061	51	18,22,23	0.30	0	26,32,35	0.56	0
1	PSU	L1	1181	1	18,21,22	0.86	1 (5%)	22,30,33	0.74	1 (4%)
7	A2M	L7	162	7,1	18,25,26	0.59	0	18,36,39	0.73	1 (5%)
2	PSU	L2	1318	2	18,21,22	0.85	1 (5%)	22,30,33	0.64	0
51	B8N	S1	1543	-	24,29,30	0.80	1 (4%)	29,42,45	0.76	0
2	A2M	L2	1384	2,92	18,25,26	0.61	0	18,36,39	0.85	1 (5%)
1	A2M	L1	407	1	18,25,26	0.60	0	18,36,39	0.85	1 (5%)
51	PSU	S1	1533	51	18,21,22	0.88	1 (5%)	22,30,33	0.71	0
2	PSU	L2	626	2	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
2	OMU	L2	1419	2	19,22,23	0.20	0	26,31,34	0.32	0
2	OMU	L2	1359	2	19,22,23	0.20	0	26,31,34	0.51	0
51	PSU	S1	1566	51	18,21,22	0.86	1 (5%)	22,30,33	0.58	0
7	PSU	L7	74	7,90	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
2	PSU	L2	565	2	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
51	PSU	S1	1539	51	18,21,22	0.86	1 (5%)	22,30,33	0.62	0
51	OMU	S1	29	51	19,22,23	0.19	0	26,31,34	0.58	0
51	OMG	S1	1647	51	18,26,27	1.00	2 (11%)	19,38,41	0.84	1 (5%)
2	PSU	L2	597	2	18,21,22	0.87	1 (5%)	22,30,33	0.65	0
1	PSU	L1	1017	1	18,21,22	0.87	1 (5%)	22,30,33	0.74	0
2	A2M	L2	95	2	18,25,26	0.61	0	18,36,39	0.75	1 (5%)
51	OMU	S1	1979	51	19,22,23	0.21	0	26,31,34	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	L2	655	2	18,26,27	1.01	2 (11%)	19,38,41	0.75	0
2	OMG	L2	534	2	18,26,27	1.01	2 (11%)	19,38,41	0.67	1 (5%)
2	OMG	L2	1078	2	18,26,27	1.01	3 (16%)	19,38,41	0.86	2 (10%)
2	A2M	L2	591	2	18,25,26	0.61	0	18,36,39	0.77	1 (5%)
1	A2M	L1	1539	2,92,1	18,25,26	0.61	0	18,36,39	0.74	1 (5%)
2	OMU	L2	667	2	19,22,23	0.20	0	26,31,34	0.60	0
51	OMU	S1	1621	51	19,22,23	0.21	0	26,31,34	0.45	0
1	OMU	L1	1659	92,1	19,22,23	0.21	0	26,31,34	0.40	0
1	PSU	L1	774	1	18,21,22	0.87	1 (5%)	22,30,33	0.75	1 (4%)
2	OMC	L2	14	2,1	19,22,23	0.27	0	26,31,34	0.33	0
2	A2M	L2	628	2	18,25,26	0.60	0	18,36,39	0.74	1 (5%)
2	5MC	L2	524	2,92	18,22,23	0.33	0	26,32,35	0.50	0
2	A2M	L2	665	2	18,25,26	0.60	0	18,36,39	0.72	1 (5%)
1	A2M	L1	955	1	18,25,26	0.59	0	18,36,39	0.78	1 (5%)
2	PSU	L2	1060	2	18,21,22	0.89	1 (5%)	22,30,33	0.83	1 (4%)
2	PSU	L2	78	2	18,21,22	0.88	1 (5%)	22,30,33	0.75	1 (4%)
1	A2M	L1	858	1	18,25,26	0.62	1 (5%)	18,36,39	0.83	1 (5%)
2	OMG	L2	1253	2	18,26,27	1.00	2 (11%)	19,38,41	0.66	1 (5%)
51	OMG	S1	1865	51	18,26,27	0.99	2 (11%)	19,38,41	0.80	0
2	OMC	L2	1317	2	19,22,23	0.27	0	26,31,34	0.33	0
7	A2M	L7	43	7	18,25,26	0.60	0	18,36,39	0.87	1 (5%)
2	OMU	L2	73	2	19,22,23	0.22	0	26,31,34	0.42	0
51	PSU	S1	1192	51	18,21,22	0.86	1 (5%)	22,30,33	0.54	0
52	MIA	S2	37	52	24,31,32	0.82	1 (4%)	26,44,47	4.50	2 (7%)
51	MA6	S1	2185	51,90	18,26,27	0.72	0	19,38,41	0.41	0
1	PSU	L1	422	1	18,21,22	0.87	1 (5%)	22,30,33	0.64	0
51	PSU	S1	2202	51	18,21,22	0.85	1 (5%)	22,30,33	0.57	0
1	OMG	L1	1524	1	18,26,27	1.02	2 (11%)	19,38,41	0.94	1 (5%)
2	PSU	L2	512	2	18,21,22	0.87	1 (5%)	22,30,33	0.73	0
51	MA6	S1	2184	51,90	18,26,27	0.75	1 (5%)	19,38,41	0.50	0
2	OMG	L2	1360	2	18,26,27	1.01	2 (11%)	19,38,41	0.66	0
51	A2M	S1	479	51	18,25,26	0.59	0	18,36,39	0.74	1 (5%)
1	OMG	L1	1540	2,1,90	18,26,27	1.02	2 (11%)	19,38,41	0.64	0
7	PSU	L7	101	7	18,21,22	0.86	1 (5%)	22,30,33	0.76	1 (4%)
2	PSU	L2	437	2	18,21,22	0.85	1 (5%)	22,30,33	0.65	0
51	A2M	S1	668	51,92	18,25,26	0.60	0	18,36,39	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L2	1265	2	18,21,22	0.87	1 (5%)	22,30,33	0.71	0
1	OMG	L1	1626	1	18,26,27	1.01	3 (16%)	19,38,41	0.69	0
2	A2M	L2	502[A]	2,51	18,25,26	0.63	0	18,36,39	1.12	3 (16%)
2	OMC	L2	359	2	19,22,23	0.27	0	26,31,34	0.41	0
2	PSU	L2	1144	2	18,21,22	0.83	1 (5%)	22,30,33	0.64	0
1	OMU	L1	1107	1	19,22,23	0.20	0	26,31,34	0.60	0
2	PSU	L2	1413	2,90	18,21,22	0.88	1 (5%)	22,30,33	0.71	1 (4%)
1	PSU	L1	1011	2,1	18,21,22	0.83	1 (5%)	22,30,33	0.74	1 (4%)
1	OMU	L1	847	1	19,22,23	0.20	0	26,31,34	0.51	0
7	OMG	L7	75	7	18,26,27	1.00	2 (11%)	19,38,41	0.75	1 (5%)
51	A2M	S1	512	51	18,25,26	0.60	0	18,36,39	0.85	1 (5%)
51	OMU	S1	661	51	19,22,23	0.20	0	26,31,34	0.39	0
2	OMU	L2	1077	2	19,22,23	0.20	0	26,31,34	0.40	0
2	PSU	L2	662	2,92	18,21,22	0.87	1 (5%)	22,30,33	0.63	0
51	OMG	S1	600	51	18,26,27	1.00	2 (11%)	19,38,41	0.68	0
1	A2M	L1	697	1	18,25,26	0.60	0	18,36,39	0.81	1 (5%)
1	OMU	L1	1371	1	19,22,23	0.28	0	26,31,34	0.99	1 (3%)
2	PSU	L2	1213	2	18,21,22	0.85	1 (5%)	22,30,33	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	L2	583	2	-	0/9/27/28	0/2/2/2
4	OMG	L4	74	4	-	2/5/27/28	0/3/3/3
2	OMG	L2	1231	2	-	0/5/27/28	0/3/3/3
2	PSU	L2	500	2	-	0/7/25/26	0/2/2/2
51	PSU	S1	2048	51	-	0/7/25/26	0/2/2/2
1	A2M	L1	305	1	-	2/5/27/28	0/3/3/3
51	PSU	S1	12	51	-	0/7/25/26	0/2/2/2
1	OMC	L1	695	1	-	0/9/27/28	0/2/2/2
51	OMU	S1	1833	51	-	2/9/27/28	0/2/2/2
2	OMG	L2	686	2	-	2/5/27/28	0/3/3/3
1	OMU	L1	1039	1	-	0/9/27/28	0/2/2/2
2	PSU	L2	472	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1194	2	-	0/7/25/26	0/2/2/2
51	OMG	S1	1478	51	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L1	940	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	1010	92,1	-	2/9/27/28	0/2/2/2
51	OMC	S1	18	51	-	1/9/27/28	0/2/2/2
2	PSU	L2	510	2	-	0/7/25/26	0/2/2/2
51	OMG	S1	1829	51,92	-	2/5/27/28	0/3/3/3
1	A2M	L1	678	2,1	-	4/5/27/28	0/3/3/3
2	A2M	L2	572	2	-	0/5/27/28	0/3/3/3
2	OMG	L2	1229	2	-	2/5/27/28	0/3/3/3
51	OMU	S1	8	51	-	6/9/27/28	0/2/2/2
1	OMG	L1	856	1	-	0/5/27/28	0/3/3/3
2	OMU	L2	560	2,91	-	3/9/27/28	0/2/2/2
1	PSU	L1	1171	1	-	2/7/25/26	0/2/2/2
51	7MG	S1	1995	51,53	-	0/7/37/38	0/3/3/3
1	PSU	L1	1529	1	-	0/7/25/26	0/2/2/2
51	PSU	S1	455	51	-	1/7/25/26	0/2/2/2
2	PSU	L2	1264	2	-	2/7/25/26	0/2/2/2
1	OMU	L1	845	1	-	3/9/27/28	0/2/2/2
2	OMG	L2	641	2	-	0/5/27/28	0/3/3/3
2	A2M	L2	1372	2	-	0/5/27/28	0/3/3/3
1	PSU	L1	1177	1	-	2/7/25/26	0/2/2/2
1	PSU	L1	1664	1	-	0/7/25/26	0/2/2/2
2	OMG	L2	71	2	-	0/5/27/28	0/3/3/3
1	A2M	L1	235	1	-	2/5/27/28	0/3/3/3
2	5MC	L2	1308	2	-	4/7/25/26	0/2/2/2
1	PSU	L1	239	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	510	1	-	3/7/25/26	0/2/2/2
2	A2M	L2	527	2	-	2/5/27/28	0/3/3/3
3	OMU	L3	13	3	-	1/9/27/28	0/2/2/2
2	PSU	L2	1284	2	-	0/7/25/26	0/2/2/2
7	PSU	L7	69	7,92	-	0/7/25/26	0/2/2/2
1	A2M	L1	69	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	959	1	-	3/5/27/28	0/3/3/3
2	A2M	L2	570	2,1	-	2/5/27/28	0/3/3/3
1	A2M	L1	681	1	-	3/5/27/28	0/3/3/3
2	PSU	L2	1303	2	-	0/7/25/26	0/2/2/2
2	OMC	L2	1159	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1841	51	-	0/7/25/26	0/2/2/2
1	1MA	L1	677	1	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	OMC	S1	2140	51	-	0/9/27/28	0/2/2/2
2	PSU	L2	802	2,92	-	2/7/25/26	0/2/2/2
2	A2M	L2	1185	2	-	2/5/27/28	0/3/3/3
51	PSU	S1	1657	51	-	2/7/25/26	0/2/2/2
51	OMC	S1	1866	51	-	0/9/27/28	0/2/2/2
2	A2M	L2	502[B]	2	-	2/5/27/28	0/3/3/3
51	PSU	S1	1246	51	-	0/7/25/26	0/2/2/2
1	OMC	L1	1527	1	-	2/9/27/28	0/2/2/2
51	5MC	S1	1544	51	-	1/7/25/26	0/2/2/2
51	PSU	S1	1156	51	-	0/7/25/26	0/2/2/2
2	OMC	L2	1397	2	-	0/9/27/28	0/2/2/2
51	OMG	S1	1550	51	-	0/5/27/28	0/3/3/3
2	PSU	L2	1152	2	-	0/7/25/26	0/2/2/2
51	PSU	S1	2046	51	-	0/7/25/26	0/2/2/2
1	A2M	L1	927	1	-	0/5/27/28	0/3/3/3
2	PSU	L2	593	2	-	2/7/25/26	0/2/2/2
51	A2M	S1	98	51,92	-	2/5/27/28	0/3/3/3
1	A2M	L1	1373	1	-	2/5/27/28	0/3/3/3
51	PSU	S1	33	51	-	0/7/25/26	0/2/2/2
2	OMC	L2	443	2,91,90	-	4/9/27/28	0/2/2/2
51	OMC	S1	38	51	-	0/9/27/28	0/2/2/2
2	PSU	L2	1382	2,92	-	0/7/25/26	0/2/2/2
51	A2M	S1	2021	51	-	2/5/27/28	0/3/3/3
51	OMG	S1	1623	51	-	0/5/27/28	0/3/3/3
2	A2M	L2	382	2	-	0/5/27/28	0/3/3/3
2	PSU	L2	1403	2	-	0/7/25/26	0/2/2/2
1	OMG	L1	1190	1	-	0/5/27/28	0/3/3/3
51	OMG	S1	2151	51	-	2/5/27/28	0/3/3/3
2	A2M	L2	604	2,1	-	0/5/27/28	0/3/3/3
2	OMG	L2	1046	2,53	-	3/5/27/28	0/3/3/3
1	PSU	L1	1528	1	-	2/7/25/26	0/2/2/2
2	OMC	L2	1248	2	-	1/9/27/28	0/2/2/2
2	PSU	L2	1058	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	1533	2,1	-	0/7/25/26	0/2/2/2
2	OMG	L2	1517	2	-	0/5/27/28	0/3/3/3
51	5MC	S1	2061	51	-	2/7/25/26	0/2/2/2
1	PSU	L1	1181	1	-	0/7/25/26	0/2/2/2
7	A2M	L7	162	7,1	-	1/5/27/28	0/3/3/3
2	PSU	L2	1318	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	B8N	S1	1543	-	-	6/16/34/35	0/2/2/2
2	A2M	L2	1384	2,92	-	1/5/27/28	0/3/3/3
1	A2M	L1	407	1	-	0/5/27/28	0/3/3/3
51	PSU	S1	1533	51	-	0/7/25/26	0/2/2/2
2	PSU	L2	626	2	-	0/7/25/26	0/2/2/2
2	OMU	L2	1419	2	-	0/9/27/28	0/2/2/2
2	OMU	L2	1359	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1566	51	-	0/7/25/26	0/2/2/2
7	PSU	L7	74	7,90	-	0/7/25/26	0/2/2/2
2	PSU	L2	565	2	-	0/7/25/26	0/2/2/2
51	PSU	S1	1539	51	-	2/7/25/26	0/2/2/2
51	OMU	S1	29	51	-	1/9/27/28	0/2/2/2
51	OMG	S1	1647	51	-	0/5/27/28	0/3/3/3
2	PSU	L2	597	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	1017	1	-	2/7/25/26	0/2/2/2
2	A2M	L2	95	2	-	1/5/27/28	0/3/3/3
51	OMU	S1	1979	51	-	1/9/27/28	0/2/2/2
2	OMG	L2	655	2	-	1/5/27/28	0/3/3/3
2	OMG	L2	534	2	-	2/5/27/28	0/3/3/3
2	OMG	L2	1078	2	-	2/5/27/28	0/3/3/3
2	A2M	L2	591	2	-	0/5/27/28	0/3/3/3
1	A2M	L1	1539	2,92,1	-	0/5/27/28	0/3/3/3
2	OMU	L2	667	2	-	1/9/27/28	0/2/2/2
51	OMU	S1	1621	51	-	0/9/27/28	0/2/2/2
1	OMU	L1	1659	92,1	-	0/9/27/28	0/2/2/2
1	PSU	L1	774	1	-	0/7/25/26	0/2/2/2
2	OMC	L2	14	2,1	-	0/9/27/28	0/2/2/2
2	A2M	L2	628	2	-	0/5/27/28	0/3/3/3
2	5MC	L2	524	2,92	-	0/7/25/26	0/2/2/2
2	A2M	L2	665	2	-	3/5/27/28	0/3/3/3
1	A2M	L1	955	1	-	1/5/27/28	0/3/3/3
2	PSU	L2	1060	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	78	2	-	0/7/25/26	0/2/2/2
1	A2M	L1	858	1	-	1/5/27/28	0/3/3/3
2	OMG	L2	1253	2	-	0/5/27/28	0/3/3/3
51	OMG	S1	1865	51	-	0/5/27/28	0/3/3/3
2	OMC	L2	1317	2	-	0/9/27/28	0/2/2/2
7	A2M	L7	43	7	-	0/5/27/28	0/3/3/3
2	OMU	L2	73	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1192	51	-	0/7/25/26	0/2/2/2
52	MIA	S2	37	52	-	4/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	MA6	S1	2185	51,90	-	4/7/29/30	0/3/3/3
1	PSU	L1	422	1	-	0/7/25/26	0/2/2/2
51	PSU	S1	2202	51	-	1/7/25/26	0/2/2/2
1	OMG	L1	1524	1	-	3/5/27/28	0/3/3/3
2	PSU	L2	512	2	-	2/7/25/26	0/2/2/2
51	MA6	S1	2184	51,90	-	3/7/29/30	0/3/3/3
2	OMG	L2	1360	2	-	1/5/27/28	0/3/3/3
51	A2M	S1	479	51	-	0/5/27/28	0/3/3/3
1	OMG	L1	1540	2,1,90	-	2/5/27/28	0/3/3/3
7	PSU	L7	101	7	-	0/7/25/26	0/2/2/2
2	PSU	L2	437	2	-	0/7/25/26	0/2/2/2
51	A2M	S1	668	51,92	-	2/5/27/28	0/3/3/3
2	PSU	L2	1265	2	-	1/7/25/26	0/2/2/2
1	OMG	L1	1626	1	-	0/5/27/28	0/3/3/3
2	A2M	L2	502[A]	2,51	-	3/5/27/28	0/3/3/3
2	OMC	L2	359	2	-	2/9/27/28	0/2/2/2
2	PSU	L2	1144	2	-	2/7/25/26	0/2/2/2
1	OMU	L1	1107	1	-	1/9/27/28	0/2/2/2
2	PSU	L2	1413	2,90	-	0/7/25/26	0/2/2/2
1	PSU	L1	1011	2,1	-	0/7/25/26	0/2/2/2
1	OMU	L1	847	1	-	0/9/27/28	0/2/2/2
7	OMG	L7	75	7	-	1/5/27/28	0/3/3/3
51	A2M	S1	512	51	-	2/5/27/28	0/3/3/3
51	OMU	S1	661	51	-	0/9/27/28	0/2/2/2
2	OMU	L2	1077	2	-	0/9/27/28	0/2/2/2
2	PSU	L2	662	2,92	-	0/7/25/26	0/2/2/2
51	OMG	S1	600	51	-	1/5/27/28	0/3/3/3
1	A2M	L1	697	1	-	0/5/27/28	0/3/3/3
1	OMU	L1	1371	1	-	5/9/27/28	0/2/2/2
2	PSU	L2	1213	2	-	0/7/25/26	0/2/2/2

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1995	7MG	C5-N7	4.26	1.40	1.35
1	L1	510	PSU	C6-C5	3.48	1.39	1.35
1	L1	1171	PSU	C6-C5	3.44	1.39	1.35
51	S1	455	PSU	C6-C5	3.41	1.39	1.35
51	S1	2048	PSU	C6-C5	3.40	1.39	1.35
51	S1	33	PSU	C6-C5	3.39	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1841	PSU	C6-C5	3.39	1.39	1.35
1	L1	1177	PSU	C6-C5	3.38	1.39	1.35
51	S1	1156	PSU	C6-C5	3.37	1.39	1.35
51	S1	2046	PSU	C6-C5	3.37	1.39	1.35
2	L2	802	PSU	C6-C5	3.36	1.39	1.35
51	S1	1533	PSU	C6-C5	3.36	1.39	1.35
51	S1	1539	PSU	C6-C5	3.36	1.39	1.35
1	L1	239	PSU	C6-C5	3.36	1.39	1.35
51	S1	1566	PSU	C6-C5	3.36	1.39	1.35
2	L2	1265	PSU	C6-C5	3.35	1.39	1.35
1	L1	1533	PSU	C6-C5	3.35	1.39	1.35
2	L2	1413	PSU	C6-C5	3.35	1.39	1.35
2	L2	1060	PSU	C6-C5	3.34	1.39	1.35
2	L2	1382	PSU	C6-C5	3.34	1.39	1.35
2	L2	78	PSU	C6-C5	3.33	1.39	1.35
2	L2	1152	PSU	C6-C5	3.33	1.39	1.35
1	L1	1181	PSU	C6-C5	3.33	1.39	1.35
2	L2	597	PSU	C6-C5	3.33	1.39	1.35
2	L2	626	PSU	C6-C5	3.33	1.39	1.35
2	L2	593	PSU	C6-C5	3.33	1.39	1.35
7	L7	74	PSU	C6-C5	3.33	1.39	1.35
51	S1	2202	PSU	C6-C5	3.32	1.39	1.35
2	L2	662	PSU	C6-C5	3.32	1.39	1.35
2	L2	1058	PSU	C6-C5	3.32	1.39	1.35
2	L2	565	PSU	C6-C5	3.32	1.39	1.35
1	L1	1528	PSU	C6-C5	3.32	1.39	1.35
2	L2	1284	PSU	C6-C5	3.32	1.39	1.35
51	S1	12	PSU	C6-C5	3.31	1.39	1.35
1	L1	1664	PSU	C6-C5	3.31	1.39	1.35
2	L2	500	PSU	C6-C5	3.31	1.39	1.35
1	L1	1017	PSU	C6-C5	3.31	1.39	1.35
7	L7	69	PSU	C6-C5	3.31	1.39	1.35
1	L1	940	PSU	C6-C5	3.31	1.39	1.35
2	L2	1403	PSU	C6-C5	3.30	1.39	1.35
2	L2	1194	PSU	C6-C5	3.30	1.39	1.35
1	L1	774	PSU	C6-C5	3.29	1.39	1.35
2	L2	510	PSU	C6-C5	3.29	1.39	1.35
7	L7	101	PSU	C6-C5	3.29	1.39	1.35
1	L1	1529	PSU	C6-C5	3.29	1.39	1.35
51	S1	1246	PSU	C6-C5	3.29	1.39	1.35
51	S1	1657	PSU	C6-C5	3.29	1.39	1.35
2	L2	1264	PSU	C6-C5	3.28	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	422	PSU	C6-C5	3.28	1.39	1.35
2	L2	512	PSU	C6-C5	3.27	1.39	1.35
2	L2	1303	PSU	C6-C5	3.27	1.39	1.35
51	S1	1192	PSU	C6-C5	3.27	1.39	1.35
1	L1	1011	PSU	C6-C5	3.26	1.39	1.35
2	L2	1318	PSU	C6-C5	3.26	1.39	1.35
2	L2	472	PSU	C6-C5	3.25	1.39	1.35
2	L2	1213	PSU	C6-C5	3.23	1.39	1.35
2	L2	437	PSU	C6-C5	3.22	1.39	1.35
2	L2	1144	PSU	C6-C5	3.18	1.39	1.35
51	S1	1543	B8N	C6-C5	2.92	1.39	1.34
2	L2	1517	OMG	C5-C6	-2.74	1.41	1.47
2	L2	1231	OMG	C5-C6	-2.72	1.41	1.47
2	L2	1229	OMG	C5-C6	-2.70	1.41	1.47
51	S1	1829	OMG	C5-C6	-2.70	1.41	1.47
1	L1	1540	OMG	C5-C6	-2.70	1.41	1.47
1	L1	959	OMG	C5-C6	-2.69	1.42	1.47
4	L4	74	OMG	C5-C6	-2.68	1.42	1.47
51	S1	600	OMG	C5-C6	-2.68	1.42	1.47
51	S1	1478	OMG	C5-C6	-2.68	1.42	1.47
2	L2	655	OMG	C5-C6	-2.68	1.42	1.47
2	L2	686	OMG	C5-C6	-2.68	1.42	1.47
2	L2	1046	OMG	C5-C6	-2.67	1.42	1.47
2	L2	534	OMG	C5-C6	-2.67	1.42	1.47
1	L1	1524	OMG	C5-C6	-2.67	1.42	1.47
51	S1	1865	OMG	C5-C6	-2.66	1.42	1.47
1	L1	856	OMG	C5-C6	-2.66	1.42	1.47
51	S1	1647	OMG	C5-C6	-2.65	1.42	1.47
7	L7	75	OMG	C5-C6	-2.65	1.42	1.47
2	L2	1360	OMG	C5-C6	-2.65	1.42	1.47
1	L1	1190	OMG	C5-C6	-2.65	1.42	1.47
51	S1	2151	OMG	C5-C6	-2.64	1.42	1.47
2	L2	1253	OMG	C5-C6	-2.63	1.42	1.47
1	L1	1626	OMG	C5-C6	-2.63	1.42	1.47
2	L2	641	OMG	C5-C6	-2.62	1.42	1.47
2	L2	1078	OMG	C5-C6	-2.62	1.42	1.47
51	S1	1623	OMG	C5-C6	-2.61	1.42	1.47
2	L2	71	OMG	C5-C6	-2.61	1.42	1.47
51	S1	1550	OMG	C5-C6	-2.59	1.42	1.47
1	L1	959	OMG	C8-N7	-2.20	1.31	1.35
51	S1	600	OMG	C8-N7	-2.18	1.31	1.35
2	L2	534	OMG	C8-N7	-2.17	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1829	OMG	C8-N7	-2.15	1.31	1.35
1	L1	1540	OMG	C8-N7	-2.15	1.31	1.35
51	S1	1478	OMG	C8-N7	-2.15	1.31	1.35
51	S1	2151	OMG	C8-N7	-2.15	1.31	1.35
2	L2	686	OMG	C8-N7	-2.15	1.31	1.35
1	L1	1626	OMG	C8-N7	-2.14	1.31	1.35
7	L7	75	OMG	C8-N7	-2.14	1.31	1.35
2	L2	1046	OMG	C8-N7	-2.14	1.31	1.35
1	L1	1524	OMG	C8-N7	-2.13	1.31	1.35
1	L1	1190	OMG	C8-N7	-2.12	1.31	1.35
2	L2	1231	OMG	C8-N7	-2.12	1.31	1.35
4	L4	74	OMG	C8-N7	-2.11	1.31	1.35
2	L2	1229	OMG	C8-N7	-2.11	1.31	1.35
2	L2	1253	OMG	C8-N7	-2.11	1.31	1.35
2	L2	655	OMG	C8-N7	-2.10	1.31	1.35
51	S1	1865	OMG	C8-N7	-2.10	1.31	1.35
1	L1	856	OMG	C8-N7	-2.10	1.31	1.35
2	L2	1360	OMG	C8-N7	-2.10	1.31	1.35
2	L2	1078	OMG	C8-N7	-2.09	1.31	1.35
51	S1	1647	OMG	C8-N7	-2.09	1.31	1.35
2	L2	1517	OMG	C8-N7	-2.09	1.31	1.35
2	L2	71	OMG	C8-N7	-2.07	1.31	1.35
51	S1	1623	OMG	C8-N7	-2.06	1.31	1.35
51	S1	1550	OMG	C8-N7	-2.06	1.31	1.35
2	L2	1231	OMG	C5-C4	-2.06	1.37	1.43
2	L2	641	OMG	C8-N7	-2.06	1.31	1.35
2	L2	1078	OMG	C5-C4	-2.05	1.37	1.43
1	L1	856	OMG	C5-C4	-2.03	1.37	1.43
1	L1	1626	OMG	C5-C4	-2.02	1.37	1.43
2	L2	1229	OMG	C5-C4	-2.01	1.37	1.43
51	S1	2184	MA6	C8-N7	-2.01	1.31	1.34
52	S2	37	MIA	C2-S10	2.01	1.77	1.75
1	L1	677	1MA	C5-C4	-2.01	1.38	1.43
51	S1	1623	OMG	C5-C4	-2.01	1.38	1.43
2	L2	641	OMG	C5-C4	-2.00	1.38	1.43
2	L2	604	A2M	C8-N7	-2.00	1.31	1.34
1	L1	858	A2M	C8-N7	-2.00	1.31	1.34

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	37	MIA	C11-S10-C2	22.64	119.17	102.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	560	OMU	O3'-C3'-C4'	3.39	120.86	111.05
52	S2	37	MIA	C5-C6-N1	-2.98	118.33	120.81
2	L2	1060	PSU	C2'-C3'-C4'	-2.59	97.60	102.64
1	L1	959	OMG	O2'-C2'-C1'	2.56	114.17	109.09
1	L1	1524	OMG	O2'-C2'-C1'	2.54	114.13	109.09
7	L7	43	A2M	C5-C6-N6	2.48	124.13	120.35
2	L2	604	A2M	C5-C6-N6	2.37	123.95	120.35
1	L1	955	A2M	C5-C6-N6	2.34	123.91	120.35
1	L1	1011	PSU	C3'-C2'-C1'	2.33	104.36	101.64
1	L1	678	A2M	C5-C6-N6	2.33	123.90	120.35
1	L1	697	A2M	C5-C6-N6	2.33	123.89	120.35
2	L2	502[A]	A2M	O3'-C3'-C2'	2.33	117.78	111.17
7	L7	101	PSU	C3'-C2'-C1'	2.32	104.33	101.64
7	L7	162	A2M	C5-C6-N6	2.31	123.87	120.35
2	L2	78	PSU	C2'-C3'-C4'	-2.31	98.16	102.64
1	L1	305	A2M	C5-C6-N6	2.30	123.84	120.35
2	L2	628	A2M	C5-C6-N6	2.29	123.83	120.35
1	L1	1539	A2M	C5-C6-N6	2.29	123.83	120.35
2	L2	502[B]	A2M	C5-C6-N6	2.29	123.83	120.35
2	L2	570	A2M	C5-C6-N6	2.29	123.83	120.35
2	L2	572	A2M	C5-C6-N6	2.29	123.83	120.35
1	L1	681	A2M	C5-C6-N6	2.28	123.81	120.35
51	S1	512	A2M	C5-C6-N6	2.27	123.81	120.35
1	L1	407	A2M	C5-C6-N6	2.27	123.80	120.35
2	L2	591	A2M	C5-C6-N6	2.27	123.80	120.35
1	L1	1373	A2M	C5-C6-N6	2.26	123.78	120.35
2	L2	95	A2M	C5-C6-N6	2.26	123.78	120.35
1	L1	927	A2M	C5-C6-N6	2.25	123.77	120.35
2	L2	1185	A2M	C5-C6-N6	2.24	123.76	120.35
51	S1	668	A2M	C5-C6-N6	2.24	123.76	120.35
2	L2	382	A2M	C5-C6-N6	2.24	123.75	120.35
1	L1	69	A2M	C5-C6-N6	2.23	123.75	120.35
2	L2	1372	A2M	C5-C6-N6	2.23	123.74	120.35
2	L2	502[A]	A2M	C5-C6-N6	2.21	123.71	120.35
1	L1	235	A2M	C5-C6-N6	2.20	123.70	120.35
2	L2	1264	PSU	C3'-C2'-C1'	2.20	104.20	101.64
2	L2	1384	A2M	C5-C6-N6	2.17	123.65	120.35
2	L2	527	A2M	C5-C6-N6	2.17	123.64	120.35
51	S1	479	A2M	C5-C6-N6	2.17	123.64	120.35
51	S1	98	A2M	C5-C6-N6	2.16	123.64	120.35
51	S1	2021	A2M	C5-C6-N6	2.16	123.63	120.35
2	L2	1308	5MC	C5-C6-N1	-2.15	121.13	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	665	A2M	C5-C6-N6	2.15	123.61	120.35
2	L2	502[A]	A2M	O2'-C2'-C1'	2.14	113.34	109.09
1	L1	1181	PSU	C2'-C3'-C4'	-2.14	98.48	102.64
2	L2	1078	OMG	C3'-C2'-C1'	-2.10	98.94	102.89
1	L1	305	A2M	C3'-C2'-C1'	-2.10	98.95	102.89
1	L1	858	A2M	C5-C6-N6	2.09	123.52	120.35
1	L1	305	A2M	O2'-C2'-C1'	2.07	113.20	109.09
1	L1	1371	OMU	C1'-N1-C2	2.06	121.31	117.57
1	L1	774	PSU	C2'-C3'-C4'	-2.06	98.65	102.64
2	L2	1229	OMG	O6-C6-C5	2.04	128.35	124.37
2	L2	502[B]	A2M	O3'-C3'-C2'	2.03	116.94	111.17
7	L7	75	OMG	O6-C6-C5	2.03	128.34	124.37
2	L2	1413	PSU	C2'-C3'-C4'	-2.02	98.71	102.64
51	S1	1647	OMG	O6-C6-C5	2.02	128.32	124.37
2	L2	1078	OMG	O6-C6-C5	2.02	128.31	124.37
2	L2	534	OMG	O6-C6-C5	2.01	128.30	124.37
1	L1	940	PSU	C2'-C3'-C4'	-2.01	98.74	102.64
51	S1	1478	OMG	O6-C6-C5	2.01	128.29	124.37
2	L2	1253	OMG	O6-C6-C5	2.00	128.28	124.37

There are no chirality outliers.

All (158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L7	75	OMG	C1'-C2'-O2'-CM2
7	L7	162	A2M	C1'-C2'-O2'-CM'
1	L1	235	A2M	O4'-C4'-C5'-O5'
1	L1	235	A2M	C3'-C4'-C5'-O5'
1	L1	510	PSU	C2'-C1'-C5-C4
1	L1	678	A2M	O4'-C4'-C5'-O5'
1	L1	678	A2M	C1'-C2'-O2'-CM'
1	L1	681	A2M	O4'-C4'-C5'-O5'
1	L1	681	A2M	C3'-C4'-C5'-O5'
1	L1	845	OMU	O4'-C1'-N1-C2
1	L1	845	OMU	O4'-C1'-N1-C6
1	L1	845	OMU	C1'-C2'-O2'-CM2
1	L1	955	A2M	C1'-C2'-O2'-CM'
1	L1	959	OMG	C1'-C2'-O2'-CM2
1	L1	1010	OMC	O4'-C4'-C5'-O5'
1	L1	1171	PSU	C3'-C4'-C5'-O5'
1	L1	1371	OMU	O4'-C1'-N1-C2
1	L1	1371	OMU	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	L1	1371	OMU	C1'-C2'-O2'-CM2
1	L1	1524	OMG	C1'-C2'-O2'-CM2
1	L1	1540	OMG	O4'-C4'-C5'-O5'
1	L1	1540	OMG	C3'-C4'-C5'-O5'
2	L2	95	A2M	C1'-C2'-O2'-CM'
2	L2	443	OMC	C2'-C1'-N1-C6
2	L2	527	A2M	O4'-C4'-C5'-O5'
2	L2	534	OMG	O4'-C4'-C5'-O5'
2	L2	534	OMG	C3'-C4'-C5'-O5'
2	L2	686	OMG	O4'-C4'-C5'-O5'
2	L2	802	PSU	C3'-C4'-C5'-O5'
2	L2	1046	OMG	O4'-C4'-C5'-O5'
2	L2	1046	OMG	C1'-C2'-O2'-CM2
2	L2	1185	A2M	C1'-C2'-O2'-CM'
2	L2	1229	OMG	O4'-C4'-C5'-O5'
2	L2	1229	OMG	C3'-C4'-C5'-O5'
2	L2	1265	PSU	O4'-C1'-C5-C6
2	L2	1384	A2M	C1'-C2'-O2'-CM'
51	S1	29	OMU	C1'-C2'-O2'-CM2
51	S1	668	A2M	O4'-C4'-C5'-O5'
51	S1	668	A2M	C3'-C4'-C5'-O5'
51	S1	1543	B8N	O4'-C4'-C5'-O5'
51	S1	1543	B8N	C3'-C4'-C5'-O5'
51	S1	1543	B8N	N34-C33-C34-O35
51	S1	1543	B8N	N3-C31-C32-C33
51	S1	1657	PSU	O4'-C1'-C5-C6
51	S1	1829	OMG	C1'-C2'-O2'-CM2
51	S1	1979	OMU	C1'-C2'-O2'-CM2
51	S1	2021	A2M	C1'-C2'-O2'-CM'
51	S1	2184	MA6	C5-C6-N6-C9
51	S1	2184	MA6	C5-C6-N6-C10
51	S1	2185	MA6	C5-C6-N6-C9
51	S1	2185	MA6	C5-C6-N6-C10
51	S1	2202	PSU	O4'-C1'-C5-C6
52	S2	37	MIA	O4'-C4'-C5'-O5'
52	S2	37	MIA	C3'-C4'-C5'-O5'
52	S2	37	MIA	N1-C2-S10-C11
52	S2	37	MIA	N3-C2-S10-C11
51	S1	1543	B8N	N34-C33-C34-O36
2	L2	443	OMC	C2'-C1'-N1-C2
1	L1	678	A2M	C3'-C4'-C5'-O5'
1	L1	1010	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L1	1371	OMU	C3'-C4'-C5'-O5'
2	L2	686	OMG	C3'-C4'-C5'-O5'
2	L2	802	PSU	O4'-C4'-C5'-O5'
51	S1	8	OMU	C3'-C4'-C5'-O5'
51	S1	512	A2M	O4'-C4'-C5'-O5'
1	L1	305	A2M	O4'-C4'-C5'-O5'
1	L1	305	A2M	C3'-C4'-C5'-O5'
1	L1	1017	PSU	C3'-C4'-C5'-O5'
1	L1	1171	PSU	O4'-C4'-C5'-O5'
1	L1	1371	OMU	O4'-C4'-C5'-O5'
2	L2	502[A]	A2M	O4'-C4'-C5'-O5'
2	L2	502[A]	A2M	C3'-C4'-C5'-O5'
2	L2	527	A2M	C3'-C4'-C5'-O5'
2	L2	665	A2M	C3'-C4'-C5'-O5'
2	L2	1046	OMG	C3'-C4'-C5'-O5'
2	L2	1144	PSU	O4'-C4'-C5'-O5'
2	L2	1264	PSU	O4'-C4'-C5'-O5'
51	S1	8	OMU	O4'-C4'-C5'-O5'
51	S1	98	A2M	O4'-C4'-C5'-O5'
51	S1	512	A2M	C3'-C4'-C5'-O5'
51	S1	1539	PSU	O4'-C4'-C5'-O5'
51	S1	2184	MA6	N1-C6-N6-C10
51	S1	2185	MA6	N1-C6-N6-C10
2	L2	1308	5MC	C2'-C1'-N1-C6
51	S1	8	OMU	C2'-C1'-N1-C6
2	L2	512	PSU	C3'-C4'-C5'-O5'
2	L2	1308	5MC	C2'-C1'-N1-C2
51	S1	8	OMU	C2'-C1'-N1-C2
1	L1	1017	PSU	O4'-C4'-C5'-O5'
2	L2	502[B]	A2M	O4'-C4'-C5'-O5'
2	L2	502[B]	A2M	C3'-C4'-C5'-O5'
2	L2	570	A2M	O4'-C4'-C5'-O5'
2	L2	570	A2M	C3'-C4'-C5'-O5'
2	L2	665	A2M	O4'-C4'-C5'-O5'
2	L2	1144	PSU	C3'-C4'-C5'-O5'
2	L2	1264	PSU	C3'-C4'-C5'-O5'
4	L4	74	OMG	C3'-C4'-C5'-O5'
51	S1	1539	PSU	C3'-C4'-C5'-O5'
1	L1	1524	OMG	O4'-C4'-C5'-O5'
1	L1	1528	PSU	O4'-C4'-C5'-O5'
2	L2	512	PSU	O4'-C4'-C5'-O5'
2	L2	593	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	L2	1078	OMG	O4'-C4'-C5'-O5'
51	S1	98	A2M	C3'-C4'-C5'-O5'
2	L2	560	OMU	C3'-C4'-C5'-O5'
2	L2	1078	OMG	C3'-C4'-C5'-O5'
51	S1	8	OMU	O4'-C1'-N1-C6
1	L1	1373	A2M	O4'-C4'-C5'-O5'
1	L1	1524	OMG	C3'-C4'-C5'-O5'
4	L4	74	OMG	O4'-C4'-C5'-O5'
2	L2	667	OMU	C1'-C2'-O2'-CM2
2	L2	560	OMU	C4'-C5'-O5'-P
1	L1	1177	PSU	C3'-C4'-C5'-O5'
1	L1	1373	A2M	C3'-C4'-C5'-O5'
51	S1	2061	5MC	C3'-C4'-C5'-O5'
2	L2	1308	5MC	O4'-C1'-N1-C2
2	L2	655	OMG	C3'-C2'-O2'-CM2
2	L2	1308	5MC	O4'-C1'-N1-C6
51	S1	1543	B8N	C4'-C5'-O5'-P
1	L1	1528	PSU	C3'-C4'-C5'-O5'
2	L2	359	OMC	C3'-C4'-C5'-O5'
51	S1	2061	5MC	O4'-C4'-C5'-O5'
51	S1	2151	OMG	C3'-C4'-C5'-O5'
2	L2	443	OMC	O4'-C1'-N1-C6
1	L1	681	A2M	C4'-C5'-O5'-P
2	L2	1248	OMC	C4'-C5'-O5'-P
51	S1	8	OMU	O4'-C1'-N1-C2
51	S1	1833	OMU	C4'-C5'-O5'-P
51	S1	2185	MA6	C4'-C5'-O5'-P
1	L1	959	OMG	O4'-C4'-C5'-O5'
2	L2	443	OMC	O4'-C1'-N1-C2
51	S1	1478	OMG	C4'-C5'-O5'-P
2	L2	359	OMC	O4'-C4'-C5'-O5'
1	L1	1107	OMU	C3'-C2'-O2'-CM2
2	L2	502[A]	A2M	C4'-C5'-O5'-P
1	L1	678	A2M	C4'-C5'-O5'-P
51	S1	1829	OMG	C4'-C5'-O5'-P
1	L1	510	PSU	O4'-C1'-C5-C4
51	S1	1657	PSU	O4'-C1'-C5-C4
2	L2	1360	OMG	C3'-C2'-O2'-CM2
51	S1	2021	A2M	C3'-C2'-O2'-CM'
1	L1	959	OMG	C3'-C4'-C5'-O5'
51	S1	600	OMG	O4'-C4'-C5'-O5'
1	L1	1177	PSU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	L2	560	OMU	O4'-C4'-C5'-O5'
51	S1	1544	5MC	O4'-C4'-C5'-O5'
2	L2	665	A2M	C1'-C2'-O2'-CM'
51	S1	18	OMC	C1'-C2'-O2'-CM2
1	L1	1527	OMC	C3'-C2'-O2'-CM2
3	L3	13	OMU	C4'-C5'-O5'-P
1	L1	858	A2M	C3'-C4'-C5'-O5'
2	L2	593	PSU	O4'-C4'-C5'-O5'
1	L1	510	PSU	O4'-C1'-C5'-C6
2	L2	1185	A2M	C4'-C5'-O5'-P
51	S1	455	PSU	C4'-C5'-O5'-P
1	L1	1527	OMC	O4'-C4'-C5'-O5'
51	S1	1833	OMU	O4'-C4'-C5'-O5'
51	S1	2151	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 299 ligands modelled in this entry, 299 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	S1	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S1	1543:B8N	O3'	1544:5MC	P	3.91
1	S1	1542:C	O3'	1543:B8N	P	3.22

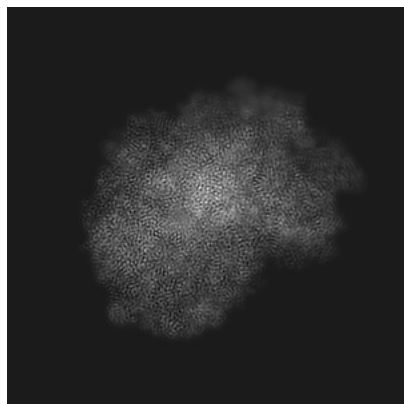
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19582. These allow visual inspection of the internal detail of the map and identification of artifacts.

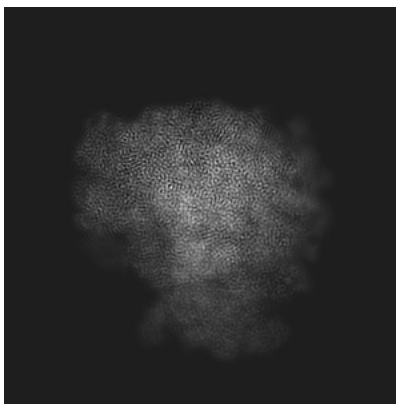
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

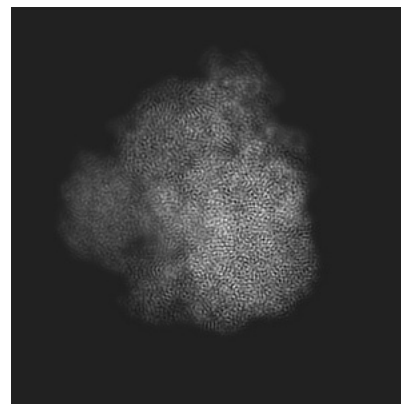
6.1.1 Primary map



X

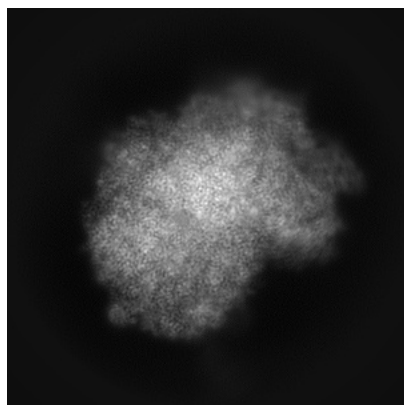


Y

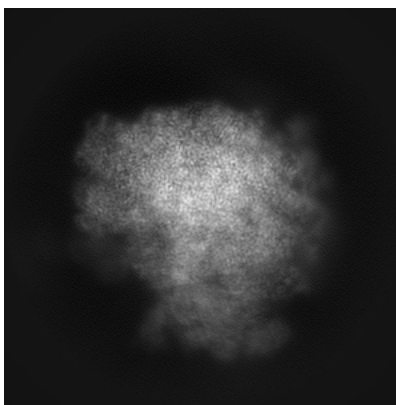


Z

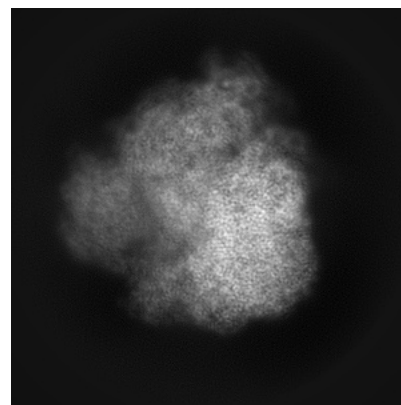
6.1.2 Raw map



X



Y

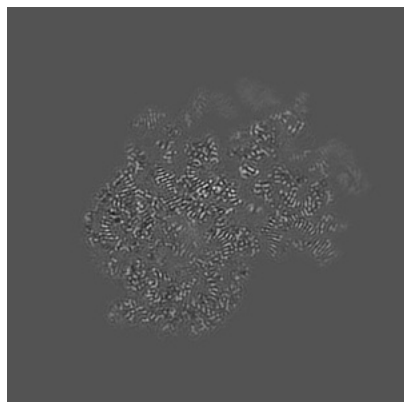


Z

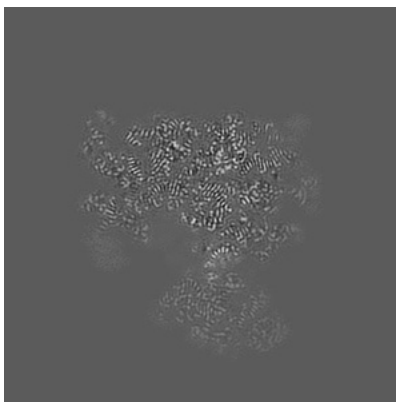
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

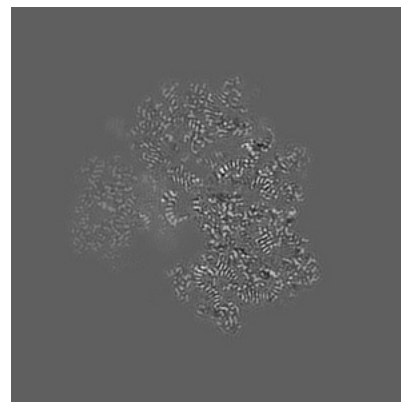
6.2.1 Primary map



X Index: 240

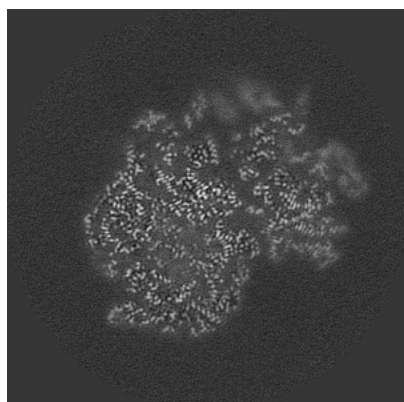


Y Index: 240

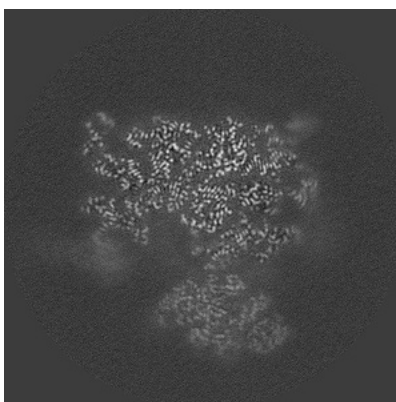


Z Index: 240

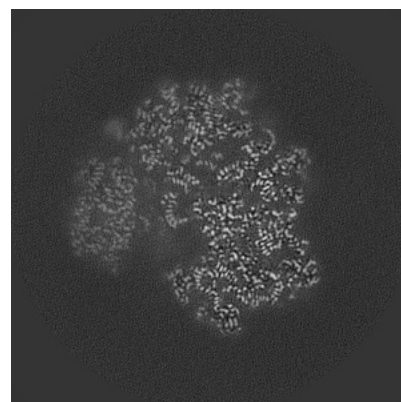
6.2.2 Raw map



X Index: 240



Y Index: 240

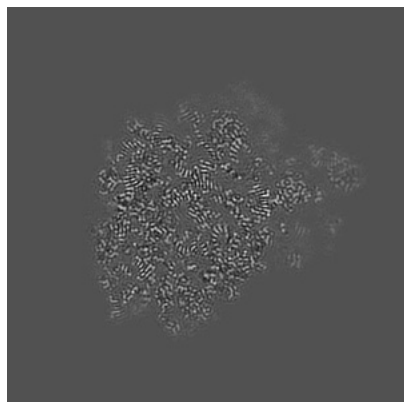


Z Index: 240

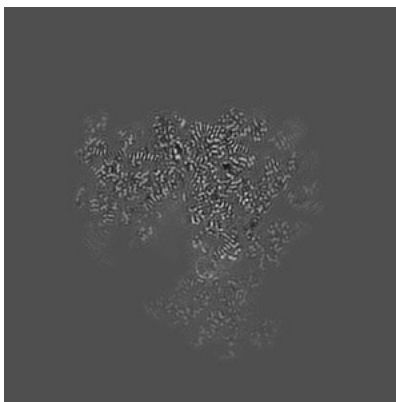
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

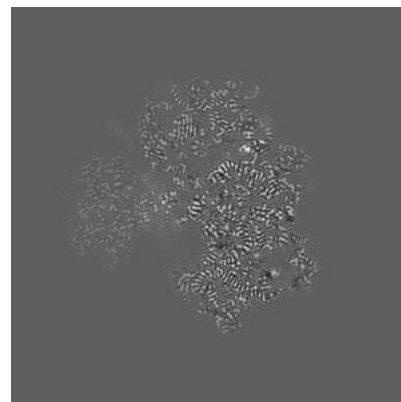
6.3.1 Primary map



X Index: 286

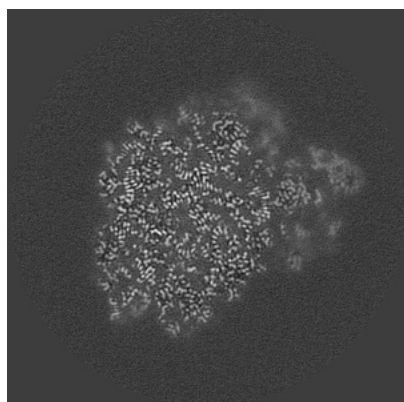


Y Index: 230

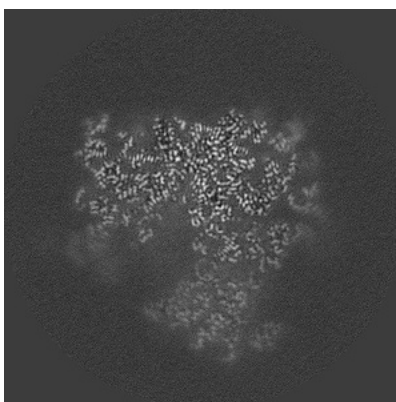


Z Index: 245

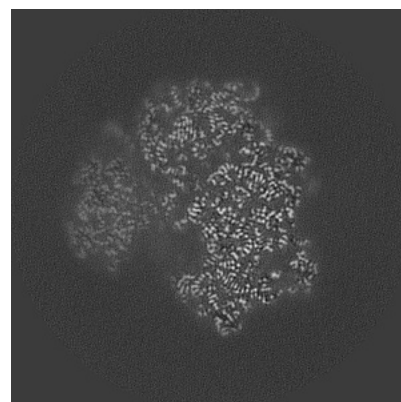
6.3.2 Raw map



X Index: 286



Y Index: 230

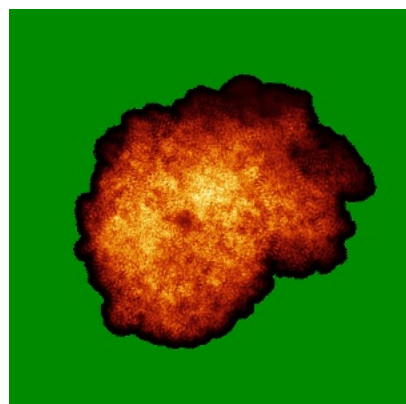


Z Index: 245

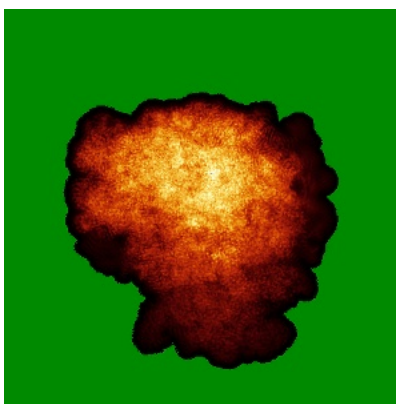
The images above show the largest variance slices of the map in three orthogonal directions.

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

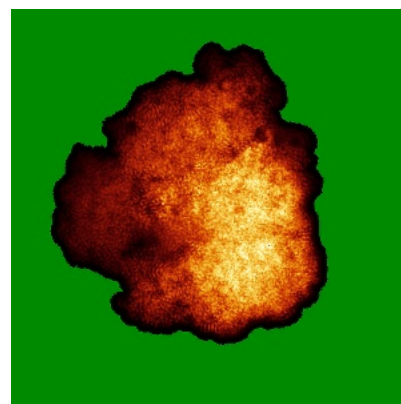
6.4.1 Primary map



X

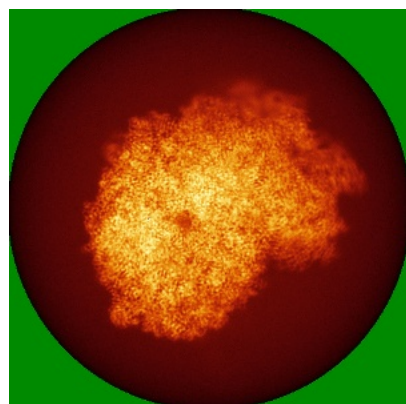


Y

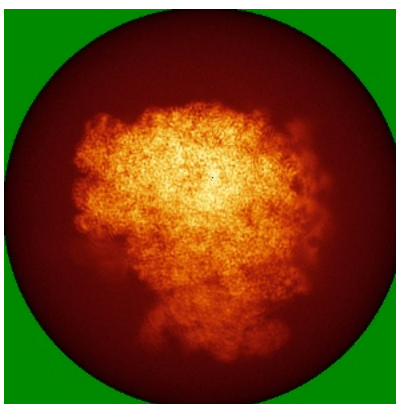


Z

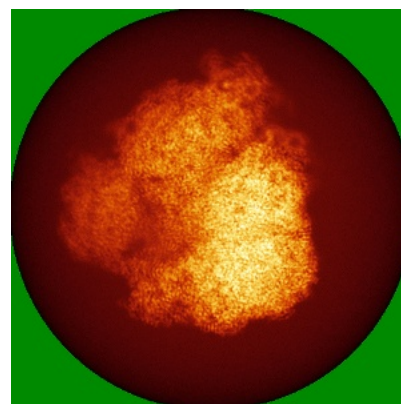
6.4.2 Raw map



X



Y

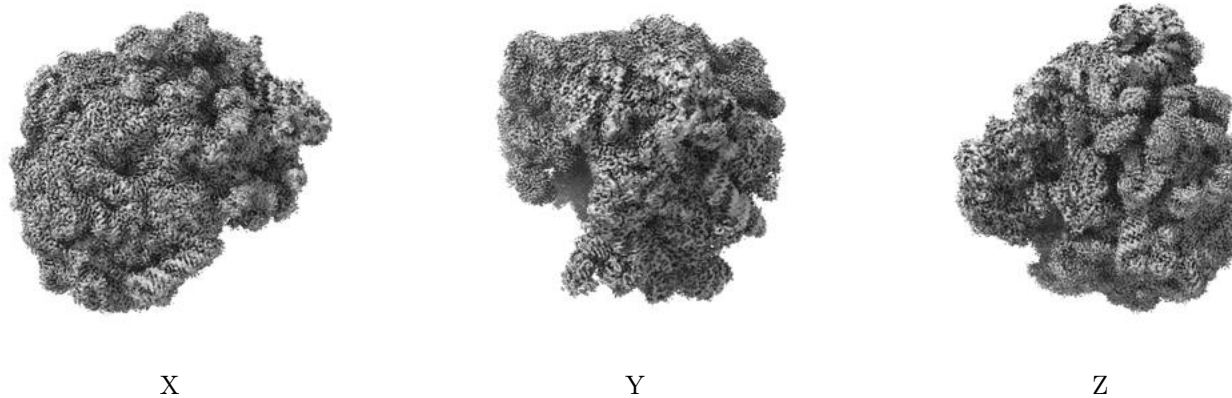


Z

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

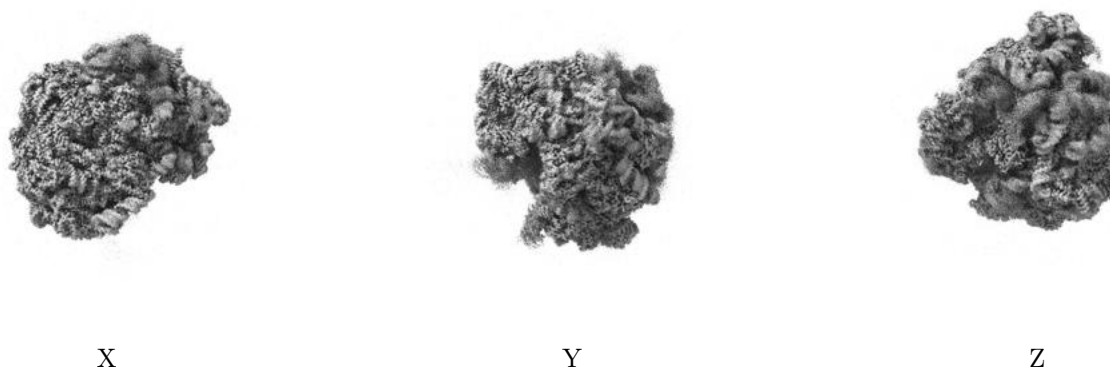
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

6.5.2 Raw map



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

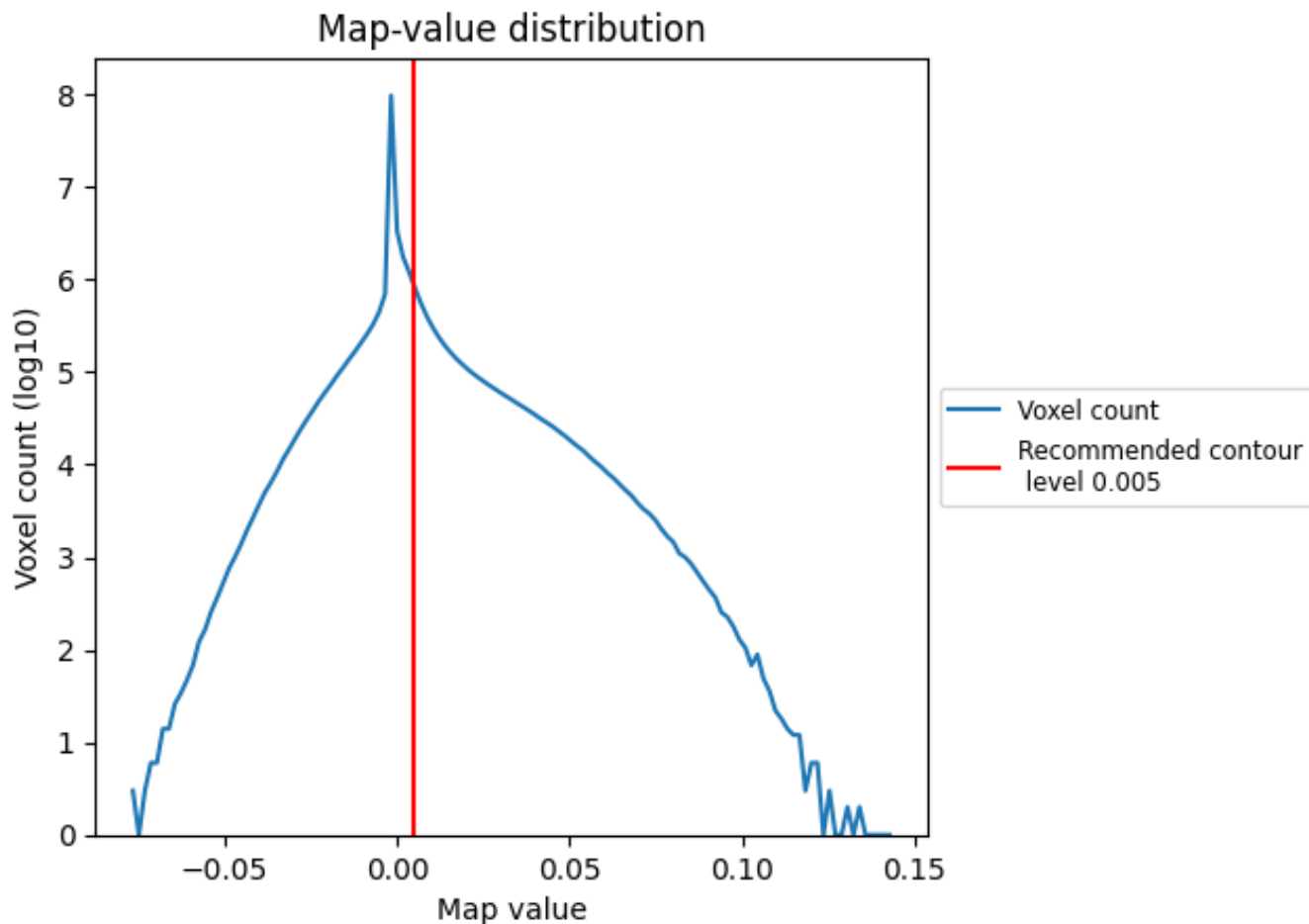
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

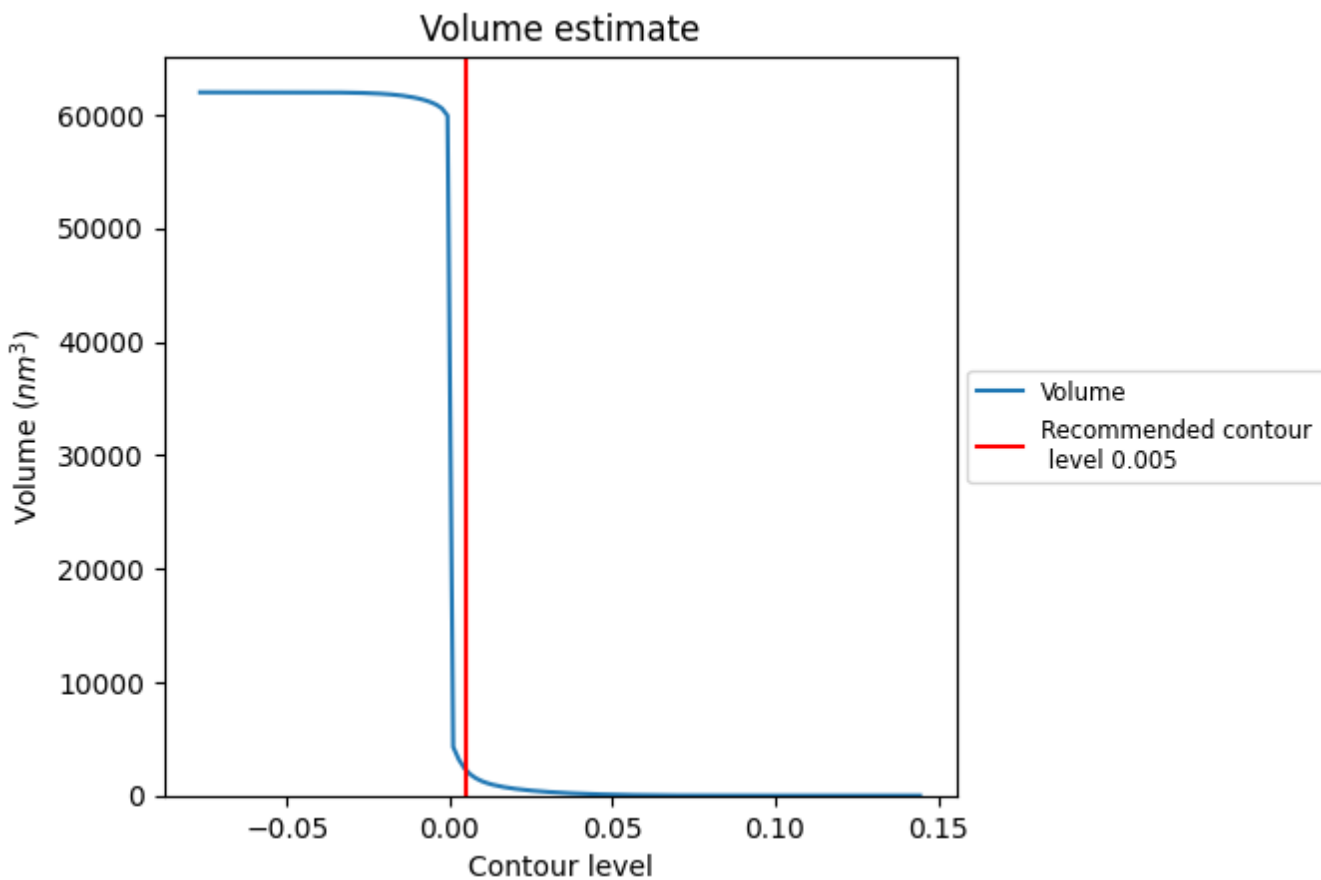
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

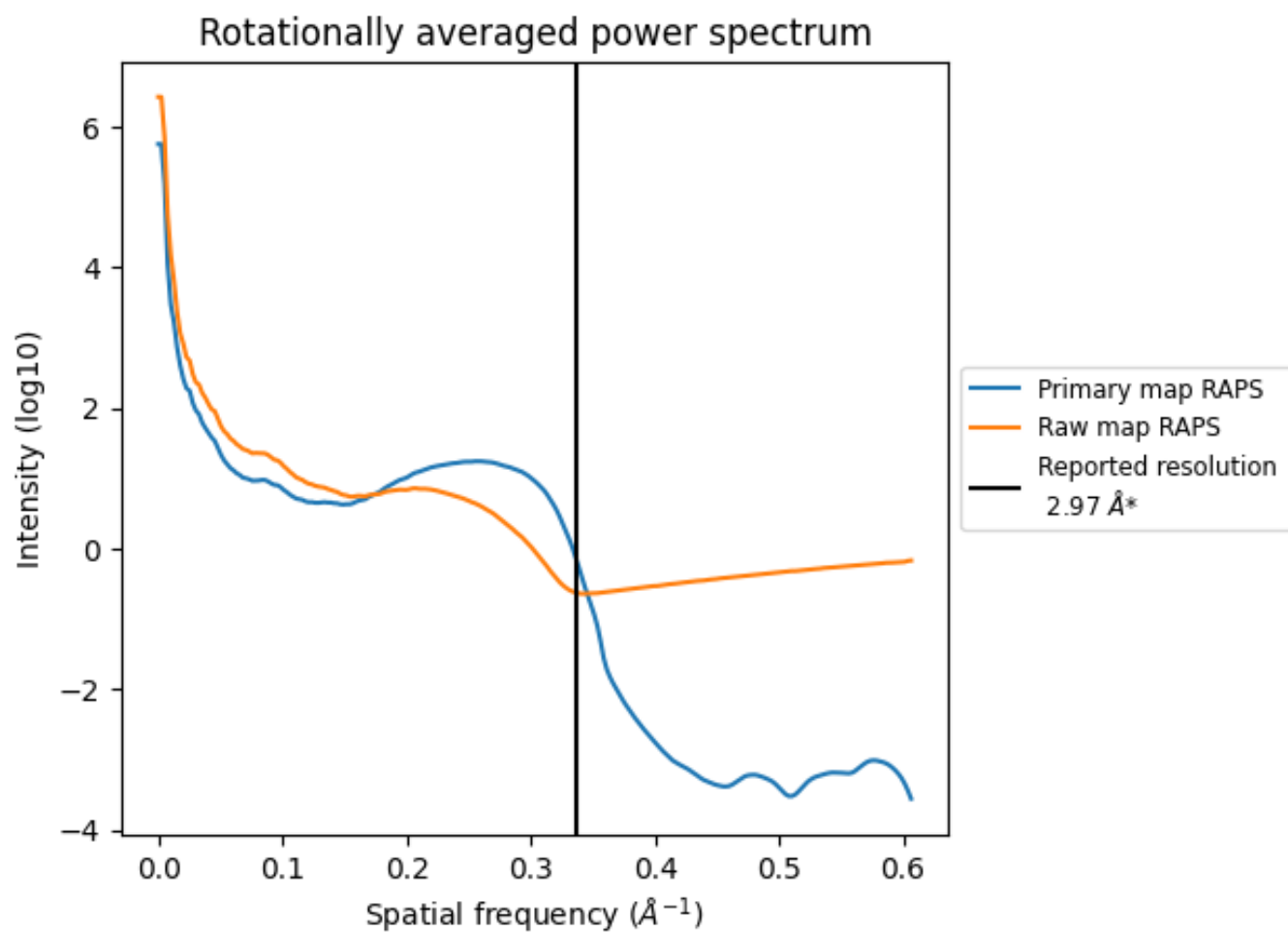
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2282 nm^3 ; this corresponds to an approximate mass of 2062 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

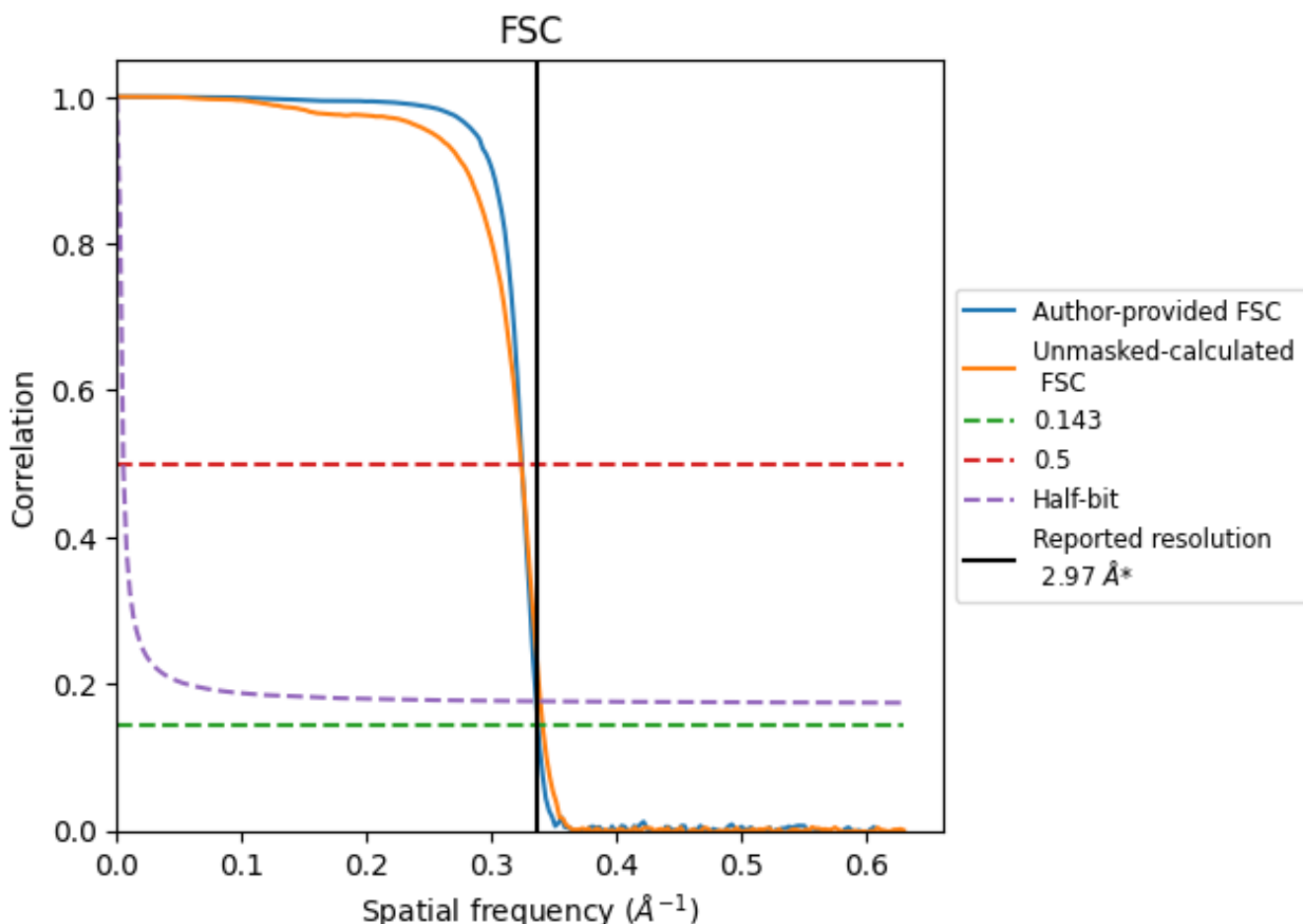


*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.337 \AA^{-1}

8.2 Resolution estimates [i](#)

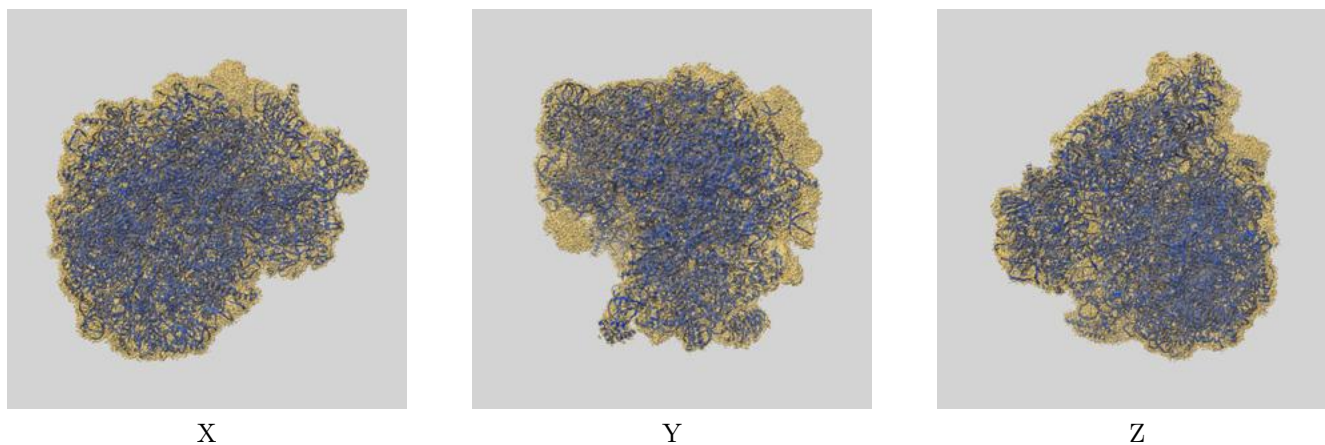
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.96	3.08	2.98
Unmasked-calculated*	2.93	3.09	2.95

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

9 Map-model fit [i](#)

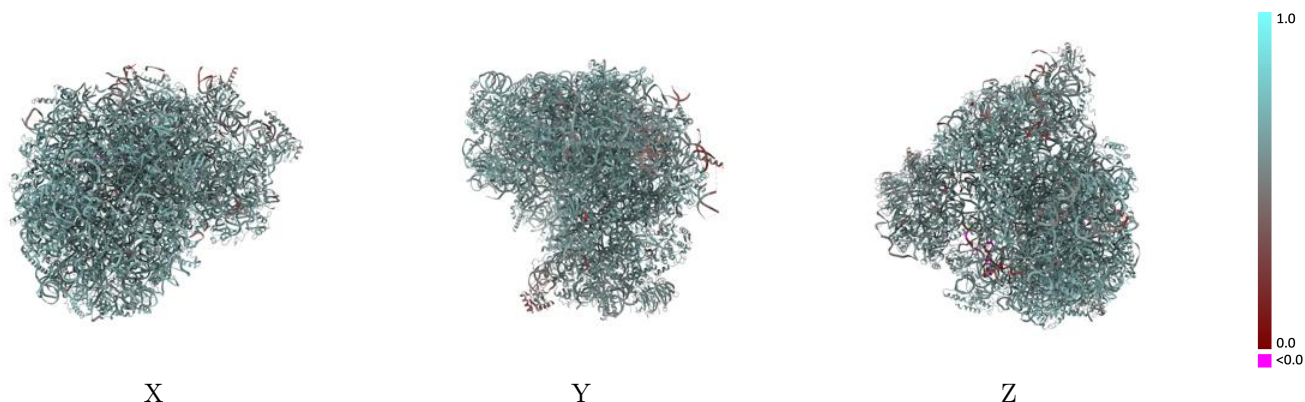
This section contains information regarding the fit between EMDB map EMD-19582 and PDB model 8RXX. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



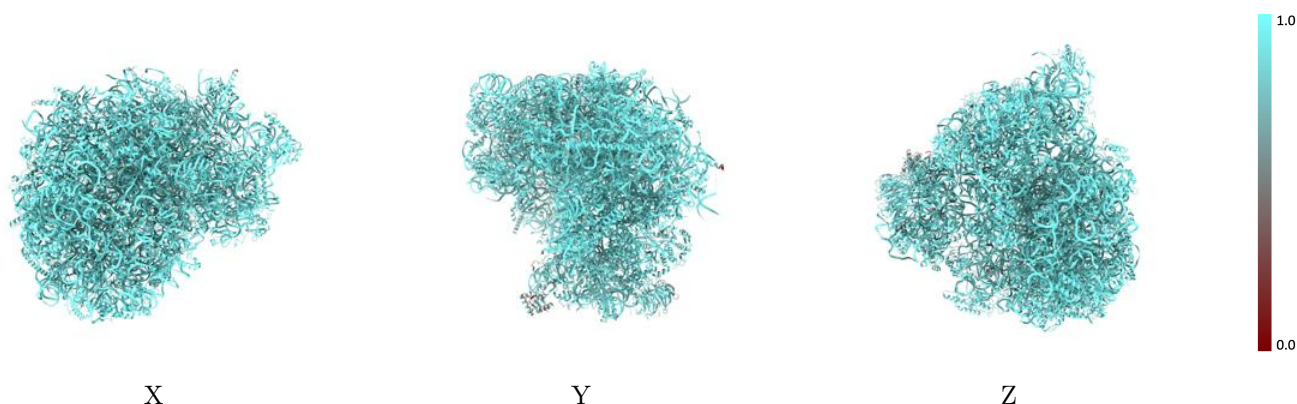
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



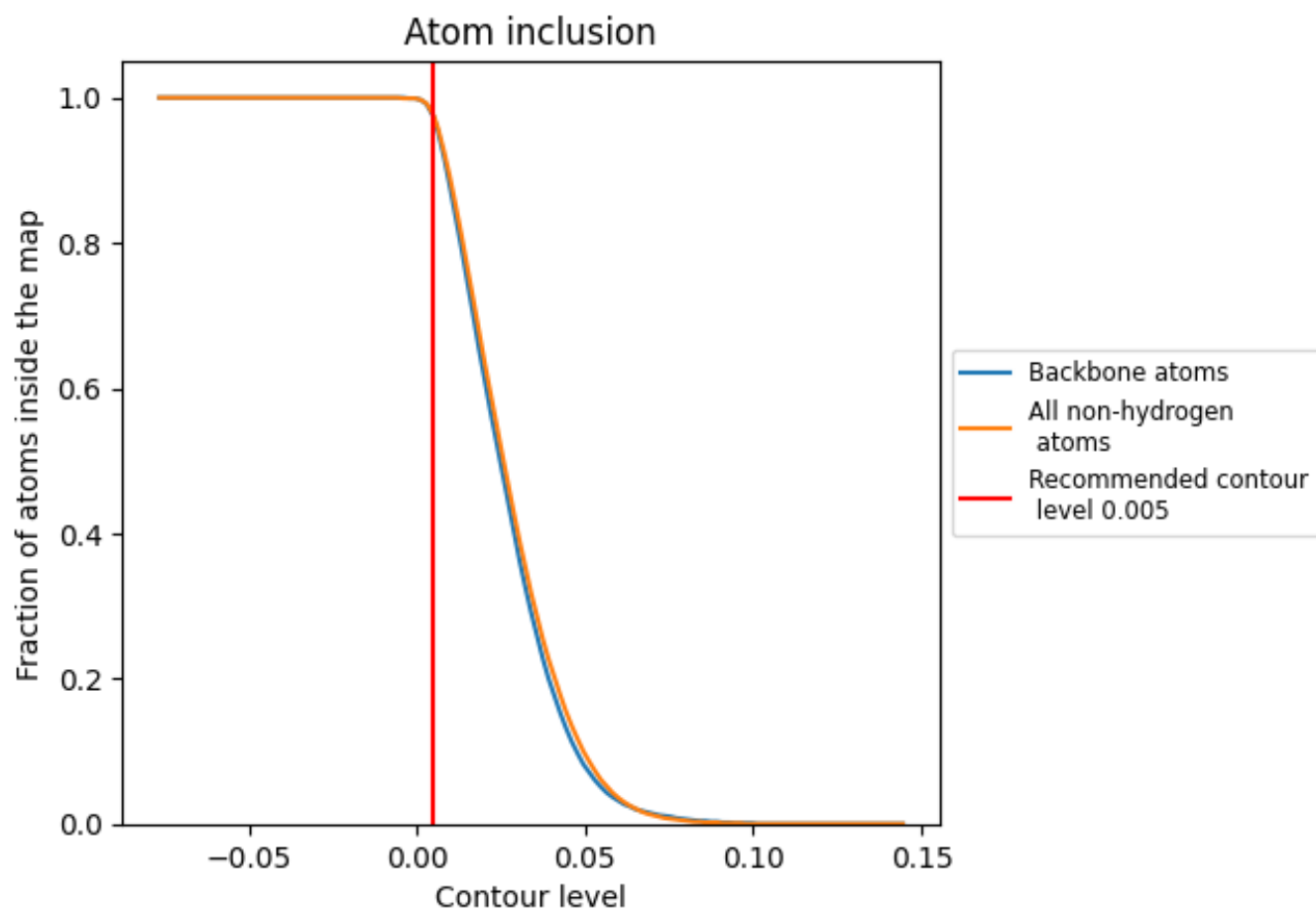
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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	 0.9750	 0.6010
L1	 0.9900	 0.6160
L2	 0.9860	 0.6050
L3	 0.9830	 0.6020
L4	 0.9940	 0.6220
L5	 0.9820	 0.6000
L6	 0.9780	 0.5990
L7	 0.9900	 0.6210
L8	 0.9950	 0.6100
LA	 0.9940	 0.6460
LB	 0.9910	 0.6410
LC	 0.9910	 0.6370
LD	 0.9760	 0.5850
LE	 0.9810	 0.6230
LF	 0.9760	 0.6200
LG	 0.9710	 0.6130
LH	 0.9880	 0.6360
LI	 0.9870	 0.6360
LJ	 0.9930	 0.6370
LK	 0.9860	 0.6210
LL	 0.9890	 0.6450
LM	 0.9950	 0.6450
LN	 0.9650	 0.6080
LO	 0.9740	 0.6110
LP	 0.9950	 0.6380
LQ	 0.9780	 0.6010
LR	 0.9890	 0.6360
LS	 0.9910	 0.6280
LT	 0.9960	 0.6440
LU	 0.9790	 0.6120
LV	 0.9860	 0.6370
LW	 0.9910	 0.6410
LX	 0.9740	 0.6200
LY	 0.9780	 0.6200
LZ	 0.9900	 0.6370





























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Chain	Atom inclusion	Q-score
La	 0.9870	 0.6300
Lb	 0.9810	 0.6270
Lc	 0.9880	 0.6380
Ld	 0.9810	 0.6110
Le	 0.9780	 0.6260
Lf	 0.9910	 0.6360
Lg	 0.9940	 0.6480
Lh	 0.9710	 0.6140
Li	 0.9600	 0.6060
Lj	 0.9920	 0.6440
Lk	 0.9810	 0.6310
Ll	 0.9930	 0.6460
Lm	 0.9820	 0.6220
Ln	 0.9930	 0.6020
Lo	 0.9930	 0.6290
Lp	 0.9920	 0.6370
S1	 0.9780	 0.5780
S2	 0.9390	 0.3690
S3	 0.9900	 0.4260
S4	 0.8410	 0.2800
S5	 1.0000	 0.5370
SA	 0.9570	 0.6080
SB	 0.9720	 0.6000
SC	 0.8880	 0.5730
SD	 0.9630	 0.6020
SE	 0.9810	 0.6170
SF	 0.9770	 0.6140
SG	 0.9670	 0.5930
SH	 0.9320	 0.5810
SI	 0.9820	 0.6100
SJ	 0.9870	 0.6230
SK	 0.9920	 0.6190
SL	 0.9600	 0.5890
SM	 0.8980	 0.5670
SN	 0.8740	 0.5500
SO	 0.9680	 0.6110
SP	 0.9770	 0.6090
SQ	 0.5140	 0.3640
SR	 0.8760	 0.5510
SS	 0.9450	 0.5940
ST	 0.9810	 0.6140
SU	 0.9930	 0.6310

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Chain	Atom inclusion	Q-score
SV	 0.9300	 0.5740
SW	 0.8330	 0.5420
SX	 0.9560	 0.5760
SY	 0.9660	 0.5940
SZ	 0.9710	 0.6020
Sa	 0.8930	 0.5580
Sb	 0.9750	 0.6120
Sc	 0.9800	 0.6050
Sd	 0.9070	 0.5710
Se	 0.9070	 0.5600
Sf	 0.7700	 0.4760
Sg	 0.8350	 0.5300
Sh	 0.9290	 0.5350