



Full wwPDB EM Validation Report ⓘ

May 12, 2024 – 10:18 am BST

PDB ID : 8RXH
EMDB ID : EMD-19576
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME
WITH A/P/E-site tRNA AND mRNA : PARENTAL STRAIN
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2024-02-07
Resolution : 2.93 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:

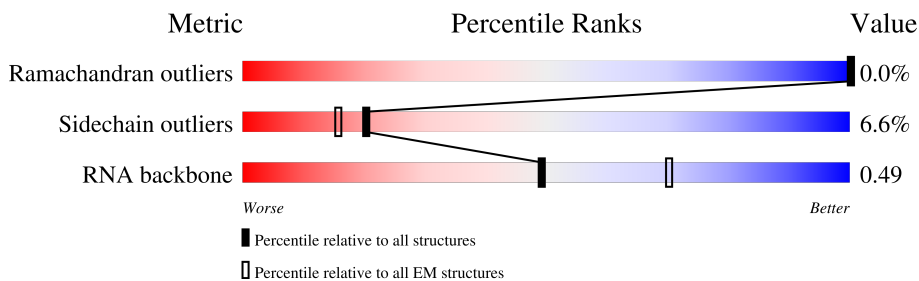
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.93 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	
2	L2	1526	
3	L3	216	
4	L4	184	
5	L5	135	
6	L6	73	
7	L7	171	
8	L8	124	

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Mol	Chain	Length	Quality of chain
9	LA	260	95% 5%
10	LB	419	94%
11	LC	373	93% 5%
12	LD	188	87% 6% 7%
13	LE	190	92% 6%
14	LF	195	72% 24%
15	LG	264	88% 9%
16	LH	222	95% 5%
17	LI	220	94%
18	LJ	139	95%
19	LK	175	92% 5%
20	LL	145	94%
21	LM	204	92% 6%
22	LN	213	86% 10%
23	LO	305	94%
24	LP	198	96%
25	LQ	254	75% 21%
26	LR	179	95%
27	LS	159	94% 5%
28	LT	166	89% 8%
29	LU	129	90% 5% 5%
30	LV	145	80% 18%
31	LW	143	82% 15%
32	LX	124	66% 31%
33	LY	134	95%

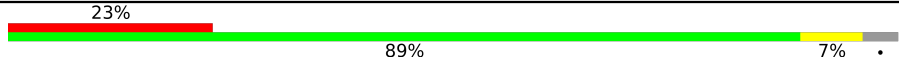
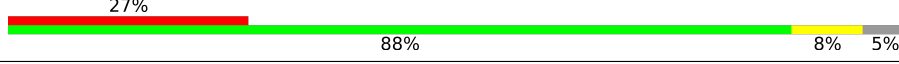
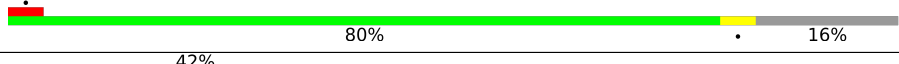

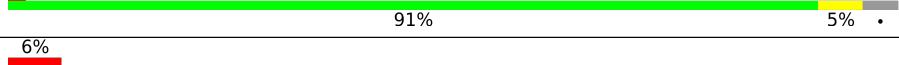
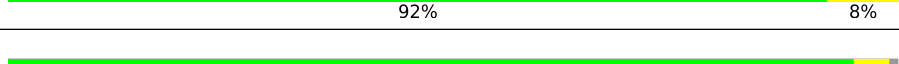
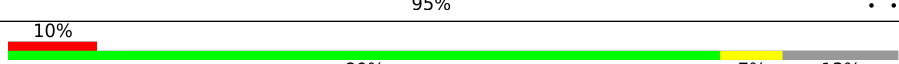
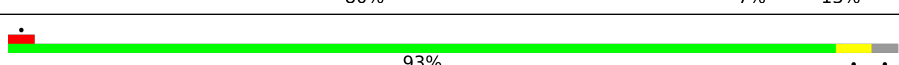
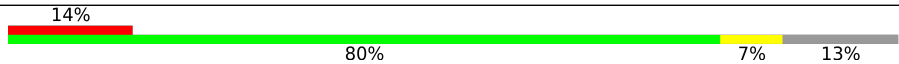

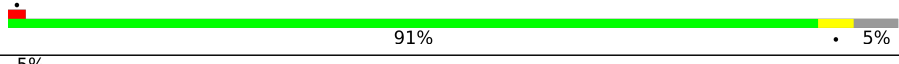
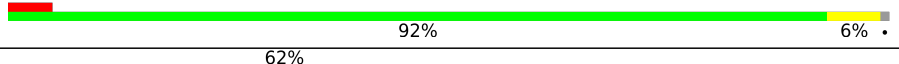
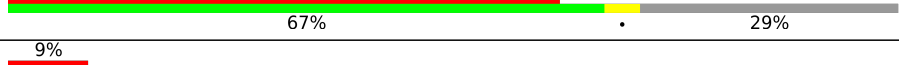

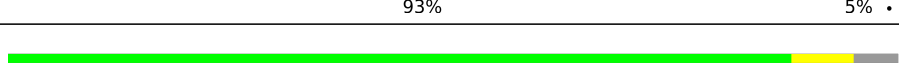



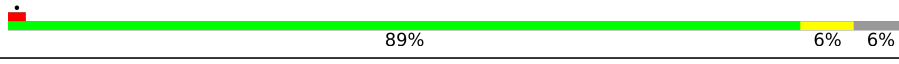
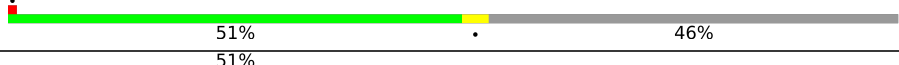





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Mol	Chain	Length	Quality of chain
34	LZ	147	95%
35	La	127	97%
36	Lb	70	90% 7%
37	Lc	252	88% 9%
38	Ld	104	90% 7%
39	Le	188	96%
40	Lf	133	94%
41	Lg	144	97%
42	Lh	168	72% 24%
43	Li	105	94%
44	Lj	83	93% 5%
45	Lk	83	92% 6%
46	Ll	51	92% 6%
47	Lm	128	38% 59%
48	Ln	34	94%
49	Lo	92	92%
50	Lp	106	86% 6% 8%
51	S1	2204	61% 22% 11% 16%
52	S2	76	62% 38% 80%
53	S3	77	71% 25% 21%
54	S4	76	46% 51% 63%
55	S5	13	46% 46% 8%
56	SA	264	88% 5% 8%
57	SB	246	83% 14%
58	SC	219	89% 8% 10%

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Mol	Chain	Length	Quality of chain
59	SD	190	
60	SE	273	
61	SF	265	
62	SG	249	
63	SH	190	
64	SI	200	
65	SJ	130	
66	SK	220	
67	SL	149	
68	SM	116	
69	SN	168	
70	SO	144	
71	SP	143	
72	SQ	141	
73	SR	153	
74	SS	57	
75	ST	151	
76	SU	173	
77	SV	143	
78	SW	152	
79	SX	161	
80	SY	164	
81	SZ	137	
82	Sa	120	
83	Sb	112	

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Mol	Chain	Length	Quality of chain
84	Sc	86	<p>91% 8%</p>
85	Sd	87	<p>10% 70% 6% 24%</p>
86	Se	66	<p>26% 86% 6% 8%</p>
87	Sf	152	<p>38% 45% 7% 47%</p>
88	Sg	312	<p>33% 90% 7%</p>
89	Sh	235	<p>40% 36% 5% 59%</p>

2 Entry composition

There are 95 unique types of molecules in this entry. The entry contains 216694 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	1677	35987	16086	6578	11645	1678	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	1155	24715	11065	4453	8042	1155	0	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	120	2555	1140	455	840	120	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	3533	1583	626	1159	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	120	2551	1141	454	836	120	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	258	1962	1223	400	329	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	404	3216	2024	638	541	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	2820	1761	561	483	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	1387	875	261	243	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	1477	936	273	262	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	1199	376	323	7	0	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	1767	1123	353	284	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	214	1695	1056	342	289	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	1012	638	191	177	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	1336	833	264	231	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	205	Total	C	N	O	S	0	0
			1665	1050	329	271	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	298	Total	C	N	O	S	0	0
			2329	1480	437	406	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
			1539	968	307	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
			1682	1035	367	274	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
			1261	803	245	209	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
			1217	761	241	205	10		

- 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
			960	624	176	157	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
			953	604	181	166	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
			967	603	200	160	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
34	LZ	145	Total	C	N	O	S	0	0
			1117	685	238	189	5		

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			608	383	119	103	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	52	Total	C	N	O	S	0	0
			417	263	85	64	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ln	33	Total	C	N	O	S	0	0
			296	181	76	37	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lp	97	Total	C	N	O	S	0	0
			784	496	158	125	5		

- Molecule 51 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S1	1844	Total	C	N	O	P	0	0
			39438	17643	7112	12839	1844		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
52	S2	76	Total	C	N	O	P	S	0	0
			1626	729	290	531	75	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S3	75	Total	C	N	O	P	0	0
			1602	714	292	521	75		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S4	74	Total	C	N	O	P	0	0
			1574	703	280	518	73		

- Molecule 55 is a RNA chain called mRNA_chain_S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S5	12	Total	C	N	O	P	0	0
			251	113	43	83	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SA	244	Total	C	N	O	S	0	0
			1943	1213	375	344	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SB	211	Total	C	N	O	S	0	0
			1661	1055	303	292	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SC	212	Total	C	N	O	S	1	0
			1646	1040	302	291	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SD	183	Total	C	N	O	S	0	0
			1508	949	305	246	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SF	222	Total	C	N	O	S	0	0
			1708	1088	301	309	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	SG	229	1829	1140	375	311	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	SH	183	1447	899	279	262	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	SI	200	1649	1050	320	271	8	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	SK	192	1550	967	320	261	2	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	SM	101	792	496	144	150	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	SN	100	818	525	143	143	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	137	1024	633	200	183	8	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	1100	694	217	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	100	670	411	121	133	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	142	1138	715	226	192	5	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	452	279	94	73	6	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	143	1167	736	231	191	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	SU	153	1257	795	251	206	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	SV	122	992	619	193	175	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	SW	115	928	591	176	157	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	SY	88	663	409	121	129	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	Sa	105	798	502	147	145	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	Sb	104	825	511	177	130	7	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Sd	66	496	301	100	91	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	Se	61	487	307	102	77	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
87	Sf	80	659	413	130	110	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
88	Sg	303	2354	1475	420	446	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
89	Sh	96	768	486	146	133	3	0	0

- Molecule 90 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	L1	116	Total 116	Mg 116	0
90	L2	74	Total 74	Mg 74	0
90	L3	4	Total 4	Mg 4	0
90	L4	4	Total 4	Mg 4	0
90	L5	1	Total 1	Mg 1	0
90	L6	1	Total 1	Mg 1	0
90	L7	9	Total 9	Mg 9	0
90	L8	5	Total 5	Mg 5	0
90	LA	1	Total 1	Mg 1	0
90	LB	1	Total 1	Mg 1	0
90	LJ	1	Total 1	Mg 1	0
90	LS	1	Total 1	Mg 1	0
90	LT	1	Total 1	Mg 1	0
90	Lf	1	Total 1	Mg 1	0
90	Lh	1	Total 1	Mg 1	0
90	Lj	1	Total 1	Mg 1	0
90	S1	64	Total 64	Mg 64	0
90	S5	2	Total 2	Mg 2	0
90	SX	1	Total 1	Mg 1	0

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

Mol	Chain	Residues	Atoms		AltConf
91	L1	29	Total 29	Na 29	0

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Mol	Chain	Residues	Atoms		AltConf
91	L2	21	Total 21	Na 21	0
91	L4	4	Total 4	Na 4	0
91	L5	3	Total 3	Na 3	0
91	L8	1	Total 1	Na 1	0
91	LA	2	Total 2	Na 2	0
91	LE	1	Total 1	Na 1	0
91	LH	1	Total 1	Na 1	0
91	LM	2	Total 2	Na 2	0
91	LN	2	Total 2	Na 2	0
91	LR	1	Total 1	Na 1	0
91	Lf	1	Total 1	Na 1	0
91	S1	16	Total 16	Na 16	0
91	SH	1	Total 1	Na 1	0
91	SP	1	Total 1	Na 1	0

- Molecule 92 is POTASSIUM ION (three-letter code: K) (formula: K).

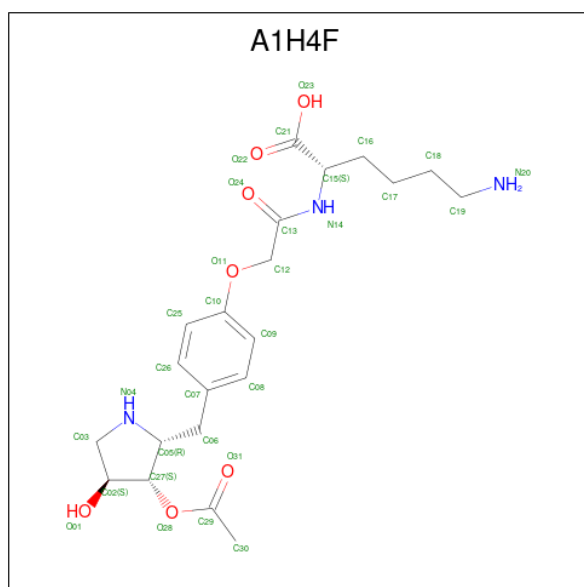
Mol	Chain	Residues	Atoms		AltConf
92	L1	55	Total 55	K 55	0
92	L2	33	Total 33	K 33	0
92	L3	2	Total 2	K 2	0
92	L4	6	Total 6	K 6	0
92	L5	2	Total 2	K 2	0

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Mol	Chain	Residues	Atoms	AltConf
92	L7	5	Total K 5 5	0
92	L8	1	Total K 1 1	0
92	LB	2	Total K 2 2	0
92	LC	2	Total K 2 2	0
92	LZ	1	Total K 1 1	0
92	Lh	1	Total K 1 1	0
92	S1	30	Total K 30 30	0
92	SS	1	Total K 1 1	0
92	ST	1	Total K 1 1	0
92	Sb	1	Total K 1 1	0

- Molecule 93 is (2S)-2-[2-[4-[[[(2R,3S,4S)-3-acetyloxy-4-oxidanyl-pyrrolidin-2-yl]methyl]phenoxy]ethanoylamino]-6-azanyl-hexanoic acid (three-letter code: A1H4F) (formula: C₂₁H₃₁N₃O₇).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
93	L2	1	31	21	3	7	0

- Molecule 94 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
94	Lp	1	1	1	0

- Molecule 95 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
95	L1	152	152	152	0
95	L2	119	119	119	0
95	L3	10	10	10	0
95	L4	11	11	11	0
95	L5	3	3	3	0
95	L7	11	11	11	0
95	L8	1	1	1	0
95	LA	7	7	7	0
95	LB	5	5	5	0
95	LC	4	4	4	0
95	LG	1	1	1	0
95	LH	2	2	2	0
95	LI	2	2	2	0
95	LL	5	5	5	0
95	LM	7	7	7	0
95	LP	2	2	2	0

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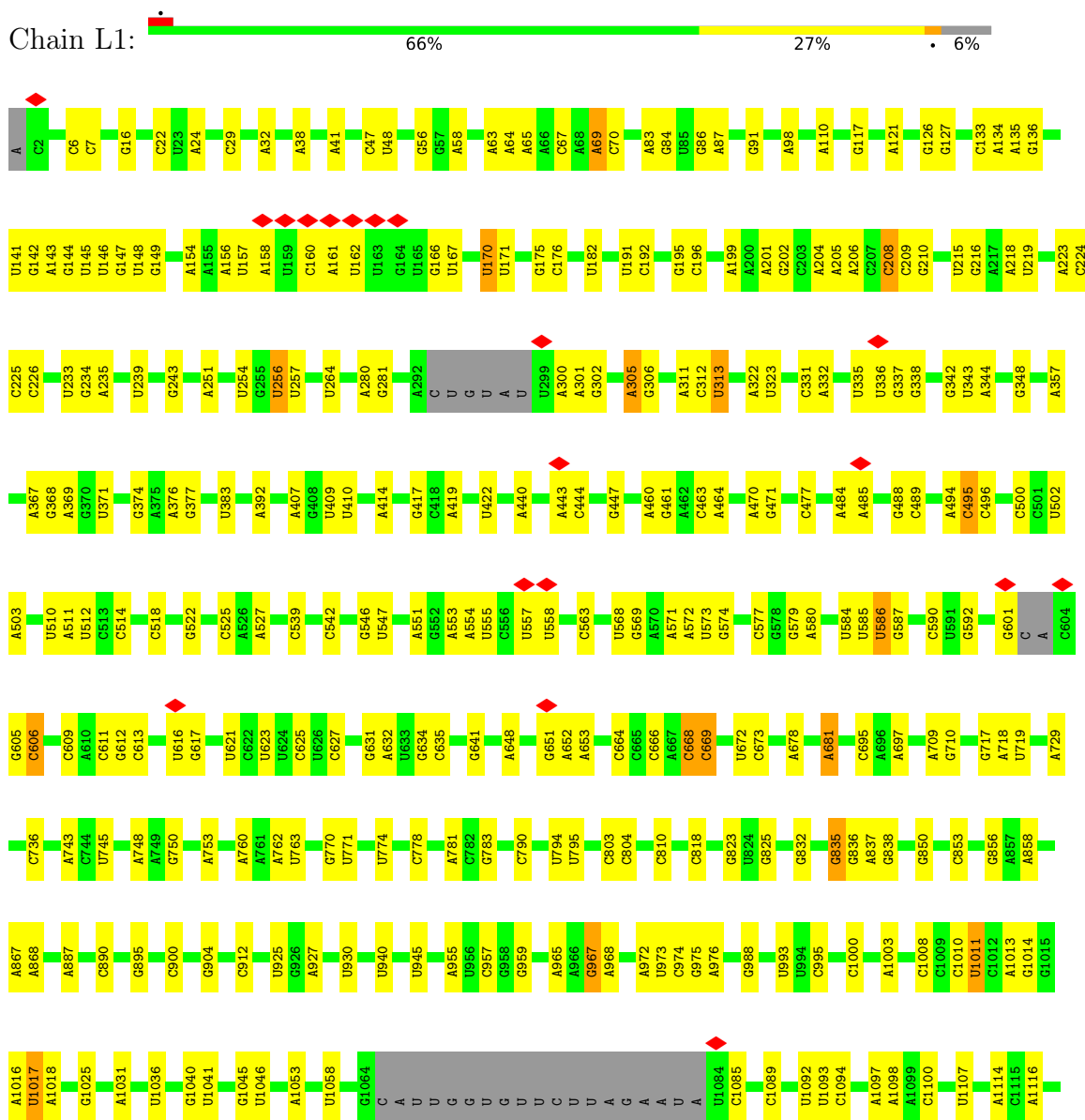
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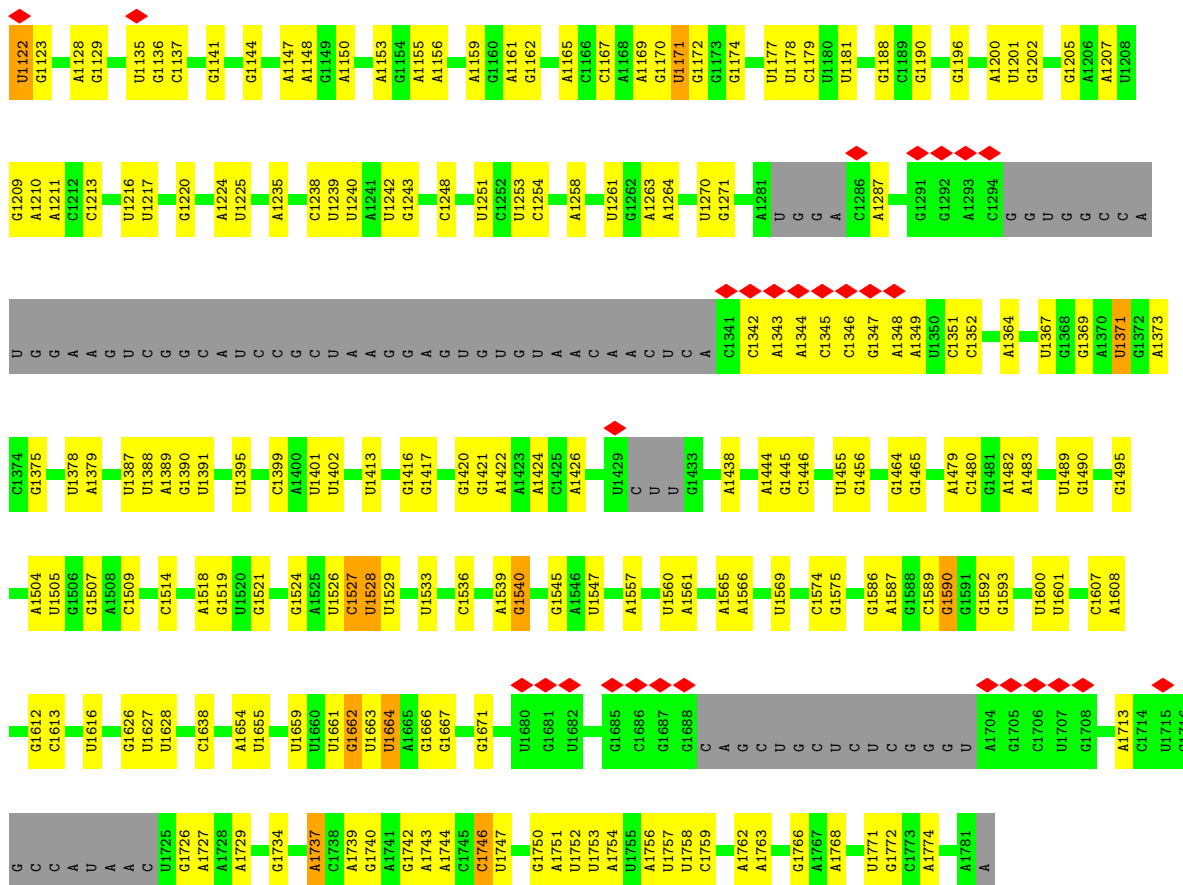
Mol	Chain	Residues	Atoms		AltConf
95	LQ	2	Total 2	O 2	0
95	LS	2	Total 2	O 2	0
95	LT	2	Total 2	O 2	0
95	LV	1	Total 1	O 1	0
95	LW	1	Total 1	O 1	0
95	La	2	Total 2	O 2	0
95	Lb	2	Total 2	O 2	0
95	Le	1	Total 1	O 1	0
95	Lf	2	Total 2	O 2	0
95	Lh	1	Total 1	O 1	0
95	Lj	4	Total 4	O 4	0
95	Lo	1	Total 1	O 1	0
95	Lp	2	Total 2	O 2	0
95	S1	47	Total 47	O 47	0
95	SA	1	Total 1	O 1	0

3 Residue-property plots

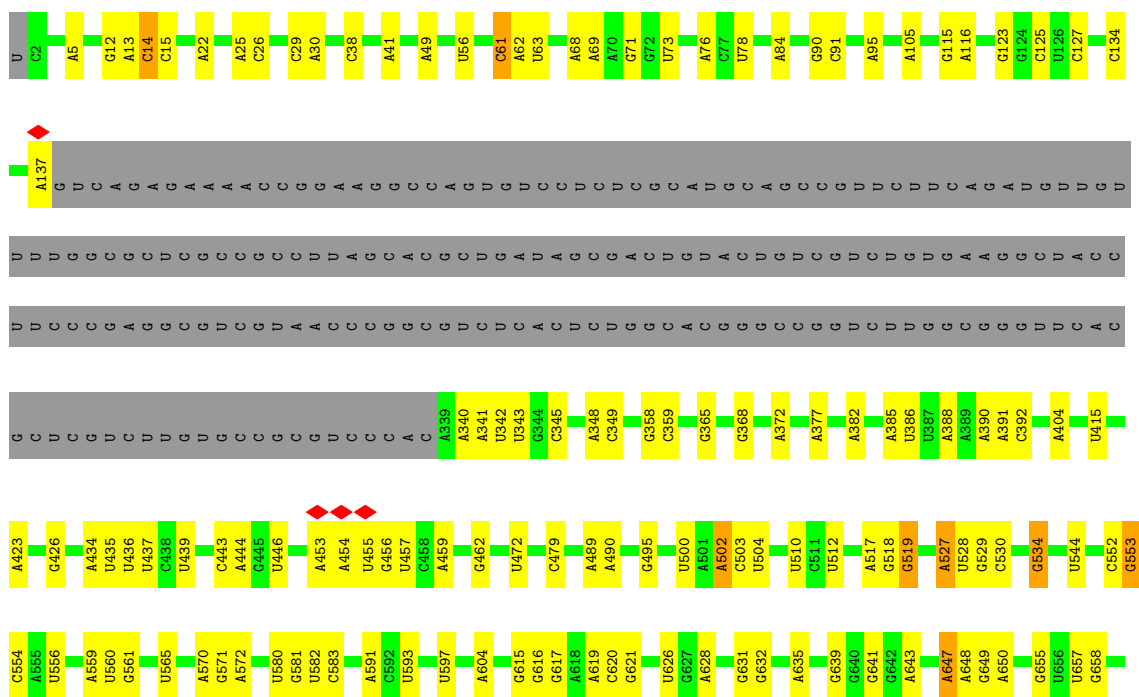
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

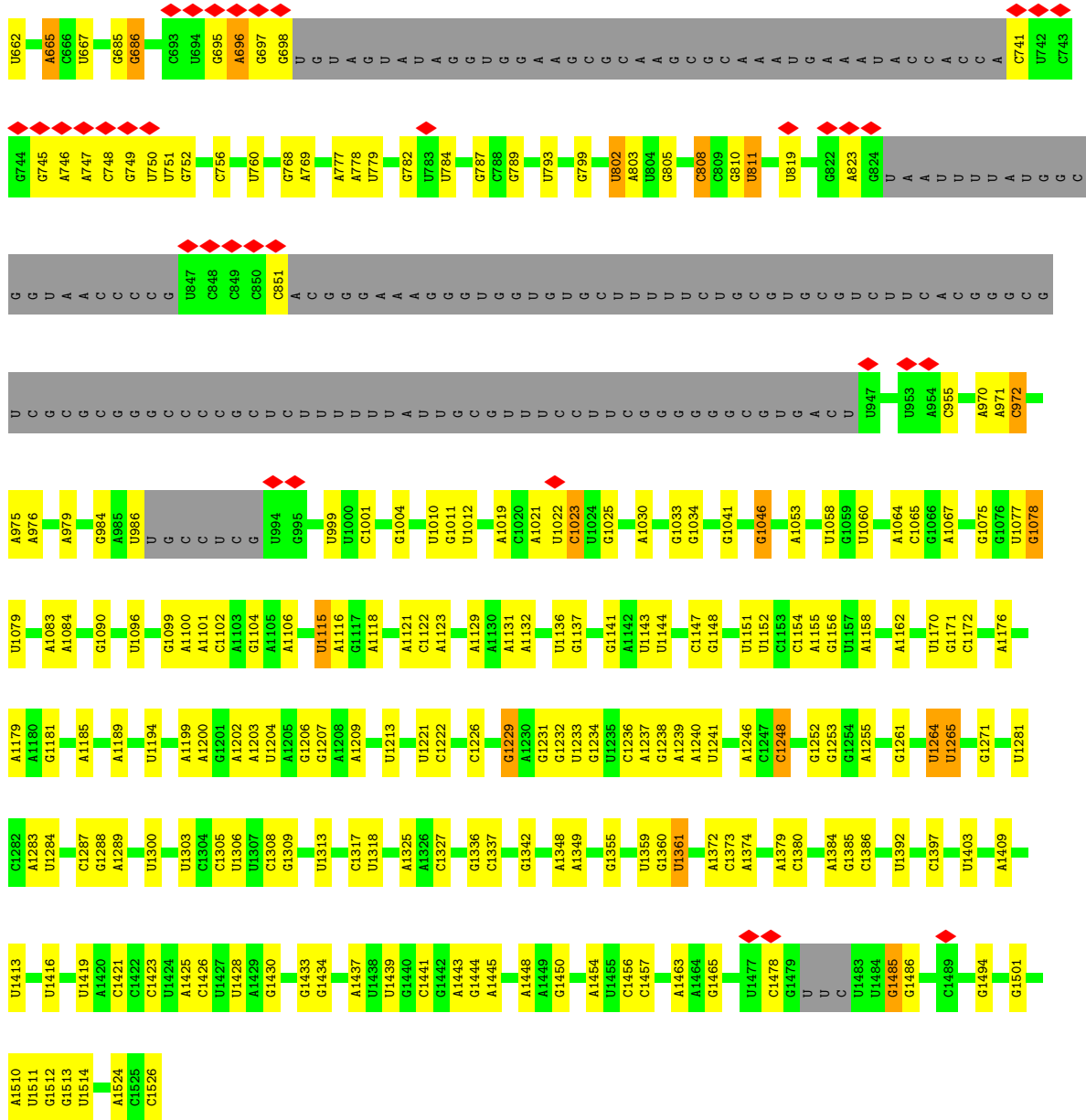
- Molecule 1: LSUa_rRNA_chain_1



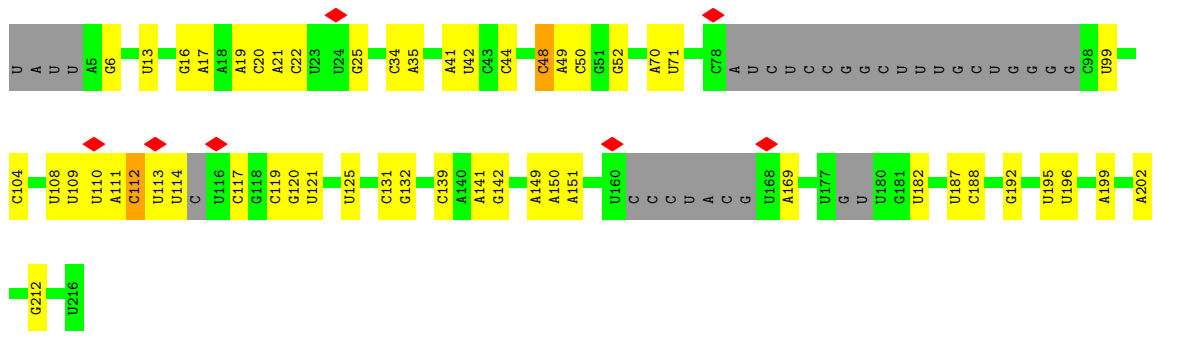


• Molecule 2: LSub_rRNA_chain_2

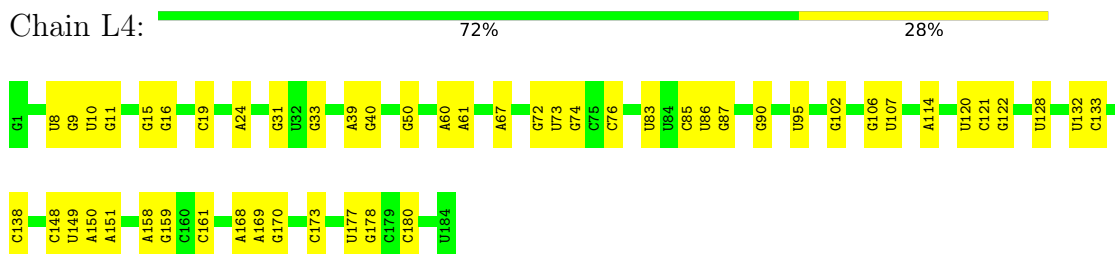




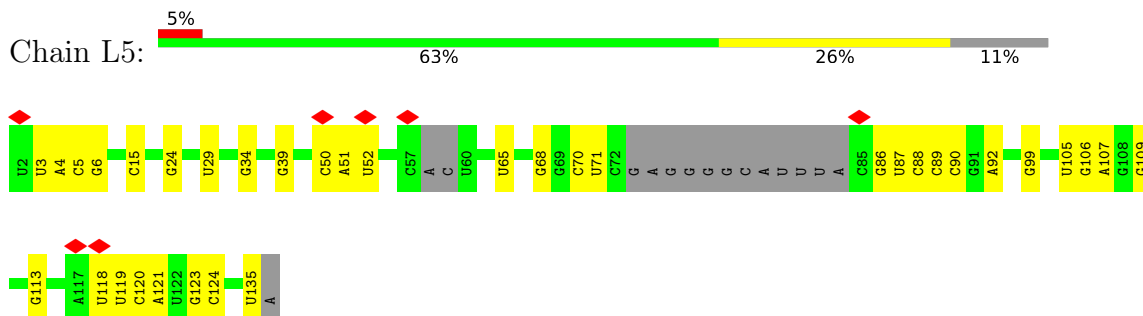
• Molecule 3: SR1_chain_3



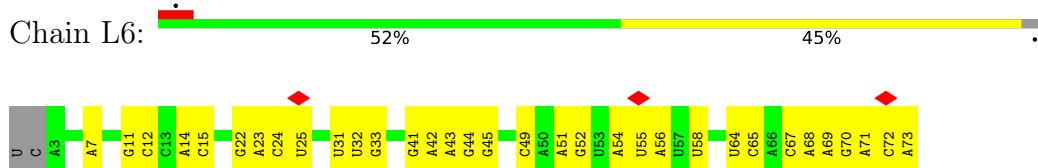
• Molecule 4: SR2_chain_4



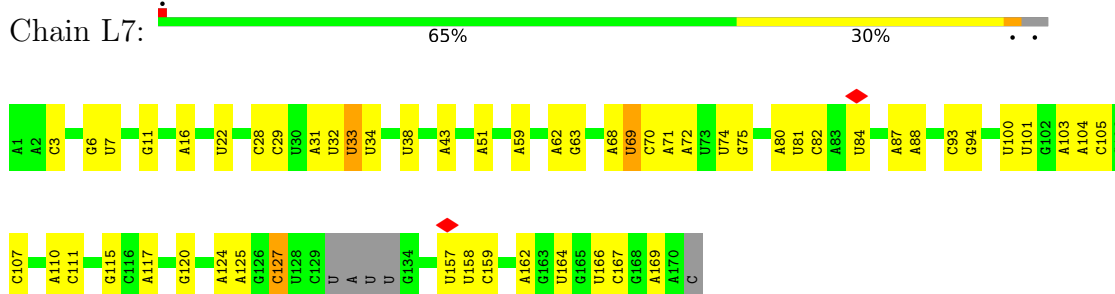
• Molecule 5: SR4_chain_5



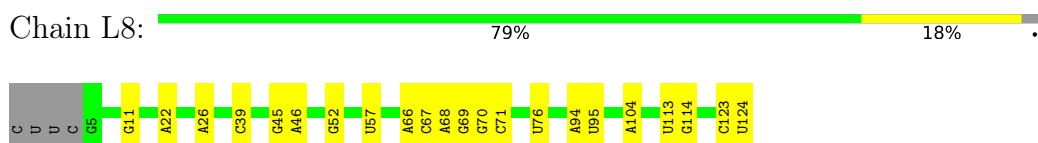
• Molecule 6: SR6_chain_6



• Molecule 7: 5.8S_rRNA_chain_7



• Molecule 8: 5S_rRNA_chain_8



• Molecule 9: Putative 60S ribosomal protein L2





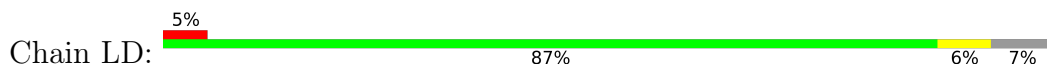
- Molecule 10: Putative ribosomal protein L3



- Molecule 11: Putative ribosomal protein L1a



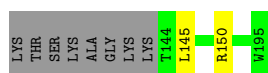
- Molecule 12: 60S ribosomal protein L11



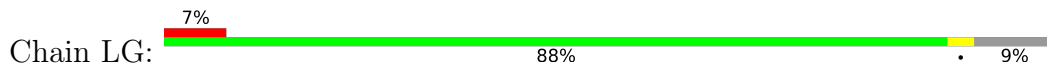
- Molecule 13: Putative 60S ribosomal protein L9



- Molecule 14: Putative 60S ribosomal protein L6



- Molecule 15: 60S ribosomal protein L7a





- Molecule 16: Putative 60S ribosomal protein L13a

Chain LH: 95% 5%



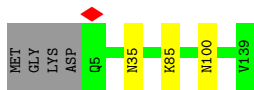
- Molecule 17: Putative 60S ribosomal protein L13

Chain LI: 94% 6%



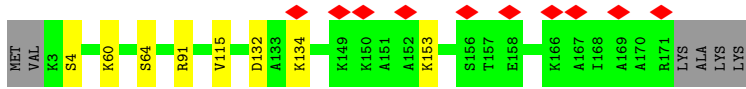
- Molecule 18: Putative 60S ribosomal protein L23

Chain LJ: 95% 6%



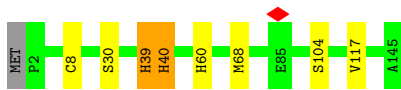
- Molecule 19: Putative 40S ribosomal protein L14

Chain LK: 6% 92% 5%



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

Chain LL: 94% 6%

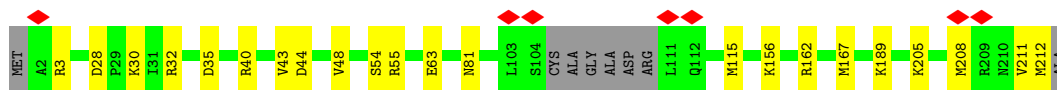
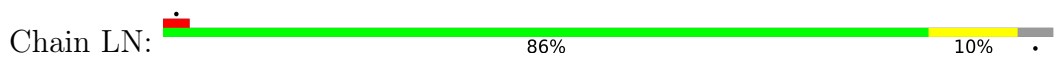


- Molecule 21: Ribosomal protein L15

Chain LM: 92% 6%



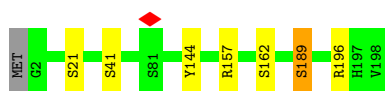
- Molecule 22: Putative 60S ribosomal protein L10



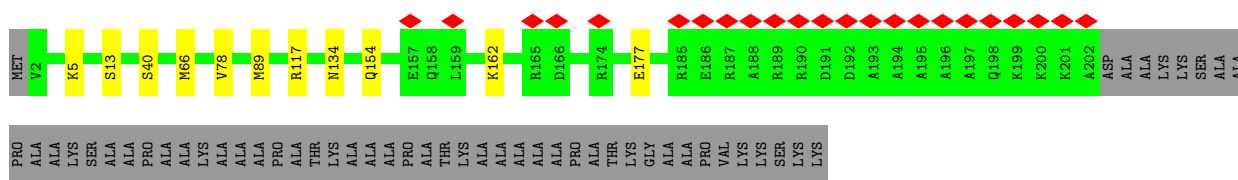
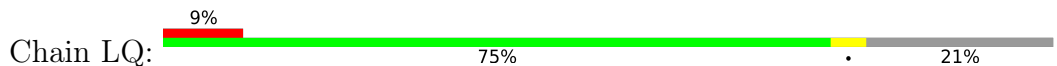
• Molecule 23: Putative 60S ribosomal protein L5



• Molecule 24: 60S ribosomal protein L18



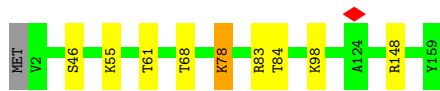
• Molecule 25: Putative 60S ribosomal protein L19



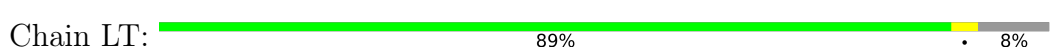
• Molecule 26: 60S ribosomal protein L18a



• Molecule 27: Putative 60S ribosomal protein L21

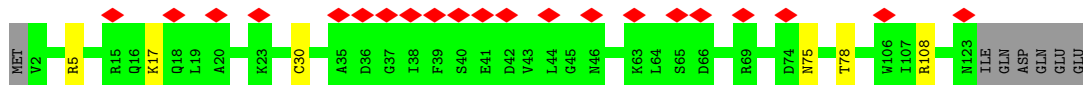
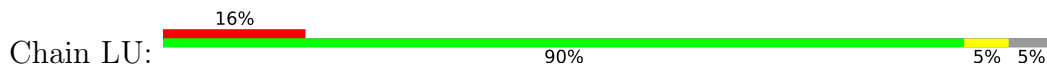


• Molecule 28: Putative 60S ribosomal protein L17

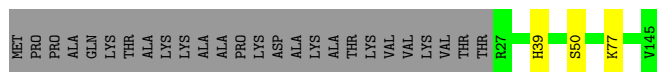
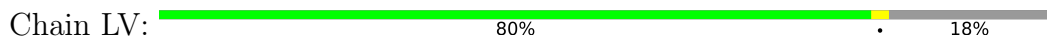




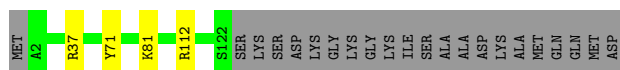
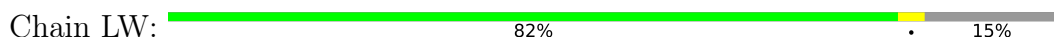
• Molecule 29: Putative 60S ribosomal protein L22



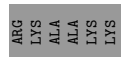
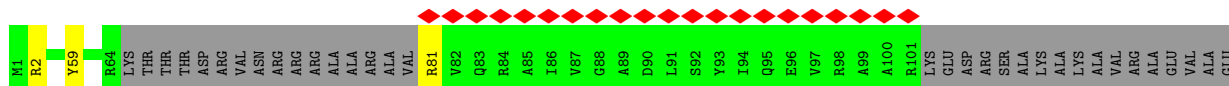
• Molecule 30: Putative 60S ribosomal protein L23a



• Molecule 31: Putative 60S ribosomal protein L26



• Molecule 32: Putative ribosomal protein L24



• Molecule 33: 60S ribosomal protein L27

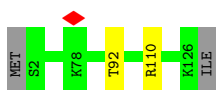


• Molecule 34: Putative 60S ribosomal protein L28



- Molecule 35: Putative 60S ribosomal protein L35

Chain La:  97%




- Molecule 36: 60S ribosomal protein L29

Chain Lb:  90%

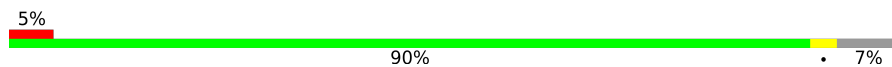


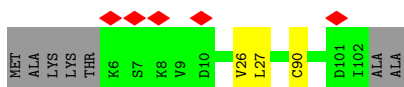
- Molecule 37: Putative 60S ribosomal protein L7

Chain Lc:  88%



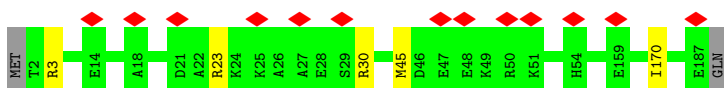
- Molecule 38: 60S ribosomal protein L30

Chain Ld:  5%



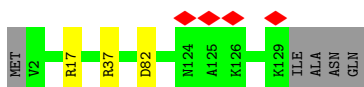
- Molecule 39: Putative 60S ribosomal subunit protein L31

Chain Le:  7%



- Molecule 40: 60S ribosomal protein L32

Chain Lf:  94%

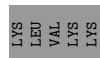
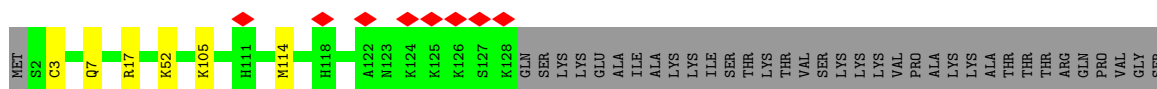
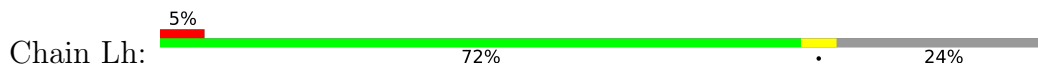


- Molecule 41: Putative ribosomal protein l35a

Chain Lg:  97%



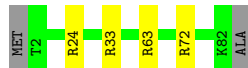
- Molecule 42: Putative 60S ribosomal protein L34



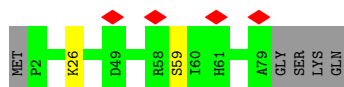
- Molecule 43: Putative 60S Ribosomal protein L36



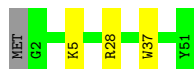
- Molecule 44: Ribosomal protein L37



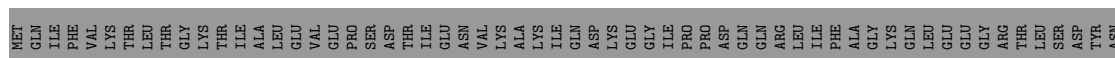
- Molecule 45: Putative ribosomal protein L38

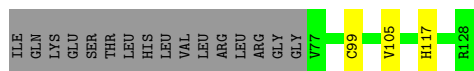


- Molecule 46: Putative 60S ribosomal protein L39



- Molecule 47: Ubiquitin-60S ribosomal protein L40

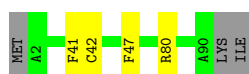




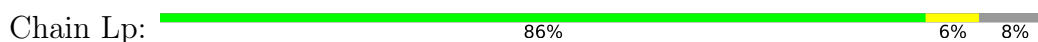
• Molecule 48: 60S ribosomal protein L41



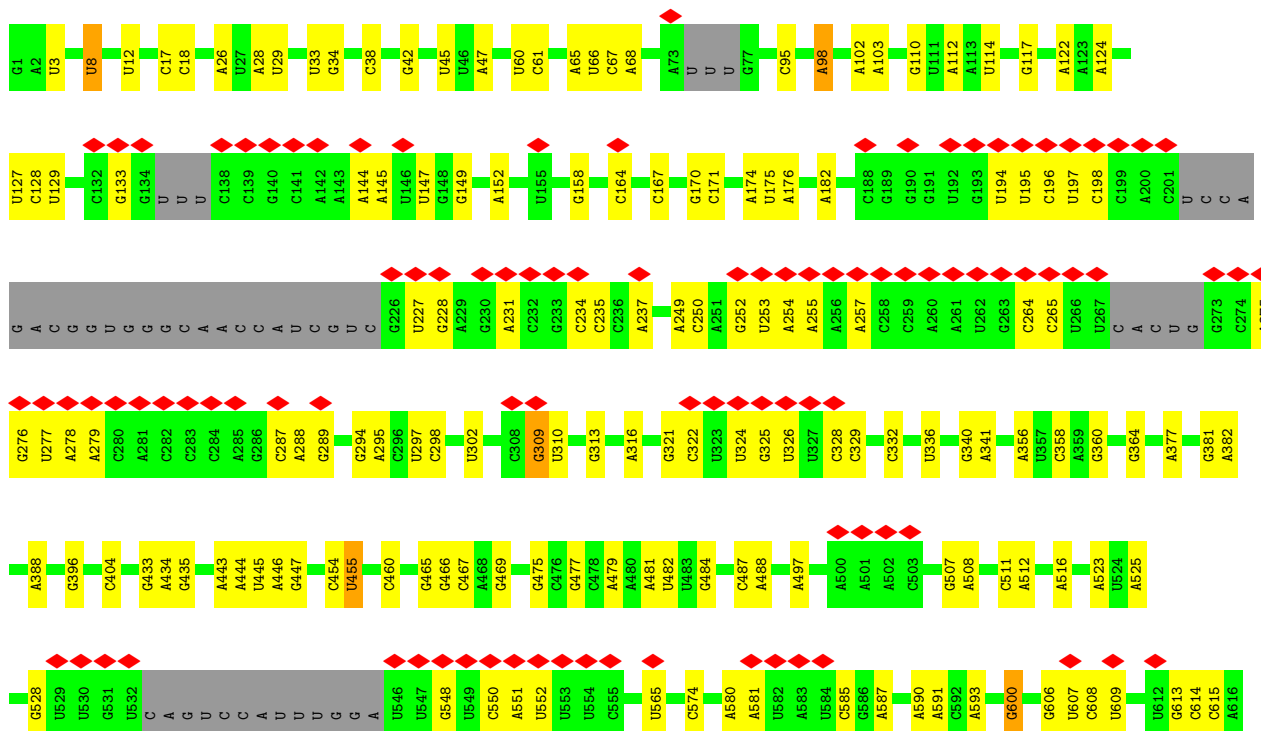
• Molecule 49: 60S ribosomal protein L37a



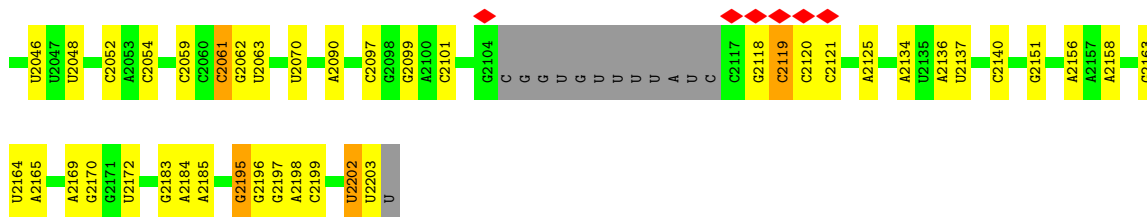
• Molecule 50: Putative 60S ribosomal protein L44



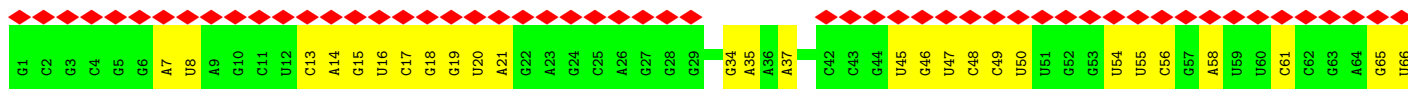
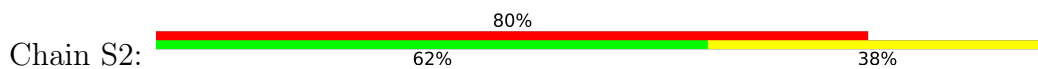
• Molecule 51: SSU_rRNA_chain_S1



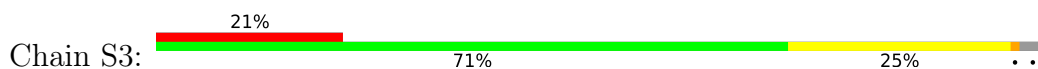




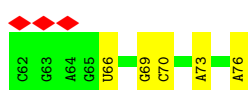
• Molecule 52: A-site_tRNA_chain_S2



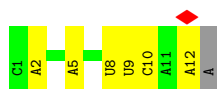
• Molecule 53: P-site_tRNA_chain_S3



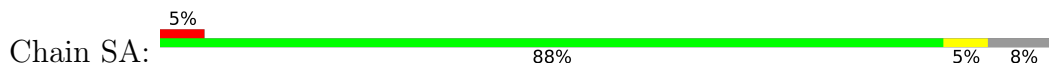
• Molecule 54: E-site_tRNA_chain_S4

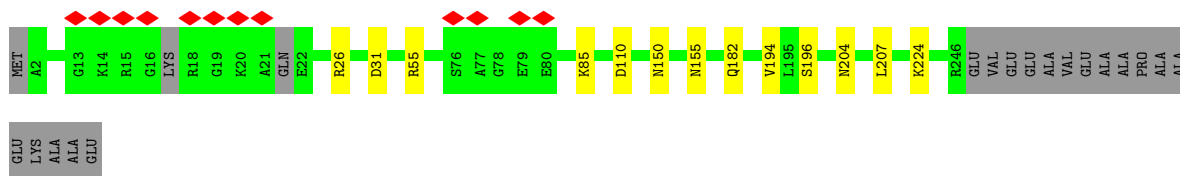


• Molecule 55: mRNA_chain_S5

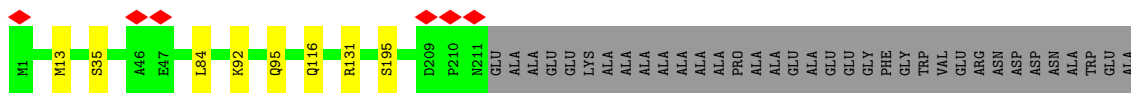
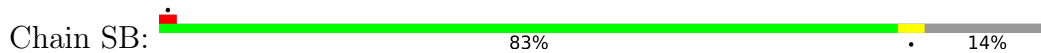


• Molecule 56: 40S ribosomal protein S3a

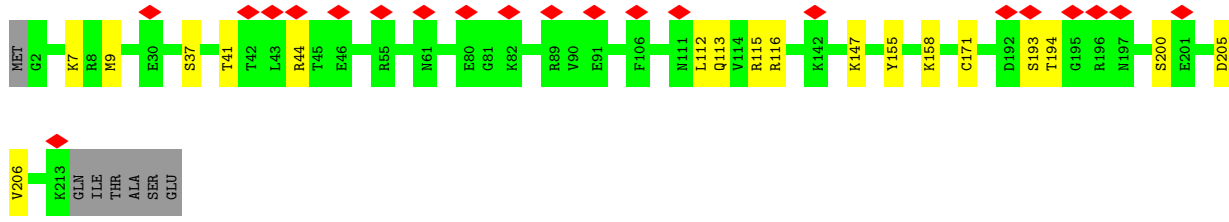
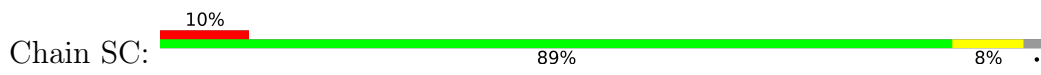




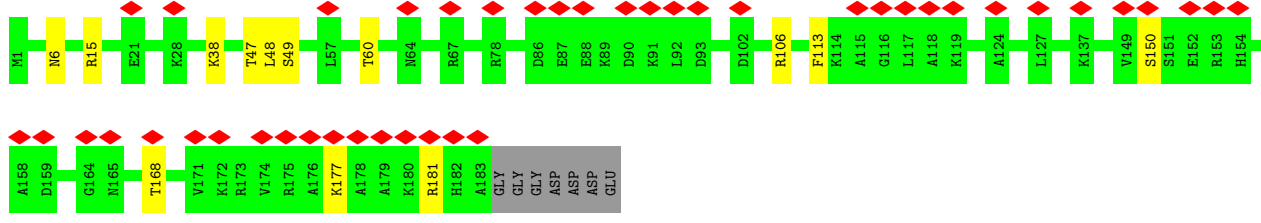
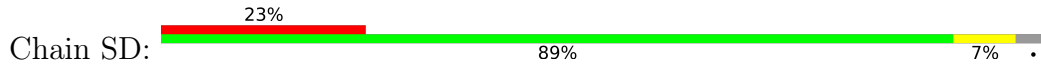
• Molecule 57: 40S ribosomal protein SA



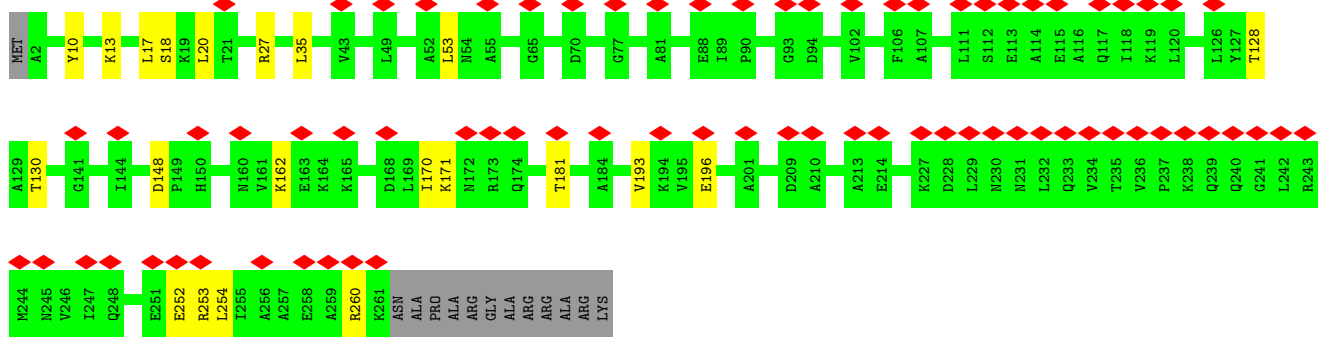
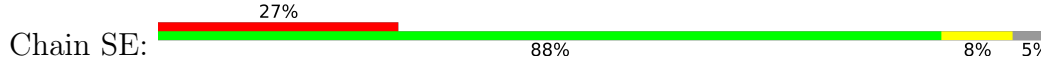
• Molecule 58: Putative 40S ribosomal protein S3



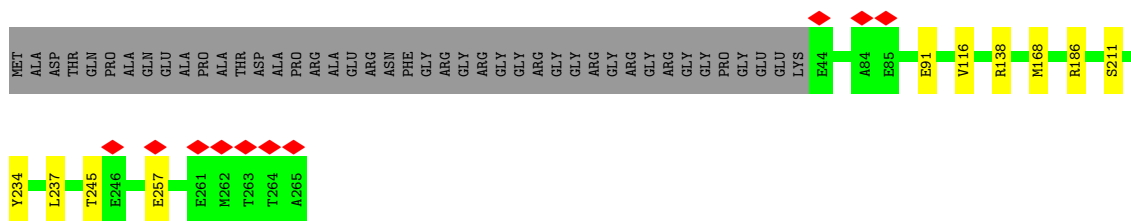
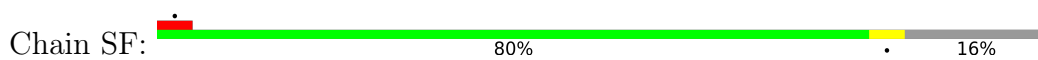
• Molecule 59: Putative 40S ribosomal protein S9



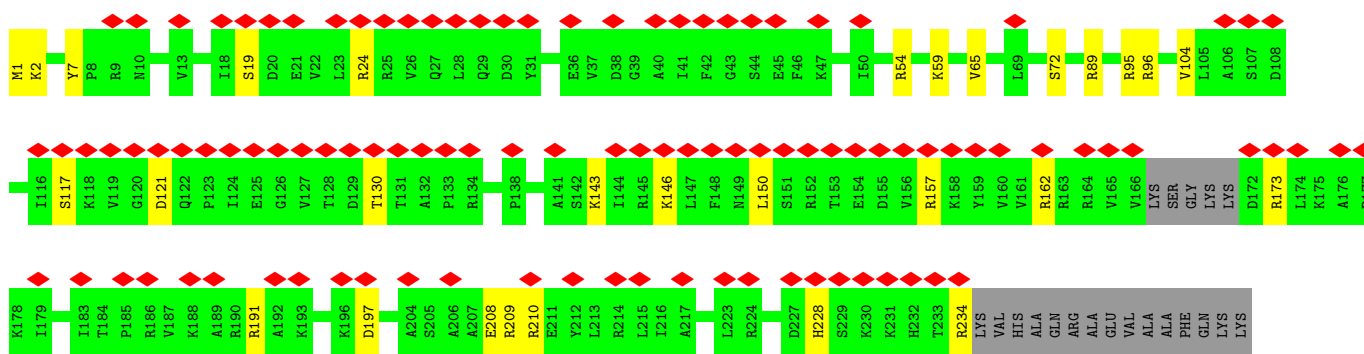
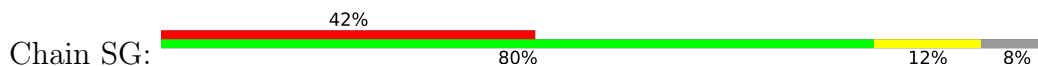
• Molecule 60: 40S ribosomal protein S4



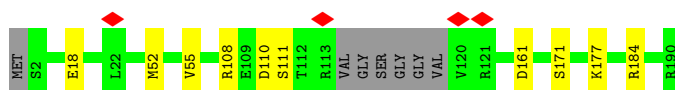
• Molecule 61: 40S ribosomal protein S2



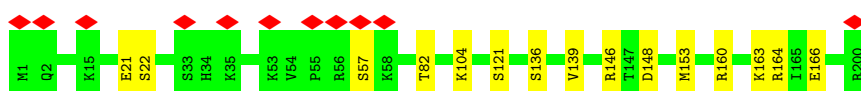
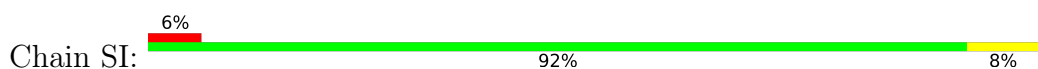
• Molecule 62: 40S ribosomal protein S6



• Molecule 63: 40S ribosomal protein S5



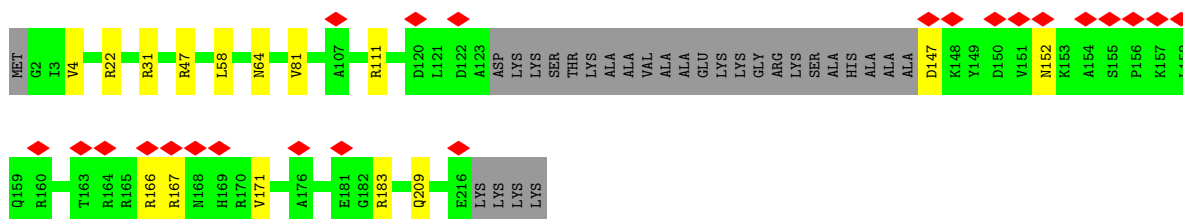
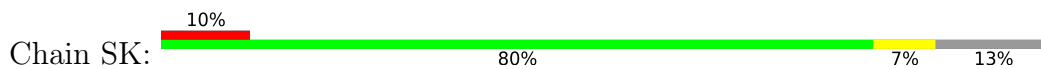
• Molecule 64: 40S ribosomal protein S7



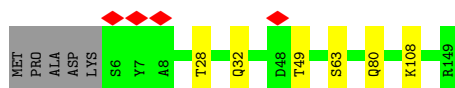
• Molecule 65: Putative 40S ribosomal protein S15A



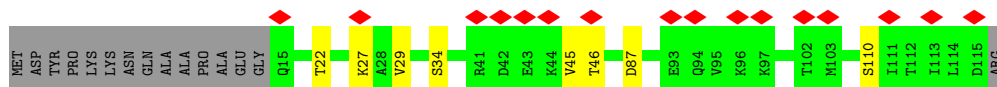
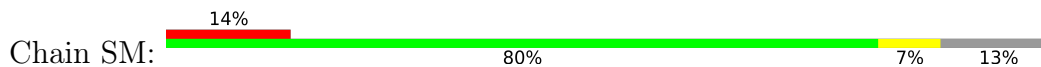
• Molecule 66: 40S ribosomal protein S8



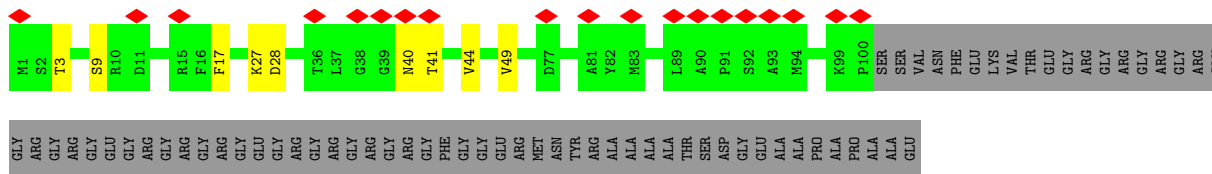
- Molecule 67: Putative 40S ribosomal protein S16



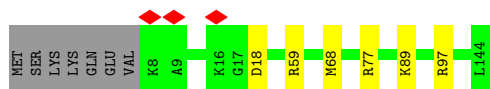
- Molecule 68: Putative ribosomal protein S20



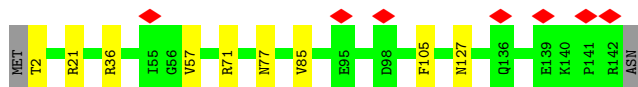
- Molecule 69: Putative 40S ribosomal protein S10



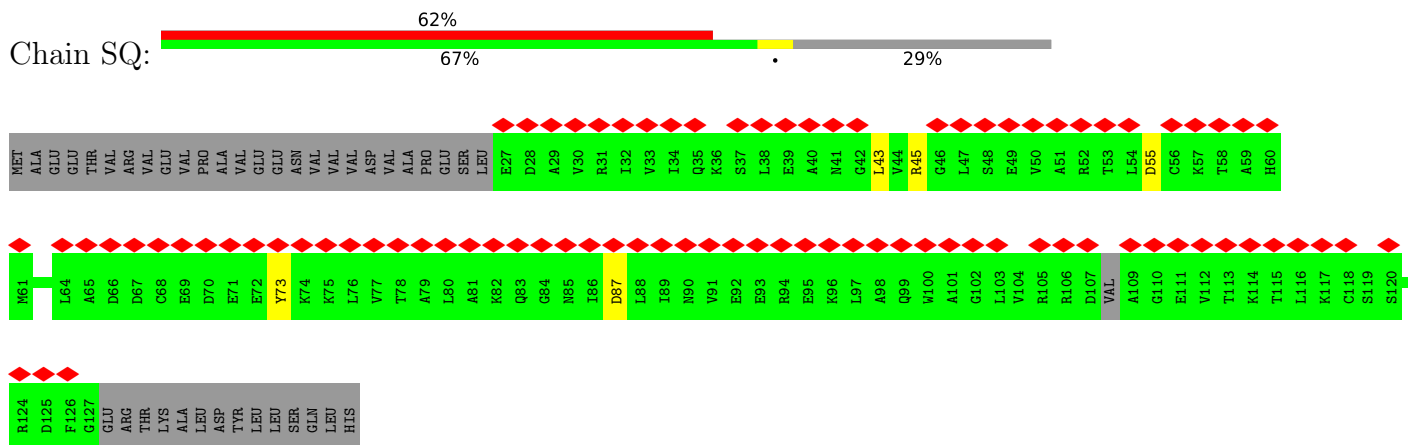
- Molecule 70: 40S ribosomal protein S14



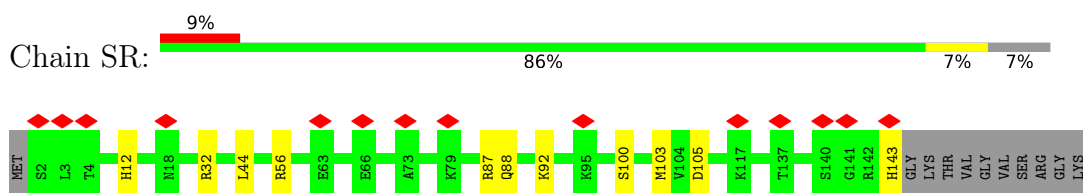
- Molecule 71: Putative 40S ribosomal protein S23



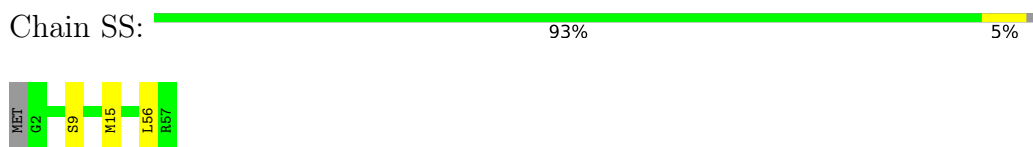
- Molecule 72: 40S ribosomal protein S12



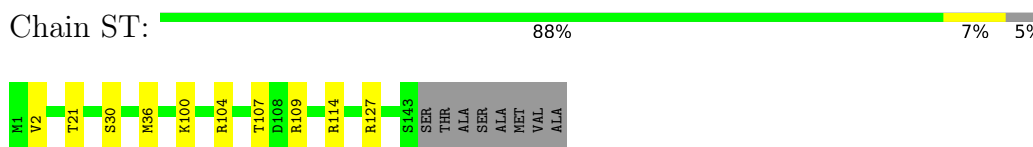
• Molecule 73: Putative 40S ribosomal protein S18



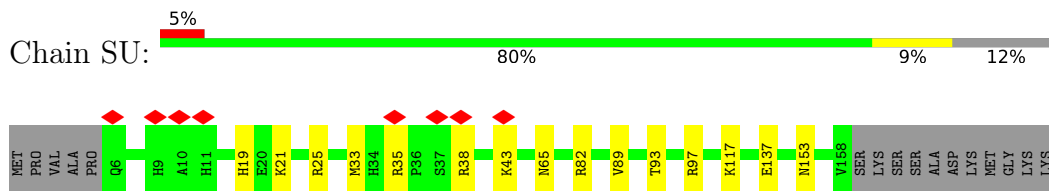
• Molecule 74: Putative ribosomal protein S29



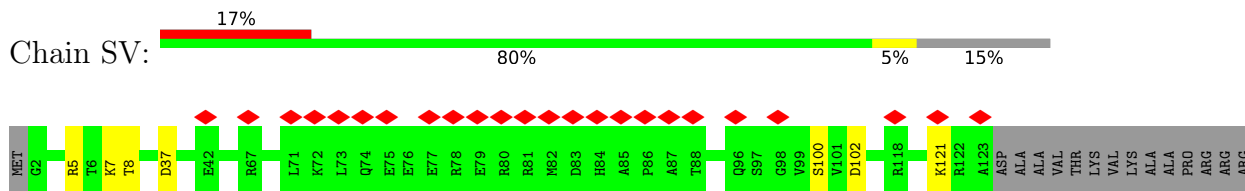
• Molecule 75: Putative 40S ribosomal protein S13



• Molecule 76: Ribosomal protein S17 family protein



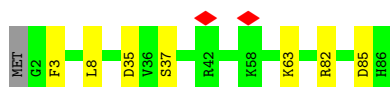
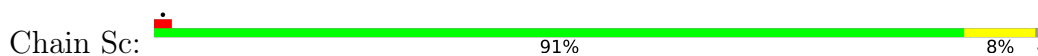
• Molecule 77: Putative 40S ribosomal protein S17



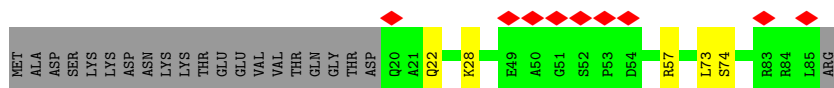
• Molecule 83: 40S ribosomal protein S26



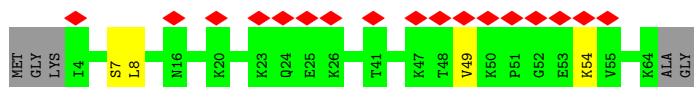
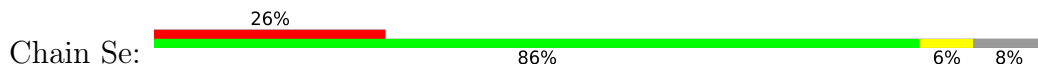
• Molecule 84: Putative 40S ribosomal protein S27-1



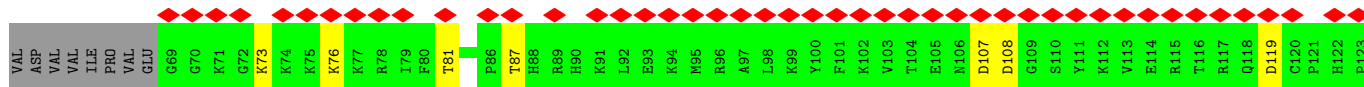
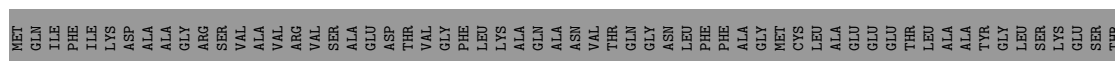
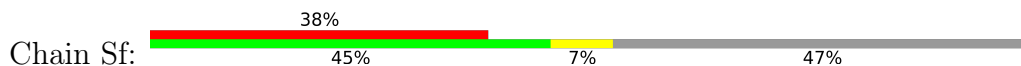
• Molecule 85: Putative 40S ribosomal protein S33



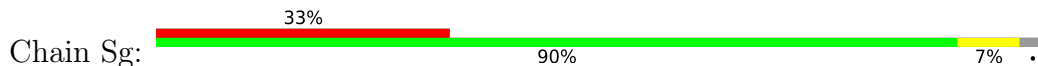
• Molecule 86: 40S ribosomal protein S30

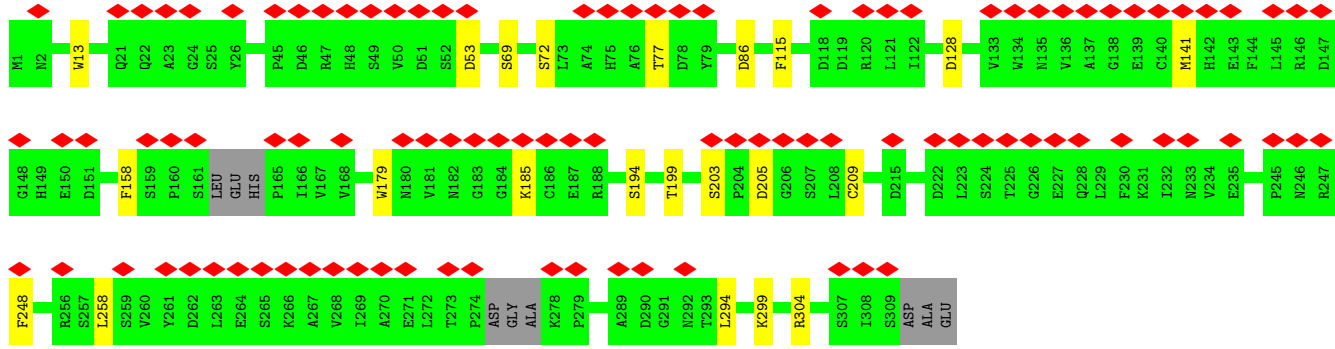


• Molecule 87: Ubiquitin-60S ribosomal protein L40

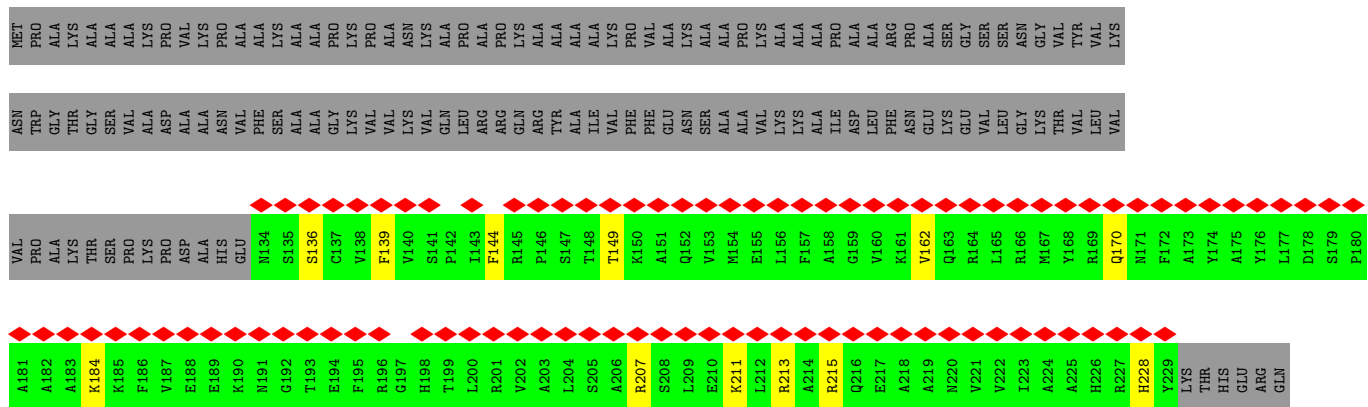
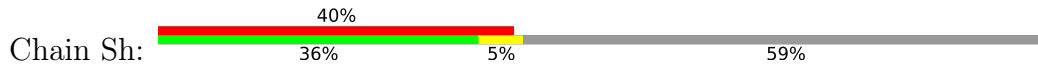


• Molecule 88: Guanine nucleotide-binding protein subunit beta-like protein





• 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	419524	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 ($e^-/\text{\AA}^2$)	0.9340390798620625	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, PSU, MA6, MG, OMC, ZN, A1H4F, 7MG, A2M, K, MIA, OMU, OMG, B8N, NA

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	0.42	0/39236	0.91	56/61175 (0.1%)
2	L2	0.42	0/25973	0.92	49/40481 (0.1%)
3	L3	0.37	0/4302	0.91	11/6687 (0.2%)
4	L4	0.41	0/4376	0.90	9/6822 (0.1%)
5	L5	0.43	0/2852	0.99	4/4438 (0.1%)
6	L6	0.35	0/1683	0.90	1/2618 (0.0%)
7	L7	0.40	0/3782	1.01	13/5889 (0.2%)
8	L8	0.42	0/2851	0.91	3/4439 (0.1%)
9	LA	0.30	0/2007	0.60	0/2696
10	LB	0.27	0/3283	0.55	0/4412
11	LC	0.26	0/2870	0.53	0/3861
12	LD	0.25	0/1410	0.51	0/1884
13	LE	0.26	0/1497	0.52	0/2017
14	LF	0.26	0/1173	0.52	0/1586
15	LG	0.25	0/1932	0.54	0/2599
16	LH	0.28	0/1803	0.54	0/2422
17	LI	0.27	0/1728	0.54	0/2313
18	LJ	0.28	0/1029	0.52	0/1388
19	LK	0.28	0/1355	0.52	0/1816
20	LL	0.30	0/1151	0.58	1/1538 (0.1%)
21	LM	0.32	0/1751	0.59	0/2338
22	LN	0.27	0/1697	0.57	0/2269
23	LO	0.27	0/2370	0.51	1/3172 (0.0%)
24	LP	0.33	0/1564	0.58	0/2092
25	LQ	0.24	0/1701	0.54	0/2250
26	LR	0.29	0/1489	0.52	0/2008
27	LS	0.31	0/1290	0.60	2/1736 (0.1%)
28	LT	0.27	0/1241	0.52	0/1665
29	LU	0.25	0/976	0.50	0/1303
30	LV	0.26	0/968	0.51	0/1302
31	LW	0.25	0/981	0.56	0/1310
32	LX	0.27	0/735	0.55	0/989

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LY	0.27	0/1088	0.53	0/1455
34	LZ	0.26	0/1133	0.55	0/1516
35	La	0.24	0/1054	0.53	0/1399
36	Lb	0.30	0/557	0.55	0/743
37	Lc	0.27	0/1896	0.53	0/2540
38	Ld	0.26	0/754	0.47	0/1019
39	Le	0.25	0/1488	0.54	0/1979
40	Lf	0.33	0/1066	0.61	0/1424
41	Lg	0.30	0/1172	0.57	0/1573
42	Lh	0.26	0/1045	0.56	0/1390
43	Li	0.26	0/822	0.53	0/1099
44	Lj	0.31	0/686	0.65	0/915
45	Lk	0.26	0/617	0.52	0/828
46	Ll	0.26	0/463	0.54	0/617
47	Lm	0.26	0/423	0.57	0/563
48	Ln	0.26	0/300	0.70	0/390
49	Lo	0.28	0/705	0.60	0/940
50	Lp	0.29	0/797	0.49	0/1053
51	S1	0.34	0/42995	0.86	33/66976 (0.0%)
52	S2	0.49	0/1783	0.95	0/2776
53	S3	0.39	0/1790	0.88	1/2789 (0.0%)
54	S4	0.26	0/1757	0.88	1/2735 (0.0%)
55	S5	0.28	0/279	0.90	0/431
56	SA	0.25	0/1967	0.55	0/2641
57	SB	0.25	0/1695	0.50	0/2292
58	SC	0.27	0/1674	0.53	0/2240
59	SD	0.25	0/1536	0.58	0/2059
60	SE	0.25	0/2092	0.54	0/2819
61	SF	0.25	0/1744	0.50	1/2362 (0.0%)
62	SG	0.25	0/1851	0.59	0/2474
63	SH	0.24	0/1469	0.51	0/1970
64	SI	0.25	0/1679	0.54	0/2255
65	SJ	0.26	0/1038	0.53	0/1391
66	SK	0.25	0/1573	0.58	0/2107
67	SL	0.28	0/1161	0.49	0/1559
68	SM	0.25	0/802	0.54	0/1088
69	SN	0.25	0/842	0.53	1/1141 (0.1%)
70	SO	0.31	0/1039	0.59	0/1395
71	SP	0.25	0/1120	0.52	0/1500
72	SQ	0.26	0/671	0.58	0/911
73	SR	0.24	0/1158	0.53	0/1553
74	SS	0.25	0/458	0.55	0/607
75	ST	0.28	0/1190	0.55	0/1594

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SU	0.26	0/1286	0.54	0/1727
77	SV	0.24	0/1002	0.51	0/1334
78	SW	0.25	0/948	0.51	0/1275
79	SX	0.29	0/1237	0.51	0/1661
80	SY	0.24	0/673	0.50	0/913
81	SZ	0.25	0/1071	0.51	0/1425
82	Sa	0.25	0/807	0.51	0/1082
83	Sb	0.26	0/842	0.58	0/1127
84	Sc	0.28	0/688	0.54	0/921
85	Sd	0.23	0/498	0.58	0/668
86	Se	0.36	0/496	0.61	0/658
87	Sf	0.26	0/674	0.52	0/892
88	Sg	0.24	0/2412	0.51	0/3276
89	Sh	0.26	0/783	0.54	0/1053
All	All	0.35	0/227902	0.78	187/334635 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	LH	0	1
21	LM	0	4
24	LP	0	1
40	Lf	0	1
44	Lj	0	2
70	SO	0	1
79	SX	0	1
All	All	0	11

There are no bond length outliers.

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L7	6	G	O3'-P-O5'	-24.52	57.42	104.00
7	L7	7	U	O5'-P-OP1	-18.18	88.89	110.70
7	L7	6	G	OP1-P-O3'	14.95	138.08	105.20
1	L1	563	C	N1-C2-O2	8.73	124.14	118.90
1	L1	563	C	C2-N1-C1'	8.11	127.72	118.80
2	L2	1485	G	P-O3'-C3'	8.06	129.37	119.70
2	L2	61	C	C2-N1-C1'	8.04	127.64	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	741	C	N3-C2-O2	-8.01	116.29	121.90
51	S1	1956	C	N1-C2-O2	7.90	123.64	118.90
27	LS	78	LYS	CB-CG-CD	7.86	132.05	111.60
51	S1	1956	C	C2-N1-C1'	7.80	127.38	118.80
27	LS	78	LYS	CA-CB-CG	7.78	130.51	113.40
51	S1	1181	C	C2-N1-C1'	7.72	127.29	118.80
1	L1	1600	U	C2-N1-C1'	7.62	126.84	117.70
2	L2	61	C	N1-C2-O2	7.42	123.35	118.90
2	L2	631	G	O4'-C1'-N9	7.41	114.13	108.20
1	L1	447	G	O4'-C1'-N9	7.37	114.09	108.20
1	L1	563	C	N3-C2-O2	-7.22	116.84	121.90
2	L2	435	U	O4'-C1'-N1	7.10	113.88	108.20
1	L1	1122	U	C2-N1-C1'	7.06	126.17	117.70
2	L2	1226	C	N3-C2-O2	-7.04	116.98	121.90
7	L7	111	C	C2-N1-C1'	6.87	126.35	118.80
1	L1	967	G	P-O3'-C3'	6.84	127.91	119.70
51	S1	2040	C	C6-N1-C2	-6.73	117.61	120.30
51	S1	1181	C	N1-C2-O2	6.67	122.90	118.90
7	L7	111	C	N1-C2-O2	6.66	122.89	118.90
2	L2	741	C	N1-C2-O2	6.60	122.86	118.90
2	L2	1236	C	OP1-P-O3'	6.41	119.30	105.20
1	L1	1216	U	C2-N1-C1'	6.32	125.29	117.70
3	L3	104	C	C2-N1-C1'	6.31	125.74	118.80
1	L1	175	G	O4'-C1'-N9	6.26	113.21	108.20
51	S1	1956	C	N3-C2-O2	-6.26	117.52	121.90
7	L7	127	C	C2-N1-C1'	6.18	125.60	118.80
2	L2	811	U	C2-N1-C1'	6.16	125.10	117.70
1	L1	166	G	O4'-C1'-N9	6.14	113.12	108.20
1	L1	1122	U	N1-C2-O2	6.14	127.10	122.80
4	L4	161	C	C2-N1-C1'	6.12	125.53	118.80
1	L1	853	C	C2-N1-C1'	6.06	125.47	118.80
1	L1	967	G	OP1-P-O3'	5.99	118.38	105.20
51	S1	511	C	C2-N1-C1'	5.99	125.39	118.80
1	L1	890	C	C2-N1-C1'	5.99	125.39	118.80
7	L7	28	C	C2-N1-C1'	5.99	125.39	118.80
2	L2	1305	C	O4'-C1'-N1	5.98	112.99	108.20
2	L2	1065	C	O4'-C1'-N1	5.98	112.98	108.20
2	L2	1222	C	C2-N1-C1'	5.95	125.34	118.80
3	L3	139	C	C2-N1-C1'	5.91	125.30	118.80
2	L2	756	C	C2-N1-C1'	5.89	125.28	118.80
1	L1	606	C	C2-N1-C1'	5.88	125.26	118.80
7	L7	29	C	C2-N1-C1'	5.87	125.26	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L7	111	C	N3-C2-O2	-5.85	117.80	121.90
2	L2	61	C	N3-C2-O2	-5.85	117.81	121.90
51	S1	2040	C	N3-C2-O2	-5.84	117.81	121.90
5	L5	90	C	C2-N1-C1'	5.80	125.19	118.80
51	S1	748	C	C2-N1-C1'	5.75	125.12	118.80
1	L1	993	U	N3-C2-O2	-5.73	118.19	122.20
51	S1	2119	C	OP1-P-O3'	5.73	117.80	105.20
4	L4	138	C	C2-N1-C1'	5.71	125.08	118.80
1	L1	256	U	OP2-P-O3'	5.70	117.74	105.20
2	L2	1485	G	OP1-P-O3'	5.69	117.72	105.20
2	L2	503	C	C2-N1-C1'	5.68	125.05	118.80
5	L5	70	C	C2-N1-C1'	5.68	125.05	118.80
3	L3	112	C	C2-N1-C1'	5.67	125.04	118.80
2	L2	382	A2M	OP2-P-O3'	5.66	117.66	105.20
1	L1	22	C	C6-N1-C2	-5.65	118.04	120.30
3	L3	20	C	C2-N1-C1'	5.64	125.01	118.80
2	L2	345	C	C2-N1-C1'	5.64	125.00	118.80
1	L1	495	C	C2-N1-C1'	5.63	124.99	118.80
3	L3	188	C	C2-N1-C1'	5.62	124.98	118.80
1	L1	1514	C	C2-N1-C1'	5.62	124.98	118.80
2	L2	479	C	C2-N1-C1'	5.61	124.97	118.80
53	S3	20	G	OP1-P-O3'	5.61	117.53	105.20
2	L2	61	C	C6-N1-C1'	-5.60	114.08	120.80
20	LL	39	HIS	CB-CA-C	-5.58	99.23	110.40
51	S1	1572	C	C6-N1-C2	-5.58	118.07	120.30
1	L1	563	C	C6-N1-C1'	-5.55	114.14	120.80
1	L1	208	C	C2-N1-C1'	5.55	124.90	118.80
51	S1	1788	U	N3-C2-O2	-5.54	118.32	122.20
51	S1	1212	C	C2-N1-C1'	5.53	124.89	118.80
51	S1	782	C	N1-C2-O2	5.51	122.20	118.90
1	L1	1600	U	N1-C2-O2	5.50	126.65	122.80
1	L1	1601	U	C2-N1-C1'	5.49	124.28	117.70
2	L2	527	A2M	OP2-P-O3'	5.48	117.26	105.20
8	L8	39	C	C2-N1-C1'	5.48	124.83	118.80
1	L1	22	C	N3-C2-O2	-5.47	118.07	121.90
61	SF	237	LEU	C-N-CA	5.46	135.35	121.70
7	L7	164	U	C2-N1-C1'	5.46	124.25	117.70
1	L1	1122	U	N3-C2-O2	-5.46	118.38	122.20
3	L3	131	C	C2-N1-C1'	5.45	124.80	118.80
2	L2	134	C	C2-N1-C1'	5.45	124.79	118.80
4	L4	169	A	OP1-P-O3'	5.44	117.18	105.20
1	L1	514	C	C2-N1-C1'	5.42	124.76	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	563	C	C6-N1-C2	-5.41	118.14	120.30
2	L2	115	G	OP2-P-O3'	5.41	117.11	105.20
2	L2	1115	U	N3-C2-O2	-5.40	118.42	122.20
5	L5	5	C	C2-N1-C1'	5.40	124.74	118.80
1	L1	1746	C	O4'-C1'-N1	5.40	112.52	108.20
51	S1	1181	C	C6-N1-C1'	-5.39	114.33	120.80
1	L1	1737	A	OP2-P-O3'	5.39	117.05	105.20
51	S1	95	C	C2-N1-C1'	5.38	124.72	118.80
69	SN	28	ASP	CB-CG-OD2	5.36	123.13	118.30
2	L2	1226	C	N1-C2-O2	5.36	122.12	118.90
2	L2	615	G	OP2-P-O3'	5.35	116.96	105.20
2	L2	811	U	N1-C2-O2	5.33	126.53	122.80
8	L8	123	C	O4'-C1'-N1	5.33	112.47	108.20
1	L1	668	C	OP2-P-O3'	5.33	116.93	105.20
51	S1	1956	C	C6-N1-C1'	-5.33	114.41	120.80
2	L2	38	C	OP2-P-O3'	5.33	116.92	105.20
4	L4	161	C	N3-C2-O2	-5.32	118.17	121.90
4	L4	95	U	C2-N1-C1'	5.32	124.08	117.70
51	S1	1572	C	C2-N1-C1'	5.32	124.65	118.80
2	L2	1305	C	C2-N1-C1'	5.32	124.65	118.80
3	L3	139	C	N3-C2-O2	-5.31	118.18	121.90
1	L1	331	C	N3-C2-O2	-5.31	118.19	121.90
51	S1	1572	C	N3-C2-O2	-5.30	118.19	121.90
1	L1	22	C	C2-N1-C1'	5.30	124.63	118.80
3	L3	119	C	C2-N1-C1'	5.27	124.60	118.80
2	L2	391	A	OP2-P-O3'	5.26	116.78	105.20
2	L2	696	A	OP1-P-O3'	5.26	116.77	105.20
1	L1	835	G	OP2-P-O3'	5.25	116.75	105.20
1	L1	170	U	P-O3'-C3'	5.25	126.00	119.70
2	L2	479	C	N1-C2-O2	5.24	122.04	118.90
1	L1	254	U	N3-C2-O2	-5.24	118.53	122.20
51	S1	1271	C	C2-N1-C1'	5.23	124.55	118.80
2	L2	553	G	OP2-P-O3'	5.22	116.69	105.20
51	S1	309	G	P-O3'-C3'	5.22	125.97	119.70
1	L1	196	C	C2-N1-C1'	5.22	124.54	118.80
51	S1	1956	C	C6-N1-C2	-5.22	118.21	120.30
1	L1	719	U	O4'-C1'-N1	5.21	112.37	108.20
2	L2	519	G	C3'-C2'-C1'	-5.21	97.33	101.50
1	L1	1008	C	OP1-P-O3'	5.21	116.66	105.20
1	L1	331	C	N1-C2-O2	5.19	122.02	118.90
2	L2	1232	G	O4'-C1'-N9	5.19	112.36	108.20
51	S1	1788	U	C2-N1-C1'	5.18	123.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	613	C	C2-N1-C1'	5.18	124.50	118.80
2	L2	808	C	N3-C2-O2	-5.18	118.28	121.90
51	S1	2195	G	OP2-P-O3'	5.18	116.59	105.20
4	L4	72	G	OP2-P-O3'	5.17	116.58	105.20
7	L7	100	U	N3-C2-O2	-5.17	118.58	122.20
51	S1	1779	U	N3-C2-O2	-5.17	118.58	122.20
4	L4	161	C	C6-N1-C2	-5.17	118.23	120.30
1	L1	460	A	OP2-P-O3'	5.16	116.56	105.20
54	S4	60	U	N3-C2-O2	-5.16	118.59	122.20
2	L2	517	A	OP2-P-O3'	5.16	116.54	105.20
51	S1	748	C	N1-C2-O2	5.15	121.99	118.90
4	L4	33	G	O4'-C1'-N9	5.15	112.32	108.20
51	S1	1181	C	N3-C2-O2	-5.14	118.30	121.90
1	L1	1171	PSU	OP2-P-O3'	5.14	116.51	105.20
1	L1	254	U	C2-N1-C1'	5.14	123.86	117.70
1	L1	1058	U	C2-N1-C1'	5.14	123.86	117.70
51	S1	302	U	C2-N1-C1'	5.13	123.86	117.70
51	S1	2040	C	C2-N1-C1'	5.13	124.44	118.80
6	L6	11	G	O4'-C1'-N9	5.12	112.30	108.20
1	L1	1600	U	N3-C2-O2	-5.12	118.62	122.20
3	L3	131	C	N1-C2-O2	5.11	121.97	118.90
51	S1	1788	U	N1-C2-O2	5.11	126.38	122.80
2	L2	1287	C	O4'-C1'-N1	5.11	112.29	108.20
1	L1	586	U	O4'-C1'-N1	5.11	112.28	108.20
2	L2	1023	C	N1-C2-O2	5.10	121.96	118.90
1	L1	835	G	P-O3'-C3'	5.10	125.82	119.70
3	L3	71	U	C2-N1-C1'	5.09	123.81	117.70
1	L1	1224	A	OP2-P-O3'	5.09	116.40	105.20
1	L1	853	C	N3-C2-O2	-5.09	118.34	121.90
2	L2	61	C	C6-N1-C2	-5.08	118.27	120.30
1	L1	331	C	C2-N1-C1'	5.08	124.38	118.80
7	L7	33	U	OP1-P-OP2	-5.08	111.99	119.60
1	L1	1590	G	OP2-P-O3'	5.07	116.35	105.20
3	L3	48	C	C2-N1-C1'	5.06	124.37	118.80
51	S1	171	C	N1-C2-O2	5.06	121.94	118.90
2	L2	1023	C	C2-N1-C1'	5.06	124.36	118.80
8	L8	66	A	OP2-P-O3'	5.06	116.33	105.20
2	L2	1151	U	N3-C2-O2	-5.06	118.66	122.20
2	L2	1115	U	C2-N1-C1'	5.05	123.77	117.70
2	L2	1222	C	N3-C2-O2	-5.05	118.36	121.90
5	L5	90	C	N3-C2-O2	-5.04	118.37	121.90
2	L2	1065	C	C2-N1-C1'	5.04	124.34	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	67	C	C2-N1-C1'	5.03	124.33	118.80
1	L1	609	C	C2-N1-C1'	5.02	124.32	118.80
51	S1	1145	A	OP1-P-O3'	5.02	116.25	105.20
1	L1	1600	U	C6-N1-C1'	-5.02	114.17	121.20
4	L4	177	U	C2-N1-C1'	5.02	123.72	117.70
1	L1	669	C	C3'-C2'-C1'	-5.01	97.49	101.50
2	L2	972	C	C2-N1-C1'	5.01	124.31	118.80
1	L1	1662	G	OP1-P-O3'	5.01	116.21	105.20
2	L2	1151	U	C6-N1-C2	-5.01	118.00	121.00
7	L7	32	U	P-O3'-C3'	5.00	125.71	119.70
23	LO	84	PRO	CA-N-CD	-5.00	104.49	111.50
2	L2	811	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	LH	108	ARG	Sidechain
21	LM	189	ARG	Sidechain
21	LM	193	ARG	Sidechain
21	LM	194	ARG	Sidechain
21	LM	71	ARG	Sidechain
24	LP	157	ARG	Sidechain
40	Lf	37	ARG	Sidechain
44	Lj	63	ARG	Sidechain
44	Lj	72	ARG	Sidechain
70	SO	59	ARG	Sidechain
79	SX	101	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	256/260 (98%)	249 (97%)	7 (3%)	0	100	100
10	LB	402/419 (96%)	390 (97%)	12 (3%)	0	100	100
11	LC	364/373 (98%)	353 (97%)	11 (3%)	0	100	100
12	LD	173/188 (92%)	170 (98%)	3 (2%)	0	100	100
13	LE	184/190 (97%)	175 (95%)	9 (5%)	0	100	100
14	LF	145/195 (74%)	138 (95%)	7 (5%)	0	100	100
15	LG	239/264 (90%)	234 (98%)	5 (2%)	0	100	100
16	LH	219/222 (99%)	216 (99%)	3 (1%)	0	100	100
17	LI	212/220 (96%)	206 (97%)	6 (3%)	0	100	100
18	LJ	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
19	LK	167/175 (95%)	161 (96%)	6 (4%)	0	100	100
20	LL	142/145 (98%)	135 (95%)	6 (4%)	1 (1%)	22	52
21	LM	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
22	LN	201/213 (94%)	195 (97%)	6 (3%)	0	100	100
23	LO	294/305 (96%)	288 (98%)	6 (2%)	0	100	100
24	LP	195/198 (98%)	190 (97%)	4 (2%)	1 (0%)	29	60
25	LQ	199/254 (78%)	198 (100%)	1 (0%)	0	100	100
26	LR	176/179 (98%)	175 (99%)	1 (1%)	0	100	100
27	LS	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
28	LT	150/166 (90%)	146 (97%)	4 (3%)	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%)	117 (98%)	2 (2%)	0	100	100
32	LX	81/124 (65%)	78 (96%)	3 (4%)	0	100	100
33	LY	131/134 (98%)	131 (100%)	0	0	100	100
34	LZ	143/147 (97%)	141 (99%)	2 (1%)	0	100	100
35	La	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
36	Lb	66/70 (94%)	63 (96%)	2 (3%)	1 (2%)	10	32
37	Lc	227/252 (90%)	221 (97%)	6 (3%)	0	100	100
38	Ld	95/104 (91%)	95 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	Le	184/188 (98%)	183 (100%)	1 (0%)	0	100	100
40	Lf	126/133 (95%)	122 (97%)	4 (3%)	0	100	100
41	Lg	141/144 (98%)	141 (100%)	0	0	100	100
42	Lh	125/168 (74%)	122 (98%)	3 (2%)	0	100	100
43	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
44	Lj	79/83 (95%)	79 (100%)	0	0	100	100
45	Lk	76/83 (92%)	75 (99%)	1 (1%)	0	100	100
46	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
47	Lm	50/128 (39%)	50 (100%)	0	0	100	100
48	Ln	31/34 (91%)	31 (100%)	0	0	100	100
49	Lo	87/92 (95%)	80 (92%)	7 (8%)	0	100	100
50	Lp	95/106 (90%)	93 (98%)	2 (2%)	0	100	100
56	SA	240/264 (91%)	232 (97%)	8 (3%)	0	100	100
57	SB	209/246 (85%)	202 (97%)	7 (3%)	0	100	100
58	SC	211/219 (96%)	207 (98%)	4 (2%)	0	100	100
59	SD	181/190 (95%)	178 (98%)	3 (2%)	0	100	100
60	SE	258/273 (94%)	253 (98%)	5 (2%)	0	100	100
61	SF	220/265 (83%)	220 (100%)	0	0	100	100
62	SG	225/249 (90%)	218 (97%)	7 (3%)	0	100	100
63	SH	179/190 (94%)	177 (99%)	2 (1%)	0	100	100
64	SI	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
65	SJ	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
66	SK	188/220 (86%)	188 (100%)	0	0	100	100
67	SL	142/149 (95%)	138 (97%)	4 (3%)	0	100	100
68	SM	99/116 (85%)	99 (100%)	0	0	100	100
69	SN	98/168 (58%)	93 (95%)	4 (4%)	1 (1%)	15	43
70	SO	135/144 (94%)	131 (97%)	4 (3%)	0	100	100
71	SP	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
72	SQ	96/141 (68%)	93 (97%)	3 (3%)	0	100	100
73	SR	140/153 (92%)	138 (99%)	2 (1%)	0	100	100
74	SS	54/57 (95%)	53 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	ST	141/151 (93%)	139 (99%)	2 (1%)	0	100	100
76	SU	151/173 (87%)	144 (95%)	7 (5%)	0	100	100
77	SV	120/143 (84%)	119 (99%)	1 (1%)	0	100	100
78	SW	113/152 (74%)	113 (100%)	0	0	100	100
79	SX	150/161 (93%)	144 (96%)	6 (4%)	0	100	100
80	SY	86/164 (52%)	86 (100%)	0	0	100	100
81	SZ	128/137 (93%)	122 (95%)	6 (5%)	0	100	100
82	Sa	103/120 (86%)	94 (91%)	9 (9%)	0	100	100
83	Sb	102/112 (91%)	101 (99%)	1 (1%)	0	100	100
84	Sc	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
85	Sd	64/87 (74%)	61 (95%)	3 (5%)	0	100	100
86	Se	59/66 (89%)	57 (97%)	2 (3%)	0	100	100
87	Sf	78/152 (51%)	73 (94%)	5 (6%)	0	100	100
88	Sg	297/312 (95%)	286 (96%)	11 (4%)	0	100	100
89	Sh	94/235 (40%)	92 (98%)	2 (2%)	0	100	100
All	All	11480/12926 (89%)	11208 (98%)	268 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
69	SN	40	ASN
36	Lb	10	HIS
20	LL	40	HIS
24	LP	189	SER

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	200/204 (98%)	188 (94%)	12 (6%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	LB	337/351 (96%)	325 (96%)	12 (4%)	35	66
11	LC	291/301 (97%)	271 (93%)	20 (7%)	15	40
12	LD	147/162 (91%)	135 (92%)	12 (8%)	11	31
13	LE	166/172 (96%)	154 (93%)	12 (7%)	14	37
14	LF	122/153 (80%)	114 (93%)	8 (7%)	16	42
15	LG	198/221 (90%)	189 (96%)	9 (4%)	27	58
16	LH	182/188 (97%)	172 (94%)	10 (6%)	21	50
17	LI	178/183 (97%)	170 (96%)	8 (4%)	27	58
18	LJ	106/111 (96%)	103 (97%)	3 (3%)	43	73
19	LK	138/145 (95%)	130 (94%)	8 (6%)	20	48
20	LL	113/114 (99%)	105 (93%)	8 (7%)	14	38
21	LM	178/180 (99%)	164 (92%)	14 (8%)	12	32
22	LN	175/179 (98%)	153 (87%)	22 (13%)	4	13
23	LO	232/242 (96%)	222 (96%)	10 (4%)	29	60
24	LP	163/164 (99%)	157 (96%)	6 (4%)	34	65
25	LQ	170/198 (86%)	159 (94%)	11 (6%)	17	43
26	LR	157/159 (99%)	149 (95%)	8 (5%)	24	53
27	LS	132/134 (98%)	123 (93%)	9 (7%)	16	40
28	LT	127/143 (89%)	122 (96%)	5 (4%)	32	63
29	LU	93/114 (82%)	87 (94%)	6 (6%)	17	43
30	LV	102/124 (82%)	99 (97%)	3 (3%)	42	73
31	LW	104/122 (85%)	100 (96%)	4 (4%)	33	64
32	LX	74/104 (71%)	71 (96%)	3 (4%)	30	61
33	LY	111/116 (96%)	105 (95%)	6 (5%)	22	51
34	LZ	114/118 (97%)	108 (95%)	6 (5%)	22	52
35	La	114/118 (97%)	112 (98%)	2 (2%)	59	82
36	Lb	56/58 (97%)	52 (93%)	4 (7%)	14	38
37	Lc	191/209 (91%)	183 (96%)	8 (4%)	30	61
38	Ld	85/89 (96%)	82 (96%)	3 (4%)	36	67
39	Le	154/158 (98%)	149 (97%)	5 (3%)	39	70
40	Lf	111/115 (96%)	109 (98%)	2 (2%)	59	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	Lg	120/121 (99%)	116 (97%)	4 (3%)	38	69
42	Lh	107/146 (73%)	101 (94%)	6 (6%)	21	50
43	Li	84/88 (96%)	81 (96%)	3 (4%)	35	66
44	Lj	68/70 (97%)	66 (97%)	2 (3%)	42	73
45	Lk	65/74 (88%)	63 (97%)	2 (3%)	40	71
46	Ll	46/47 (98%)	43 (94%)	3 (6%)	17	43
47	Lm	43/113 (38%)	40 (93%)	3 (7%)	15	39
48	Ln	31/32 (97%)	30 (97%)	1 (3%)	39	70
49	Lo	69/74 (93%)	65 (94%)	4 (6%)	20	48
50	Lp	83/92 (90%)	77 (93%)	6 (7%)	14	37
56	SA	206/222 (93%)	193 (94%)	13 (6%)	18	44
57	SB	178/202 (88%)	170 (96%)	8 (4%)	27	58
58	SC	176/184 (96%)	157 (89%)	19 (11%)	6	19
59	SD	159/164 (97%)	146 (92%)	13 (8%)	11	31
60	SE	216/225 (96%)	195 (90%)	21 (10%)	8	24
61	SF	182/208 (88%)	173 (95%)	9 (5%)	25	55
62	SG	190/208 (91%)	161 (85%)	29 (15%)	2	8
63	SH	153/159 (96%)	143 (94%)	10 (6%)	17	43
64	SI	181/186 (97%)	166 (92%)	15 (8%)	11	30
65	SJ	110/111 (99%)	105 (96%)	5 (4%)	27	58
66	SK	157/176 (89%)	142 (90%)	15 (10%)	8	24
67	SL	116/120 (97%)	110 (95%)	6 (5%)	23	53
68	SM	92/104 (88%)	84 (91%)	8 (9%)	10	29
69	SN	88/128 (69%)	81 (92%)	7 (8%)	12	32
70	SO	104/113 (92%)	99 (95%)	5 (5%)	25	56
71	SP	114/117 (97%)	105 (92%)	9 (8%)	12	32
72	SQ	57/120 (48%)	52 (91%)	5 (9%)	10	28
73	SR	120/130 (92%)	109 (91%)	11 (9%)	9	26
74	SS	47/49 (96%)	44 (94%)	3 (6%)	17	43
75	ST	126/132 (96%)	116 (92%)	10 (8%)	12	32
76	SU	135/152 (89%)	120 (89%)	15 (11%)	6	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	SV	109/126 (86%)	102 (94%)	7 (6%)	17	43
78	SW	98/130 (75%)	94 (96%)	4 (4%)	30	61
79	SX	122/131 (93%)	114 (93%)	8 (7%)	16	42
80	SY	72/116 (62%)	67 (93%)	5 (7%)	15	40
81	SZ	111/118 (94%)	97 (87%)	14 (13%)	4	13
82	Sa	83/95 (87%)	73 (88%)	10 (12%)	5	15
83	Sb	85/93 (91%)	78 (92%)	7 (8%)	11	31
84	Sc	75/76 (99%)	68 (91%)	7 (9%)	9	25
85	Sd	52/75 (69%)	47 (90%)	5 (10%)	8	24
86	Se	52/54 (96%)	48 (92%)	4 (8%)	13	34
87	Sf	70/126 (56%)	59 (84%)	11 (16%)	2	7
88	Sg	259/265 (98%)	237 (92%)	22 (8%)	10	29
89	Sh	79/177 (45%)	67 (85%)	12 (15%)	3	8
All	All	9711/10798 (90%)	9066 (93%)	645 (7%)	20	42

All (645) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	LA	30	ARG
9	LA	46	LYS
9	LA	76	MET
9	LA	122	ASP
9	LA	148	LEU
9	LA	155	LYS
9	LA	157	SER
9	LA	185	SER
9	LA	190	ARG
9	LA	202	VAL
9	LA	242	ARG
9	LA	245	ARG
10	LB	40	LYS
10	LB	59	ASP
10	LB	66	LYS
10	LB	79	LEU
10	LB	87	VAL
10	LB	171	LEU
10	LB	206	LYS

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Mol	Chain	Res	Type
10	LB	307	LEU
10	LB	339	ARG
10	LB	360	LYS
10	LB	376	ARG
10	LB	392	LYS
11	LC	13	SER
11	LC	15	ASP
11	LC	55	ARG
11	LC	56	LEU
11	LC	70	ARG
11	LC	83	THR
11	LC	94	MET
11	LC	107	PHE
11	LC	121	PHE
11	LC	204	ARG
11	LC	213	ASN
11	LC	214	LYS
11	LC	253	SER
11	LC	259	ASP
11	LC	276	THR
11	LC	285	THR
11	LC	312	ARG
11	LC	326	ARG
11	LC	337	THR
11	LC	353	ARG
12	LD	6	LYS
12	LD	31	ARG
12	LD	46	THR
12	LD	50	SER
12	LD	62	ARG
12	LD	71	CYS
12	LD	80	GLU
12	LD	83	GLU
12	LD	95	SER
12	LD	127	MET
12	LD	153	SER
12	LD	178	LYS
13	LE	6	SER
13	LE	7	LEU
13	LE	16	VAL
13	LE	56	VAL
13	LE	81	THR

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Mol	Chain	Res	Type
13	LE	92	ARG
13	LE	130	LYS
13	LE	137	SER
13	LE	155	ARG
13	LE	171	ILE
13	LE	176	ASP
13	LE	182	THR
14	LF	31	LYS
14	LF	66	SER
14	LF	70	LYS
14	LF	77	ARG
14	LF	81	SER
14	LF	84	VAL
14	LF	145	LEU
14	LF	150	ARG
15	LG	66	LEU
15	LG	87	SER
15	LG	118	LYS
15	LG	128	LYS
15	LG	167	MET
15	LG	175	LYS
15	LG	183	ASP
15	LG	209	GLU
15	LG	254	ASN
16	LH	67	ARG
16	LH	77	ARG
16	LH	85	THR
16	LH	133	THR
16	LH	136	ARG
16	LH	141	ARG
16	LH	149	ARG
16	LH	150	SER
16	LH	155	THR
16	LH	169	SER
17	LI	39	ARG
17	LI	57	LYS
17	LI	60	ARG
17	LI	68	VAL
17	LI	81	SER
17	LI	140	LYS
17	LI	170	SER
17	LI	184	MET

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Mol	Chain	Res	Type
18	LJ	35	ASN
18	LJ	85	LYS
18	LJ	100	ASN
19	LK	4	SER
19	LK	60	LYS
19	LK	64	SER
19	LK	91	ARG
19	LK	115	VAL
19	LK	132	ASP
19	LK	134	LYS
19	LK	153	LYS
20	LL	8	CYS
20	LL	30	SER
20	LL	39	HIS
20	LL	40	HIS
20	LL	60	HIS
20	LL	68	MET
20	LL	104	SER
20	LL	117	VAL
21	LM	46	GLU
21	LM	61	VAL
21	LM	80	THR
21	LM	96	LYS
21	LM	117	ASN
21	LM	124	ASP
21	LM	155	VAL
21	LM	159	ARG
21	LM	182	SER
21	LM	183	LYS
21	LM	187	SER
21	LM	189	ARG
21	LM	193	ARG
21	LM	194	ARG
22	LN	3	ARG
22	LN	28	ASP
22	LN	30	LYS
22	LN	32	ARG
22	LN	35	ASP
22	LN	40	ARG
22	LN	43	VAL
22	LN	44	ASP
22	LN	48	VAL

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Mol	Chain	Res	Type
22	LN	54	SER
22	LN	55	ARG
22	LN	63	GLU
22	LN	81	ASN
22	LN	115	MET
22	LN	156	LYS
22	LN	162	ARG
22	LN	167	MET
22	LN	189	LYS
22	LN	205	LYS
22	LN	208	MET
22	LN	211	VAL
22	LN	212	MET
23	LO	5	LYS
23	LO	15	ARG
23	LO	31	HIS
23	LO	139	GLU
23	LO	142	ASP
23	LO	185	ARG
23	LO	223	SER
23	LO	224	ASN
23	LO	228	LYS
23	LO	246	GLU
24	LP	21	SER
24	LP	41	SER
24	LP	144	TYR
24	LP	162	SER
24	LP	189	SER
24	LP	196	ARG
25	LQ	5	LYS
25	LQ	13	SER
25	LQ	40	SER
25	LQ	66	MET
25	LQ	78	VAL
25	LQ	89	MET
25	LQ	117	ARG
25	LQ	134	ASN
25	LQ	154	GLN
25	LQ	162	LYS
25	LQ	177	GLU
26	LR	19	GLU
26	LR	41	SER

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Mol	Chain	Res	Type
26	LR	50	LYS
26	LR	61	LEU
26	LR	65	VAL
26	LR	75	ASN
26	LR	98	ASP
26	LR	156	ARG
27	LS	46	SER
27	LS	55	LYS
27	LS	61	THR
27	LS	68	THR
27	LS	78	LYS
27	LS	83	ARG
27	LS	84	THR
27	LS	98	LYS
27	LS	148	ARG
28	LT	37	ASN
28	LT	57	CYS
28	LT	75	GLU
28	LT	126	ARG
28	LT	128	ARG
29	LU	5	ARG
29	LU	17	LYS
29	LU	30	CYS
29	LU	75	ASN
29	LU	78	THR
29	LU	108	ARG
30	LV	39	HIS
30	LV	50	SER
30	LV	77	LYS
31	LW	37	ARG
31	LW	71	TYR
31	LW	81	LYS
31	LW	112	ARG
32	LX	2	ARG
32	LX	59	TYR
32	LX	81	ARG
33	LY	9	LYS
33	LY	47	LYS
33	LY	59	LYS
33	LY	89	MET
33	LY	103	SER
33	LY	104	LYS

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Mol	Chain	Res	Type
34	LZ	14	GLN
34	LZ	17	ARG
34	LZ	62	CYS
34	LZ	81	THR
34	LZ	93	SER
34	LZ	138	SER
35	La	92	THR
35	La	110	ARG
36	Lb	14	SER
36	Lb	33	LYS
36	Lb	34	ARG
36	Lb	53	LYS
37	Lc	72	LEU
37	Lc	123	ASN
37	Lc	141	GLU
37	Lc	157	MET
37	Lc	175	ASP
37	Lc	188	ILE
37	Lc	237	TYR
37	Lc	241	ASP
38	Ld	26	VAL
38	Ld	27	LEU
38	Ld	90	CYS
39	Le	3	ARG
39	Le	23	ARG
39	Le	30	ARG
39	Le	45	MET
39	Le	170	ILE
40	Lf	17	ARG
40	Lf	82	ASP
41	Lg	21	THR
41	Lg	26	ARG
41	Lg	76	CYS
41	Lg	142	SER
42	Lh	3	CYS
42	Lh	7	GLN
42	Lh	17	ARG
42	Lh	52	LYS
42	Lh	105	LYS
42	Lh	114	MET
43	Li	1	MET
43	Li	5	THR

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Mol	Chain	Res	Type
43	Li	91	SER
44	Lj	24	ARG
44	Lj	33	ARG
45	Lk	26	LYS
45	Lk	59	SER
46	Ll	5	LYS
46	Ll	28	ARG
46	Ll	37	TRP
47	Lm	99	CYS
47	Lm	105	VAL
47	Lm	117	HIS
48	Ln	8	ARG
49	Lo	41	PHE
49	Lo	42	CYS
49	Lo	47	PHE
49	Lo	80	ARG
50	Lp	2	VAL
50	Lp	26	VAL
50	Lp	61	LYS
50	Lp	72	LEU
50	Lp	78	LYS
50	Lp	79	SER
56	SA	26	ARG
56	SA	31	ASP
56	SA	55	ARG
56	SA	85	LYS
56	SA	110	ASP
56	SA	150	ASN
56	SA	155	ASN
56	SA	182	GLN
56	SA	194	VAL
56	SA	196	SER
56	SA	204	ASN
56	SA	207	LEU
56	SA	224	LYS
57	SB	13	MET
57	SB	35	SER
57	SB	84	LEU
57	SB	92	LYS
57	SB	95	GLN
57	SB	116	GLN
57	SB	131	ARG

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Mol	Chain	Res	Type
57	SB	195	SER
58	SC	7	LYS
58	SC	9	MET
58	SC	37	SER
58	SC	41	THR
58	SC	44	ARG
58	SC	112	LEU
58	SC	113	GLN
58	SC	115	ARG
58	SC	116	ARG
58	SC	147	LYS
58	SC	155	TYR
58	SC	158	LYS
58	SC	171[A]	CYS
58	SC	171[B]	CYS
58	SC	193	SER
58	SC	194	THR
58	SC	200	SER
58	SC	205	ASP
58	SC	206	VAL
59	SD	6	ASN
59	SD	15	ARG
59	SD	38	LYS
59	SD	47	THR
59	SD	48	LEU
59	SD	49	SER
59	SD	60	THR
59	SD	106	ARG
59	SD	113	PHE
59	SD	150	SER
59	SD	168	THR
59	SD	177	LYS
59	SD	181	ARG
60	SE	10	TYR
60	SE	13	LYS
60	SE	17	LEU
60	SE	18	SER
60	SE	20	LEU
60	SE	27	ARG
60	SE	35	LEU
60	SE	53	LEU
60	SE	128	THR

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Mol	Chain	Res	Type
60	SE	130	THR
60	SE	148	ASP
60	SE	162	LYS
60	SE	170	ILE
60	SE	171	LYS
60	SE	181	THR
60	SE	193	VAL
60	SE	196	GLU
60	SE	252	GLU
60	SE	253	ARG
60	SE	254	LEU
60	SE	260	ARG
61	SF	91	GLU
61	SF	116	VAL
61	SF	138	ARG
61	SF	168	MET
61	SF	186	ARG
61	SF	211	SER
61	SF	234	TYR
61	SF	245	THR
61	SF	257	GLU
62	SG	1	MET
62	SG	2	LYS
62	SG	7	TYR
62	SG	19	SER
62	SG	24	ARG
62	SG	54	ARG
62	SG	59	LYS
62	SG	65	VAL
62	SG	72	SER
62	SG	89	ARG
62	SG	95	ARG
62	SG	96	ARG
62	SG	104	VAL
62	SG	117	SER
62	SG	121	ASP
62	SG	130	THR
62	SG	143	LYS
62	SG	146	LYS
62	SG	150	LEU
62	SG	157	ARG
62	SG	162	ARG

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Mol	Chain	Res	Type
62	SG	173	ARG
62	SG	191	ARG
62	SG	197	ASP
62	SG	208	GLU
62	SG	209	ARG
62	SG	210	ARG
62	SG	228	HIS
62	SG	234	ARG
63	SH	18	GLU
63	SH	52	MET
63	SH	55	VAL
63	SH	108	ARG
63	SH	110	ASP
63	SH	111	SER
63	SH	161	ASP
63	SH	171	SER
63	SH	177	LYS
63	SH	184	ARG
64	SI	21	GLU
64	SI	22	SER
64	SI	57	SER
64	SI	82	THR
64	SI	104	LYS
64	SI	121	SER
64	SI	136	SER
64	SI	139	VAL
64	SI	146	ARG
64	SI	148	ASP
64	SI	153	MET
64	SI	160	ARG
64	SI	163	LYS
64	SI	164	ARG
64	SI	166	GLU
65	SJ	22	LYS
65	SJ	30	SER
65	SJ	78	ARG
65	SJ	88	LYS
65	SJ	124	LYS
66	SK	4	VAL
66	SK	22	ARG
66	SK	31	ARG
66	SK	47	ARG

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Mol	Chain	Res	Type
66	SK	58	LEU
66	SK	64	ASN
66	SK	81	VAL
66	SK	111	ARG
66	SK	147	ASP
66	SK	152	ASN
66	SK	166	ARG
66	SK	167	ARG
66	SK	171	VAL
66	SK	183	ARG
66	SK	209	GLN
67	SL	28	THR
67	SL	32	GLN
67	SL	49	THR
67	SL	63	SER
67	SL	80	GLN
67	SL	108	LYS
68	SM	22	THR
68	SM	27	LYS
68	SM	29	VAL
68	SM	34	SER
68	SM	45	VAL
68	SM	46	THR
68	SM	87	ASP
68	SM	110	SER
69	SN	3	THR
69	SN	9	SER
69	SN	17	PHE
69	SN	27	LYS
69	SN	41	THR
69	SN	44	VAL
69	SN	49	VAL
70	SO	18	ASP
70	SO	68	MET
70	SO	77	ARG
70	SO	89	LYS
70	SO	97	ARG
71	SP	2	THR
71	SP	21	ARG
71	SP	36	ARG
71	SP	57	VAL
71	SP	71	ARG

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Mol	Chain	Res	Type
71	SP	77	ASN
71	SP	85	VAL
71	SP	105	PHE
71	SP	127	ASN
72	SQ	43	LEU
72	SQ	45	ARG
72	SQ	55	ASP
72	SQ	73	TYR
72	SQ	87	ASP
73	SR	12	HIS
73	SR	32	ARG
73	SR	44	LEU
73	SR	56	ARG
73	SR	87	ARG
73	SR	88	GLN
73	SR	92	LYS
73	SR	100	SER
73	SR	103	MET
73	SR	105	ASP
73	SR	143	HIS
74	SS	9	SER
74	SS	15	MET
74	SS	56	LEU
75	ST	2	VAL
75	ST	21	THR
75	ST	30	SER
75	ST	36	MET
75	ST	100	LYS
75	ST	104	ARG
75	ST	107	THR
75	ST	109	ARG
75	ST	114	ARG
75	ST	127	ARG
76	SU	19	HIS
76	SU	21	LYS
76	SU	25	ARG
76	SU	33	MET
76	SU	35	ARG
76	SU	38	ARG
76	SU	43	LYS
76	SU	65	ASN
76	SU	82	ARG

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Mol	Chain	Res	Type
76	SU	89	VAL
76	SU	93	THR
76	SU	97	ARG
76	SU	117	LYS
76	SU	137	GLU
76	SU	153	ASN
77	SV	5	ARG
77	SV	7	LYS
77	SV	8	THR
77	SV	37	ASP
77	SV	100	SER
77	SV	102	ASP
77	SV	121	LYS
78	SW	22	PHE
78	SW	73	HIS
78	SW	75	LYS
78	SW	107	HIS
79	SX	7	LYS
79	SX	10	ARG
79	SX	13	LYS
79	SX	21	ASP
79	SX	33	ARG
79	SX	80	ARG
79	SX	100	SER
79	SX	142	LYS
80	SY	15	ASP
80	SY	40	SER
80	SY	55	THR
80	SY	62	TYR
80	SY	80	ARG
81	SZ	28	PHE
81	SZ	50	LEU
81	SZ	52	THR
81	SZ	55	LYS
81	SZ	60	SER
81	SZ	69	THR
81	SZ	81	LEU
81	SZ	91	ARG
81	SZ	103	PHE
81	SZ	112	LYS
81	SZ	116	GLU
81	SZ	120	ARG

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Mol	Chain	Res	Type
81	SZ	125	ARG
81	SZ	127	LYS
82	Sa	9	LYS
82	Sa	17	ASN
82	Sa	32	SER
82	Sa	33	ARG
82	Sa	43	ASP
82	Sa	51	ARG
82	Sa	58	LYS
82	Sa	87	LYS
82	Sa	94	CYS
82	Sa	98	THR
83	Sb	2	THR
83	Sb	32	THR
83	Sb	42	VAL
83	Sb	59	SER
83	Sb	78	CYS
83	Sb	87	THR
83	Sb	88	VAL
84	Sc	3	PHE
84	Sc	8	LEU
84	Sc	35	ASP
84	Sc	37	SER
84	Sc	63	LYS
84	Sc	82	ARG
84	Sc	85	ASP
85	Sd	22	GLN
85	Sd	28	LYS
85	Sd	57	ARG
85	Sd	73	LEU
85	Sd	74	SER
86	Se	7	SER
86	Se	8	LEU
86	Se	49	VAL
86	Se	54	LYS
87	Sf	73	LYS
87	Sf	76	LYS
87	Sf	81	THR
87	Sf	87	THR
87	Sf	107	ASP
87	Sf	108	ASP
87	Sf	119	ASP

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Mol	Chain	Res	Type
87	Sf	125	CYS
87	Sf	135	LYS
87	Sf	137	ARG
87	Sf	143	CYS
88	Sg	13	TRP
88	Sg	53	ASP
88	Sg	69	SER
88	Sg	72	SER
88	Sg	77	THR
88	Sg	86	ASP
88	Sg	115	PHE
88	Sg	128	ASP
88	Sg	141	MET
88	Sg	158	PHE
88	Sg	179	TRP
88	Sg	185	LYS
88	Sg	194	SER
88	Sg	199	THR
88	Sg	203	SER
88	Sg	205	ASP
88	Sg	209	CYS
88	Sg	248	PHE
88	Sg	258	LEU
88	Sg	294	LEU
88	Sg	299	LYS
88	Sg	304	ARG
89	Sh	136	SER
89	Sh	139	PHE
89	Sh	144	PHE
89	Sh	149	THR
89	Sh	162	VAL
89	Sh	170	GLN
89	Sh	184	LYS
89	Sh	207	ARG
89	Sh	211	LYS
89	Sh	213	ARG
89	Sh	215	ARG
89	Sh	228	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
17	L1	93	GLN
18	LJ	35	ASN
18	LJ	106	ASN
23	LO	120	GLN
34	LZ	35	ASN
34	LZ	37	ASN
35	La	114	GLN
41	Lg	25	ASN
59	SD	3	ASN
80	SY	66	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1667/1782 (93%)	447 (26%)	18 (1%)
2	L2	1148/1526 (75%)	279 (24%)	14 (1%)
3	L3	178/216 (82%)	44 (24%)	3 (1%)
4	L4	183/184 (99%)	43 (23%)	2 (1%)
5	L5	117/135 (86%)	32 (27%)	3 (2%)
51	S1	1819/2204 (82%)	436 (23%)	26 (1%)
52	S2	74/76 (97%)	27 (36%)	8 (10%)
53	S3	74/77 (96%)	19 (25%)	2 (2%)
54	S4	72/76 (94%)	37 (51%)	1 (1%)
55	S5	11/13 (84%)	6 (54%)	0
6	L6	70/73 (95%)	32 (45%)	1 (1%)
7	L7	164/171 (95%)	40 (24%)	2 (1%)
8	L8	119/124 (95%)	19 (15%)	1 (0%)
All	All	5696/6657 (85%)	1461 (25%)	81 (1%)

All (1461) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	6	C
1	L1	7	C
1	L1	16	G
1	L1	24	A
1	L1	29	C
1	L1	32	A
1	L1	38	A
1	L1	41	A
1	L1	47	C
1	L1	56	G

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Mol	Chain	Res	Type
1	L1	58	A
1	L1	63	A
1	L1	64	A
1	L1	65	A
1	L1	67	C
1	L1	69	A2M
1	L1	70	C
1	L1	83	A
1	L1	84	G
1	L1	86	G
1	L1	87	A
1	L1	91	G
1	L1	98	A
1	L1	110	A
1	L1	117	G
1	L1	121	A
1	L1	126	G
1	L1	127	G
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	145	U
1	L1	146	U
1	L1	147	G
1	L1	148	U
1	L1	149	G
1	L1	154	A
1	L1	156	A
1	L1	157	U
1	L1	158	A
1	L1	160	C
1	L1	161	A
1	L1	162	U
1	L1	167	U
1	L1	170	U
1	L1	171	U
1	L1	176	C

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Mol	Chain	Res	Type
1	L1	182	U
1	L1	191	U
1	L1	192	C
1	L1	195	G
1	L1	199	A
1	L1	201	A
1	L1	202	G
1	L1	204	A
1	L1	205	A
1	L1	206	A
1	L1	209	C
1	L1	210	G
1	L1	215	U
1	L1	216	G
1	L1	218	A
1	L1	219	U
1	L1	223	A
1	L1	224	C
1	L1	225	C
1	L1	226	C
1	L1	233	U
1	L1	234	G
1	L1	243	G
1	L1	251	A
1	L1	256	U
1	L1	257	U
1	L1	264	U
1	L1	280	A
1	L1	281	G
1	L1	300	A
1	L1	301	A
1	L1	302	G
1	L1	305	A2M
1	L1	306	G
1	L1	311	A
1	L1	312	C
1	L1	313	PSU
1	L1	322	A
1	L1	323	U
1	L1	332	A
1	L1	335	U
1	L1	336	U

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Mol	Chain	Res	Type
1	L1	337	G
1	L1	338	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	374	G
1	L1	376	A
1	L1	377	G
1	L1	383	U
1	L1	392	A
1	L1	409	U
1	L1	410	U
1	L1	414	A
1	L1	417	G
1	L1	419	A
1	L1	440	A
1	L1	443	A
1	L1	444	C
1	L1	461	G
1	L1	463	C
1	L1	464	A
1	L1	470	A
1	L1	471	G
1	L1	477	C
1	L1	484	A
1	L1	485	A
1	L1	488	G
1	L1	489	C
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	511	A
1	L1	512	U

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Mol	Chain	Res	Type
1	L1	518	C
1	L1	522	G
1	L1	525	C
1	L1	527	A
1	L1	539	C
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	568	U
1	L1	569	G
1	L1	571	A
1	L1	572	A
1	L1	573	U
1	L1	574	G
1	L1	577	C
1	L1	579	G
1	L1	580	A
1	L1	584	U
1	L1	585	U
1	L1	586	U
1	L1	587	G
1	L1	590	C
1	L1	592	G
1	L1	601	G
1	L1	605	G
1	L1	606	C
1	L1	611	C
1	L1	612	G
1	L1	616	U
1	L1	617	G
1	L1	621	U
1	L1	623	U
1	L1	625	C
1	L1	627	C
1	L1	631	G
1	L1	632	A

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Mol	Chain	Res	Type
1	L1	634	G
1	L1	635	C
1	L1	641	G
1	L1	648	A
1	L1	651	G
1	L1	652	A
1	L1	653	A
1	L1	664	C
1	L1	666	C
1	L1	668	C
1	L1	669	C
1	L1	673	C
1	L1	681	A2M
1	L1	709	A
1	L1	710	G
1	L1	717	G
1	L1	718	A
1	L1	729	A
1	L1	736	C
1	L1	743	A
1	L1	745	U
1	L1	748	A
1	L1	750	G
1	L1	753	A
1	L1	760	A
1	L1	762	A
1	L1	763	U
1	L1	770	G
1	L1	771	U
1	L1	778	C
1	L1	781	A
1	L1	783	G
1	L1	790	C
1	L1	794	U
1	L1	795	U
1	L1	803	C
1	L1	804	C
1	L1	810	C
1	L1	818	C
1	L1	823	G
1	L1	825	G
1	L1	832	G

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Mol	Chain	Res	Type
1	L1	836	G
1	L1	838	G
1	L1	850	G
1	L1	867	A
1	L1	868	A
1	L1	887	A
1	L1	895	G
1	L1	900	C
1	L1	904	G
1	L1	912	C
1	L1	925	U
1	L1	930	U
1	L1	945	U
1	L1	957	C
1	L1	965	A
1	L1	967	G
1	L1	968	A
1	L1	972	A
1	L1	973	U
1	L1	974	C
1	L1	975	G
1	L1	976	A
1	L1	988	G
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	1014	G
1	L1	1016	A
1	L1	1017	PSU
1	L1	1018	A
1	L1	1025	G
1	L1	1031	A
1	L1	1036	U
1	L1	1040	G
1	L1	1041	U
1	L1	1045	G
1	L1	1046	U
1	L1	1053	A
1	L1	1085	C

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Mol	Chain	Res	Type
1	L1	1089	C
1	L1	1092	U
1	L1	1093	U
1	L1	1094	C
1	L1	1097	A
1	L1	1098	A
1	L1	1100	C
1	L1	1114	A
1	L1	1116	A
1	L1	1122	U
1	L1	1123	G
1	L1	1128	A
1	L1	1129	G
1	L1	1135	U
1	L1	1136	G
1	L1	1137	C
1	L1	1141	G
1	L1	1144	G
1	L1	1147	A
1	L1	1148	A
1	L1	1150	A
1	L1	1153	A
1	L1	1155	A
1	L1	1156	A
1	L1	1159	A
1	L1	1161	A
1	L1	1162	G
1	L1	1165	A
1	L1	1167	C
1	L1	1169	A
1	L1	1170	G
1	L1	1171	PSU
1	L1	1172	G
1	L1	1174	G
1	L1	1178	U
1	L1	1179	C
1	L1	1188	G
1	L1	1196	G
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	1209	G
1	L1	1210	A
1	L1	1211	A
1	L1	1213	C
1	L1	1217	U
1	L1	1220	G
1	L1	1225	U
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	1263	A
1	L1	1264	A
1	L1	1270	U
1	L1	1271	G
1	L1	1287	A
1	L1	1342	C
1	L1	1343	A
1	L1	1344	A
1	L1	1345	C
1	L1	1346	C
1	L1	1348	A
1	L1	1349	A
1	L1	1351	C
1	L1	1352	C
1	L1	1364	A
1	L1	1367	U
1	L1	1369	G
1	L1	1371	OMU
1	L1	1375	G
1	L1	1378	U
1	L1	1379	A
1	L1	1387	U
1	L1	1388	U

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Mol	Chain	Res	Type
1	L1	1389	A
1	L1	1390	G
1	L1	1391	U
1	L1	1395	U
1	L1	1399	C
1	L1	1401	U
1	L1	1402	U
1	L1	1413	U
1	L1	1416	G
1	L1	1417	G
1	L1	1420	G
1	L1	1421	G
1	L1	1422	A
1	L1	1424	A
1	L1	1426	A
1	L1	1438	A
1	L1	1444	A
1	L1	1445	G
1	L1	1446	C
1	L1	1455	U
1	L1	1456	G
1	L1	1464	G
1	L1	1465	G
1	L1	1480	C
1	L1	1482	A
1	L1	1483	A
1	L1	1489	U
1	L1	1490	G
1	L1	1495	G
1	L1	1504	A
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	1527	OMC
1	L1	1528	PSU
1	L1	1536	C
1	L1	1540	OMG
1	L1	1545	G
1	L1	1547	U

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Mol	Chain	Res	Type
1	L1	1557	A
1	L1	1560	U
1	L1	1561	A
1	L1	1566	A
1	L1	1569	U
1	L1	1574	C
1	L1	1575	G
1	L1	1586	G
1	L1	1587	A
1	L1	1589	C
1	L1	1590	G
1	L1	1592	G
1	L1	1593	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	1638	C
1	L1	1654	A
1	L1	1655	U
1	L1	1661	U
1	L1	1662	G
1	L1	1663	U
1	L1	1664	PSU
1	L1	1666	G
1	L1	1667	G
1	L1	1671	G
1	L1	1713	A
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	1746	C

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Mol	Chain	Res	Type
1	L1	1747	U
1	L1	1750	G
1	L1	1751	A
1	L1	1752	U
1	L1	1753	U
1	L1	1754	A
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	1766	G
1	L1	1768	A
1	L1	1771	U
1	L1	1772	G
1	L1	1774	A
2	L2	5	A
2	L2	12	G
2	L2	13	A
2	L2	14	OMC
2	L2	15	C
2	L2	22	A
2	L2	25	A
2	L2	26	C
2	L2	29	C
2	L2	30	A
2	L2	41	A
2	L2	49	A
2	L2	61	C
2	L2	62	A
2	L2	63	U
2	L2	68	A
2	L2	69	A
2	L2	76	A
2	L2	84	A
2	L2	90	G
2	L2	91	C
2	L2	105	A
2	L2	116	A
2	L2	123	G
2	L2	125	C

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Mol	Chain	Res	Type
2	L2	127	C
2	L2	137	A
2	L2	340	A
2	L2	341	A
2	L2	342	U
2	L2	343	U
2	L2	348	A
2	L2	349	C
2	L2	358	G
2	L2	365	G
2	L2	368	G
2	L2	372	A
2	L2	377	A
2	L2	385	A
2	L2	386	U
2	L2	388	A
2	L2	390	A
2	L2	392	C
2	L2	404	A
2	L2	415	U
2	L2	423	A
2	L2	426	G
2	L2	434	A
2	L2	436	U
2	L2	439	U
2	L2	443	OMC
2	L2	444	A
2	L2	446	U
2	L2	453	A
2	L2	454	A
2	L2	455	U
2	L2	456	G
2	L2	457	U
2	L2	459	A
2	L2	462	G
2	L2	489	A
2	L2	490	A
2	L2	495	G
2	L2	502	A2M
2	L2	518	G
2	L2	519	G
2	L2	527	A2M

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Mol	Chain	Res	Type
2	L2	528	U
2	L2	529	G
2	L2	530	C
2	L2	534	OMG
2	L2	544	U
2	L2	552	C
2	L2	553	G
2	L2	554	C
2	L2	556	U
2	L2	559	A
2	L2	561	G
2	L2	571	G
2	L2	580	U
2	L2	581	G
2	L2	582	U
2	L2	616	G
2	L2	617	G
2	L2	619	A
2	L2	620	C
2	L2	621	G
2	L2	632	G
2	L2	635	A
2	L2	639	G
2	L2	643	A
2	L2	647	A2M
2	L2	648	A
2	L2	649	G
2	L2	650	A
2	L2	657	U
2	L2	658	G
2	L2	665	A2M
2	L2	685	G
2	L2	686	OMG
2	L2	695	G
2	L2	696	A
2	L2	697	G
2	L2	698	G
2	L2	745	G
2	L2	746	A
2	L2	747	A
2	L2	749	G
2	L2	750	U

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Mol	Chain	Res	Type
2	L2	751	U
2	L2	752	G
2	L2	760	U
2	L2	768	G
2	L2	769	A
2	L2	777	A
2	L2	778	A
2	L2	779	U
2	L2	782	G
2	L2	784	U
2	L2	787	G
2	L2	789	G
2	L2	793	U
2	L2	799	G
2	L2	802	PSU
2	L2	803	A
2	L2	805	G
2	L2	808	C
2	L2	810	G
2	L2	811	U
2	L2	819	U
2	L2	823	A
2	L2	851	C
2	L2	955	C
2	L2	970	A
2	L2	971	A
2	L2	972	C
2	L2	975	A
2	L2	976	A
2	L2	979	A
2	L2	984	G
2	L2	986	U
2	L2	999	U
2	L2	1001	C
2	L2	1004	G
2	L2	1010	U
2	L2	1011	G
2	L2	1012	U
2	L2	1019	A
2	L2	1021	A
2	L2	1022	U
2	L2	1023	C

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Mol	Chain	Res	Type
2	L2	1025	G
2	L2	1030	A
2	L2	1033	G
2	L2	1034	G
2	L2	1041	G
2	L2	1046	OMG
2	L2	1053	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	1090	G
2	L2	1096	U
2	L2	1099	G
2	L2	1100	A
2	L2	1102	C
2	L2	1104	G
2	L2	1106	A
2	L2	1115	U
2	L2	1116	A
2	L2	1118	A
2	L2	1121	A
2	L2	1122	C
2	L2	1123	A
2	L2	1129	A
2	L2	1132	A
2	L2	1137	G
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	1158	A
2	L2	1162	A
2	L2	1171	G
2	L2	1172	C
2	L2	1176	A
2	L2	1179	A

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Mol	Chain	Res	Type
2	L2	1181	G
2	L2	1189	A
2	L2	1199	A
2	L2	1200	A
2	L2	1202	A
2	L2	1203	A
2	L2	1204	U
2	L2	1206	G
2	L2	1207	G
2	L2	1209	A
2	L2	1221	U
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	1246	A
2	L2	1248	OMC
2	L2	1252	G
2	L2	1255	A
2	L2	1261	G
2	L2	1264	PSU
2	L2	1265	PSU
2	L2	1271	G
2	L2	1281	U
2	L2	1283	A
2	L2	1288	G
2	L2	1289	A
2	L2	1300	U
2	L2	1306	U
2	L2	1309	G
2	L2	1313	U
2	L2	1325	A
2	L2	1327	C
2	L2	1336	G
2	L2	1337	C
2	L2	1342	G
2	L2	1348	A
2	L2	1349	A

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Mol	Chain	Res	Type
2	L2	1355	G
2	L2	1361	PSU
2	L2	1373	C
2	L2	1374	A
2	L2	1379	A
2	L2	1380	C
2	L2	1385	G
2	L2	1386	C
2	L2	1392	U
2	L2	1409	A
2	L2	1416	U
2	L2	1421	C
2	L2	1423	C
2	L2	1425	A
2	L2	1426	C
2	L2	1428	U
2	L2	1430	G
2	L2	1433	G
2	L2	1434	G
2	L2	1437	A
2	L2	1439	U
2	L2	1441	C
2	L2	1443	A
2	L2	1444	G
2	L2	1445	A
2	L2	1448	A
2	L2	1450	G
2	L2	1454	A
2	L2	1456	C
2	L2	1457	C
2	L2	1463	A
2	L2	1465	G
2	L2	1478	C
2	L2	1485	G
2	L2	1486	G
2	L2	1494	G
2	L2	1501	G
2	L2	1510	A
2	L2	1511	U
2	L2	1512	G
2	L2	1513	G
2	L2	1514	U

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Mol	Chain	Res	Type
2	L2	1524	A
2	L2	1526	C
3	L3	6	G
3	L3	16	G
3	L3	17	A
3	L3	19	A
3	L3	21	A
3	L3	22	C
3	L3	25	G
3	L3	34	C
3	L3	35	A
3	L3	41	A
3	L3	42	U
3	L3	44	C
3	L3	48	C
3	L3	49	A
3	L3	50	C
3	L3	52	G
3	L3	70	A
3	L3	99	U
3	L3	108	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	120	G
3	L3	121	U
3	L3	125	U
3	L3	132	G
3	L3	141	A
3	L3	142	G
3	L3	149	A
3	L3	150	A
3	L3	151	A
3	L3	169	A
3	L3	182	U
3	L3	187	U
3	L3	192	G
3	L3	195	U

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Mol	Chain	Res	Type
3	L3	196	U
3	L3	199	A
3	L3	202	A
3	L3	212	G
4	L4	8	U
4	L4	9	G
4	L4	10	U
4	L4	11	G
4	L4	15	G
4	L4	16	G
4	L4	19	C
4	L4	24	A
4	L4	31	G
4	L4	39	A
4	L4	40	G
4	L4	50	G
4	L4	60	A
4	L4	61	A
4	L4	67	A
4	L4	73	U
4	L4	76	C
4	L4	83	U
4	L4	85	C
4	L4	86	U
4	L4	87	G
4	L4	90	G
4	L4	102	G
4	L4	106	G
4	L4	107	U
4	L4	114	A
4	L4	120	U
4	L4	121	C
4	L4	122	G
4	L4	128	U
4	L4	132	U
4	L4	133	C
4	L4	148	C
4	L4	149	U
4	L4	150	A
4	L4	151	A
4	L4	158	A
4	L4	159	G

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Mol	Chain	Res	Type
4	L4	168	A
4	L4	170	G
4	L4	173	C
4	L4	178	G
4	L4	180	C
5	L5	3	U
5	L5	4	A
5	L5	6	G
5	L5	15	C
5	L5	24	G
5	L5	29	U
5	L5	34	G
5	L5	39	G
5	L5	50	C
5	L5	51	A
5	L5	52	U
5	L5	65	U
5	L5	68	G
5	L5	71	U
5	L5	86	G
5	L5	87	U
5	L5	88	C
5	L5	89	C
5	L5	92	A
5	L5	99	G
5	L5	105	U
5	L5	106	G
5	L5	107	A
5	L5	109	G
5	L5	113	G
5	L5	118	U
5	L5	119	U
5	L5	120	C
5	L5	121	A
5	L5	123	G
5	L5	124	C
5	L5	135	U
6	L6	7	A
6	L6	12	C
6	L6	14	A
6	L6	15	C
6	L6	22	G

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Mol	Chain	Res	Type
6	L6	23	A
6	L6	24	C
6	L6	25	U
6	L6	31	U
6	L6	32	U
6	L6	33	G
6	L6	41	G
6	L6	42	A
6	L6	43	A
6	L6	44	G
6	L6	45	G
6	L6	49	C
6	L6	51	A
6	L6	52	G
6	L6	54	A
6	L6	55	U
6	L6	56	A
6	L6	58	U
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	11	G
7	L7	16	A
7	L7	22	U
7	L7	31	A
7	L7	33	U
7	L7	34	U
7	L7	38	U
7	L7	51	A
7	L7	59	A
7	L7	62	A
7	L7	63	G
7	L7	68	A
7	L7	69	PSU
7	L7	70	C

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Mol	Chain	Res	Type
7	L7	71	A
7	L7	72	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	94	G
7	L7	103	A
7	L7	104	A
7	L7	105	C
7	L7	107	C
7	L7	110	A
7	L7	115	G
7	L7	117	A
7	L7	120	G
7	L7	124	A
7	L7	125	A
7	L7	127	C
7	L7	157	U
7	L7	158	U
7	L7	159	C
7	L7	167	C
7	L7	169	A
8	L8	11	G
8	L8	22	A
8	L8	26	A
8	L8	45	G
8	L8	46	A
8	L8	52	G
8	L8	57	U
8	L8	67	C
8	L8	68	A
8	L8	69	G
8	L8	70	G
8	L8	71	C
8	L8	76	U
8	L8	94	A
8	L8	95	U
8	L8	104	A
8	L8	113	U

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Mol	Chain	Res	Type
8	L8	114	G
8	L8	124	U
51	S1	3	U
51	S1	8	OMU
51	S1	17	C
51	S1	26	A
51	S1	34	G
51	S1	42	G
51	S1	45	U
51	S1	47	A
51	S1	60	U
51	S1	61	C
51	S1	65	A
51	S1	66	U
51	S1	68	A
51	S1	98	A2M
51	S1	102	A
51	S1	103	A
51	S1	110	G
51	S1	112	A
51	S1	114	U
51	S1	117	G
51	S1	122	A
51	S1	124	A
51	S1	127	U
51	S1	129	U
51	S1	133	G
51	S1	144	A
51	S1	145	A
51	S1	147	U
51	S1	149	G
51	S1	152	A
51	S1	158	G
51	S1	164	C
51	S1	167	C
51	S1	170	G
51	S1	174	A
51	S1	175	U
51	S1	176	A
51	S1	182	A
51	S1	194	U
51	S1	195	U

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Mol	Chain	Res	Type
51	S1	196	C
51	S1	197	U
51	S1	198	C
51	S1	227	U
51	S1	228	G
51	S1	231	A
51	S1	234	C
51	S1	235	C
51	S1	237	A
51	S1	249	A
51	S1	250	C
51	S1	252	G
51	S1	253	U
51	S1	254	A
51	S1	255	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	287	C
51	S1	288	A
51	S1	289	G
51	S1	295	A
51	S1	297	U
51	S1	298	C
51	S1	309	G
51	S1	310	U
51	S1	313	G
51	S1	316	A
51	S1	321	G
51	S1	322	C
51	S1	324	U
51	S1	325	G
51	S1	326	U
51	S1	329	C
51	S1	332	C
51	S1	336	U
51	S1	340	G

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Mol	Chain	Res	Type
51	S1	341	A
51	S1	356	A
51	S1	358	C
51	S1	360	G
51	S1	364	G
51	S1	377	A
51	S1	381	G
51	S1	382	A
51	S1	388	A
51	S1	396	G
51	S1	404	C
51	S1	433	G
51	S1	434	A
51	S1	435	G
51	S1	443	A
51	S1	444	A
51	S1	445	U
51	S1	446	A
51	S1	447	G
51	S1	454	C
51	S1	455	PSU
51	S1	460	C
51	S1	465	G
51	S1	466	G
51	S1	467	C
51	S1	469	G
51	S1	475	G
51	S1	477	G
51	S1	481	A
51	S1	482	U
51	S1	484	G
51	S1	487	C
51	S1	488	A
51	S1	497	A
51	S1	507	G
51	S1	508	A
51	S1	516	A
51	S1	523	A
51	S1	525	A
51	S1	528	G
51	S1	548	G
51	S1	551	A

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Mol	Chain	Res	Type
51	S1	552	U
51	S1	565	U
51	S1	574	C
51	S1	580	A
51	S1	581	A
51	S1	585	C
51	S1	587	A
51	S1	590	A
51	S1	591	A
51	S1	593	A
51	S1	600	OMG
51	S1	606	G
51	S1	607	U
51	S1	608	C
51	S1	609	U
51	S1	613	G
51	S1	614	C
51	S1	615	C
51	S1	617	G
51	S1	627	U
51	S1	628	A
51	S1	629	A
51	S1	630	U
51	S1	631	U
51	S1	632	C
51	S1	643	A
51	S1	659	G
51	S1	660	U
51	S1	666	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	678	U
51	S1	687	U
51	S1	688	G
51	S1	689	U
51	S1	690	G
51	S1	697	G
51	S1	698	C

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Mol	Chain	Res	Type
51	S1	699	A
51	S1	749	U
51	S1	755	C
51	S1	757	C
51	S1	758	G
51	S1	762	A
51	S1	775	C
51	S1	778	G
51	S1	782	C
51	S1	784	C
51	S1	788	A
51	S1	789	G
51	S1	790	U
51	S1	791	G
51	S1	792	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	819	G
51	S1	820	C
51	S1	825	C
51	S1	826	A
51	S1	830	G
51	S1	832	C
51	S1	833	G
51	S1	841	U
51	S1	844	U
51	S1	845	U
51	S1	856	A
51	S1	866	G
51	S1	867	A
51	S1	868	C
51	S1	869	U
51	S1	879	A
51	S1	880	U
51	S1	883	G
51	S1	886	U
51	S1	887	U
51	S1	890	A

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Mol	Chain	Res	Type
51	S1	892	U
51	S1	895	A
51	S1	914	G
51	S1	919	G
51	S1	923	C
51	S1	925	A
51	S1	926	G
51	S1	930	A
51	S1	935	U
51	S1	936	U
51	S1	937	C
51	S1	938	G
51	S1	944	U
51	S1	945	G
51	S1	950	U
51	S1	951	U
51	S1	952	U
51	S1	955	A
51	S1	956	A
51	S1	959	U
51	S1	969	A
51	S1	970	U
51	S1	971	U
51	S1	972	A
51	S1	973	U
51	S1	974	G
51	S1	1101	A
51	S1	1102	G
51	S1	1103	G
51	S1	1105	A
51	S1	1109	A
51	S1	1119	U
51	S1	1123	G
51	S1	1139	G
51	S1	1148	G
51	S1	1161	G
51	S1	1180	A
51	S1	1182	A
51	S1	1197	C
51	S1	1198	A
51	S1	1199	A
51	S1	1207	U

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Mol	Chain	Res	Type
51	S1	1210	C
51	S1	1211	U
51	S1	1213	A
51	S1	1217	A
51	S1	1232	G
51	S1	1235	A
51	S1	1239	A
51	S1	1240	A
51	S1	1251	A
51	S1	1270	G
51	S1	1271	C
51	S1	1272	A
51	S1	1273	A
51	S1	1275	C
51	S1	1359	C
51	S1	1360	U
51	S1	1361	U
51	S1	1365	U
51	S1	1371	U
51	S1	1398	C
51	S1	1399	G
51	S1	1431	A
51	S1	1443	U
51	S1	1444	G
51	S1	1448	U
51	S1	1449	U
51	S1	1452	A
51	S1	1466	G
51	S1	1467	U
51	S1	1490	A
51	S1	1502	G
51	S1	1503	A
51	S1	1510	C
51	S1	1531	G
51	S1	1537	U
51	S1	1546	A
51	S1	1548	A
51	S1	1551	G
51	S1	1552	G
51	S1	1554	A
51	S1	1565	A
51	S1	1566	PSU

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Mol	Chain	Res	Type
51	S1	1569	G
51	S1	1570	G
51	S1	1579	A
51	S1	1582	A
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	1609	U
51	S1	1611	C
51	S1	1612	C
51	S1	1613	C
51	S1	1614	U
51	S1	1622	G
51	S1	1625	G
51	S1	1637	A
51	S1	1638	U
51	S1	1640	G
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	1675	C
51	S1	1677	G
51	S1	1689	G
51	S1	1690	C
51	S1	1699	A
51	S1	1706	A
51	S1	1712	G
51	S1	1713	C
51	S1	1715	C
51	S1	1718	A
51	S1	1719	G
51	S1	1720	G
51	S1	1724	G
51	S1	1725	C
51	S1	1762	A
51	S1	1764	U

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Mol	Chain	Res	Type
51	S1	1766	G
51	S1	1768	U
51	S1	1769	C
51	S1	1770	G
51	S1	1784	G
51	S1	1788	U
51	S1	1789	U
51	S1	1794	U
51	S1	1795	G
51	S1	1799	U
51	S1	1800	U
51	S1	1801	G
51	S1	1806	A
51	S1	1814	U
51	S1	1816	U
51	S1	1825	A
51	S1	1826	G
51	S1	1828	A
51	S1	1829	OMG
51	S1	1833	OMU
51	S1	1837	A
51	S1	1846	A
51	S1	1847	A
51	S1	1848	U
51	S1	1858	G
51	S1	1860	C
51	S1	1861	A
51	S1	1867	A
51	S1	1872	A
51	S1	1874	U
51	S1	1878	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	1905	C
51	S1	1906	G
51	S1	1907	A
51	S1	1916	G
51	S1	1917	A

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Mol	Chain	Res	Type
51	S1	1918	U
51	S1	1919	C
51	S1	1920	A
51	S1	1923	A
51	S1	1933	A
51	S1	1944	C
51	S1	1948	U
51	S1	1949	A
51	S1	1950	G
51	S1	1956	C
51	S1	1961	G
51	S1	1962	A
51	S1	1976	U
51	S1	1978	A
51	S1	1988	C
51	S1	1989	A
51	S1	1995	7MG
51	S1	2003	C
51	S1	2004	G
51	S1	2010	G
51	S1	2015	U
51	S1	2016	C
51	S1	2020	A
51	S1	2021	A2M
51	S1	2031	A
51	S1	2036	G
51	S1	2052	C
51	S1	2054	C
51	S1	2061	5MC
51	S1	2062	G
51	S1	2063	U
51	S1	2070	U
51	S1	2090	A
51	S1	2097	C
51	S1	2099	G
51	S1	2101	C
51	S1	2118	G
51	S1	2119	C
51	S1	2120	C
51	S1	2121	C
51	S1	2125	A
51	S1	2134	A

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Mol	Chain	Res	Type
51	S1	2136	A
51	S1	2137	U
51	S1	2156	A
51	S1	2158	A
51	S1	2163	G
51	S1	2164	U
51	S1	2165	A
51	S1	2169	A
51	S1	2170	G
51	S1	2172	U
51	S1	2183	G
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	7	A
52	S2	8	U
52	S2	14	A
52	S2	15	G
52	S2	16	U
52	S2	17	C
52	S2	18	G
52	S2	19	G
52	S2	20	U
52	S2	21	A
52	S2	34	G
52	S2	35	A
52	S2	45	U
52	S2	46	G
52	S2	47	U
52	S2	48	C
52	S2	49	C
52	S2	50	U
52	S2	54	U
52	S2	55	U
52	S2	56	C
52	S2	58	A
52	S2	61	C
52	S2	65	G

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Mol	Chain	Res	Type
52	S2	66	U
52	S2	67	C
52	S2	74	C
53	S3	8	U
53	S3	10	G
53	S3	16	C
53	S3	17	C
53	S3	18	U
53	S3	19	G
53	S3	20	G
53	S3	21	A
53	S3	22	G
53	S3	47	U
53	S3	48	C
53	S3	49	G
53	S3	52	G
53	S3	61	C
53	S3	66	C
53	S3	68	C
53	S3	72	A
53	S3	74	C
53	S3	75	C
54	S4	2	C
54	S4	3	G
54	S4	4	C
54	S4	7	A
54	S4	8	U
54	S4	9	A
54	S4	10	G
54	S4	14	A
54	S4	15	G
54	S4	16	U
54	S4	17	C
54	S4	18	G
54	S4	19	G
54	S4	20	U
54	S4	21	A
54	S4	29	G
54	S4	30	G
54	S4	32	U
54	S4	33	U
54	S4	38	A

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Mol	Chain	Res	Type
54	S4	39	U
54	S4	44	G
54	S4	45	U
54	S4	47	U
54	S4	49	C
54	S4	51	U
54	S4	54	U
54	S4	55	U
54	S4	56	C
54	S4	57	G
54	S4	59	U
54	S4	61	C
54	S4	66	U
54	S4	69	G
54	S4	70	C
54	S4	73	A
54	S4	76	A
55	S5	2	A
55	S5	5	A
55	S5	8	U
55	S5	9	U
55	S5	10	C
55	S5	12	A

All (81) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	141	U
1	L1	170	U
1	L1	191	U
1	L1	208	C
1	L1	554	A
1	L1	557	U
1	L1	584	U
1	L1	835	G
1	L1	837	A
1	L1	967	G
1	L1	1200	A
1	L1	1347	G
1	L1	1390	G
1	L1	1479	A
1	L1	1565	A

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Mol	Chain	Res	Type
1	L1	1574	C
1	L1	1612	G
1	L1	1662	G
2	L2	443	OMC
2	L2	454	A
2	L2	620	C
2	L2	696	A
2	L2	748	C
2	L2	1083	A
2	L2	1101	A
2	L2	1131	A
2	L2	1136	U
2	L2	1170	U
2	L2	1237	A
2	L2	1437	A
2	L2	1485	G
2	L2	1512	G
3	L3	34	C
3	L3	35	A
3	L3	149	A
4	L4	148	C
4	L4	149	U
5	L5	51	A
5	L5	106	G
5	L5	119	U
6	L6	51	A
7	L7	71	A
7	L7	93	C
8	L8	113	U
51	S1	128	C
51	S1	254	A
51	S1	276	G
51	S1	294	G
51	S1	309	G
51	S1	328	C
51	S1	550	C
51	S1	613	G
51	S1	628	A
51	S1	629	A
51	S1	631	U
51	S1	777	A
51	S1	889	A

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Mol	Chain	Res	Type
51	S1	937	C
51	S1	958	G
51	S1	1209	C
51	S1	1360	U
51	S1	1608	A
51	S1	1672	C
51	S1	1717	U
51	S1	1761	C
51	S1	1858	G
51	S1	1889	G
51	S1	1915	U
51	S1	1931	G
51	S1	2119	C
52	S2	7	A
52	S2	13	C
52	S2	34	G
52	S2	45	U
52	S2	47	U
52	S2	48	C
52	S2	49	C
52	S2	54	U
53	S3	20	G
53	S3	60	U
54	S4	13	C

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

170 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	$\# Z > 2$
51	PSU	S1	1292	90,91,51	18,21,22	4.42	7 (38%)	22,30,33	1.77	5 (22%)
51	OMC	S1	1866	51	19,22,23	2.96	8 (42%)	26,31,34	0.79	0
51	PSU	S1	2048	51	18,21,22	0.87	1 (5%)	22,30,33	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	OMG	L7	75	7	18,26,27	2.56	8 (44%)	19,38,41	1.53	4 (21%)
51	OMC	S1	38	51	19,22,23	3.00	8 (42%)	26,31,34	0.84	0
2	PSU	L2	512	2	18,21,22	4.49	7 (38%)	22,30,33	1.78	5 (22%)
2	A2M	L2	1185	2	18,25,26	4.19	6 (33%)	18,36,39	2.72	3 (16%)
51	MA6	S1	2185	90,51	18,26,27	1.11	1 (5%)	19,38,41	3.17	2 (10%)
7	PSU	L7	166	7,1	18,21,22	4.49	7 (38%)	22,30,33	1.81	5 (22%)
2	OMU	L2	667	2	19,22,23	2.99	8 (42%)	26,31,34	1.72	4 (15%)
2	PSU	L2	1194	2	18,21,22	4.46	7 (38%)	22,30,33	1.77	4 (18%)
2	OMC	L2	583	2	19,22,23	2.93	8 (42%)	26,31,34	0.70	0
2	A2M	L2	570	2,1	18,25,26	4.24	6 (33%)	18,36,39	2.75	3 (16%)
2	PSU	L2	626	2	18,21,22	4.43	7 (38%)	22,30,33	1.71	4 (18%)
2	PSU	L2	1144	2	18,21,22	4.44	7 (38%)	22,30,33	1.88	5 (22%)
1	OMG	L1	1190	90,1	18,26,27	2.51	8 (44%)	19,38,41	1.69	5 (26%)
1	PSU	L1	1533	2,1	18,21,22	4.45	7 (38%)	22,30,33	1.87	5 (22%)
2	A2M	L2	502	2	18,25,26	4.22	8 (44%)	18,36,39	2.71	3 (16%)
2	PSU	L2	1361	92,2,52	18,21,22	4.48	7 (38%)	22,30,33	1.80	5 (22%)
1	OMU	L1	1659	90,1	19,22,23	2.97	8 (42%)	26,31,34	1.68	4 (15%)
51	OMU	S1	8	51	19,22,23	0.24	0	26,31,34	0.60	1 (3%)
2	PSU	L2	1152	2	18,21,22	4.45	7 (38%)	22,30,33	1.93	5 (22%)
51	OMG	S1	2151	51	18,26,27	2.53	8 (44%)	19,38,41	1.57	5 (26%)
2	PSU	L2	510	2	18,21,22	4.45	7 (38%)	22,30,33	1.77	5 (22%)
1	A2M	L1	1539	90,2,1	18,25,26	4.22	7 (38%)	18,36,39	2.73	3 (16%)
2	A2M	L2	1384	90,2	18,25,26	4.24	6 (33%)	18,36,39	2.66	3 (16%)
2	A2M	L2	604	2,1	18,25,26	4.26	6 (33%)	18,36,39	2.63	3 (16%)
2	PSU	L2	1403	2	18,21,22	4.47	7 (38%)	22,30,33	1.87	6 (27%)
51	A2M	S1	28	51	18,25,26	4.27	7 (38%)	18,36,39	2.58	3 (16%)
1	PSU	L1	1177	1	18,21,22	4.46	7 (38%)	22,30,33	1.73	5 (22%)
1	PSU	L1	1181	1	18,21,22	4.47	7 (38%)	22,30,33	1.81	5 (22%)
2	PSU	L2	1060	2	18,21,22	4.44	7 (38%)	22,30,33	1.93	5 (22%)
3	OMU	L3	13	3	19,22,23	3.01	8 (42%)	26,31,34	1.76	4 (15%)
51	OMG	S1	1829	90,51	18,26,27	1.03	3 (16%)	19,38,41	0.64	0
7	PSU	L7	74	7	18,21,22	4.49	7 (38%)	22,30,33	1.82	5 (22%)
2	A2M	L2	1067	2	18,25,26	0.64	1 (5%)	18,36,39	0.75	1 (5%)
2	A2M	L2	591	92,2	18,25,26	4.26	7 (38%)	18,36,39	2.60	3 (16%)
2	OMG	L2	1253	2	18,26,27	2.47	8 (44%)	19,38,41	1.59	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L1	1017	91,1	18,21,22	4.43	7 (38%)	22,30,33	1.82	5 (22%)
2	OMC	L2	14	2,1	19,22,23	0.30	0	26,31,34	0.65	1 (3%)
51	PSU	S1	1657	51	18,21,22	4.46	7 (38%)	22,30,33	1.77	5 (22%)
7	A2M	L7	43	90,7	18,25,26	4.26	6 (33%)	18,36,39	2.82	3 (16%)
1	PSU	L1	1664	1	18,21,22	0.89	1 (5%)	22,30,33	0.65	0
2	OMU	L2	56	2,1	19,22,23	3.01	8 (42%)	26,31,34	1.72	4 (15%)
51	OMU	S1	1979	51	19,22,23	3.05	8 (42%)	26,31,34	1.71	4 (15%)
51	MA6	S1	2184	51	18,26,27	1.16	2 (11%)	19,38,41	2.91	2 (10%)
1	A2M	L1	407	1	18,25,26	4.25	6 (33%)	18,36,39	2.64	3 (16%)
2	OMU	L2	1077	2	19,22,23	3.01	8 (42%)	26,31,34	1.70	4 (15%)
51	PSU	S1	1533	51	18,21,22	4.49	7 (38%)	22,30,33	1.81	5 (22%)
1	OMG	L1	856	1	18,26,27	2.53	8 (44%)	19,38,41	1.55	5 (26%)
1	PSU	L1	510	1	18,21,22	0.90	1 (5%)	22,30,33	0.64	0
51	PSU	S1	2202	51	18,21,22	4.43	8 (44%)	22,30,33	1.71	5 (22%)
51	OMC	S1	2140	51	19,22,23	3.02	8 (42%)	26,31,34	0.78	0
2	A2M	L2	382	2	18,25,26	4.27	6 (33%)	18,36,39	2.64	3 (16%)
1	A2M	L1	235	1	18,25,26	4.24	7 (38%)	18,36,39	2.67	3 (16%)
2	A2M	L2	527	90,2	18,25,26	4.09	7 (38%)	18,36,39	2.77	4 (22%)
51	PSU	S1	455	51	18,21,22	4.53	7 (38%)	22,30,33	1.72	4 (18%)
2	PSU	L2	437	2	18,21,22	0.85	1 (5%)	22,30,33	0.67	0
2	OMC	L2	359	2	19,22,23	2.99	8 (42%)	26,31,34	0.70	0
7	PSU	L7	69	90,7	18,21,22	4.44	7 (38%)	22,30,33	1.82	6 (27%)
1	PSU	L1	239	1	18,21,22	0.88	1 (5%)	22,30,33	0.65	0
2	PSU	L2	1264	91,2	18,21,22	4.41	8 (44%)	22,30,33	1.70	4 (18%)
51	OMU	S1	1833	51	19,22,23	3.02	8 (42%)	26,31,34	1.81	5 (19%)
51	PSU	S1	2046	51	18,21,22	4.47	7 (38%)	22,30,33	1.82	5 (22%)
51	PSU	S1	12	51	18,21,22	0.88	1 (5%)	22,30,33	0.63	0
2	PSU	L2	662	90,2	18,21,22	4.40	7 (38%)	22,30,33	1.75	5 (22%)
2	OMG	L2	1078	2	18,26,27	2.50	8 (44%)	19,38,41	1.72	5 (26%)
2	OMU	L2	560	2	19,22,23	0.26	0	26,31,34	1.21	3 (11%)
7	PSU	L7	101	7	18,21,22	4.40	8 (44%)	22,30,33	1.81	6 (27%)
51	OMG	S1	1865	51	18,26,27	2.59	8 (44%)	19,38,41	1.57	4 (21%)
2	5MC	L2	524	90,2	18,22,23	0.34	0	26,32,35	0.53	0
51	OMG	S1	1647	51	18,26,27	2.58	8 (44%)	19,38,41	1.62	4 (21%)
1	OMC	L1	695	1	19,22,23	2.90	8 (42%)	26,31,34	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	L2	1317	2	19,22,23	2.92	8 (42%)	26,31,34	0.75	0
51	7MG	S1	1995	51,53	22,26,27	4.24	10 (45%)	29,39,42	2.06	9 (31%)
1	A2M	L1	697	1	18,25,26	4.24	7 (38%)	18,36,39	2.65	3 (16%)
2	PSU	L2	1318	2	18,21,22	4.44	7 (38%)	22,30,33	1.85	5 (22%)
4	OMG	L4	74	4	18,26,27	1.03	3 (16%)	19,38,41	0.65	0
51	PSU	S1	1539	51	18,21,22	4.48	7 (38%)	22,30,33	1.79	5 (22%)
2	A2M	L2	665	2	18,25,26	4.23	7 (38%)	18,36,39	2.69	3 (16%)
2	OMU	L2	73	92,2	19,22,23	3.02	8 (42%)	26,31,34	1.67	4 (15%)
1	A2M	L1	678	2,1	18,25,26	0.63	1 (5%)	18,36,39	0.77	1 (5%)
2	OMG	L2	534	2	18,26,27	2.53	8 (44%)	19,38,41	1.48	4 (21%)
2	PSU	L2	500	2	18,21,22	4.47	7 (38%)	22,30,33	1.80	5 (22%)
2	A2M	L2	572	2	18,25,26	4.26	7 (38%)	18,36,39	2.66	3 (16%)
51	OMG	S1	1623	91,51	18,26,27	2.55	8 (44%)	19,38,41	1.52	4 (21%)
1	OMG	L1	959	1	18,26,27	1.03	3 (16%)	19,38,41	0.98	1 (5%)
2	PSU	L2	1303	2	18,21,22	4.48	7 (38%)	22,30,33	1.86	6 (27%)
1	PSU	L1	1526	1	18,21,22	4.46	8 (44%)	22,30,33	1.85	6 (27%)
51	OMU	S1	29	51	19,22,23	3.04	8 (42%)	26,31,34	1.71	5 (19%)
2	OMC	L2	1248	2	19,22,23	2.97	8 (42%)	26,31,34	0.86	0
1	A2M	L1	69	1	18,25,26	4.14	6 (33%)	18,36,39	2.82	5 (27%)
1	A2M	L1	927	1	18,25,26	4.23	7 (38%)	18,36,39	2.60	3 (16%)
1	OMU	L1	1371	1	19,22,23	3.08	8 (42%)	26,31,34	1.87	6 (23%)
2	PSU	L2	1265	2	18,21,22	4.45	7 (38%)	22,30,33	1.70	4 (18%)
1	A2M	L1	681	1	18,25,26	0.60	0	18,36,39	0.74	1 (5%)
2	A2M	L2	1372	2	18,25,26	4.25	6 (33%)	18,36,39	2.72	3 (16%)
2	A2M	L2	647	2	18,25,26	4.19	8 (44%)	18,36,39	2.68	3 (16%)
1	A2M	L1	1373	1	18,25,26	4.22	6 (33%)	18,36,39	2.70	3 (16%)
1	OMU	L1	1107	1	19,22,23	3.01	8 (42%)	26,31,34	1.75	4 (15%)
51	PSU	S1	1192	51	18,21,22	4.46	7 (38%)	22,30,33	1.72	5 (22%)
51	A2M	S1	897	51	18,25,26	4.25	6 (33%)	18,36,39	2.71	3 (16%)
1	OMU	L1	48	1	19,22,23	0.35	0	26,31,34	1.03	2 (7%)
1	OMU	L1	845	1	19,22,23	0.35	0	26,31,34	0.84	0
2	OMU	L2	1359	92,2	19,22,23	2.99	8 (42%)	26,31,34	1.68	4 (15%)
2	A2M	L2	628	2	18,25,26	0.63	1 (5%)	18,36,39	0.73	1 (5%)
1	OMU	L1	847	1	19,22,23	0.23	0	26,31,34	0.62	0
2	OMG	L2	641	2	18,26,27	2.52	8 (44%)	19,38,41	1.60	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L1	774	1	18,21,22	0.87	1 (5%)	22,30,33	0.79	1 (4%)
7	A2M	L7	162	7,1	18,25,26	4.27	6 (33%)	18,36,39	2.62	3 (16%)
1	OMG	L1	1540	2,1	18,26,27	1.04	3 (16%)	19,38,41	0.67	0
2	OMG	L2	1229	2	18,26,27	2.55	8 (44%)	19,38,41	1.53	4 (21%)
51	OMG	S1	1478	51	18,26,27	2.53	8 (44%)	19,38,41	1.59	5 (26%)
2	OMC	L2	1397	2	19,22,23	2.93	8 (42%)	26,31,34	0.79	0
51	OMG	S1	1550	51	18,26,27	1.02	3 (16%)	19,38,41	0.68	0
51	OMG	S1	600	51	18,26,27	2.55	8 (44%)	19,38,41	1.52	4 (21%)
51	OMU	S1	661	51	19,22,23	2.99	8 (42%)	26,31,34	1.67	5 (19%)
2	PSU	L2	1413	2	18,21,22	4.37	7 (38%)	22,30,33	1.82	5 (22%)
2	OMC	L2	1159	2	19,22,23	0.29	0	26,31,34	0.49	0
1	OMG	L1	1626	1	18,26,27	1.01	3 (16%)	19,38,41	0.83	1 (5%)
51	A2M	S1	2021	51	18,25,26	0.61	0	18,36,39	0.81	1 (5%)
2	OMC	L2	443	90,91,2	19,22,23	0.37	0	26,31,34	0.58	0
2	PSU	L2	472	2	18,21,22	4.45	7 (38%)	22,30,33	1.76	5 (22%)
51	OMC	S1	18	51	19,22,23	2.93	8 (42%)	26,31,34	0.80	0
51	A2M	S1	512	51	18,25,26	4.27	7 (38%)	18,36,39	2.61	3 (16%)
2	PSU	L2	1058	2	18,21,22	4.46	7 (38%)	22,30,33	1.95	5 (22%)
2	PSU	L2	802	2	18,21,22	4.49	7 (38%)	22,30,33	1.81	6 (27%)
2	5MC	L2	1308	2	18,22,23	4.65	12 (66%)	26,32,35	1.26	2 (7%)
2	OMG	L2	1360	2,52	18,26,27	2.55	8 (44%)	19,38,41	1.49	4 (21%)
2	OMG	L2	71	92,2	18,26,27	2.58	8 (44%)	19,38,41	1.60	4 (21%)
2	OMU	L2	1419	2	19,22,23	2.97	8 (42%)	26,31,34	1.67	4 (15%)
51	PSU	S1	1246	51	18,21,22	4.49	7 (38%)	22,30,33	1.82	5 (22%)
1	A2M	L1	955	1	18,25,26	0.63	1 (5%)	18,36,39	0.77	1 (5%)
1	PSU	L1	1528	1	18,21,22	4.46	7 (38%)	22,30,33	1.80	5 (22%)
1	OMC	L1	1010	90,91,1	19,22,23	0.31	0	26,31,34	0.44	0
1	PSU	L1	1529	1	18,21,22	4.44	7 (38%)	22,30,33	1.81	5 (22%)
2	PSU	L2	1284	2	18,21,22	4.50	7 (38%)	22,30,33	1.80	5 (22%)
51	PSU	S1	1566	51	18,21,22	4.52	8 (44%)	22,30,33	1.72	4 (18%)
51	A2M	S1	668	90,51	18,25,26	4.14	7 (38%)	18,36,39	2.75	4 (22%)
1	OMG	L1	1524	1	18,26,27	2.56	8 (44%)	19,38,41	1.74	6 (31%)
2	PSU	L2	597	2	18,21,22	4.42	7 (38%)	22,30,33	1.78	5 (22%)
1	PSU	L1	672	90,1	18,21,22	0.85	1 (5%)	22,30,33	0.61	0
1	OMC	L1	1527	90,1	19,22,23	2.95	8 (42%)	26,31,34	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	5MC	S1	1544	51	18,22,23	0.32	0	26,32,35	0.52	0
51	5MC	S1	2061	51	18,22,23	3.48	7 (38%)	26,32,35	0.94	1 (3%)
1	PSU	L1	1171	91,1	18,21,22	4.46	8 (44%)	22,30,33	1.77	4 (18%)
1	A2M	L1	305	1	18,25,26	4.17	8 (44%)	18,36,39	2.76	5 (27%)
2	OMG	L2	686	2	18,26,27	2.57	8 (44%)	19,38,41	1.55	5 (26%)
2	PSU	L2	593	92,2	18,21,22	4.41	7 (38%)	22,30,33	1.70	5 (22%)
51	PSU	S1	33	51	18,21,22	4.52	7 (38%)	22,30,33	1.80	5 (22%)
52	MIA	S2	37	52	24,31,32	2.43	3 (12%)	26,44,47	4.88	10 (38%)
51	OMU	S1	1662	51	19,22,23	3.02	8 (42%)	26,31,34	1.68	4 (15%)
1	PSU	L1	422	1	18,21,22	4.47	7 (38%)	22,30,33	1.73	5 (22%)
1	PSU	L1	940	1	18,21,22	4.45	7 (38%)	22,30,33	1.80	5 (22%)
2	PSU	L2	78	2	18,21,22	4.43	7 (38%)	22,30,33	1.81	5 (22%)
2	OMG	L2	1046	90,2,53	18,26,27	2.53	8 (44%)	19,38,41	1.50	4 (21%)
2	PSU	L2	1213	2	18,21,22	4.43	7 (38%)	22,30,33	1.84	5 (22%)
51	OMC	S1	2059	51	19,22,23	2.99	8 (42%)	26,31,34	1.22	2 (7%)
2	PSU	L2	565	2	18,21,22	0.87	1 (5%)	22,30,33	0.72	1 (4%)
51	B8N	S1	1543	-	24,29,30	4.25	14 (58%)	29,42,45	2.00	7 (24%)
1	PSU	L1	1011	2,1	18,21,22	0.79	1 (5%)	22,30,33	0.75	0
2	OMG	L2	1231	2	18,26,27	2.52	8 (44%)	19,38,41	1.54	5 (26%)
1	PSU	L1	313	1	18,21,22	4.44	7 (38%)	22,30,33	1.71	4 (18%)
1	A2M	L1	858	1	18,25,26	4.23	6 (33%)	18,36,39	2.70	3 (16%)
2	A2M	L2	95	2	18,25,26	4.25	7 (38%)	18,36,39	2.68	3 (16%)
2	PSU	L2	504	2	18,21,22	4.52	7 (38%)	22,30,33	1.84	5 (22%)
51	OMU	S1	1621	90,51	19,22,23	3.02	8 (42%)	26,31,34	1.72	5 (19%)
51	A2M	S1	479	51	18,25,26	4.24	7 (38%)	18,36,39	2.66	3 (16%)
51	A2M	S1	98	90,51	18,25,26	4.26	7 (38%)	18,36,39	2.60	3 (16%)
2	OMG	L2	655	2	18,26,27	2.55	8 (44%)	19,38,41	1.63	6 (31%)

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
51	PSU	S1	1292	90,91,51	-	0/7/25/26	0/2/2/2
51	OMC	S1	1866	51	-	0/9/27/28	0/2/2/2
51	PSU	S1	2048	51	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OMG	L7	75	7	-	0/5/27/28	0/3/3/3
51	OMC	S1	38	51	-	0/9/27/28	0/2/2/2
2	PSU	L2	512	2	-	0/7/25/26	0/2/2/2
2	A2M	L2	1185	2	-	2/5/27/28	0/3/3/3
51	MA6	S1	2185	90,51	-	1/7/29/30	0/3/3/3
7	PSU	L7	166	7,1	-	0/7/25/26	0/2/2/2
2	OMU	L2	667	2	-	0/9/27/28	0/2/2/2
2	PSU	L2	1194	2	-	0/7/25/26	0/2/2/2
2	OMC	L2	583	2	-	0/9/27/28	0/2/2/2
2	A2M	L2	570	2,1	-	0/5/27/28	0/3/3/3
2	PSU	L2	626	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1144	2	-	0/7/25/26	0/2/2/2
1	OMG	L1	1190	90,1	-	0/5/27/28	0/3/3/3
1	PSU	L1	1533	2,1	-	0/7/25/26	0/2/2/2
2	A2M	L2	502	2	-	2/5/27/28	0/3/3/3
2	PSU	L2	1361	92,2,52	-	5/7/25/26	0/2/2/2
1	OMU	L1	1659	90,1	-	0/9/27/28	0/2/2/2
51	OMU	S1	8	51	-	7/9/27/28	0/2/2/2
2	PSU	L2	1152	2	-	0/7/25/26	0/2/2/2
51	OMG	S1	2151	51	-	2/5/27/28	0/3/3/3
2	PSU	L2	510	2	-	0/7/25/26	0/2/2/2
1	A2M	L1	1539	90,2,1	-	1/5/27/28	0/3/3/3
2	A2M	L2	1384	90,2	-	0/5/27/28	0/3/3/3
2	A2M	L2	604	2,1	-	0/5/27/28	0/3/3/3
2	PSU	L2	1403	2	-	0/7/25/26	0/2/2/2
51	A2M	S1	28	51	-	0/5/27/28	0/3/3/3
1	PSU	L1	1177	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	1181	1	-	0/7/25/26	0/2/2/2
2	PSU	L2	1060	2	-	0/7/25/26	0/2/2/2
3	OMU	L3	13	3	-	1/9/27/28	0/2/2/2
51	OMG	S1	1829	90,51	-	2/5/27/28	0/3/3/3
7	PSU	L7	74	7	-	0/7/25/26	0/2/2/2
2	A2M	L2	1067	2	-	0/5/27/28	0/3/3/3
2	A2M	L2	591	92,2	-	0/5/27/28	0/3/3/3
2	OMG	L2	1253	2	-	0/5/27/28	0/3/3/3
1	PSU	L1	1017	91,1	-	2/7/25/26	0/2/2/2
2	OMC	L2	14	2,1	-	2/9/27/28	0/2/2/2
51	PSU	S1	1657	51	-	1/7/25/26	0/2/2/2
7	A2M	L7	43	90,7	-	0/5/27/28	0/3/3/3
1	PSU	L1	1664	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	L2	56	2,1	-	1/9/27/28	0/2/2/2
51	OMU	S1	1979	51	-	1/9/27/28	0/2/2/2
51	MA6	S1	2184	51	-	0/7/29/30	0/3/3/3
1	A2M	L1	407	1	-	0/5/27/28	0/3/3/3
2	OMU	L2	1077	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1533	51	-	0/7/25/26	0/2/2/2
1	OMG	L1	856	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	510	1	-	3/7/25/26	0/2/2/2
51	PSU	S1	2202	51	-	1/7/25/26	0/2/2/2
51	OMC	S1	2140	51	-	3/9/27/28	0/2/2/2
2	A2M	L2	382	2	-	0/5/27/28	0/3/3/3
1	A2M	L1	235	1	-	0/5/27/28	0/3/3/3
2	A2M	L2	527	90,2	-	3/5/27/28	0/3/3/3
51	PSU	S1	455	51	-	2/7/25/26	0/2/2/2
2	PSU	L2	437	2	-	0/7/25/26	0/2/2/2
2	OMC	L2	359	2	-	0/9/27/28	0/2/2/2
7	PSU	L7	69	90,7	-	0/7/25/26	0/2/2/2
1	PSU	L1	239	1	-	0/7/25/26	0/2/2/2
2	PSU	L2	1264	91,2	-	2/7/25/26	0/2/2/2
51	OMU	S1	1833	51	-	1/9/27/28	0/2/2/2
51	PSU	S1	2046	51	-	0/7/25/26	0/2/2/2
51	PSU	S1	12	51	-	0/7/25/26	0/2/2/2
2	PSU	L2	662	90,2	-	0/7/25/26	0/2/2/2
2	OMG	L2	1078	2	-	2/5/27/28	0/3/3/3
2	OMU	L2	560	2	-	3/9/27/28	0/2/2/2
7	PSU	L7	101	7	-	0/7/25/26	0/2/2/2
51	OMG	S1	1865	51	-	0/5/27/28	0/3/3/3
2	5MC	L2	524	90,2	-	0/7/25/26	0/2/2/2
51	OMG	S1	1647	51	-	0/5/27/28	0/3/3/3
1	OMC	L1	695	1	-	1/9/27/28	0/2/2/2
2	OMC	L2	1317	2	-	0/9/27/28	0/2/2/2
51	7MG	S1	1995	51,53	-	2/7/37/38	0/3/3/3
1	A2M	L1	697	1	-	0/5/27/28	0/3/3/3
2	PSU	L2	1318	2	-	0/7/25/26	0/2/2/2
4	OMG	L4	74	4	-	3/5/27/28	0/3/3/3
51	PSU	S1	1539	51	-	0/7/25/26	0/2/2/2
2	A2M	L2	665	2	-	2/5/27/28	0/3/3/3
2	OMU	L2	73	92,2	-	0/9/27/28	0/2/2/2
1	A2M	L1	678	2,1	-	0/5/27/28	0/3/3/3
2	OMG	L2	534	2	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L2	500	2	-	0/7/25/26	0/2/2/2
2	A2M	L2	572	2	-	0/5/27/28	0/3/3/3
51	OMG	S1	1623	91,51	-	0/5/27/28	0/3/3/3
1	OMG	L1	959	1	-	3/5/27/28	0/3/3/3
2	PSU	L2	1303	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	1526	1	-	4/7/25/26	0/2/2/2
51	OMU	S1	29	51	-	1/9/27/28	0/2/2/2
2	OMC	L2	1248	2	-	1/9/27/28	0/2/2/2
1	A2M	L1	69	1	-	2/5/27/28	0/3/3/3
1	A2M	L1	927	1	-	0/5/27/28	0/3/3/3
1	OMU	L1	1371	1	-	3/9/27/28	0/2/2/2
2	PSU	L2	1265	2	-	0/7/25/26	0/2/2/2
1	A2M	L1	681	1	-	4/5/27/28	0/3/3/3
2	A2M	L2	1372	2	-	0/5/27/28	0/3/3/3
2	A2M	L2	647	2	-	3/5/27/28	0/3/3/3
1	A2M	L1	1373	1	-	0/5/27/28	0/3/3/3
1	OMU	L1	1107	1	-	0/9/27/28	0/2/2/2
51	PSU	S1	1192	51	-	2/7/25/26	0/2/2/2
51	A2M	S1	897	51	-	0/5/27/28	0/3/3/3
1	OMU	L1	48	1	-	2/9/27/28	0/2/2/2
1	OMU	L1	845	1	-	3/9/27/28	0/2/2/2
2	OMU	L2	1359	92,2	-	0/9/27/28	0/2/2/2
2	A2M	L2	628	2	-	0/5/27/28	0/3/3/3
1	OMU	L1	847	1	-	0/9/27/28	0/2/2/2
2	OMG	L2	641	2	-	0/5/27/28	0/3/3/3
1	PSU	L1	774	1	-	0/7/25/26	0/2/2/2
7	A2M	L7	162	7,1	-	1/5/27/28	0/3/3/3
1	OMG	L1	1540	2,1	-	2/5/27/28	0/3/3/3
2	OMG	L2	1229	2	-	2/5/27/28	0/3/3/3
51	OMG	S1	1478	51	-	1/5/27/28	0/3/3/3
2	OMC	L2	1397	2	-	0/9/27/28	0/2/2/2
51	OMG	S1	1550	51	-	1/5/27/28	0/3/3/3
51	OMG	S1	600	51	-	2/5/27/28	0/3/3/3
51	OMU	S1	661	51	-	0/9/27/28	0/2/2/2
2	PSU	L2	1413	2	-	0/7/25/26	0/2/2/2
2	OMC	L2	1159	2	-	0/9/27/28	0/2/2/2
1	OMG	L1	1626	1	-	0/5/27/28	0/3/3/3
51	A2M	S1	2021	51	-	1/5/27/28	0/3/3/3
2	OMC	L2	443	90,91,2	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L2	472	2	-	0/7/25/26	0/2/2/2
51	OMC	S1	18	51	-	1/9/27/28	0/2/2/2
51	A2M	S1	512	51	-	2/5/27/28	0/3/3/3
2	PSU	L2	1058	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	802	2	-	2/7/25/26	0/2/2/2
2	5MC	L2	1308	2	-	4/7/25/26	0/2/2/2
2	OMG	L2	1360	2,52	-	0/5/27/28	0/3/3/3
2	OMG	L2	71	92,2	-	0/5/27/28	0/3/3/3
2	OMU	L2	1419	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1246	51	-	0/7/25/26	0/2/2/2
1	A2M	L1	955	1	-	1/5/27/28	0/3/3/3
1	PSU	L1	1528	1	-	2/7/25/26	0/2/2/2
1	OMC	L1	1010	90,91,1	-	2/9/27/28	0/2/2/2
1	PSU	L1	1529	1	-	0/7/25/26	0/2/2/2
2	PSU	L2	1284	2	-	0/7/25/26	0/2/2/2
51	PSU	S1	1566	51	-	2/7/25/26	0/2/2/2
51	A2M	S1	668	90,51	-	3/5/27/28	0/3/3/3
1	OMG	L1	1524	1	-	1/5/27/28	0/3/3/3
2	PSU	L2	597	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	672	90,1	-	0/7/25/26	0/2/2/2
1	OMC	L1	1527	90,1	-	1/9/27/28	0/2/2/2
51	5MC	S1	1544	51	-	0/7/25/26	0/2/2/2
51	5MC	S1	2061	51	-	2/7/25/26	0/2/2/2
1	PSU	L1	1171	91,1	-	2/7/25/26	0/2/2/2
1	A2M	L1	305	1	-	2/5/27/28	0/3/3/3
2	OMG	L2	686	2	-	2/5/27/28	0/3/3/3
2	PSU	L2	593	92,2	-	0/7/25/26	0/2/2/2
51	PSU	S1	33	51	-	2/7/25/26	0/2/2/2
52	MIA	S2	37	52	-	0/11/33/34	0/3/3/3
51	OMU	S1	1662	51	-	1/9/27/28	0/2/2/2
1	PSU	L1	422	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	940	1	-	0/7/25/26	0/2/2/2
2	PSU	L2	78	2	-	0/7/25/26	0/2/2/2
2	OMG	L2	1046	90,2,53	-	3/5/27/28	0/3/3/3
2	PSU	L2	1213	2	-	0/7/25/26	0/2/2/2
51	OMC	S1	2059	51	-	3/9/27/28	0/2/2/2
2	PSU	L2	565	2	-	0/7/25/26	0/2/2/2
51	B8N	S1	1543	-	-	10/16/34/35	0/2/2/2
1	PSU	L1	1011	2,1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L2	1231	2	-	0/5/27/28	0/3/3/3
1	PSU	L1	313	1	-	2/7/25/26	0/2/2/2
1	A2M	L1	858	1	-	0/5/27/28	0/3/3/3
2	A2M	L2	95	2	-	1/5/27/28	0/3/3/3
2	PSU	L2	504	2	-	0/7/25/26	0/2/2/2
51	OMU	S1	1621	90,51	-	0/9/27/28	0/2/2/2
51	A2M	S1	479	51	-	0/5/27/28	0/3/3/3
51	A2M	S1	98	90,51	-	2/5/27/28	0/3/3/3
2	OMG	L2	655	2	-	0/5/27/28	0/3/3/3

All (1036) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	512	A2M	O4'-C1'	15.43	1.62	1.41
51	S1	28	A2M	O4'-C1'	15.40	1.62	1.41
2	L2	572	A2M	O4'-C1'	15.37	1.62	1.41
2	L2	604	A2M	O4'-C1'	15.34	1.62	1.41
1	L1	407	A2M	O4'-C1'	15.34	1.62	1.41
2	L2	382	A2M	O4'-C1'	15.32	1.62	1.41
7	L7	162	A2M	O4'-C1'	15.32	1.62	1.41
7	L7	43	A2M	O4'-C1'	15.32	1.62	1.41
51	S1	897	A2M	O4'-C1'	15.32	1.62	1.41
2	L2	591	A2M	O4'-C1'	15.30	1.62	1.41
51	S1	98	A2M	O4'-C1'	15.29	1.62	1.41
2	L2	1372	A2M	O4'-C1'	15.27	1.62	1.41
51	S1	479	A2M	O4'-C1'	15.24	1.62	1.41
2	L2	95	A2M	O4'-C1'	15.21	1.62	1.41
1	L1	697	A2M	O4'-C1'	15.20	1.62	1.41
2	L2	570	A2M	O4'-C1'	15.20	1.62	1.41
2	L2	1384	A2M	O4'-C1'	15.18	1.62	1.41
1	L1	235	A2M	O4'-C1'	15.17	1.62	1.41
2	L2	502	A2M	O4'-C1'	15.16	1.62	1.41
1	L1	1373	A2M	O4'-C1'	15.14	1.62	1.41
2	L2	665	A2M	O4'-C1'	15.13	1.62	1.41
1	L1	927	A2M	O4'-C1'	15.11	1.62	1.41
1	L1	1539	A2M	O4'-C1'	15.09	1.62	1.41
1	L1	858	A2M	O4'-C1'	15.07	1.62	1.41
1	L1	305	A2M	O4'-C1'	14.91	1.61	1.41
2	L2	1185	A2M	O4'-C1'	14.86	1.61	1.41
1	L1	69	A2M	O4'-C1'	14.82	1.61	1.41
2	L2	647	A2M	O4'-C1'	14.80	1.61	1.41
51	S1	668	A2M	O4'-C1'	14.55	1.61	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	527	A2M	O4'-C1'	14.37	1.61	1.41
51	S1	1566	PSU	C6-C5	11.84	1.49	1.35
7	L7	166	PSU	C6-C5	11.78	1.49	1.35
2	L2	504	PSU	C6-C5	11.77	1.49	1.35
1	L1	1171	PSU	C6-C5	11.73	1.49	1.35
1	L1	313	PSU	C6-C5	11.72	1.49	1.35
51	S1	455	PSU	C6-C5	11.71	1.49	1.35
1	L1	1528	PSU	C6-C5	11.69	1.48	1.35
1	L1	1529	PSU	C6-C5	11.68	1.48	1.35
51	S1	33	PSU	C6-C5	11.67	1.48	1.35
1	L1	1177	PSU	C6-C5	11.67	1.48	1.35
2	L2	1265	PSU	C6-C5	11.65	1.48	1.35
2	L2	512	PSU	C6-C5	11.64	1.48	1.35
1	L1	1181	PSU	C6-C5	11.62	1.48	1.35
2	L2	1058	PSU	C6-C5	11.62	1.48	1.35
51	S1	1533	PSU	C6-C5	11.61	1.48	1.35
2	L2	1284	PSU	C6-C5	11.59	1.48	1.35
51	S1	2046	PSU	C6-C5	11.57	1.48	1.35
2	L2	1194	PSU	C6-C5	11.57	1.48	1.35
2	L2	1361	PSU	C6-C5	11.57	1.48	1.35
51	S1	1192	PSU	C6-C5	11.56	1.48	1.35
2	L2	1303	PSU	C6-C5	11.55	1.48	1.35
2	L2	802	PSU	C6-C5	11.55	1.48	1.35
1	L1	1017	PSU	C6-C5	11.53	1.48	1.35
2	L2	626	PSU	C6-C5	11.53	1.48	1.35
51	S1	1539	PSU	C6-C5	11.53	1.48	1.35
1	L1	422	PSU	C6-C5	11.53	1.48	1.35
2	L2	472	PSU	C6-C5	11.52	1.48	1.35
2	L2	500	PSU	C6-C5	11.51	1.48	1.35
2	L2	1403	PSU	C6-C5	11.51	1.48	1.35
2	L2	1318	PSU	C6-C5	11.51	1.48	1.35
51	S1	1246	PSU	C6-C5	11.51	1.48	1.35
2	L2	510	PSU	C6-C5	11.51	1.48	1.35
1	L1	940	PSU	C6-C5	11.50	1.48	1.35
51	S1	1657	PSU	C6-C5	11.49	1.48	1.35
2	L2	1144	PSU	C6-C5	11.49	1.48	1.35
7	L7	69	PSU	C6-C5	11.48	1.48	1.35
2	L2	593	PSU	C6-C5	11.48	1.48	1.35
2	L2	1060	PSU	C6-C5	11.48	1.48	1.35
7	L7	74	PSU	C6-C5	11.47	1.48	1.35
2	L2	597	PSU	C6-C5	11.47	1.48	1.35
2	L2	1213	PSU	C6-C5	11.46	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1152	PSU	C6-C5	11.46	1.48	1.35
2	L2	78	PSU	C6-C5	11.46	1.48	1.35
2	L2	662	PSU	C6-C5	11.45	1.48	1.35
51	S1	1292	PSU	C6-C5	11.43	1.48	1.35
1	L1	1533	PSU	C6-C5	11.39	1.48	1.35
7	L7	101	PSU	C6-C5	11.37	1.48	1.35
51	S1	2202	PSU	C6-C5	11.35	1.48	1.35
1	L1	1526	PSU	C6-C5	11.35	1.48	1.35
2	L2	1264	PSU	C6-C5	11.33	1.48	1.35
2	L2	1413	PSU	C6-C5	11.19	1.48	1.35
51	S1	1995	7MG	C8-N9	11.08	1.52	1.46
51	S1	1543	B8N	C2'-C3'	-10.38	1.24	1.53
51	S1	33	PSU	C2-N1	9.78	1.50	1.36
51	S1	1246	PSU	C2-N1	9.78	1.50	1.36
51	S1	1539	PSU	C2-N1	9.74	1.49	1.36
51	S1	455	PSU	C2-N1	9.71	1.49	1.36
51	S1	1533	PSU	C2-N1	9.70	1.49	1.36
2	L2	1152	PSU	C2-N1	9.69	1.49	1.36
7	L7	74	PSU	C2-N1	9.67	1.49	1.36
1	L1	1526	PSU	C2-N1	9.65	1.49	1.36
2	L2	1303	PSU	C2-N1	9.64	1.49	1.36
2	L2	802	PSU	C2-N1	9.64	1.49	1.36
1	L1	1533	PSU	C2-N1	9.63	1.49	1.36
1	L1	422	PSU	C2-N1	9.63	1.49	1.36
1	L1	940	PSU	C2-N1	9.63	1.49	1.36
2	L2	500	PSU	C2-N1	9.62	1.49	1.36
51	S1	2046	PSU	C2-N1	9.62	1.49	1.36
2	L2	1403	PSU	C2-N1	9.61	1.49	1.36
2	L2	1284	PSU	C2-N1	9.59	1.49	1.36
2	L2	512	PSU	C2-N1	9.59	1.49	1.36
1	L1	1181	PSU	C2-N1	9.58	1.49	1.36
2	L2	504	PSU	C2-N1	9.56	1.49	1.36
7	L7	166	PSU	C2-N1	9.55	1.49	1.36
2	L2	1318	PSU	C2-N1	9.53	1.49	1.36
2	L2	1060	PSU	C2-N1	9.53	1.49	1.36
1	L1	1017	PSU	C2-N1	9.53	1.49	1.36
2	L2	1213	PSU	C2-N1	9.52	1.49	1.36
2	L2	1361	PSU	C2-N1	9.52	1.49	1.36
2	L2	78	PSU	C2-N1	9.52	1.49	1.36
51	S1	1657	PSU	C2-N1	9.52	1.49	1.36
2	L2	472	PSU	C2-N1	9.51	1.49	1.36
2	L2	1144	PSU	C2-N1	9.51	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	510	PSU	C2-N1	9.51	1.49	1.36
2	L2	1194	PSU	C2-N1	9.51	1.49	1.36
51	S1	1566	PSU	C2-N1	9.50	1.49	1.36
51	S1	2202	PSU	C2-N1	9.49	1.49	1.36
2	L2	626	PSU	C2-N1	9.48	1.49	1.36
1	L1	1177	PSU	C2-N1	9.47	1.49	1.36
7	L7	69	PSU	C2-N1	9.47	1.49	1.36
2	L2	1058	PSU	C2-N1	9.46	1.49	1.36
2	L2	597	PSU	C2-N1	9.44	1.49	1.36
2	L2	593	PSU	C2-N1	9.44	1.49	1.36
1	L1	1529	PSU	C2-N1	9.44	1.49	1.36
1	L1	1528	PSU	C2-N1	9.44	1.49	1.36
51	S1	1292	PSU	C2-N1	9.42	1.49	1.36
51	S1	1192	PSU	C2-N1	9.38	1.49	1.36
2	L2	662	PSU	C2-N1	9.37	1.49	1.36
2	L2	1264	PSU	C2-N1	9.35	1.49	1.36
2	L2	1413	PSU	C2-N1	9.34	1.49	1.36
51	S1	1995	7MG	C5-N7	9.32	1.46	1.35
2	L2	1265	PSU	C2-N1	9.32	1.49	1.36
7	L7	101	PSU	C2-N1	9.30	1.49	1.36
1	L1	1171	PSU	C2-N1	9.24	1.49	1.36
1	L1	313	PSU	C2-N1	9.23	1.49	1.36
2	L2	1308	5MC	C6-C5	9.15	1.49	1.34
51	S1	2061	5MC	C6-C5	8.86	1.49	1.34
2	L2	1308	5MC	C3'-C4'	-8.69	1.30	1.53
52	S2	37	MIA	C2-S10	8.64	1.83	1.75
51	S1	1543	B8N	C4-N3	-7.72	1.26	1.40
2	L2	1284	PSU	C2-N3	7.67	1.50	1.37
51	S1	455	PSU	C2-N3	7.67	1.50	1.37
2	L2	504	PSU	C2-N3	7.65	1.50	1.37
2	L2	1361	PSU	C2-N3	7.64	1.50	1.37
51	S1	1566	PSU	C2-N3	7.60	1.50	1.37
51	S1	33	PSU	C2-N3	7.58	1.50	1.37
1	L1	1371	OMU	C2-N1	7.57	1.50	1.38
2	L2	512	PSU	C2-N3	7.56	1.50	1.37
51	S1	1192	PSU	C2-N3	7.55	1.50	1.37
51	S1	1543	B8N	C6-N1	7.54	1.55	1.36
51	S1	1246	PSU	C2-N3	7.54	1.50	1.37
2	L2	1265	PSU	C2-N3	7.54	1.50	1.37
1	L1	1533	PSU	C2-N3	7.53	1.50	1.37
2	L2	802	PSU	C2-N3	7.52	1.50	1.37
7	L7	74	PSU	C2-N3	7.52	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1171	PSU	C2-N3	7.50	1.50	1.37
51	S1	1657	PSU	C2-N3	7.50	1.50	1.37
51	S1	1995	7MG	C4-N9	7.49	1.46	1.37
7	L7	166	PSU	C2-N3	7.49	1.50	1.37
2	L2	1303	PSU	C2-N3	7.49	1.50	1.37
2	L2	500	PSU	C2-N3	7.49	1.50	1.37
51	S1	1533	PSU	C2-N3	7.48	1.50	1.37
2	L2	510	PSU	C2-N3	7.48	1.50	1.37
51	S1	2046	PSU	C2-N3	7.48	1.50	1.37
51	S1	2202	PSU	C2-N3	7.47	1.50	1.37
1	L1	1528	PSU	C2-N3	7.47	1.50	1.37
2	L2	1152	PSU	C2-N3	7.47	1.50	1.37
2	L2	472	PSU	C2-N3	7.46	1.50	1.37
2	L2	1213	PSU	C2-N3	7.45	1.50	1.37
2	L2	1403	PSU	C2-N3	7.45	1.50	1.37
1	L1	1181	PSU	C2-N3	7.45	1.50	1.37
51	S1	1539	PSU	C2-N3	7.44	1.50	1.37
2	L2	1264	PSU	C2-N3	7.43	1.50	1.37
1	L1	1526	PSU	C2-N3	7.43	1.50	1.37
51	S1	1292	PSU	C2-N3	7.43	1.50	1.37
7	L7	69	PSU	C2-N3	7.42	1.50	1.37
1	L1	313	PSU	C2-N3	7.42	1.50	1.37
1	L1	422	PSU	C2-N3	7.41	1.50	1.37
2	L2	1194	PSU	C2-N3	7.41	1.50	1.37
1	L1	1177	PSU	C2-N3	7.41	1.50	1.37
1	L1	940	PSU	C2-N3	7.41	1.50	1.37
2	L2	1318	PSU	C2-N3	7.40	1.50	1.37
2	L2	1413	PSU	C2-N3	7.38	1.50	1.37
2	L2	1058	PSU	C2-N3	7.37	1.50	1.37
7	L7	101	PSU	C2-N3	7.36	1.50	1.37
2	L2	597	PSU	C2-N3	7.36	1.50	1.37
2	L2	1060	PSU	C2-N3	7.35	1.50	1.37
1	L1	1529	PSU	C2-N3	7.35	1.50	1.37
2	L2	626	PSU	C2-N3	7.35	1.50	1.37
1	L1	1017	PSU	C2-N3	7.33	1.50	1.37
2	L2	78	PSU	C2-N3	7.33	1.50	1.37
2	L2	1144	PSU	C2-N3	7.31	1.50	1.37
2	L2	1308	5MC	O4'-C4'	7.30	1.61	1.45
2	L2	662	PSU	C2-N3	7.26	1.49	1.37
2	L2	593	PSU	C2-N3	7.25	1.49	1.37
51	S1	1979	OMU	C2-N1	7.03	1.49	1.38
2	L2	1077	OMU	C2-N1	7.03	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	56	OMU	C2-N1	7.03	1.49	1.38
2	L2	73	OMU	C2-N1	7.02	1.49	1.38
51	S1	29	OMU	C2-N1	7.00	1.49	1.38
1	L1	1107	OMU	C2-N1	6.98	1.49	1.38
51	S1	1833	OMU	C2-N1	6.96	1.49	1.38
51	S1	1662	OMU	C2-N1	6.92	1.49	1.38
2	L2	667	OMU	C2-N1	6.92	1.49	1.38
51	S1	1621	OMU	C2-N1	6.92	1.49	1.38
2	L2	1359	OMU	C2-N1	6.91	1.49	1.38
3	L3	13	OMU	C2-N1	6.90	1.49	1.38
51	S1	1979	OMU	C2-N3	6.90	1.50	1.38
2	L2	1419	OMU	C2-N1	6.88	1.49	1.38
1	L1	1659	OMU	C2-N1	6.88	1.49	1.38
51	S1	29	OMU	C2-N3	6.86	1.50	1.38
51	S1	1662	OMU	C2-N3	6.86	1.50	1.38
51	S1	1621	OMU	C2-N3	6.85	1.50	1.38
51	S1	1833	OMU	C2-N3	6.84	1.50	1.38
51	S1	661	OMU	C2-N1	6.82	1.49	1.38
2	L2	73	OMU	C2-N3	6.78	1.50	1.38
3	L3	13	OMU	C2-N3	6.77	1.50	1.38
2	L2	56	OMU	C2-N3	6.75	1.50	1.38
1	L1	1107	OMU	C2-N3	6.74	1.50	1.38
2	L2	1077	OMU	C2-N3	6.74	1.50	1.38
51	S1	668	A2M	O4'-C4'	-6.74	1.29	1.45
1	L1	1371	OMU	C2-N3	6.73	1.50	1.38
52	S2	37	MIA	C6-N6	6.69	1.46	1.34
2	L2	1359	OMU	C2-N3	6.68	1.49	1.38
2	L2	1419	OMU	C2-N3	6.68	1.49	1.38
51	S1	661	OMU	C2-N3	6.66	1.49	1.38
2	L2	667	OMU	C2-N3	6.64	1.49	1.38
1	L1	1659	OMU	C2-N3	6.63	1.49	1.38
1	L1	858	A2M	O4'-C4'	-6.59	1.30	1.45
2	L2	647	A2M	O4'-C4'	-6.56	1.30	1.45
2	L2	1185	A2M	O4'-C4'	-6.55	1.30	1.45
2	L2	1384	A2M	O4'-C4'	-6.52	1.30	1.45
1	L1	69	A2M	O4'-C4'	-6.51	1.30	1.45
1	L1	1539	A2M	O4'-C4'	-6.51	1.30	1.45
1	L1	927	A2M	O4'-C4'	-6.48	1.30	1.45
1	L1	235	A2M	O4'-C4'	-6.47	1.30	1.45
2	L2	95	A2M	O4'-C4'	-6.45	1.30	1.45
2	L2	527	A2M	O4'-C4'	-6.45	1.30	1.45
2	L2	665	A2M	O4'-C4'	-6.41	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	479	A2M	O4'-C4'	-6.40	1.30	1.45
51	S1	2061	5MC	C4-N3	6.39	1.44	1.34
51	S1	1543	B8N	O4'-C4'	-6.39	1.30	1.45
7	L7	162	A2M	O4'-C4'	-6.38	1.30	1.45
2	L2	591	A2M	O4'-C4'	-6.38	1.30	1.45
2	L2	1372	A2M	O4'-C4'	-6.38	1.30	1.45
2	L2	382	A2M	O4'-C4'	-6.38	1.30	1.45
1	L1	1373	A2M	O4'-C4'	-6.36	1.30	1.45
7	L7	43	A2M	O4'-C4'	-6.36	1.30	1.45
1	L1	305	A2M	O4'-C4'	-6.36	1.30	1.45
2	L2	570	A2M	O4'-C4'	-6.36	1.30	1.45
1	L1	697	A2M	O4'-C4'	-6.35	1.30	1.45
2	L2	604	A2M	O4'-C4'	-6.33	1.30	1.45
2	L2	359	OMC	C2-N3	6.33	1.49	1.36
51	S1	897	A2M	O4'-C4'	-6.32	1.30	1.45
51	S1	2140	OMC	C2-N3	6.32	1.49	1.36
51	S1	98	A2M	O4'-C4'	-6.32	1.30	1.45
51	S1	28	A2M	O4'-C4'	-6.32	1.30	1.45
51	S1	38	OMC	C2-N3	6.31	1.49	1.36
2	L2	1248	OMC	C2-N3	6.28	1.49	1.36
51	S1	1866	OMC	C2-N3	6.25	1.49	1.36
1	L1	407	A2M	O4'-C4'	-6.25	1.31	1.45
2	L2	572	A2M	O4'-C4'	-6.24	1.31	1.45
51	S1	2059	OMC	C2-N3	6.22	1.49	1.36
51	S1	1995	7MG	C2-N3	6.22	1.48	1.33
2	L2	502	A2M	O4'-C4'	-6.21	1.31	1.45
51	S1	18	OMC	C2-N3	6.18	1.48	1.36
1	L1	695	OMC	C2-N3	6.17	1.48	1.36
51	S1	512	A2M	O4'-C4'	-6.16	1.31	1.45
1	L1	1527	OMC	C2-N3	6.15	1.48	1.36
2	L2	583	OMC	C2-N3	6.12	1.48	1.36
2	L2	1397	OMC	C2-N3	6.12	1.48	1.36
2	L2	1317	OMC	C2-N3	6.08	1.48	1.36
2	L2	1248	OMC	C6-C5	5.99	1.49	1.35
51	S1	2140	OMC	C6-C5	5.99	1.49	1.35
51	S1	38	OMC	C6-C5	5.99	1.49	1.35
2	L2	1308	5MC	C4-N3	5.96	1.44	1.34
2	L2	359	OMC	C6-C5	5.93	1.48	1.35
1	L1	1527	OMC	C6-C5	5.92	1.48	1.35
51	S1	2061	5MC	C2-N3	5.92	1.48	1.36
51	S1	1866	OMC	C6-C5	5.91	1.48	1.35
2	L2	1317	OMC	C6-C5	5.91	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1397	OMC	C6-C5	5.90	1.48	1.35
2	L2	583	OMC	C6-C5	5.88	1.48	1.35
51	S1	2059	OMC	C6-C5	5.88	1.48	1.35
51	S1	18	OMC	C6-C5	5.83	1.48	1.35
1	L1	695	OMC	C6-C5	5.82	1.48	1.35
2	L2	1308	5MC	C2-N3	5.79	1.48	1.36
51	S1	29	OMU	C6-C5	5.74	1.48	1.35
51	S1	1979	OMU	C6-C5	5.70	1.48	1.35
1	L1	1107	OMU	C6-C5	5.68	1.48	1.35
51	S1	1621	OMU	C6-C5	5.68	1.48	1.35
51	S1	1662	OMU	C6-C5	5.64	1.48	1.35
1	L1	1371	OMU	C6-C5	5.63	1.48	1.35
2	L2	73	OMU	C6-C5	5.63	1.48	1.35
51	S1	661	OMU	C6-C5	5.63	1.48	1.35
2	L2	667	OMU	C6-C5	5.62	1.48	1.35
3	L3	13	OMU	C6-C5	5.60	1.48	1.35
2	L2	56	OMU	C6-C5	5.59	1.48	1.35
2	L2	1077	OMU	C6-C5	5.59	1.48	1.35
2	L2	1359	OMU	C6-C5	5.59	1.48	1.35
51	S1	1833	OMU	C6-C5	5.58	1.48	1.35
1	L1	1659	OMU	C6-C5	5.54	1.47	1.35
2	L2	1419	OMU	C6-C5	5.53	1.47	1.35
51	S1	1995	7MG	C4-N3	5.41	1.47	1.34
7	L7	74	PSU	C6-N1	5.40	1.45	1.36
2	L2	802	PSU	C6-N1	5.37	1.45	1.36
51	S1	1533	PSU	C6-N1	5.36	1.45	1.36
51	S1	33	PSU	C6-N1	5.34	1.45	1.36
2	L2	500	PSU	C6-N1	5.34	1.45	1.36
51	S1	1657	PSU	C6-N1	5.33	1.45	1.36
51	S1	1539	PSU	C6-N1	5.33	1.45	1.36
51	S1	455	PSU	C6-N1	5.32	1.45	1.36
51	S1	1865	OMG	C2-N3	5.32	1.46	1.33
2	L2	1403	PSU	C6-N1	5.31	1.45	1.36
1	L1	422	PSU	C6-N1	5.29	1.45	1.36
2	L2	597	PSU	C6-N1	5.29	1.45	1.36
2	L2	1194	PSU	C6-N1	5.29	1.45	1.36
2	L2	472	PSU	C6-N1	5.28	1.45	1.36
2	L2	626	PSU	C6-N1	5.28	1.45	1.36
51	S1	1566	PSU	C6-N1	5.28	1.45	1.36
51	S1	1192	PSU	C6-N1	5.28	1.45	1.36
2	L2	512	PSU	C6-N1	5.27	1.45	1.36
1	L1	1526	PSU	C6-N1	5.27	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1543	B8N	C2-N1	5.27	1.54	1.39
2	L2	1284	PSU	C6-N1	5.27	1.45	1.36
2	L2	1303	PSU	C6-N1	5.26	1.45	1.36
2	L2	1152	PSU	C6-N1	5.26	1.45	1.36
1	L1	1524	OMG	C2-N3	5.26	1.46	1.33
51	S1	1623	OMG	C2-N3	5.25	1.46	1.33
51	S1	1246	PSU	C6-N1	5.25	1.45	1.36
2	L2	510	PSU	C6-N1	5.25	1.44	1.36
7	L7	69	PSU	C6-N1	5.24	1.44	1.36
7	L7	166	PSU	C6-N1	5.24	1.44	1.36
2	L2	504	PSU	C6-N1	5.23	1.44	1.36
2	L2	71	OMG	C2-N3	5.22	1.45	1.33
51	S1	2046	PSU	C6-N1	5.22	1.44	1.36
2	L2	1361	PSU	C6-N1	5.22	1.44	1.36
2	L2	1058	PSU	C6-N1	5.22	1.44	1.36
2	L2	686	OMG	C2-N3	5.22	1.45	1.33
51	S1	2140	OMC	C4-N3	5.21	1.45	1.34
1	L1	1528	PSU	C6-N1	5.21	1.44	1.36
51	S1	1647	OMG	C2-N3	5.21	1.45	1.33
2	L2	1360	OMG	C2-N3	5.21	1.45	1.33
2	L2	78	PSU	C6-N1	5.21	1.44	1.36
1	L1	940	PSU	C6-N1	5.21	1.44	1.36
2	L2	662	PSU	C6-N1	5.20	1.44	1.36
2	L2	1144	PSU	C6-N1	5.20	1.44	1.36
1	L1	1181	PSU	C6-N1	5.20	1.44	1.36
51	S1	2202	PSU	C6-N1	5.20	1.44	1.36
1	L1	1177	PSU	C6-N1	5.19	1.44	1.36
51	S1	1292	PSU	C6-N1	5.18	1.44	1.36
2	L2	359	OMC	C4-N3	5.17	1.44	1.34
51	S1	1543	B8N	C3'-C4'	5.17	1.66	1.53
51	S1	38	OMC	C4-N3	5.17	1.44	1.34
7	L7	75	OMG	C2-N3	5.16	1.45	1.33
2	L2	593	PSU	C6-N1	5.16	1.44	1.36
2	L2	1318	PSU	C6-N1	5.16	1.44	1.36
51	S1	600	OMG	C2-N3	5.16	1.45	1.33
2	L2	1213	PSU	C6-N1	5.15	1.44	1.36
2	L2	1046	OMG	C2-N3	5.14	1.45	1.33
2	L2	655	OMG	C2-N3	5.14	1.45	1.33
1	L1	1533	PSU	C6-N1	5.13	1.44	1.36
2	L2	1264	PSU	C6-N1	5.12	1.44	1.36
2	L2	534	OMG	C2-N3	5.12	1.45	1.33
7	L7	101	PSU	C6-N1	5.11	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1231	OMG	C2-N3	5.11	1.45	1.33
1	L1	1527	OMC	C4-N3	5.10	1.44	1.34
2	L2	1265	PSU	C6-N1	5.09	1.44	1.36
1	L1	856	OMG	C2-N3	5.08	1.45	1.33
2	L2	583	OMC	C4-N3	5.08	1.44	1.34
2	L2	1060	PSU	C6-N1	5.08	1.44	1.36
51	S1	1866	OMC	C4-N3	5.07	1.44	1.34
2	L2	1229	OMG	C2-N3	5.07	1.45	1.33
1	L1	313	PSU	C6-N1	5.07	1.44	1.36
1	L1	1171	PSU	C6-N1	5.06	1.44	1.36
1	L1	1017	PSU	C6-N1	5.05	1.44	1.36
1	L1	1529	PSU	C6-N1	5.05	1.44	1.36
2	L2	1413	PSU	C6-N1	5.04	1.44	1.36
51	S1	2151	OMG	C2-N3	5.04	1.45	1.33
51	S1	18	OMC	C4-N3	5.00	1.44	1.34
1	L1	695	OMC	C4-N3	4.97	1.44	1.34
2	L2	1253	OMG	C2-N3	4.96	1.45	1.33
2	L2	1397	OMC	C4-N3	4.96	1.44	1.34
51	S1	1478	OMG	C2-N3	4.96	1.45	1.33
2	L2	1248	OMC	C4-N3	4.95	1.44	1.34
51	S1	1865	OMG	C4-N3	4.94	1.49	1.37
2	L2	71	OMG	C4-N3	4.92	1.49	1.37
51	S1	2059	OMC	C4-N3	4.91	1.44	1.34
2	L2	641	OMG	C2-N3	4.91	1.45	1.33
2	L2	1317	OMC	C4-N3	4.91	1.44	1.34
51	S1	1647	OMG	C4-N3	4.90	1.49	1.37
2	L2	1046	OMG	C4-N3	4.88	1.49	1.37
2	L2	1308	5MC	O4'-C1'	-4.88	1.30	1.42
2	L2	1360	OMG	C4-N3	4.85	1.49	1.37
1	L1	856	OMG	C4-N3	4.85	1.49	1.37
7	L7	75	OMG	C4-N3	4.84	1.49	1.37
51	S1	38	OMC	C4-N4	4.83	1.45	1.33
2	L2	359	OMC	C4-N4	4.83	1.45	1.33
2	L2	655	OMG	C4-N3	4.82	1.49	1.37
51	S1	1623	OMG	C4-N3	4.82	1.49	1.37
51	S1	600	OMG	C4-N3	4.82	1.49	1.37
2	L2	534	OMG	C4-N3	4.81	1.49	1.37
51	S1	2059	OMC	C4-N4	4.81	1.45	1.33
1	L1	1524	OMG	C4-N3	4.81	1.49	1.37
2	L2	686	OMG	C4-N3	4.81	1.49	1.37
51	S1	2140	OMC	C4-N4	4.80	1.45	1.33
2	L2	1229	OMG	C4-N3	4.80	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1527	OMC	C4-N4	4.79	1.45	1.33
51	S1	1866	OMC	C4-N4	4.79	1.45	1.33
51	S1	2059	OMC	C2-N1	4.79	1.50	1.40
51	S1	18	OMC	C4-N4	4.79	1.45	1.33
51	S1	2151	OMG	C4-N3	4.79	1.49	1.37
2	L2	1078	OMG	C2-N3	4.78	1.44	1.33
2	L2	1397	OMC	C4-N4	4.77	1.45	1.33
2	L2	1248	OMC	C4-N4	4.76	1.45	1.33
1	L1	1190	OMG	C2-N3	4.76	1.44	1.33
2	L2	1231	OMG	C4-N3	4.72	1.48	1.37
51	S1	1865	OMG	C2-N2	4.71	1.45	1.34
1	L1	695	OMC	C4-N4	4.70	1.45	1.33
2	L2	583	OMC	C4-N4	4.69	1.45	1.33
2	L2	71	OMG	C2-N2	4.69	1.45	1.34
51	S1	1647	OMG	C2-N2	4.67	1.45	1.34
2	L2	1317	OMC	C4-N4	4.67	1.44	1.33
51	S1	1478	OMG	C4-N3	4.66	1.48	1.37
2	L2	686	OMG	C2-N2	4.65	1.45	1.34
51	S1	1543	B8N	C1'-C5	-4.65	1.39	1.50
7	L7	75	OMG	C2-N2	4.65	1.45	1.34
2	L2	1229	OMG	C2-N2	4.64	1.45	1.34
2	L2	1360	OMG	C2-N2	4.64	1.45	1.34
2	L2	655	OMG	C2-N2	4.64	1.45	1.34
51	S1	1623	OMG	C2-N2	4.64	1.45	1.34
51	S1	600	OMG	C2-N2	4.62	1.45	1.34
2	L2	1046	OMG	C2-N2	4.61	1.45	1.34
2	L2	641	OMG	C4-N3	4.61	1.48	1.37
51	S1	2151	OMG	C2-N2	4.60	1.45	1.34
1	L1	1190	OMG	C4-N3	4.59	1.48	1.37
2	L2	1253	OMG	C4-N3	4.59	1.48	1.37
2	L2	1060	PSU	C1'-C5	-4.59	1.39	1.50
1	L1	1524	OMG	C2-N2	4.59	1.45	1.34
2	L2	1231	OMG	C2-N2	4.58	1.45	1.34
2	L2	534	OMG	C2-N2	4.58	1.45	1.34
51	S1	1543	B8N	O4'-C1'	4.57	1.50	1.43
51	S1	1478	OMG	C2-N2	4.56	1.45	1.34
2	L2	1058	PSU	C1'-C5	-4.55	1.39	1.50
51	S1	2140	OMC	C2-N1	4.55	1.49	1.40
2	L2	641	OMG	C2-N2	4.54	1.45	1.34
2	L2	1308	5MC	C6-N1	4.53	1.45	1.38
1	L1	1190	OMG	C2-N2	4.53	1.45	1.34
2	L2	1078	OMG	C4-N3	4.52	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1543	B8N	C6-C5	4.51	1.41	1.34
1	L1	856	OMG	C2-N2	4.51	1.44	1.34
2	L2	1078	OMG	C2-N2	4.50	1.44	1.34
7	L7	74	PSU	C1'-C5	-4.49	1.39	1.50
51	S1	38	OMC	C2-N1	4.47	1.49	1.40
51	S1	2061	5MC	C6-N1	4.47	1.45	1.38
2	L2	1248	OMC	C2-N1	4.45	1.49	1.40
2	L2	1413	PSU	C1'-C5	-4.45	1.40	1.50
1	L1	1526	PSU	C1'-C5	-4.44	1.40	1.50
1	L1	1017	PSU	C1'-C5	-4.43	1.40	1.50
2	L2	1144	PSU	C1'-C5	-4.41	1.40	1.50
2	L2	1253	OMG	C2-N2	4.41	1.44	1.34
51	S1	1543	B8N	C2'-C1'	4.40	1.59	1.53
2	L2	1213	PSU	C1'-C5	-4.40	1.40	1.50
1	L1	940	PSU	C1'-C5	-4.39	1.40	1.50
51	S1	1539	PSU	C1'-C5	-4.39	1.40	1.50
2	L2	78	PSU	C1'-C5	-4.39	1.40	1.50
2	L2	802	PSU	C1'-C5	-4.38	1.40	1.50
1	L1	1181	PSU	C1'-C5	-4.38	1.40	1.50
7	L7	101	PSU	C1'-C5	-4.37	1.40	1.50
2	L2	597	PSU	C1'-C5	-4.37	1.40	1.50
2	L2	510	PSU	C1'-C5	-4.37	1.40	1.50
51	S1	2061	5MC	C4-N4	4.36	1.45	1.34
1	L1	1533	PSU	C1'-C5	-4.35	1.40	1.50
1	L1	422	PSU	C1'-C5	-4.35	1.40	1.50
1	L1	1529	PSU	C1'-C5	-4.35	1.40	1.50
2	L2	472	PSU	C1'-C5	-4.34	1.40	1.50
2	L2	1317	OMC	C2-N1	4.33	1.49	1.40
51	S1	1866	OMC	C2-N1	4.33	1.49	1.40
1	L1	1177	PSU	C1'-C5	-4.33	1.40	1.50
2	L2	1403	PSU	C1'-C5	-4.32	1.40	1.50
51	S1	1292	PSU	C1'-C5	-4.32	1.40	1.50
51	S1	1246	PSU	C1'-C5	-4.32	1.40	1.50
51	S1	1533	PSU	C1'-C5	-4.32	1.40	1.50
51	S1	18	OMC	C2-N1	4.32	1.49	1.40
51	S1	2046	PSU	C1'-C5	-4.31	1.40	1.50
2	L2	1152	PSU	C1'-C5	-4.31	1.40	1.50
2	L2	1361	PSU	C1'-C5	-4.31	1.40	1.50
2	L2	500	PSU	C1'-C5	-4.30	1.40	1.50
51	S1	1657	PSU	C1'-C5	-4.30	1.40	1.50
2	L2	662	PSU	C1'-C5	-4.30	1.40	1.50
1	L1	1527	OMC	C2-N1	4.30	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	593	PSU	C1'-C5	-4.29	1.40	1.50
2	L2	359	OMC	C2-N1	4.29	1.49	1.40
2	L2	504	PSU	C1'-C5	-4.29	1.40	1.50
2	L2	1194	PSU	C1'-C5	-4.29	1.40	1.50
2	L2	1303	PSU	C1'-C5	-4.28	1.40	1.50
2	L2	1284	PSU	C1'-C5	-4.28	1.40	1.50
51	S1	33	PSU	C1'-C5	-4.26	1.40	1.50
7	L7	69	PSU	C1'-C5	-4.26	1.40	1.50
7	L7	166	PSU	C1'-C5	-4.26	1.40	1.50
2	L2	1308	5MC	C4-N4	4.26	1.45	1.34
51	S1	1192	PSU	C1'-C5	-4.25	1.40	1.50
2	L2	512	PSU	C1'-C5	-4.25	1.40	1.50
2	L2	1318	PSU	C1'-C5	-4.25	1.40	1.50
2	L2	1397	OMC	C2-N1	4.24	1.49	1.40
2	L2	626	PSU	C1'-C5	-4.22	1.40	1.50
51	S1	1662	OMU	C4-N3	4.19	1.46	1.38
1	L1	1528	PSU	C1'-C5	-4.19	1.40	1.50
2	L2	583	OMC	C2-N1	4.19	1.49	1.40
51	S1	29	OMU	C4-N3	4.18	1.46	1.38
1	L1	695	OMC	C2-N1	4.17	1.49	1.40
51	S1	1621	OMU	C4-N3	4.17	1.46	1.38
51	S1	455	PSU	C1'-C5	-4.15	1.40	1.50
51	S1	2202	PSU	C1'-C5	-4.15	1.40	1.50
51	S1	1566	PSU	C1'-C5	-4.13	1.40	1.50
51	S1	1833	OMU	C4-N3	4.12	1.45	1.38
51	S1	661	OMU	C4-N3	4.08	1.45	1.38
3	L3	13	OMU	C4-N3	4.08	1.45	1.38
2	L2	1077	OMU	C4-N3	4.07	1.45	1.38
51	S1	1979	OMU	C4-N3	4.06	1.45	1.38
2	L2	73	OMU	C4-N3	4.06	1.45	1.38
2	L2	56	OMU	C4-N3	4.05	1.45	1.38
1	L1	313	PSU	C1'-C5	-4.04	1.41	1.50
2	L2	1419	OMU	C4-N3	4.04	1.45	1.38
2	L2	504	PSU	C4-N3	4.01	1.46	1.38
51	S1	1566	PSU	C4-N3	4.00	1.46	1.38
2	L2	1265	PSU	C1'-C5	-4.00	1.41	1.50
1	L1	1171	PSU	C1'-C5	-3.99	1.41	1.50
1	L1	1659	OMU	C4-N3	3.98	1.45	1.38
2	L2	1359	OMU	C4-N3	3.97	1.45	1.38
51	S1	2061	5MC	C2-N1	3.97	1.48	1.40
2	L2	1284	PSU	C4-N3	3.95	1.46	1.38
51	S1	455	PSU	C4-N3	3.94	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1246	PSU	C4-N3	3.93	1.46	1.38
1	L1	1107	OMU	C4-N3	3.93	1.45	1.38
51	S1	2202	PSU	C4-N3	3.93	1.46	1.38
51	S1	33	PSU	C4-N3	3.92	1.46	1.38
2	L2	667	OMU	C4-N3	3.92	1.45	1.38
51	S1	1192	PSU	C4-N3	3.91	1.46	1.38
2	L2	1308	5MC	C2-N1	3.88	1.48	1.40
1	L1	1190	OMG	C6-N1	3.88	1.43	1.37
1	L1	1181	PSU	C4-N3	3.88	1.46	1.38
2	L2	1264	PSU	C4-N3	3.87	1.46	1.38
2	L2	1265	PSU	C4-N3	3.87	1.46	1.38
2	L2	1361	PSU	C4-N3	3.87	1.46	1.38
2	L2	472	PSU	C4-N3	3.87	1.46	1.38
1	L1	1533	PSU	C4-N3	3.86	1.46	1.38
2	L2	500	PSU	C4-N3	3.86	1.46	1.38
51	S1	1478	OMG	C6-N1	3.85	1.43	1.37
7	L7	74	PSU	C4-N3	3.85	1.46	1.38
2	L2	512	PSU	C4-N3	3.85	1.46	1.38
1	L1	422	PSU	C4-N3	3.84	1.46	1.38
2	L2	1264	PSU	C1'-C5	-3.84	1.41	1.50
7	L7	166	PSU	C4-N3	3.83	1.45	1.38
51	S1	1533	PSU	C4-N3	3.83	1.45	1.38
1	L1	1371	OMU	C4-N3	3.83	1.45	1.38
51	S1	1292	PSU	C4-N3	3.83	1.45	1.38
2	L2	1078	OMG	C6-N1	3.83	1.43	1.37
2	L2	802	PSU	C4-N3	3.83	1.45	1.38
51	S1	2046	PSU	C4-N3	3.82	1.45	1.38
51	S1	1657	PSU	C4-N3	3.82	1.45	1.38
2	L2	641	OMG	C6-N1	3.82	1.43	1.37
2	L2	1194	PSU	C4-N3	3.82	1.45	1.38
1	L1	1524	OMG	C6-N1	3.81	1.43	1.37
1	L1	1526	PSU	C4-N3	3.81	1.45	1.38
51	S1	1539	PSU	C4-N3	3.81	1.45	1.38
2	L2	510	PSU	C4-N3	3.80	1.45	1.38
1	L1	1177	PSU	C4-N3	3.80	1.45	1.38
1	L1	1171	PSU	C4-N3	3.78	1.45	1.38
2	L2	1413	PSU	C4-N3	3.78	1.45	1.38
1	L1	1528	PSU	C4-N3	3.78	1.45	1.38
2	L2	78	PSU	C4-N3	3.77	1.45	1.38
2	L2	1403	PSU	C4-N3	3.77	1.45	1.38
1	L1	313	PSU	C4-N3	3.76	1.45	1.38
2	L2	662	PSU	C4-N3	3.76	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1213	PSU	C4-N3	3.76	1.45	1.38
2	L2	1303	PSU	C4-N3	3.76	1.45	1.38
2	L2	626	PSU	C4-N3	3.75	1.45	1.38
1	L1	940	PSU	C4-N3	3.75	1.45	1.38
2	L2	1229	OMG	C6-N1	3.75	1.43	1.37
2	L2	686	OMG	C6-N1	3.75	1.43	1.37
51	S1	1623	OMG	C6-N1	3.74	1.43	1.37
1	L1	1529	PSU	C4-N3	3.74	1.45	1.38
7	L7	69	PSU	C4-N3	3.74	1.45	1.38
2	L2	593	PSU	C4-N3	3.74	1.45	1.38
2	L2	1144	PSU	C4-N3	3.73	1.45	1.38
7	L7	101	PSU	C4-N3	3.73	1.45	1.38
2	L2	1360	OMG	C6-N1	3.72	1.43	1.37
2	L2	1318	PSU	C4-N3	3.72	1.45	1.38
51	S1	1865	OMG	C6-N1	3.72	1.43	1.37
2	L2	597	PSU	C4-N3	3.71	1.45	1.38
51	S1	600	OMG	C6-N1	3.71	1.43	1.37
2	L2	655	OMG	C6-N1	3.69	1.43	1.37
51	S1	1647	OMG	C6-N1	3.69	1.43	1.37
2	L2	534	OMG	C6-N1	3.68	1.43	1.37
1	L1	1017	PSU	C4-N3	3.68	1.45	1.38
2	L2	1060	PSU	C4-N3	3.68	1.45	1.38
2	L2	71	OMG	C6-N1	3.67	1.43	1.37
7	L7	75	OMG	C6-N1	3.66	1.43	1.37
51	S1	2151	OMG	C6-N1	3.66	1.43	1.37
2	L2	1058	PSU	C4-N3	3.65	1.45	1.38
2	L2	1152	PSU	C4-N3	3.64	1.45	1.38
2	L2	1253	OMG	C6-N1	3.63	1.43	1.37
2	L2	1046	OMG	C6-N1	3.63	1.43	1.37
2	L2	1231	OMG	C6-N1	3.60	1.43	1.37
1	L1	856	OMG	C6-N1	3.60	1.43	1.37
51	S1	1995	7MG	C6-N1	3.54	1.45	1.38
51	S1	1995	7MG	C2-N1	3.50	1.46	1.37
51	S1	1995	7MG	C5-C6	3.44	1.52	1.43
51	S1	2140	OMC	C6-N1	3.32	1.46	1.38
1	L1	510	PSU	C6-C5	3.30	1.39	1.35
51	S1	1995	7MG	C2-N2	3.30	1.42	1.34
2	L2	359	OMC	C6-N1	3.28	1.45	1.38
2	L2	565	PSU	C6-C5	3.27	1.39	1.35
51	S1	12	PSU	C6-C5	3.27	1.39	1.35
1	L1	1664	PSU	C6-C5	3.26	1.39	1.35
51	S1	2048	PSU	C6-C5	3.25	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1524	OMG	C5-C6	3.24	1.54	1.47
1	L1	239	PSU	C6-C5	3.24	1.39	1.35
2	L2	1248	OMC	C6-N1	3.23	1.45	1.38
1	L1	1527	OMC	C6-N1	3.21	1.45	1.38
2	L2	583	OMC	C6-N1	3.20	1.45	1.38
1	L1	774	PSU	C6-C5	3.20	1.39	1.35
2	L2	1397	OMC	C6-N1	3.17	1.45	1.38
51	S1	1866	OMC	C6-N1	3.16	1.45	1.38
2	L2	686	OMG	C5-C6	3.16	1.53	1.47
2	L2	1078	OMG	C5-C6	3.16	1.53	1.47
51	S1	2059	OMC	C6-N1	3.16	1.45	1.38
51	S1	38	OMC	C6-N1	3.15	1.45	1.38
51	S1	600	OMG	C5-C6	3.14	1.53	1.47
51	S1	512	A2M	C6-N6	3.14	1.45	1.34
2	L2	1317	OMC	C6-N1	3.14	1.45	1.38
51	S1	479	A2M	C6-N6	3.13	1.45	1.34
7	L7	43	A2M	O3'-C3'	-3.13	1.35	1.43
1	L1	672	PSU	C6-C5	3.13	1.39	1.35
2	L2	1231	OMG	C5-C6	3.13	1.53	1.47
2	L2	647	A2M	O2'-C2'	3.13	1.50	1.42
51	S1	1833	OMU	O4-C4	-3.12	1.18	1.24
2	L2	382	A2M	O3'-C3'	-3.12	1.35	1.43
3	L3	13	OMU	O4-C4	-3.12	1.18	1.24
2	L2	502	A2M	C6-N6	3.12	1.45	1.34
2	L2	95	A2M	C6-N6	3.11	1.45	1.34
2	L2	71	OMG	C5-C6	3.11	1.53	1.47
51	S1	2151	OMG	C5-C6	3.11	1.53	1.47
51	S1	1647	OMG	C5-C6	3.10	1.53	1.47
1	L1	858	A2M	C6-N6	3.10	1.45	1.34
51	S1	897	A2M	O3'-C3'	-3.10	1.35	1.43
51	S1	28	A2M	C6-N6	3.10	1.45	1.34
51	S1	897	A2M	C6-N6	3.10	1.45	1.34
51	S1	512	A2M	O3'-C3'	-3.09	1.35	1.43
1	L1	69	A2M	C6-N6	3.09	1.45	1.34
7	L7	75	OMG	C5-C6	3.09	1.53	1.47
2	L2	437	PSU	C6-C5	3.09	1.38	1.35
2	L2	667	OMU	O4-C4	-3.09	1.18	1.24
7	L7	162	A2M	O3'-C3'	-3.09	1.35	1.43
51	S1	1865	OMG	C5-C6	3.09	1.53	1.47
1	L1	1011	PSU	C6-C5	3.09	1.38	1.35
2	L2	502	A2M	O3'-C3'	-3.09	1.35	1.43
2	L2	1372	A2M	C6-N6	3.09	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	534	OMG	C5-C6	3.09	1.53	1.47
7	L7	162	A2M	C6-N6	3.09	1.45	1.34
2	L2	572	A2M	O3'-C3'	-3.08	1.35	1.43
2	L2	1185	A2M	C6-N6	3.08	1.45	1.34
1	L1	858	A2M	O3'-C3'	-3.08	1.35	1.43
1	L1	927	A2M	O3'-C3'	-3.07	1.35	1.43
51	S1	18	OMC	C6-N1	3.07	1.45	1.38
1	L1	305	A2M	C6-N6	3.07	1.45	1.34
1	L1	927	A2M	C6-N6	3.06	1.45	1.34
51	S1	1478	OMG	C5-C6	3.06	1.53	1.47
2	L2	570	A2M	C6-N6	3.06	1.45	1.34
2	L2	1384	A2M	C6-N6	3.06	1.45	1.34
2	L2	572	A2M	C6-N6	3.06	1.45	1.34
51	S1	1995	7MG	O6-C6	-3.06	1.17	1.23
51	S1	661	OMU	O4-C4	-3.06	1.18	1.24
2	L2	647	A2M	C6-N6	3.06	1.45	1.34
51	S1	668	A2M	C6-N6	3.06	1.45	1.34
1	L1	235	A2M	C6-N6	3.06	1.45	1.34
51	S1	28	A2M	O3'-C3'	-3.05	1.35	1.43
1	L1	695	OMC	C6-N1	3.05	1.45	1.38
1	L1	1373	A2M	O3'-C3'	-3.05	1.35	1.43
2	L2	56	OMU	O4-C4	-3.05	1.18	1.24
7	L7	43	A2M	C6-N6	3.05	1.45	1.34
2	L2	591	A2M	C6-N6	3.05	1.45	1.34
2	L2	665	A2M	C6-N6	3.05	1.45	1.34
2	L2	382	A2M	C6-N6	3.05	1.45	1.34
51	S1	98	A2M	C6-N6	3.05	1.45	1.34
2	L2	604	A2M	C6-N6	3.04	1.45	1.34
1	L1	1659	OMU	O4-C4	-3.04	1.18	1.24
1	L1	697	A2M	O3'-C3'	-3.04	1.35	1.43
1	L1	1107	OMU	O4-C4	-3.04	1.18	1.24
2	L2	95	A2M	O3'-C3'	-3.04	1.35	1.43
1	L1	697	A2M	C6-N6	3.04	1.45	1.34
2	L2	591	A2M	O3'-C3'	-3.03	1.35	1.43
51	S1	1623	OMG	C5-C6	3.02	1.53	1.47
1	L1	856	OMG	C5-C6	3.02	1.53	1.47
1	L1	407	A2M	O3'-C3'	-3.02	1.35	1.43
1	L1	407	A2M	C6-N6	3.02	1.45	1.34
2	L2	1229	OMG	C5-C6	3.02	1.53	1.47
2	L2	655	OMG	C5-C6	3.02	1.53	1.47
1	L1	1190	OMG	C5-C4	-3.02	1.35	1.43
1	L1	1371	OMU	O4-C4	-3.01	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	665	A2M	O3'-C3'	-3.01	1.35	1.43
1	L1	1190	OMG	C5-C6	3.01	1.53	1.47
1	L1	1539	A2M	C6-N6	3.01	1.45	1.34
51	S1	98	A2M	O3'-C3'	-3.01	1.35	1.43
2	L2	1419	OMU	O4-C4	-3.00	1.18	1.24
2	L2	1253	OMG	C5-C6	3.00	1.53	1.47
51	S1	1979	OMU	O4-C4	-3.00	1.18	1.24
1	L1	1373	A2M	C6-N6	3.00	1.45	1.34
2	L2	641	OMG	C5-C6	3.00	1.53	1.47
2	L2	527	A2M	C6-N6	3.00	1.45	1.34
2	L2	1077	OMU	O4-C4	-2.99	1.18	1.24
2	L2	73	OMU	O4-C4	-2.98	1.18	1.24
51	S1	2059	OMC	O2-C2	-2.98	1.18	1.23
2	L2	1078	OMG	C5-C4	-2.97	1.35	1.43
1	L1	235	A2M	O3'-C3'	-2.96	1.36	1.43
51	S1	1662	OMU	O4-C4	-2.96	1.18	1.24
2	L2	1360	OMG	C5-C6	2.96	1.53	1.47
2	L2	527	A2M	O3'-C3'	-2.96	1.36	1.43
2	L2	1185	A2M	O3'-C3'	-2.96	1.36	1.43
1	L1	1371	OMU	C6-N1	2.95	1.45	1.38
2	L2	1359	OMU	O4-C4	-2.95	1.18	1.24
2	L2	641	OMG	C5-C4	-2.94	1.35	1.43
2	L2	570	A2M	O3'-C3'	-2.94	1.36	1.43
2	L2	604	A2M	O3'-C3'	-2.94	1.36	1.43
2	L2	1308	5MC	O3'-C3'	2.94	1.49	1.43
2	L2	1308	5MC	O2'-C2'	-2.94	1.36	1.43
51	S1	1621	OMU	O4-C4	-2.93	1.18	1.24
2	L2	1308	5MC	O2-C2	-2.93	1.18	1.23
2	L2	527	A2M	C5-C4	-2.93	1.33	1.40
51	S1	668	A2M	O2'-C2'	2.92	1.50	1.42
2	L2	1372	A2M	O3'-C3'	-2.92	1.36	1.43
2	L2	1046	OMG	C5-C6	2.92	1.53	1.47
1	L1	1539	A2M	O3'-C3'	-2.91	1.36	1.43
51	S1	1979	OMU	C6-N1	2.91	1.45	1.38
2	L2	527	A2M	O2'-C2'	2.90	1.50	1.42
7	L7	162	A2M	O2'-C2'	2.90	1.50	1.42
51	S1	1478	OMG	C5-C4	-2.90	1.35	1.43
2	L2	570	A2M	O2'-C2'	2.90	1.50	1.42
51	S1	1621	OMU	C6-N1	2.90	1.45	1.38
2	L2	647	A2M	O3'-C3'	-2.89	1.36	1.43
2	L2	1317	OMC	O2-C2	-2.88	1.18	1.23
3	L3	13	OMU	C6-N1	2.88	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	661	OMU	C6-N1	2.88	1.44	1.38
7	L7	43	A2M	C5-C4	-2.88	1.33	1.40
2	L2	1384	A2M	O3'-C3'	-2.87	1.36	1.43
51	S1	29	OMU	O4-C4	-2.87	1.18	1.24
2	L2	583	OMC	O2-C2	-2.87	1.18	1.23
2	L2	1359	OMU	C6-N1	2.86	1.44	1.38
51	S1	1662	OMU	C6-N1	2.86	1.44	1.38
2	L2	73	OMU	C6-N1	2.86	1.44	1.38
2	L2	1397	OMC	O2-C2	-2.86	1.18	1.23
2	L2	1229	OMG	C5-C4	-2.86	1.35	1.43
2	L2	95	A2M	O2'-C2'	2.86	1.49	1.42
2	L2	665	A2M	C5-C4	-2.86	1.33	1.40
1	L1	305	A2M	O3'-C3'	-2.85	1.36	1.43
1	L1	697	A2M	C5-C4	-2.85	1.33	1.40
51	S1	1647	OMG	C5-C4	-2.85	1.35	1.43
2	L2	655	OMG	C5-C4	-2.84	1.35	1.43
2	L2	1231	OMG	C5-C4	-2.84	1.35	1.43
1	L1	1107	OMU	C6-N1	2.84	1.44	1.38
2	L2	382	A2M	O2'-C2'	2.83	1.49	1.42
2	L2	570	A2M	C5-C4	-2.83	1.33	1.40
2	L2	1372	A2M	O2'-C2'	2.83	1.49	1.42
51	S1	600	OMG	C2-N1	2.83	1.44	1.37
1	L1	856	OMG	C5-C4	-2.83	1.35	1.43
51	S1	512	A2M	O2'-C2'	2.83	1.49	1.42
2	L2	1077	OMU	C6-N1	2.82	1.44	1.38
51	S1	668	A2M	O3'-C3'	-2.82	1.36	1.43
7	L7	162	A2M	C5-C4	-2.82	1.33	1.40
51	S1	668	A2M	C5-C4	-2.82	1.33	1.40
2	L2	1384	A2M	C5-C4	-2.82	1.33	1.40
2	L2	591	A2M	O2'-C2'	2.82	1.49	1.42
51	S1	29	OMU	C6-N1	2.82	1.44	1.38
1	L1	1373	A2M	C5-C4	-2.82	1.33	1.40
7	L7	101	PSU	O4-C4	-2.81	1.18	1.23
2	L2	1253	OMG	C5-C4	-2.81	1.35	1.43
2	L2	641	OMG	C2-N1	2.81	1.44	1.37
2	L2	572	A2M	C5-C4	-2.81	1.33	1.40
7	L7	75	OMG	C2-N1	2.81	1.44	1.37
1	L1	1190	OMG	C2-N1	2.81	1.44	1.37
2	L2	604	A2M	O2'-C2'	2.80	1.49	1.42
1	L1	407	A2M	C5-C4	-2.80	1.33	1.40
1	L1	1373	A2M	O2'-C2'	2.80	1.49	1.42
2	L2	686	OMG	C2-N1	2.80	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1384	A2M	O2'-C2'	2.80	1.49	1.42
51	S1	98	A2M	O2'-C2'	2.80	1.49	1.42
2	L2	359	OMC	O2-C2	-2.80	1.18	1.23
51	S1	1833	OMU	C6-N1	2.80	1.44	1.38
2	L2	591	A2M	C5-C4	-2.80	1.33	1.40
2	L2	502	A2M	O2'-C2'	2.80	1.49	1.42
1	L1	858	A2M	C5-C4	-2.80	1.33	1.40
1	L1	1527	OMC	O2-C2	-2.80	1.18	1.23
2	L2	71	OMG	C5-C4	-2.80	1.35	1.43
51	S1	2151	OMG	C5-C4	-2.80	1.35	1.43
4	L4	74	OMG	C5-C6	-2.79	1.41	1.47
2	L2	665	A2M	O2'-C2'	2.79	1.49	1.42
51	S1	479	A2M	O3'-C3'	-2.79	1.36	1.43
1	L1	1540	OMG	C5-C6	-2.79	1.41	1.47
2	L2	1185	A2M	C5-C4	-2.79	1.33	1.40
51	S1	98	A2M	C5-C4	-2.79	1.33	1.40
2	L2	78	PSU	O4-C4	-2.79	1.18	1.23
2	L2	1185	A2M	O2'-C2'	2.79	1.49	1.42
1	L1	1539	A2M	C5-C4	-2.78	1.33	1.40
1	L1	235	A2M	O2'-C2'	2.78	1.49	1.42
2	L2	667	OMU	C6-N1	2.78	1.44	1.38
2	L2	1372	A2M	C5-C4	-2.78	1.33	1.40
2	L2	382	A2M	C5-C4	-2.78	1.33	1.40
2	L2	1078	OMG	C2-N1	2.78	1.44	1.37
51	S1	1865	OMG	C2-N1	2.78	1.44	1.37
1	L1	927	A2M	O2'-C2'	2.78	1.49	1.42
1	L1	305	A2M	C5-C4	-2.78	1.33	1.40
2	L2	686	OMG	C5-C4	-2.78	1.36	1.43
2	L2	56	OMU	C6-N1	2.77	1.44	1.38
1	L1	1017	PSU	O4-C4	-2.77	1.18	1.23
1	L1	1524	OMG	C5-C4	-2.77	1.36	1.43
2	L2	604	A2M	C5-C4	-2.77	1.33	1.40
2	L2	1229	OMG	C2-N1	2.77	1.44	1.37
51	S1	897	A2M	C5-C4	-2.76	1.33	1.40
51	S1	479	A2M	O2'-C2'	2.76	1.49	1.42
1	L1	695	OMC	O2-C2	-2.76	1.18	1.23
51	S1	1829	OMG	C5-C6	-2.76	1.41	1.47
2	L2	1194	PSU	O4-C4	-2.76	1.18	1.23
1	L1	1659	OMU	C6-N1	2.76	1.44	1.38
1	L1	858	A2M	O2'-C2'	2.76	1.49	1.42
2	L2	1046	OMG	C5-C4	-2.76	1.36	1.43
51	S1	1478	OMG	C2-N1	2.75	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	407	A2M	O2'-C2'	2.75	1.49	1.42
1	L1	1539	A2M	O2'-C2'	2.75	1.49	1.42
51	S1	28	A2M	C5-C4	-2.75	1.33	1.40
1	L1	927	A2M	C5-C4	-2.75	1.33	1.40
2	L2	534	OMG	C2-N1	2.74	1.44	1.37
51	S1	1623	OMG	C2-N1	2.74	1.44	1.37
1	L1	69	A2M	O2'-C2'	2.74	1.49	1.42
2	L2	1318	PSU	O4-C4	-2.74	1.18	1.23
1	L1	697	A2M	O2'-C2'	2.74	1.49	1.42
2	L2	1419	OMU	C6-N1	2.74	1.44	1.38
1	L1	69	A2M	C5-C4	-2.74	1.33	1.40
51	S1	18	OMC	O2-C2	-2.74	1.18	1.23
2	L2	1360	OMG	C5-C4	-2.74	1.36	1.43
51	S1	38	OMC	O2-C2	-2.74	1.18	1.23
51	S1	28	A2M	O2'-C2'	2.74	1.49	1.42
52	S2	37	MIA	C5-C4	-2.73	1.33	1.40
1	L1	856	OMG	C2-N1	2.73	1.44	1.37
51	S1	1865	OMG	C5-C4	-2.73	1.36	1.43
2	L2	502	A2M	C5-C4	-2.73	1.33	1.40
2	L2	1360	OMG	C2-N1	2.73	1.44	1.37
2	L2	95	A2M	C5-C4	-2.73	1.33	1.40
1	L1	959	OMG	C5-C6	-2.73	1.41	1.47
51	S1	2185	MA6	C5-C4	-2.73	1.33	1.40
51	S1	2184	MA6	C5-C4	-2.73	1.33	1.40
1	L1	1526	PSU	O4-C4	-2.73	1.18	1.23
51	S1	2151	OMG	C2-N1	2.73	1.44	1.37
7	L7	43	A2M	O2'-C2'	2.73	1.49	1.42
51	S1	2140	OMC	O2-C2	-2.73	1.18	1.23
51	S1	1647	OMG	C2-N1	2.72	1.44	1.37
2	L2	1303	PSU	O4-C4	-2.72	1.18	1.23
1	L1	940	PSU	O4-C4	-2.72	1.18	1.23
51	S1	1550	OMG	C5-C6	-2.72	1.41	1.47
2	L2	1248	OMC	O2-C2	-2.72	1.18	1.23
51	S1	512	A2M	C5-C4	-2.72	1.33	1.40
7	L7	75	OMG	C5-C4	-2.72	1.36	1.43
1	L1	313	PSU	O4-C4	-2.71	1.18	1.23
1	L1	235	A2M	C5-C4	-2.71	1.33	1.40
2	L2	572	A2M	O2'-C2'	2.71	1.49	1.42
2	L2	655	OMG	C2-N1	2.70	1.44	1.37
2	L2	1231	OMG	C2-N1	2.70	1.44	1.37
1	L1	1529	PSU	O4-C4	-2.70	1.18	1.23
2	L2	1361	PSU	O4-C4	-2.70	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1152	PSU	O4-C4	-2.69	1.18	1.23
1	L1	1524	OMG	C2-N1	2.69	1.44	1.37
2	L2	1253	OMG	C2-N1	2.69	1.44	1.37
2	L2	1144	PSU	O4-C4	-2.69	1.18	1.23
51	S1	600	OMG	C5-C4	-2.69	1.36	1.43
51	S1	1657	PSU	O4-C4	-2.69	1.18	1.23
2	L2	1060	PSU	O4-C4	-2.68	1.18	1.23
2	L2	534	OMG	C5-C4	-2.68	1.36	1.43
2	L2	1403	PSU	O4-C4	-2.68	1.18	1.23
1	L1	1171	PSU	O4-C4	-2.68	1.18	1.23
51	S1	1246	PSU	O4-C4	-2.68	1.18	1.23
1	L1	422	PSU	O4-C4	-2.67	1.18	1.23
2	L2	1046	OMG	C2-N1	2.67	1.44	1.37
2	L2	662	PSU	O4-C4	-2.67	1.18	1.23
2	L2	1264	PSU	O4-C4	-2.66	1.18	1.23
2	L2	71	OMG	C2-N1	2.66	1.44	1.37
51	S1	1533	PSU	O4-C4	-2.66	1.18	1.23
1	L1	1626	OMG	C5-C6	-2.66	1.42	1.47
51	S1	1866	OMC	O2-C2	-2.66	1.18	1.23
51	S1	479	A2M	C5-C4	-2.66	1.33	1.40
1	L1	305	A2M	O2'-C2'	2.66	1.49	1.42
2	L2	1265	PSU	O4-C4	-2.66	1.18	1.23
51	S1	1543	B8N	O2'-C2'	2.66	1.49	1.43
7	L7	69	PSU	O4-C4	-2.65	1.18	1.23
2	L2	626	PSU	O4-C4	-2.65	1.18	1.23
51	S1	897	A2M	O2'-C2'	2.65	1.49	1.42
2	L2	512	PSU	O4-C4	-2.65	1.18	1.23
2	L2	1413	PSU	O4-C4	-2.65	1.18	1.23
7	L7	166	PSU	O4-C4	-2.65	1.18	1.23
51	S1	1623	OMG	C5-C4	-2.64	1.36	1.43
2	L2	597	PSU	O4-C4	-2.64	1.18	1.23
51	S1	1292	PSU	O4-C4	-2.64	1.18	1.23
51	S1	1566	PSU	O4-C4	-2.64	1.18	1.23
7	L7	74	PSU	O4-C4	-2.63	1.18	1.23
1	L1	1181	PSU	O4-C4	-2.63	1.18	1.23
1	L1	1533	PSU	O4-C4	-2.63	1.18	1.23
2	L2	593	PSU	O4-C4	-2.62	1.18	1.23
2	L2	1213	PSU	O4-C4	-2.62	1.18	1.23
51	S1	2061	5MC	O2-C2	-2.61	1.18	1.23
1	L1	1528	PSU	O4-C4	-2.61	1.18	1.23
2	L2	1058	PSU	O4-C4	-2.60	1.18	1.23
2	L2	1284	PSU	O4-C4	-2.60	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1177	PSU	O4-C4	-2.60	1.18	1.23
2	L2	802	PSU	O4-C4	-2.59	1.18	1.23
51	S1	2202	PSU	O4-C4	-2.59	1.18	1.23
51	S1	1192	PSU	O4-C4	-2.58	1.18	1.23
2	L2	647	A2M	C5-C4	-2.58	1.34	1.40
51	S1	2046	PSU	O4-C4	-2.57	1.18	1.23
51	S1	1539	PSU	O4-C4	-2.57	1.18	1.23
2	L2	510	PSU	O4-C4	-2.56	1.18	1.23
51	S1	455	PSU	O4-C4	-2.56	1.18	1.23
2	L2	500	PSU	O4-C4	-2.56	1.18	1.23
51	S1	33	PSU	O4-C4	-2.56	1.18	1.23
2	L2	472	PSU	O4-C4	-2.55	1.18	1.23
2	L2	1264	PSU	O4'-C1'	-2.52	1.40	1.43
2	L2	504	PSU	O4-C4	-2.51	1.18	1.23
1	L1	1659	OMU	O2-C2	-2.50	1.18	1.23
51	S1	1543	B8N	O2-C2	-2.49	1.18	1.22
2	L2	1359	OMU	O2-C2	-2.47	1.18	1.23
51	S1	661	OMU	O2-C2	-2.46	1.18	1.23
51	S1	2140	OMC	C5-C4	2.46	1.48	1.42
51	S1	38	OMC	C5-C4	2.45	1.48	1.42
51	S1	29	OMU	C5-C4	2.44	1.49	1.43
2	L2	73	OMU	O2-C2	-2.43	1.18	1.23
1	L1	1171	PSU	O4'-C1'	-2.43	1.40	1.43
1	L1	1371	OMU	O2-C2	-2.42	1.18	1.23
3	L3	13	OMU	O2-C2	-2.41	1.18	1.23
2	L2	667	OMU	O2-C2	-2.41	1.18	1.23
2	L2	1397	OMC	C5-C4	2.39	1.48	1.42
2	L2	359	OMC	C5-C4	2.39	1.48	1.42
2	L2	56	OMU	O2-C2	-2.38	1.18	1.23
51	S1	2059	OMC	C5-C4	2.38	1.48	1.42
2	L2	1253	OMG	O6-C6	-2.38	1.18	1.23
51	S1	1866	OMC	C5-C4	2.37	1.48	1.42
2	L2	1248	OMC	C5-C4	2.37	1.48	1.42
51	S1	1979	OMU	O2-C2	-2.37	1.18	1.23
2	L2	71	OMG	O6-C6	-2.37	1.18	1.23
51	S1	1833	OMU	O2-C2	-2.36	1.18	1.23
1	L1	1107	OMU	O2-C2	-2.36	1.18	1.23
51	S1	1621	OMU	O2-C2	-2.36	1.18	1.23
1	L1	856	OMG	O6-C6	-2.35	1.18	1.23
1	L1	1107	OMU	C5-C4	2.35	1.48	1.43
51	S1	1621	OMU	C5-C4	2.35	1.48	1.43
51	S1	1478	OMG	O6-C6	-2.35	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	655	OMG	O6-C6	-2.34	1.18	1.23
2	L2	1419	OMU	O2-C2	-2.34	1.18	1.23
2	L2	1317	OMC	C5-C4	2.34	1.48	1.42
2	L2	1229	OMG	O6-C6	-2.33	1.18	1.23
51	S1	1662	OMU	O2-C2	-2.33	1.18	1.23
1	L1	1190	OMG	O6-C6	-2.33	1.18	1.23
2	L2	1077	OMU	O2-C2	-2.33	1.18	1.23
2	L2	583	OMC	C5-C4	2.32	1.48	1.42
2	L2	1078	OMG	O6-C6	-2.31	1.18	1.23
51	S1	1979	OMU	C5-C4	2.31	1.48	1.43
2	L2	1046	OMG	O6-C6	-2.31	1.18	1.23
2	L2	667	OMU	C5-C4	2.30	1.48	1.43
51	S1	1662	OMU	C5-C4	2.30	1.48	1.43
1	L1	1371	OMU	C5-C4	2.30	1.48	1.43
2	L2	1077	OMU	C5-C4	2.30	1.48	1.43
2	L2	534	OMG	O6-C6	-2.29	1.18	1.23
51	S1	661	OMU	C5-C4	2.29	1.48	1.43
7	L7	75	OMG	O6-C6	-2.29	1.18	1.23
2	L2	1231	OMG	O6-C6	-2.29	1.18	1.23
2	L2	641	OMG	O6-C6	-2.28	1.18	1.23
51	S1	1647	OMG	O6-C6	-2.28	1.18	1.23
51	S1	1543	B8N	O3'-C3'	2.28	1.48	1.43
2	L2	1359	OMU	C5-C4	2.28	1.48	1.43
51	S1	2151	OMG	O6-C6	-2.27	1.18	1.23
1	L1	1540	OMG	C8-N7	-2.27	1.31	1.35
2	L2	56	OMU	C5-C4	2.27	1.48	1.43
1	L1	959	OMG	C8-N7	-2.27	1.31	1.35
51	S1	1833	OMU	C5-C4	2.26	1.48	1.43
2	L2	1360	OMG	O6-C6	-2.26	1.18	1.23
51	S1	18	OMC	C5-C4	2.26	1.48	1.42
2	L2	73	OMU	C5-C4	2.26	1.48	1.43
1	L1	1659	OMU	C5-C4	2.26	1.48	1.43
51	S1	1865	OMG	O6-C6	-2.24	1.18	1.23
51	S1	1623	OMG	O6-C6	-2.23	1.18	1.23
51	S1	600	OMG	O6-C6	-2.23	1.18	1.23
2	L2	647	A2M	C2-N3	2.22	1.35	1.32
2	L2	686	OMG	O6-C6	-2.22	1.18	1.23
2	L2	647	A2M	O5'-C5'	-2.22	1.39	1.44
1	L1	695	OMC	C5-C4	2.21	1.48	1.42
51	S1	29	OMU	O2-C2	-2.20	1.19	1.23
51	S1	512	A2M	C2-N3	2.20	1.35	1.32
4	L4	74	OMG	C8-N7	-2.19	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1524	OMG	O6-C6	-2.19	1.18	1.23
2	L2	1419	OMU	C5-C4	2.19	1.48	1.43
2	L2	527	A2M	O5'-C5'	-2.19	1.39	1.44
1	L1	1527	OMC	C5-C4	2.18	1.47	1.42
51	S1	1829	OMG	C8-N7	-2.18	1.31	1.35
51	S1	479	A2M	C2-N3	2.18	1.35	1.32
3	L3	13	OMU	C5-C4	2.15	1.48	1.43
51	S1	1550	OMG	C8-N7	-2.15	1.31	1.35
1	L1	1626	OMG	C8-N7	-2.15	1.31	1.35
51	S1	668	A2M	O5'-C5'	-2.12	1.39	1.44
2	L2	1067	A2M	C8-N7	-2.11	1.30	1.34
51	S1	2184	MA6	C2-N3	2.11	1.35	1.32
2	L2	502	A2M	C2-N3	2.11	1.35	1.32
51	S1	1566	PSU	C4-C5	2.10	1.50	1.44
1	L1	235	A2M	C2-N3	2.10	1.35	1.32
1	L1	1540	OMG	C5-C4	-2.09	1.37	1.43
1	L1	678	A2M	C8-N7	-2.07	1.31	1.34
1	L1	1526	PSU	O4'-C1'	-2.06	1.41	1.43
2	L2	572	A2M	O5'-C5'	-2.06	1.39	1.44
4	L4	74	OMG	C5-C4	-2.06	1.37	1.43
1	L1	305	A2M	C2-N3	2.06	1.35	1.32
1	L1	955	A2M	C8-N7	-2.05	1.31	1.34
7	L7	101	PSU	O4'-C1'	-2.05	1.41	1.43
2	L2	95	A2M	C2-N3	2.05	1.35	1.32
2	L2	502	A2M	O5'-C5'	-2.05	1.39	1.44
51	S1	98	A2M	C2-N3	2.04	1.35	1.32
1	L1	1539	A2M	O5'-C5'	-2.04	1.39	1.44
2	L2	628	A2M	C8-N7	-2.04	1.31	1.34
1	L1	69	A2M	C2-N3	2.04	1.35	1.32
1	L1	927	A2M	O5'-C5'	-2.04	1.39	1.44
51	S1	1550	OMG	C5-C4	-2.03	1.37	1.43
51	S1	1543	B8N	O4-C4	-2.03	1.18	1.23
1	L1	305	A2M	O5'-C5'	-2.03	1.39	1.44
1	L1	697	A2M	O5'-C5'	-2.03	1.39	1.44
1	L1	1626	OMG	C5-C4	-2.02	1.37	1.43
51	S1	28	A2M	C2-N3	2.01	1.35	1.32
2	L2	591	A2M	O5'-C5'	-2.01	1.39	1.44
51	S1	2202	PSU	C4-C5	2.01	1.49	1.44
1	L1	959	OMG	C5-C4	-2.00	1.38	1.43
51	S1	1829	OMG	C5-C4	-2.00	1.38	1.43
2	L2	665	A2M	O5'-C5'	-2.00	1.39	1.44

All (568) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	37	MIA	C1'-N9-C4	17.12	156.72	126.64
51	S1	2185	MA6	N1-C6-N6	-12.27	104.14	117.06
52	S2	37	MIA	C11-S10-C2	11.54	110.89	102.27
51	S1	2184	MA6	N1-C6-N6	-11.14	105.33	117.06
52	S2	37	MIA	S10-C2-N3	8.91	147.02	116.10
7	L7	43	A2M	C5-C6-N6	8.33	133.02	120.35
1	L1	1539	A2M	C5-C6-N6	8.15	132.74	120.35
2	L2	1372	A2M	C5-C6-N6	8.08	132.64	120.35
2	L2	1185	A2M	C5-C6-N6	8.08	132.63	120.35
1	L1	1373	A2M	C5-C6-N6	8.08	132.63	120.35
2	L2	95	A2M	C5-C6-N6	8.05	132.59	120.35
51	S1	668	A2M	C5-C6-N6	8.05	132.58	120.35
2	L2	570	A2M	C5-C6-N6	8.01	132.53	120.35
2	L2	527	A2M	C5-C6-N6	7.99	132.49	120.35
2	L2	382	A2M	C5-C6-N6	7.98	132.49	120.35
1	L1	305	A2M	C5-C6-N6	7.97	132.46	120.35
51	S1	897	A2M	C5-C6-N6	7.96	132.46	120.35
2	L2	502	A2M	C5-C6-N6	7.90	132.36	120.35
1	L1	858	A2M	C5-C6-N6	7.90	132.36	120.35
2	L2	604	A2M	C5-C6-N6	7.87	132.32	120.35
2	L2	572	A2M	C5-C6-N6	7.87	132.32	120.35
2	L2	1384	A2M	C5-C6-N6	7.86	132.30	120.35
1	L1	235	A2M	C5-C6-N6	7.86	132.29	120.35
1	L1	69	A2M	C5-C6-N6	7.83	132.25	120.35
1	L1	697	A2M	C5-C6-N6	7.81	132.22	120.35
1	L1	407	A2M	C5-C6-N6	7.81	132.22	120.35
51	S1	479	A2M	C5-C6-N6	7.80	132.20	120.35
2	L2	591	A2M	C5-C6-N6	7.79	132.19	120.35
2	L2	665	A2M	C5-C6-N6	7.78	132.18	120.35
1	L1	927	A2M	C5-C6-N6	7.76	132.15	120.35
51	S1	98	A2M	C5-C6-N6	7.76	132.14	120.35
7	L7	162	A2M	C5-C6-N6	7.71	132.07	120.35
2	L2	647	A2M	C5-C6-N6	7.71	132.07	120.35
51	S1	512	A2M	C5-C6-N6	7.70	132.05	120.35
51	S1	28	A2M	C5-C6-N6	7.60	131.90	120.35
52	S2	37	MIA	S10-C2-N1	-6.45	93.71	116.01
7	L7	43	A2M	N3-C2-N1	-6.02	119.28	128.68
2	L2	572	A2M	N3-C2-N1	-5.71	119.76	128.68
51	S1	512	A2M	N3-C2-N1	-5.69	119.78	128.68
51	S1	2185	MA6	N3-C2-N1	-5.69	119.78	128.68
7	L7	162	A2M	N3-C2-N1	-5.69	119.79	128.68
2	L2	665	A2M	N3-C2-N1	-5.67	119.82	128.68
1	L1	1373	A2M	N3-C2-N1	-5.66	119.82	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	2184	MA6	N3-C2-N1	-5.65	119.85	128.68
51	S1	28	A2M	N3-C2-N1	-5.64	119.87	128.68
1	L1	697	A2M	N3-C2-N1	-5.63	119.87	128.68
51	S1	897	A2M	N3-C2-N1	-5.61	119.92	128.68
2	L2	1372	A2M	N3-C2-N1	-5.59	119.94	128.68
1	L1	69	A2M	N3-C2-N1	-5.59	119.94	128.68
2	L2	1384	A2M	N3-C2-N1	-5.59	119.94	128.68
2	L2	502	A2M	N3-C2-N1	-5.58	119.95	128.68
1	L1	1539	A2M	N3-C2-N1	-5.58	119.95	128.68
2	L2	570	A2M	N3-C2-N1	-5.55	120.00	128.68
2	L2	527	A2M	N3-C2-N1	-5.55	120.01	128.68
51	S1	1833	OMU	C4-N3-C2	-5.55	119.26	126.58
1	L1	1539	A2M	N6-C6-N1	-5.54	107.07	118.57
2	L2	1185	A2M	N3-C2-N1	-5.52	120.06	128.68
2	L2	527	A2M	N6-C6-N1	-5.51	107.14	118.57
51	S1	479	A2M	N3-C2-N1	-5.50	120.08	128.68
1	L1	407	A2M	N3-C2-N1	-5.49	120.10	128.68
2	L2	591	A2M	N3-C2-N1	-5.47	120.13	128.68
1	L1	235	A2M	N3-C2-N1	-5.46	120.14	128.68
51	S1	98	A2M	N3-C2-N1	-5.46	120.14	128.68
7	L7	43	A2M	N6-C6-N1	-5.46	107.24	118.57
1	L1	927	A2M	N3-C2-N1	-5.46	120.15	128.68
1	L1	1373	A2M	N6-C6-N1	-5.45	107.26	118.57
1	L1	305	A2M	N3-C2-N1	-5.44	120.17	128.68
51	S1	668	A2M	N3-C2-N1	-5.42	120.21	128.68
2	L2	604	A2M	N3-C2-N1	-5.42	120.21	128.68
1	L1	858	A2M	N3-C2-N1	-5.41	120.22	128.68
2	L2	382	A2M	N6-C6-N1	-5.39	107.38	118.57
2	L2	647	A2M	N3-C2-N1	-5.39	120.25	128.68
2	L2	570	A2M	N6-C6-N1	-5.39	107.39	118.57
2	L2	95	A2M	N6-C6-N1	-5.37	107.43	118.57
51	S1	668	A2M	N6-C6-N1	-5.36	107.46	118.57
1	L1	235	A2M	N6-C6-N1	-5.35	107.48	118.57
2	L2	667	OMU	C4-N3-C2	-5.35	119.53	126.58
51	S1	897	A2M	N6-C6-N1	-5.34	107.48	118.57
1	L1	305	A2M	N6-C6-N1	-5.33	107.52	118.57
2	L2	95	A2M	N3-C2-N1	-5.32	120.36	128.68
1	L1	69	A2M	N6-C6-N1	-5.31	107.55	118.57
2	L2	604	A2M	N6-C6-N1	-5.31	107.56	118.57
2	L2	1185	A2M	N6-C6-N1	-5.30	107.57	118.57
2	L2	665	A2M	N6-C6-N1	-5.30	107.58	118.57
2	L2	1077	OMU	C4-N3-C2	-5.29	119.60	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	502	A2M	N6-C6-N1	-5.29	107.59	118.57
1	L1	1107	OMU	C4-N3-C2	-5.29	119.60	126.58
2	L2	56	OMU	C4-N3-C2	-5.29	119.60	126.58
51	S1	1621	OMU	C4-N3-C2	-5.29	119.61	126.58
1	L1	697	A2M	N6-C6-N1	-5.27	107.63	118.57
1	L1	858	A2M	N6-C6-N1	-5.27	107.63	118.57
2	L2	1372	A2M	N6-C6-N1	-5.27	107.64	118.57
51	S1	29	OMU	C4-N3-C2	-5.26	119.65	126.58
3	L3	13	OMU	C4-N3-C2	-5.25	119.65	126.58
1	L1	407	A2M	N6-C6-N1	-5.25	107.68	118.57
51	S1	479	A2M	N6-C6-N1	-5.25	107.69	118.57
2	L2	647	A2M	N6-C6-N1	-5.23	107.71	118.57
2	L2	1384	A2M	N6-C6-N1	-5.23	107.72	118.57
2	L2	572	A2M	N6-C6-N1	-5.21	107.77	118.57
1	L1	927	A2M	N6-C6-N1	-5.20	107.78	118.57
51	S1	98	A2M	N6-C6-N1	-5.19	107.80	118.57
2	L2	591	A2M	N6-C6-N1	-5.19	107.80	118.57
2	L2	1359	OMU	C4-N3-C2	-5.18	119.74	126.58
51	S1	661	OMU	C4-N3-C2	-5.18	119.75	126.58
51	S1	512	A2M	N6-C6-N1	-5.17	107.85	118.57
51	S1	1662	OMU	C4-N3-C2	-5.16	119.77	126.58
51	S1	1979	OMU	C4-N3-C2	-5.16	119.78	126.58
7	L7	162	A2M	N6-C6-N1	-5.16	107.87	118.57
2	L2	382	A2M	N3-C2-N1	-5.14	120.65	128.68
1	L1	1659	OMU	C4-N3-C2	-5.13	119.82	126.58
51	S1	28	A2M	N6-C6-N1	-5.10	107.99	118.57
2	L2	1419	OMU	C4-N3-C2	-5.04	119.93	126.58
2	L2	73	OMU	C4-N3-C2	-4.97	120.02	126.58
51	S1	1995	7MG	C5-C6-N1	4.93	119.69	110.99
1	L1	1371	OMU	C4-N3-C2	-4.83	120.21	126.58
51	S1	1543	B8N	C5-C4-N3	4.79	125.04	116.17
2	L2	1058	PSU	N1-C2-N3	4.69	120.45	115.13
1	L1	1533	PSU	C4-N3-C2	-4.64	119.65	126.34
2	L2	1318	PSU	C4-N3-C2	-4.63	119.67	126.34
2	L2	1152	PSU	C4-N3-C2	-4.62	119.68	126.34
2	L2	1060	PSU	C4-N3-C2	-4.62	119.68	126.34
2	L2	1144	PSU	C4-N3-C2	-4.60	119.71	126.34
51	S1	1246	PSU	C4-N3-C2	-4.60	119.71	126.34
1	L1	940	PSU	C4-N3-C2	-4.57	119.75	126.34
51	S1	1657	PSU	C4-N3-C2	-4.56	119.78	126.34
1	L1	1526	PSU	C4-N3-C2	-4.55	119.78	126.34
2	L2	1303	PSU	C4-N3-C2	-4.55	119.78	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1403	PSU	C4-N3-C2	-4.55	119.78	126.34
51	S1	1533	PSU	C4-N3-C2	-4.55	119.79	126.34
2	L2	1058	PSU	C4-N3-C2	-4.55	119.79	126.34
2	L2	78	PSU	C4-N3-C2	-4.55	119.79	126.34
2	L2	1194	PSU	C4-N3-C2	-4.55	119.79	126.34
7	L7	74	PSU	C4-N3-C2	-4.54	119.80	126.34
2	L2	1213	PSU	C4-N3-C2	-4.53	119.82	126.34
51	S1	2046	PSU	C4-N3-C2	-4.52	119.83	126.34
1	L1	1529	PSU	C4-N3-C2	-4.51	119.83	126.34
1	L1	1017	PSU	C4-N3-C2	-4.51	119.84	126.34
2	L2	1413	PSU	C4-N3-C2	-4.50	119.86	126.34
2	L2	1284	PSU	C4-N3-C2	-4.49	119.87	126.34
2	L2	500	PSU	C4-N3-C2	-4.47	119.89	126.34
7	L7	101	PSU	C4-N3-C2	-4.46	119.91	126.34
2	L2	1361	PSU	C4-N3-C2	-4.46	119.91	126.34
2	L2	512	PSU	C4-N3-C2	-4.46	119.92	126.34
1	L1	1528	PSU	C4-N3-C2	-4.46	119.92	126.34
2	L2	802	PSU	C4-N3-C2	-4.45	119.92	126.34
51	S1	1995	7MG	C2-N3-C4	4.45	120.23	112.30
2	L2	1060	PSU	N1-C2-N3	4.44	120.17	115.13
7	L7	166	PSU	C4-N3-C2	-4.44	119.94	126.34
1	L1	1181	PSU	C4-N3-C2	-4.44	119.94	126.34
2	L2	1144	PSU	N1-C2-N3	4.44	120.16	115.13
51	S1	1292	PSU	C4-N3-C2	-4.42	119.97	126.34
2	L2	504	PSU	C4-N3-C2	-4.41	119.99	126.34
51	S1	1539	PSU	C4-N3-C2	-4.40	120.01	126.34
1	L1	422	PSU	C4-N3-C2	-4.38	120.02	126.34
2	L2	597	PSU	C4-N3-C2	-4.37	120.04	126.34
51	S1	33	PSU	C4-N3-C2	-4.37	120.05	126.34
2	L2	1318	PSU	N1-C2-N3	4.36	120.07	115.13
2	L2	510	PSU	C4-N3-C2	-4.36	120.06	126.34
2	L2	1152	PSU	N1-C2-N3	4.35	120.05	115.13
2	L2	472	PSU	C4-N3-C2	-4.34	120.09	126.34
2	L2	504	PSU	N1-C2-N3	4.33	120.04	115.13
2	L2	1303	PSU	N1-C2-N3	4.32	120.03	115.13
2	L2	626	PSU	C4-N3-C2	-4.32	120.11	126.34
51	S1	455	PSU	C4-N3-C2	-4.31	120.13	126.34
2	L2	662	PSU	C4-N3-C2	-4.30	120.14	126.34
1	L1	1533	PSU	N1-C2-N3	4.30	120.00	115.13
51	S1	2202	PSU	C4-N3-C2	-4.29	120.16	126.34
7	L7	69	PSU	C4-N3-C2	-4.28	120.17	126.34
1	L1	1177	PSU	C4-N3-C2	-4.28	120.17	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	1543	B8N	C4-N3-C2	-4.27	120.06	125.46
1	L1	1528	PSU	N1-C2-N3	4.27	119.96	115.13
7	L7	69	PSU	N1-C2-N3	4.24	119.94	115.13
51	S1	1192	PSU	C4-N3-C2	-4.23	120.24	126.34
1	L1	1171	PSU	C4-N3-C2	-4.23	120.25	126.34
1	L1	313	PSU	C4-N3-C2	-4.22	120.26	126.34
2	L2	1264	PSU	C4-N3-C2	-4.22	120.26	126.34
2	L2	1403	PSU	N1-C2-N3	4.22	119.91	115.13
1	L1	1181	PSU	N1-C2-N3	4.22	119.91	115.13
51	S1	1657	PSU	N1-C2-N3	4.22	119.91	115.13
2	L2	1213	PSU	N1-C2-N3	4.21	119.90	115.13
2	L2	593	PSU	C4-N3-C2	-4.21	120.28	126.34
51	S1	2046	PSU	N1-C2-N3	4.20	119.89	115.13
51	S1	1566	PSU	C4-N3-C2	-4.20	120.28	126.34
1	L1	1529	PSU	N1-C2-N3	4.20	119.89	115.13
1	L1	1017	PSU	N1-C2-N3	4.20	119.89	115.13
52	S2	37	MIA	N3-C2-N1	-4.19	119.27	126.98
7	L7	166	PSU	N1-C2-N3	4.19	119.88	115.13
2	L2	78	PSU	N1-C2-N3	4.17	119.85	115.13
2	L2	1413	PSU	N1-C2-N3	4.17	119.85	115.13
7	L7	74	PSU	N1-C2-N3	4.17	119.85	115.13
2	L2	1265	PSU	C4-N3-C2	-4.16	120.35	126.34
2	L2	1265	PSU	N1-C2-N3	4.15	119.84	115.13
51	S1	33	PSU	N1-C2-N3	4.15	119.83	115.13
51	S1	1533	PSU	N1-C2-N3	4.14	119.82	115.13
1	L1	1171	PSU	N1-C2-N3	4.14	119.82	115.13
2	L2	1284	PSU	N1-C2-N3	4.14	119.82	115.13
51	S1	1995	7MG	C5-C4-N3	-4.14	120.25	128.13
2	L2	500	PSU	N1-C2-N3	4.13	119.81	115.13
7	L7	101	PSU	N1-C2-N3	4.13	119.81	115.13
2	L2	1194	PSU	N1-C2-N3	4.12	119.80	115.13
2	L2	512	PSU	N1-C2-N3	4.12	119.80	115.13
51	S1	1246	PSU	N1-C2-N3	4.12	119.80	115.13
51	S1	1566	PSU	N1-C2-N3	4.12	119.80	115.13
51	S1	2202	PSU	N1-C2-N3	4.12	119.80	115.13
1	L1	940	PSU	N1-C2-N3	4.11	119.79	115.13
2	L2	802	PSU	N1-C2-N3	4.10	119.77	115.13
1	L1	1526	PSU	N1-C2-N3	4.09	119.76	115.13
1	L1	313	PSU	N1-C2-N3	4.08	119.75	115.13
2	L2	1361	PSU	N1-C2-N3	4.08	119.75	115.13
51	S1	1539	PSU	N1-C2-N3	4.08	119.75	115.13
2	L2	472	PSU	N1-C2-N3	4.08	119.75	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	510	PSU	N1-C2-N3	4.07	119.74	115.13
1	L1	1177	PSU	N1-C2-N3	4.07	119.74	115.13
2	L2	597	PSU	N1-C2-N3	4.06	119.73	115.13
51	S1	1292	PSU	N1-C2-N3	4.06	119.73	115.13
2	L2	560	OMU	O3'-C3'-C4'	4.06	122.78	111.05
2	L2	662	PSU	N1-C2-N3	4.03	119.70	115.13
51	S1	1192	PSU	N1-C2-N3	4.03	119.70	115.13
51	S1	455	PSU	N1-C2-N3	4.03	119.70	115.13
2	L2	593	PSU	N1-C2-N3	3.97	119.63	115.13
1	L1	422	PSU	N1-C2-N3	3.97	119.62	115.13
2	L2	626	PSU	N1-C2-N3	3.93	119.59	115.13
1	L1	1371	OMU	C1'-N1-C2	3.93	124.69	117.57
1	L1	1659	OMU	N3-C2-N1	3.92	120.09	114.89
1	L1	1107	OMU	N3-C2-N1	3.85	120.00	114.89
1	L1	1371	OMU	N3-C2-N1	3.84	119.98	114.89
2	L2	1308	5MC	C5-C6-N1	-3.83	119.40	123.34
2	L2	667	OMU	N3-C2-N1	3.82	119.97	114.89
2	L2	1359	OMU	N3-C2-N1	3.82	119.96	114.89
2	L2	1264	PSU	N1-C2-N3	3.82	119.45	115.13
51	S1	661	OMU	N3-C2-N1	3.78	119.91	114.89
51	S1	1979	OMU	N3-C2-N1	3.78	119.91	114.89
51	S1	29	OMU	N3-C2-N1	3.75	119.86	114.89
2	L2	56	OMU	N3-C2-N1	3.74	119.85	114.89
51	S1	1621	OMU	N3-C2-N1	3.73	119.84	114.89
2	L2	73	OMU	N3-C2-N1	3.72	119.83	114.89
51	S1	1543	B8N	C3'-C2'-C1'	3.72	105.97	101.64
52	S2	37	MIA	C2-N3-C4	3.72	120.45	115.32
51	S1	1833	OMU	C5-C4-N3	3.69	120.36	114.84
3	L3	13	OMU	N3-C2-N1	3.67	119.76	114.89
2	L2	1419	OMU	N3-C2-N1	3.65	119.74	114.89
1	L1	1171	PSU	C6-N1-C2	-3.64	118.96	122.68
51	S1	1543	B8N	C2'-C3'-C4'	3.64	109.72	102.64
51	S1	1833	OMU	N3-C2-N1	3.64	119.72	114.89
51	S1	1662	OMU	N3-C2-N1	3.63	119.71	114.89
2	L2	1077	OMU	N3-C2-N1	3.59	119.65	114.89
2	L2	71	OMG	C5-C6-N1	3.56	120.24	113.95
3	L3	13	OMU	C5-C4-N3	3.54	120.14	114.84
2	L2	1253	OMG	C5-C6-N1	3.52	120.17	113.95
2	L2	1077	OMU	C5-C4-N3	3.51	120.10	114.84
2	L2	655	OMG	C5-C6-N1	3.51	120.15	113.95
2	L2	1058	PSU	C6-N1-C2	-3.49	119.12	122.68
2	L2	1078	OMG	C5-C6-N1	3.46	120.06	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	667	OMU	C5-C4-N3	3.45	120.01	114.84
1	L1	856	OMG	C5-C6-N1	3.45	120.04	113.95
51	S1	1865	OMG	C5-C6-N1	3.45	120.04	113.95
1	L1	1107	OMU	C5-C4-N3	3.44	119.98	114.84
1	L1	1524	OMG	C5-C6-N1	3.43	120.02	113.95
51	S1	1647	OMG	C5-C6-N1	3.43	120.01	113.95
7	L7	75	OMG	C5-C6-N1	3.42	119.99	113.95
1	L1	1190	OMG	C5-C6-N1	3.42	119.98	113.95
52	S2	37	MIA	C12-C13-C14	-3.41	120.50	127.14
2	L2	1265	PSU	C6-N1-C2	-3.41	119.19	122.68
51	S1	1623	OMG	C5-C6-N1	3.41	119.98	113.95
51	S1	1833	OMU	O4-C4-C5	-3.41	119.16	125.16
51	S1	1621	OMU	C5-C4-N3	3.41	119.94	114.84
2	L2	1046	OMG	C5-C6-N1	3.40	119.96	113.95
2	L2	1231	OMG	C5-C6-N1	3.40	119.96	113.95
51	S1	2151	OMG	C5-C6-N1	3.40	119.95	113.95
51	S1	1979	OMU	C5-C4-N3	3.40	119.92	114.84
1	L1	313	PSU	C6-N1-C2	-3.39	119.21	122.68
2	L2	1359	OMU	C5-C4-N3	3.39	119.92	114.84
51	S1	1662	OMU	C5-C4-N3	3.39	119.91	114.84
51	S1	1478	OMG	C5-C6-N1	3.38	119.92	113.95
2	L2	1229	OMG	C5-C6-N1	3.37	119.91	113.95
51	S1	661	OMU	C5-C4-N3	3.37	119.88	114.84
2	L2	56	OMU	C5-C4-N3	3.36	119.87	114.84
2	L2	686	OMG	C5-C6-N1	3.36	119.88	113.95
51	S1	600	OMG	C5-C6-N1	3.34	119.84	113.95
2	L2	1360	OMG	C5-C6-N1	3.32	119.82	113.95
51	S1	1995	7MG	C4-C5-N7	3.32	110.14	105.53
7	L7	69	PSU	C6-N1-C2	-3.31	119.30	122.68
2	L2	504	PSU	C6-N1-C2	-3.31	119.30	122.68
51	S1	29	OMU	C5-C4-N3	3.31	119.79	114.84
2	L2	1144	PSU	C6-N1-C2	-3.30	119.31	122.68
2	L2	534	OMG	C5-C6-N1	3.30	119.78	113.95
2	L2	1419	OMU	C5-C4-N3	3.28	119.74	114.84
51	S1	1543	B8N	N3-C2-N1	3.28	121.38	116.76
2	L2	641	OMG	C5-C6-N1	3.27	119.72	113.95
2	L2	73	OMU	C5-C4-N3	3.26	119.72	114.84
2	L2	1152	PSU	C6-C5-C4	3.26	120.47	118.20
51	S1	1192	PSU	C6-N1-C2	-3.23	119.38	122.68
2	L2	1058	PSU	C6-C5-C4	3.21	120.44	118.20
1	L1	1371	OMU	C5-C4-N3	3.21	119.64	114.84
1	L1	1659	OMU	C5-C4-N3	3.20	119.63	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	455	PSU	C6-N1-C2	-3.19	119.42	122.68
2	L2	1264	PSU	C6-N1-C2	-3.19	119.42	122.68
2	L2	1060	PSU	C6-C5-C4	3.15	120.40	118.20
1	L1	1528	PSU	C6-N1-C2	-3.15	119.46	122.68
2	L2	1060	PSU	C6-N1-C2	-3.15	119.46	122.68
51	S1	1995	7MG	C5-C4-N9	3.14	110.42	106.35
2	L2	1413	PSU	C6-N1-C2	-3.13	119.48	122.68
3	L3	13	OMU	O4-C4-C5	-3.13	119.65	125.16
51	S1	1566	PSU	C6-N1-C2	-3.13	119.49	122.68
7	L7	166	PSU	C6-N1-C2	-3.12	119.49	122.68
1	L1	1181	PSU	C6-N1-C2	-3.12	119.49	122.68
2	L2	1284	PSU	C6-N1-C2	-3.08	119.53	122.68
51	S1	1647	OMG	C8-N7-C5	3.08	108.86	102.99
51	S1	2202	PSU	C6-N1-C2	-3.08	119.53	122.68
2	L2	1318	PSU	C6-N1-C2	-3.07	119.54	122.68
1	L1	1177	PSU	C6-N1-C2	-3.07	119.55	122.68
2	L2	1303	PSU	C6-N1-C2	-3.06	119.55	122.68
2	L2	1253	OMG	C2-N1-C6	-3.06	119.46	125.10
1	L1	1533	PSU	C6-N1-C2	-3.05	119.56	122.68
2	L2	510	PSU	C6-N1-C2	-3.05	119.56	122.68
51	S1	1657	PSU	C6-N1-C2	-3.05	119.57	122.68
51	S1	1292	PSU	C6-N1-C2	-3.05	119.57	122.68
2	L2	1194	PSU	C6-N1-C2	-3.04	119.57	122.68
2	L2	597	PSU	C6-N1-C2	-3.04	119.58	122.68
51	S1	1539	PSU	C6-N1-C2	-3.03	119.58	122.68
2	L2	1152	PSU	C6-N1-C2	-3.03	119.59	122.68
51	S1	2059	OMC	O2-C2-N3	-3.03	117.41	122.33
51	S1	2046	PSU	C6-N1-C2	-3.02	119.60	122.68
7	L7	74	PSU	C6-N1-C2	-3.01	119.60	122.68
51	S1	1979	OMU	O4-C4-C5	-3.01	119.87	125.16
2	L2	1213	PSU	C6-N1-C2	-3.01	119.61	122.68
2	L2	512	PSU	C6-N1-C2	-3.00	119.61	122.68
2	L2	1403	PSU	C6-N1-C2	-3.00	119.61	122.68
51	S1	33	PSU	C6-N1-C2	-3.00	119.61	122.68
2	L2	662	PSU	C6-N1-C2	-3.00	119.62	122.68
2	L2	1361	PSU	C6-N1-C2	-3.00	119.62	122.68
51	S1	1662	OMU	O4-C4-C5	-2.98	119.91	125.16
2	L2	593	PSU	C6-N1-C2	-2.98	119.63	122.68
51	S1	2059	OMC	C1'-N1-C2	2.98	125.08	118.42
2	L2	1077	OMU	O4-C4-C5	-2.98	119.92	125.16
1	L1	1529	PSU	C6-N1-C2	-2.98	119.64	122.68
51	S1	1621	OMU	O4-C4-C5	-2.97	119.93	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	472	PSU	C6-N1-C2	-2.97	119.65	122.68
7	L7	101	PSU	C6-N1-C2	-2.97	119.65	122.68
2	L2	626	PSU	C6-N1-C2	-2.96	119.66	122.68
2	L2	56	OMU	O4-C4-C5	-2.96	119.96	125.16
2	L2	1419	OMU	O4-C4-C5	-2.96	119.96	125.16
1	L1	1017	PSU	C6-N1-C2	-2.96	119.66	122.68
2	L2	73	OMU	O4-C4-C5	-2.94	119.99	125.16
1	L1	1526	PSU	C6-N1-C2	-2.93	119.69	122.68
1	L1	1524	OMG	C2-N1-C6	-2.93	119.70	125.10
1	L1	940	PSU	C6-N1-C2	-2.93	119.69	122.68
51	S1	1623	OMG	C2-N1-C6	-2.93	119.71	125.10
1	L1	422	PSU	C6-N1-C2	-2.92	119.70	122.68
1	L1	1190	OMG	C8-N7-C5	2.92	108.55	102.99
51	S1	1533	PSU	C6-N1-C2	-2.92	119.70	122.68
2	L2	500	PSU	C6-N1-C2	-2.91	119.71	122.68
2	L2	78	PSU	C6-N1-C2	-2.90	119.71	122.68
1	L1	959	OMG	O2'-C2'-C1'	2.90	114.85	109.09
51	S1	600	OMG	C8-N7-C5	2.90	108.51	102.99
2	L2	686	OMG	C8-N7-C5	2.89	108.50	102.99
51	S1	1478	OMG	C8-N7-C5	2.89	108.49	102.99
51	S1	1246	PSU	C6-N1-C2	-2.89	119.73	122.68
2	L2	802	PSU	C6-N1-C2	-2.88	119.73	122.68
1	L1	1524	OMG	C8-N7-C5	2.88	108.48	102.99
2	L2	1229	OMG	C8-N7-C5	2.87	108.46	102.99
2	L2	655	OMG	C8-N7-C5	2.87	108.46	102.99
2	L2	641	OMG	C8-N7-C5	2.87	108.45	102.99
51	S1	1865	OMG	C8-N7-C5	2.86	108.44	102.99
2	L2	1078	OMG	C8-N7-C5	2.86	108.44	102.99
2	L2	71	OMG	C2-N1-C6	-2.86	119.83	125.10
1	L1	856	OMG	C8-N7-C5	2.86	108.43	102.99
2	L2	504	PSU	O2-C2-N1	-2.85	119.66	122.79
51	S1	1995	7MG	C2-N1-C6	-2.85	119.91	125.10
2	L2	1231	OMG	C2-N1-C6	-2.85	119.86	125.10
2	L2	667	OMU	O4-C4-C5	-2.85	120.16	125.16
1	L1	1107	OMU	O4-C4-C5	-2.84	120.16	125.16
51	S1	1478	OMG	C2-N1-C6	-2.84	119.86	125.10
2	L2	1403	PSU	C6-C5-C4	2.84	120.19	118.20
2	L2	802	PSU	C6-C5-C4	2.84	120.18	118.20
51	S1	2151	OMG	C8-N7-C5	2.83	108.39	102.99
51	S1	600	OMG	C2-N1-C6	-2.83	119.89	125.10
2	L2	1213	PSU	C6-C5-C4	2.83	120.17	118.20
51	S1	2151	OMG	C2-N1-C6	-2.82	119.90	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	686	OMG	C2-N1-C6	-2.81	119.92	125.10
2	L2	1359	OMU	O4-C4-C5	-2.81	120.21	125.16
2	L2	1078	OMG	C2-N1-C6	-2.81	119.92	125.10
7	L7	75	OMG	C2-N1-C6	-2.80	119.94	125.10
51	S1	661	OMU	O4-C4-C5	-2.79	120.25	125.16
51	S1	1647	OMG	C2-N1-C6	-2.79	119.97	125.10
2	L2	1046	OMG	C8-N7-C5	2.79	108.30	102.99
1	L1	1526	PSU	C6-C5-C4	2.78	120.14	118.20
51	S1	29	OMU	O4-C4-C5	-2.78	120.27	125.16
1	L1	1533	PSU	O2-C2-N1	-2.77	119.74	122.79
2	L2	1231	OMG	C8-N7-C5	2.77	108.27	102.99
2	L2	1046	OMG	C2-N1-C6	-2.77	119.99	125.10
2	L2	655	OMG	C2-N1-C6	-2.77	120.00	125.10
1	L1	1659	OMU	O4-C4-C5	-2.76	120.30	125.16
2	L2	71	OMG	C8-N7-C5	2.76	108.25	102.99
1	L1	1190	OMG	C2-N1-C6	-2.76	120.02	125.10
2	L2	1078	OMG	N2-C2-N1	2.76	122.59	116.71
51	S1	1995	7MG	O6-C6-C5	-2.74	120.83	127.54
2	L2	1360	OMG	C2-N1-C6	-2.73	120.06	125.10
51	S1	1865	OMG	C2-N1-C6	-2.73	120.06	125.10
51	S1	33	PSU	C6-C5-C4	2.73	120.11	118.20
51	S1	1623	OMG	C8-N7-C5	2.73	108.19	102.99
1	L1	856	OMG	C2-N1-C6	-2.73	120.07	125.10
2	L2	1229	OMG	C2-N1-C6	-2.73	120.08	125.10
7	L7	75	OMG	C8-N7-C5	2.73	108.19	102.99
2	L2	1360	OMG	C8-N7-C5	2.72	108.18	102.99
1	L1	1190	OMG	N2-C2-N1	2.72	122.51	116.71
2	L2	534	OMG	C8-N7-C5	2.71	108.16	102.99
2	L2	641	OMG	C2-N1-C6	-2.70	120.12	125.10
2	L2	1253	OMG	C8-N7-C5	2.70	108.13	102.99
1	L1	1533	PSU	C6-C5-C4	2.70	120.08	118.20
52	S2	37	MIA	C12-N6-C6	-2.69	118.56	122.55
51	S1	2202	PSU	O2-C2-N1	-2.69	119.83	122.79
2	L2	534	OMG	C2-N1-C6	-2.68	120.16	125.10
2	L2	1413	PSU	O2-C2-N1	-2.68	119.84	122.79
2	L2	1303	PSU	C6-C5-C4	2.68	120.07	118.20
51	S1	1246	PSU	C6-C5-C4	2.67	120.07	118.20
2	L2	1144	PSU	O2-C2-N1	-2.67	119.86	122.79
1	L1	1171	PSU	O2-C2-N1	-2.66	119.87	122.79
7	L7	74	PSU	C6-C5-C4	2.65	120.05	118.20
51	S1	2061	5MC	C5-C6-N1	-2.64	120.63	123.34
2	L2	500	PSU	C6-C5-C4	2.62	120.03	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	1657	PSU	O2-C2-N1	-2.62	119.91	122.79
51	S1	1995	7MG	N9-C8-N7	2.62	107.12	103.38
51	S1	1539	PSU	C6-C5-C4	2.61	120.03	118.20
51	S1	1566	PSU	O2-C2-N1	-2.61	119.92	122.79
2	L2	1284	PSU	O2-C2-N1	-2.61	119.92	122.79
1	L1	1371	OMU	O4-C4-C5	-2.60	120.59	125.16
2	L2	1152	PSU	O2-C2-N1	-2.58	119.95	122.79
51	S1	1995	7MG	N9-C4-N3	2.58	129.33	125.47
2	L2	1265	PSU	O2-C2-N1	-2.58	119.95	122.79
2	L2	1361	PSU	C6-C5-C4	2.56	119.99	118.20
51	S1	2046	PSU	O2-C2-N1	-2.56	119.97	122.79
51	S1	1533	PSU	C6-C5-C4	2.55	119.98	118.20
2	L2	1361	PSU	O2-C2-N1	-2.55	119.99	122.79
51	S1	1543	B8N	O4-C4-N3	-2.54	115.66	119.98
2	L2	1303	PSU	O2-C2-N1	-2.54	119.99	122.79
1	L1	1529	PSU	O2-C2-N1	-2.54	120.00	122.79
2	L2	641	OMG	N2-C2-N1	2.53	122.10	116.71
1	L1	1017	PSU	C6-C5-C4	2.51	119.96	118.20
7	L7	166	PSU	O2-C2-N1	-2.51	120.03	122.79
1	L1	313	PSU	O2-C2-N1	-2.50	120.03	122.79
1	L1	1017	PSU	O2-C2-N1	-2.50	120.03	122.79
2	L2	510	PSU	O2-C2-N1	-2.50	120.04	122.79
1	L1	1181	PSU	O2-C2-N1	-2.50	120.04	122.79
2	L2	504	PSU	C6-C5-C4	2.49	119.94	118.20
7	L7	69	PSU	O2-C2-N1	-2.48	120.06	122.79
2	L2	500	PSU	O2-C2-N1	-2.48	120.06	122.79
2	L2	512	PSU	C6-C5-C4	2.48	119.93	118.20
2	L2	1318	PSU	C6-C5-C4	2.48	119.93	118.20
7	L7	69	PSU	C6-C5-C4	2.47	119.92	118.20
2	L2	472	PSU	O2-C2-N1	-2.47	120.07	122.79
51	S1	1192	PSU	O2-C2-N1	-2.47	120.08	122.79
7	L7	101	PSU	C6-C5-C4	2.46	119.92	118.20
2	L2	593	PSU	O2-C2-N1	-2.46	120.08	122.79
7	L7	101	PSU	O2-C2-N1	-2.46	120.08	122.79
2	L2	1144	PSU	C6-C5-C4	2.46	119.92	118.20
2	L2	78	PSU	C6-C5-C4	2.45	119.91	118.20
51	S1	455	PSU	O2-C2-N1	-2.44	120.10	122.79
2	L2	1308	5MC	C4'-O4'-C1'	-2.44	104.09	109.47
51	S1	33	PSU	O2-C2-N1	-2.44	120.10	122.79
2	L2	597	PSU	O2-C2-N1	-2.43	120.11	122.79
2	L2	560	OMU	O4'-C4'-C3'	-2.43	100.31	105.11
2	L2	1264	PSU	O2-C2-N1	-2.42	120.13	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	1657	PSU	C6-C5-C4	2.41	119.88	118.20
2	L2	1194	PSU	O2-C2-N1	-2.41	120.14	122.79
2	L2	1318	PSU	O2-C2-N1	-2.41	120.14	122.79
2	L2	1253	OMG	N2-C2-N1	2.41	121.83	116.71
51	S1	1533	PSU	O2-C2-N1	-2.40	120.14	122.79
2	L2	802	PSU	O2-C2-N1	-2.40	120.15	122.79
2	L2	78	PSU	O2-C2-N1	-2.40	120.15	122.79
1	L1	305	A2M	O2'-C2'-C1'	2.39	113.84	109.09
1	L1	1177	PSU	O2-C2-N1	-2.39	120.16	122.79
1	L1	48	OMU	C1'-N1-C2	2.39	121.89	117.57
1	L1	1529	PSU	C6-C5-C4	2.37	119.86	118.20
2	L2	1284	PSU	C6-C5-C4	2.37	119.85	118.20
2	L2	1060	PSU	O2-C2-N1	-2.36	120.19	122.79
7	L7	74	PSU	O2-C2-N1	-2.36	120.19	122.79
51	S1	1246	PSU	O2-C2-N1	-2.35	120.20	122.79
1	L1	1181	PSU	C6-C5-C4	2.35	119.84	118.20
51	S1	1292	PSU	O2-C2-N1	-2.35	120.20	122.79
2	L2	510	PSU	C6-C5-C4	2.35	119.84	118.20
1	L1	1528	PSU	O2-C2-N1	-2.35	120.21	122.79
2	L2	1403	PSU	O2-C2-N1	-2.34	120.21	122.79
2	L2	472	PSU	C6-C5-C4	2.34	119.83	118.20
2	L2	512	PSU	O2-C2-N1	-2.33	120.22	122.79
1	L1	940	PSU	O2-C2-N1	-2.33	120.22	122.79
2	L2	1213	PSU	O2-C2-N1	-2.32	120.23	122.79
51	S1	1478	OMG	N2-C2-N1	2.32	121.65	116.71
7	L7	166	PSU	C6-C5-C4	2.32	119.82	118.20
51	S1	2046	PSU	C6-C5-C4	2.31	119.82	118.20
51	S1	8	OMU	C3'-C2'-C1'	-2.31	98.55	102.89
2	L2	662	PSU	O2-C2-N1	-2.31	120.25	122.79
51	S1	1292	PSU	C6-C5-C4	2.31	119.81	118.20
2	L2	1253	OMG	O6-C6-C5	-2.30	119.87	124.37
2	L2	1413	PSU	C6-C5-C4	2.28	119.79	118.20
1	L1	940	PSU	C6-C5-C4	2.28	119.79	118.20
2	L2	662	PSU	C6-C5-C4	2.28	119.79	118.20
51	S1	2202	PSU	C6-C5-C4	2.27	119.78	118.20
1	L1	955	A2M	C5-C6-N6	2.26	123.79	120.35
51	S1	1623	OMG	O6-C6-C5	-2.25	119.97	124.37
51	S1	668	A2M	C3'-C2'-C1'	2.25	107.12	102.89
1	L1	1526	PSU	O2-C2-N1	-2.25	120.31	122.79
1	L1	1524	OMG	O2'-C2'-C1'	2.25	113.55	109.09
1	L1	681	A2M	C5-C6-N6	2.25	123.77	120.35
1	L1	48	OMU	O4'-C1'-N1	2.25	113.50	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1403	PSU	O4'-C1'-C2'	2.24	108.30	105.14
51	S1	1539	PSU	O2-C2-N1	-2.24	120.33	122.79
51	S1	2021	A2M	C5-C6-N6	2.24	123.75	120.35
1	L1	1528	PSU	C6-C5-C4	2.23	119.76	118.20
1	L1	422	PSU	C6-C5-C4	2.23	119.76	118.20
1	L1	1526	PSU	O4'-C1'-C2'	2.23	108.28	105.14
1	L1	305	A2M	O4'-C1'-C2'	-2.22	102.73	106.59
2	L2	628	A2M	C5-C6-N6	2.22	123.73	120.35
51	S1	1865	OMG	O6-C6-C5	-2.22	120.03	124.37
1	L1	678	A2M	C5-C6-N6	2.22	123.72	120.35
1	L1	422	PSU	O2-C2-N1	-2.21	120.36	122.79
2	L2	597	PSU	C6-C5-C4	2.21	119.74	118.20
2	L2	1360	OMG	O6-C6-C5	-2.21	120.06	124.37
52	S2	37	MIA	C16-C14-C15	2.21	119.47	114.60
51	S1	1478	OMG	O6-C6-C5	-2.20	120.07	124.37
1	L1	69	A2M	C3'-C2'-C1'	2.20	107.03	102.89
2	L2	71	OMG	O6-C6-C5	-2.19	120.09	124.37
2	L2	1058	PSU	O2-C2-N1	-2.19	120.38	122.79
2	L2	527	A2M	O4'-C1'-C2'	-2.17	102.82	106.59
2	L2	686	OMG	O6-C6-C5	-2.17	120.13	124.37
2	L2	1046	OMG	O6-C6-C5	-2.17	120.14	124.37
51	S1	2151	OMG	N2-C2-N1	2.17	121.33	116.71
1	L1	774	PSU	C2'-C3'-C4'	-2.16	98.44	102.64
7	L7	75	OMG	O6-C6-C5	-2.15	120.16	124.37
1	L1	1177	PSU	C6-C5-C4	2.15	119.70	118.20
2	L2	1229	OMG	O6-C6-C5	-2.15	120.18	124.37
2	L2	655	OMG	O6-C6-C5	-2.14	120.19	124.37
51	S1	1833	OMU	O2-C2-N1	-2.14	119.95	122.79
2	L2	14	OMC	O3'-C3'-C2'	2.14	117.23	111.17
2	L2	641	OMG	O6-C6-C5	-2.14	120.20	124.37
7	L7	101	PSU	O4'-C1'-C2'	2.13	108.15	105.14
1	L1	1190	OMG	O6-C6-C5	-2.12	120.23	124.37
51	S1	2151	OMG	O6-C6-C5	-2.11	120.25	124.37
51	S1	29	OMU	O2-C2-N1	-2.11	119.98	122.79
2	L2	1231	OMG	O6-C6-C5	-2.11	120.25	124.37
51	S1	1647	OMG	O6-C6-C5	-2.10	120.27	124.37
2	L2	1303	PSU	O4'-C1'-C2'	2.10	108.11	105.14
2	L2	1067	A2M	C5-C6-N6	2.09	123.53	120.35
51	S1	1621	OMU	O2-C2-N1	-2.09	120.01	122.79
52	S2	37	MIA	C4-C5-N7	-2.09	107.22	109.40
51	S1	600	OMG	O6-C6-C5	-2.08	120.32	124.37
2	L2	686	OMG	N2-C2-N1	2.07	121.12	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	802	PSU	O4'-C1'-C2'	2.07	108.06	105.14
1	L1	856	OMG	O6-C6-C5	-2.07	120.34	124.37
51	S1	1543	B8N	C5'-C4'-C3'	-2.06	107.47	115.18
2	L2	560	OMU	C2'-C3'-C4'	-2.06	97.52	101.99
2	L2	534	OMG	O6-C6-C5	-2.06	120.35	124.37
2	L2	655	OMG	N2-C2-N1	2.06	121.09	116.71
1	L1	69	A2M	O3'-C3'-C4'	2.05	116.99	111.05
2	L2	626	PSU	O2-C2-N1	-2.05	120.53	122.79
1	L1	1524	OMG	O6-C6-C5	-2.05	120.37	124.37
1	L1	856	OMG	N2-C2-N1	2.04	121.07	116.71
1	L1	1371	OMU	O2-C2-N3	-2.04	117.70	121.50
51	S1	1192	PSU	C6-C5-C4	2.04	119.62	118.20
2	L2	1231	OMG	N2-C2-N1	2.04	121.06	116.71
1	L1	1626	OMG	O6-C6-C5	2.03	128.34	124.37
2	L2	1078	OMG	O6-C6-C5	-2.02	120.42	124.37
2	L2	655	OMG	N1-C2-N3	-2.02	119.54	123.32
7	L7	69	PSU	O4'-C1'-C2'	2.02	107.99	105.14
1	L1	1524	OMG	N2-C2-N1	2.01	121.00	116.71
51	S1	661	OMU	O2-C2-N1	-2.01	120.12	122.79
2	L2	593	PSU	C6-C5-C4	2.00	119.60	118.20
2	L2	565	PSU	C2'-C3'-C4'	-2.00	98.75	102.64

There are no chirality outliers.

All (157) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L7	162	A2M	C1'-C2'-O2'-CM'
1	L1	48	OMU	O4'-C1'-N1-C2
1	L1	48	OMU	O4'-C1'-N1-C6
1	L1	305	A2M	O4'-C4'-C5'-O5'
1	L1	510	PSU	C2'-C1'-C5-C6
1	L1	681	A2M	O4'-C4'-C5'-O5'
1	L1	681	A2M	C1'-C2'-O2'-CM'
1	L1	695	OMC	C1'-C2'-O2'-CM2
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	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	1524	OMG	C1'-C2'-O2'-CM2
1	L1	1540	OMG	O4'-C4'-C5'-O5'
2	L2	95	A2M	C1'-C2'-O2'-CM'
2	L2	443	OMC	C2'-C1'-N1-C6
2	L2	502	A2M	O4'-C4'-C5'-O5'
2	L2	502	A2M	C3'-C4'-C5'-O5'
2	L2	534	OMG	O4'-C4'-C5'-O5'
2	L2	534	OMG	C3'-C4'-C5'-O5'
2	L2	560	OMU	C1'-C2'-O2'-CM2
2	L2	647	A2M	O4'-C4'-C5'-O5'
2	L2	647	A2M	C1'-C2'-O2'-CM'
2	L2	686	OMG	O4'-C4'-C5'-O5'
2	L2	686	OMG	C3'-C4'-C5'-O5'
2	L2	802	PSU	C3'-C4'-C5'-O5'
2	L2	802	PSU	O4'-C4'-C5'-O5'
2	L2	1046	OMG	O4'-C4'-C5'-O5'
2	L2	1046	OMG	C1'-C2'-O2'-CM2
2	L2	1229	OMG	O4'-C4'-C5'-O5'
2	L2	1229	OMG	C3'-C4'-C5'-O5'
2	L2	1264	PSU	C3'-C4'-C5'-O5'
2	L2	1264	PSU	O4'-C4'-C5'-O5'
2	L2	1361	PSU	C3'-C4'-C5'-O5'
51	S1	18	OMC	C1'-C2'-O2'-CM2
51	S1	29	OMU	C1'-C2'-O2'-CM2
51	S1	455	PSU	C3'-C4'-C5'-O5'
51	S1	512	A2M	C1'-C2'-O2'-CM'
51	S1	600	OMG	O4'-C4'-C5'-O5'
51	S1	668	A2M	C3'-C4'-C5'-O5'
51	S1	668	A2M	C1'-C2'-O2'-CM'
51	S1	1543	B8N	N34-C33-C34-O35
51	S1	1543	B8N	N3-C31-C32-C33
51	S1	1543	B8N	C31-C32-C33-N34
51	S1	1566	PSU	C3'-C4'-C5'-O5'
51	S1	1566	PSU	O4'-C4'-C5'-O5'
51	S1	1662	OMU	C1'-C2'-O2'-CM2
51	S1	1829	OMG	C1'-C2'-O2'-CM2
51	S1	2021	A2M	C1'-C2'-O2'-CM'
51	S1	2059	OMC	O4'-C1'-N1-C2
51	S1	2059	OMC	O4'-C1'-N1-C6
51	S1	1543	B8N	N34-C33-C34-O36
2	L2	443	OMC	C2'-C1'-N1-C2
1	L1	313	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L1	681	A2M	C3'-C4'-C5'-O5'
1	L1	1010	OMC	C3'-C4'-C5'-O5'
1	L1	1010	OMC	O4'-C4'-C5'-O5'
1	L1	1528	PSU	O4'-C4'-C5'-O5'
1	L1	1540	OMG	C3'-C4'-C5'-O5'
2	L2	14	OMC	C3'-C4'-C5'-O5'
2	L2	1046	OMG	C3'-C4'-C5'-O5'
2	L2	1361	PSU	O4'-C4'-C5'-O5'
51	S1	8	OMU	O4'-C4'-C5'-O5'
51	S1	600	OMG	C3'-C4'-C5'-O5'
51	S1	668	A2M	O4'-C4'-C5'-O5'
1	L1	305	A2M	C3'-C4'-C5'-O5'
1	L1	1171	PSU	O4'-C4'-C5'-O5'
2	L2	14	OMC	O4'-C4'-C5'-O5'
2	L2	647	A2M	C3'-C4'-C5'-O5'
2	L2	665	A2M	C3'-C4'-C5'-O5'
51	S1	98	A2M	O4'-C4'-C5'-O5'
51	S1	1995	7MG	C3'-C4'-C5'-O5'
51	S1	2061	5MC	O4'-C4'-C5'-O5'
51	S1	2061	5MC	C3'-C4'-C5'-O5'
51	S1	2151	OMG	C3'-C4'-C5'-O5'
51	S1	8	OMU	C2'-C1'-N1-C6
1	L1	1528	PSU	C3'-C4'-C5'-O5'
1	L1	1664	PSU	C3'-C4'-C5'-O5'
4	L4	74	OMG	C3'-C4'-C5'-O5'
51	S1	1995	7MG	O4'-C4'-C5'-O5'
51	S1	1543	B8N	C32-C33-C34-O36
51	S1	1543	B8N	C32-C33-C34-O35
1	L1	313	PSU	O4'-C4'-C5'-O5'
1	L1	1017	PSU	O4'-C4'-C5'-O5'
1	L1	1664	PSU	O4'-C4'-C5'-O5'
2	L2	665	A2M	O4'-C4'-C5'-O5'
2	L2	1185	A2M	C3'-C4'-C5'-O5'
51	S1	455	PSU	O4'-C4'-C5'-O5'
51	S1	2151	OMG	O4'-C4'-C5'-O5'
2	L2	1308	5MC	C2'-C1'-N1-C6
1	L1	959	OMG	C3'-C4'-C5'-O5'
1	L1	69	A2M	C3'-C4'-C5'-O5'
1	L1	1017	PSU	C3'-C4'-C5'-O5'
51	S1	8	OMU	C3'-C4'-C5'-O5'
51	S1	1543	B8N	C3'-C4'-C5'-O5'
1	L1	959	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L1	69	A2M	O4'-C4'-C5'-O5'
4	L4	74	OMG	O4'-C4'-C5'-O5'
51	S1	2140	OMC	O4'-C4'-C5'-O5'
51	S1	1543	B8N	C31-C32-C33-C34
2	L2	443	OMC	O4'-C1'-N1-C2
2	L2	443	OMC	O4'-C1'-N1-C6
51	S1	8	OMU	O4'-C1'-N1-C6
51	S1	1543	B8N	C4'-C5'-O5'-P
2	L2	527	A2M	C3'-C4'-C5'-O5'
2	L2	1078	OMG	O4'-C4'-C5'-O5'
51	S1	8	OMU	C2'-C1'-N1-C2
1	L1	681	A2M	C4'-C5'-O5'-P
51	S1	33	PSU	O4'-C4'-C5'-O5'
51	S1	512	A2M	C3'-C4'-C5'-O5'
2	L2	1248	OMC	C4'-C5'-O5'-P
51	S1	1478	OMG	C4'-C5'-O5'-P
51	S1	2185	MA6	C4'-C5'-O5'-P
2	L2	1308	5MC	O4'-C1'-N1-C6
2	L2	560	OMU	C3'-C4'-C5'-O5'
51	S1	1192	PSU	O4'-C4'-C5'-O5'
2	L2	1308	5MC	C2'-C1'-N1-C2
2	L2	527	A2M	C3'-C2'-O2'-CM'
51	S1	8	OMU	C3'-C2'-O2'-CM2
51	S1	1550	OMG	C3'-C2'-O2'-CM2
2	L2	560	OMU	C4'-C5'-O5'-P
2	L2	1361	PSU	C4'-C5'-O5'-P
51	S1	1829	OMG	C4'-C5'-O5'-P
1	L1	1526	PSU	C3'-C4'-C5'-O5'
1	L1	1526	PSU	O4'-C4'-C5'-O5'
51	S1	8	OMU	O4'-C1'-N1-C2
2	L2	527	A2M	O4'-C4'-C5'-O5'
51	S1	1192	PSU	C3'-C4'-C5'-O5'
1	L1	510	PSU	O4'-C1'-C5-C4
1	L1	1526	PSU	O4'-C1'-C5-C4
2	L2	1361	PSU	O4'-C1'-C5-C4
51	S1	1657	PSU	O4'-C1'-C5-C4
2	L2	1308	5MC	O4'-C1'-N1-C2
1	L1	1371	OMU	C3'-C4'-C5'-O5'
2	L2	1078	OMG	C3'-C4'-C5'-O5'
51	S1	98	A2M	C3'-C4'-C5'-O5'
51	S1	1543	B8N	O4'-C4'-C5'-O5'
51	S1	1833	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
51	S1	2059	OMC	O4'-C4'-C5'-O5'
51	S1	1979	OMU	C4'-C5'-O5'-P
4	L4	74	OMG	C1'-C2'-O2'-CM2
51	S1	2140	OMC	C1'-C2'-O2'-CM2
1	L1	510	PSU	O4'-C1'-C5-C6
2	L2	1361	PSU	O4'-C1'-C5-C6
51	S1	2202	PSU	O4'-C1'-C5-C6
1	L1	1526	PSU	C4'-C5'-O5'-P
1	L1	1527	OMC	O4'-C4'-C5'-O5'
2	L2	56	OMU	O4'-C4'-C5'-O5'
51	S1	2140	OMC	C3'-C4'-C5'-O5'
1	L1	1539	A2M	C3'-C2'-O2'-CM'
2	L2	1185	A2M	O4'-C4'-C5'-O5'
51	S1	33	PSU	C3'-C4'-C5'-O5'
3	L3	13	OMU	C2'-C1'-N1-C2

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 520 ligands modelled in this entry, 519 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
93	A1H4F	L2	1601	-	32,32,32	4.25	11 (34%)	37,42,42	1.42	5 (13%)

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
93	A1H4F	L2	1601	-	-	9/26/39/39	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
93	L2	1601	A1H4F	C03-C02	-16.85	1.28	1.53
93	L2	1601	A1H4F	C27-C05	-11.96	1.29	1.53
93	L2	1601	A1H4F	C13-N14	6.04	1.46	1.34
93	L2	1601	A1H4F	C02-C27	5.95	1.65	1.53
93	L2	1601	A1H4F	O28-C29	3.78	1.43	1.35
93	L2	1601	A1H4F	C05-N04	3.58	1.55	1.48
93	L2	1601	A1H4F	C06-C05	2.94	1.59	1.53
93	L2	1601	A1H4F	C03-N04	2.61	1.56	1.47
93	L2	1601	A1H4F	C06-C07	2.51	1.57	1.51
93	L2	1601	A1H4F	O11-C10	2.21	1.42	1.37
93	L2	1601	A1H4F	C12-C13	2.04	1.55	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	L2	1601	A1H4F	O28-C29-C30	5.01	120.30	111.09
93	L2	1601	A1H4F	C12-C13-N14	3.01	121.61	116.37
93	L2	1601	A1H4F	C12-O11-C10	-2.90	112.57	117.67
93	L2	1601	A1H4F	O23-C21-C15	2.26	120.92	113.40
93	L2	1601	A1H4F	O23-C21-O22	-2.08	119.36	124.09

There are no chirality outliers.

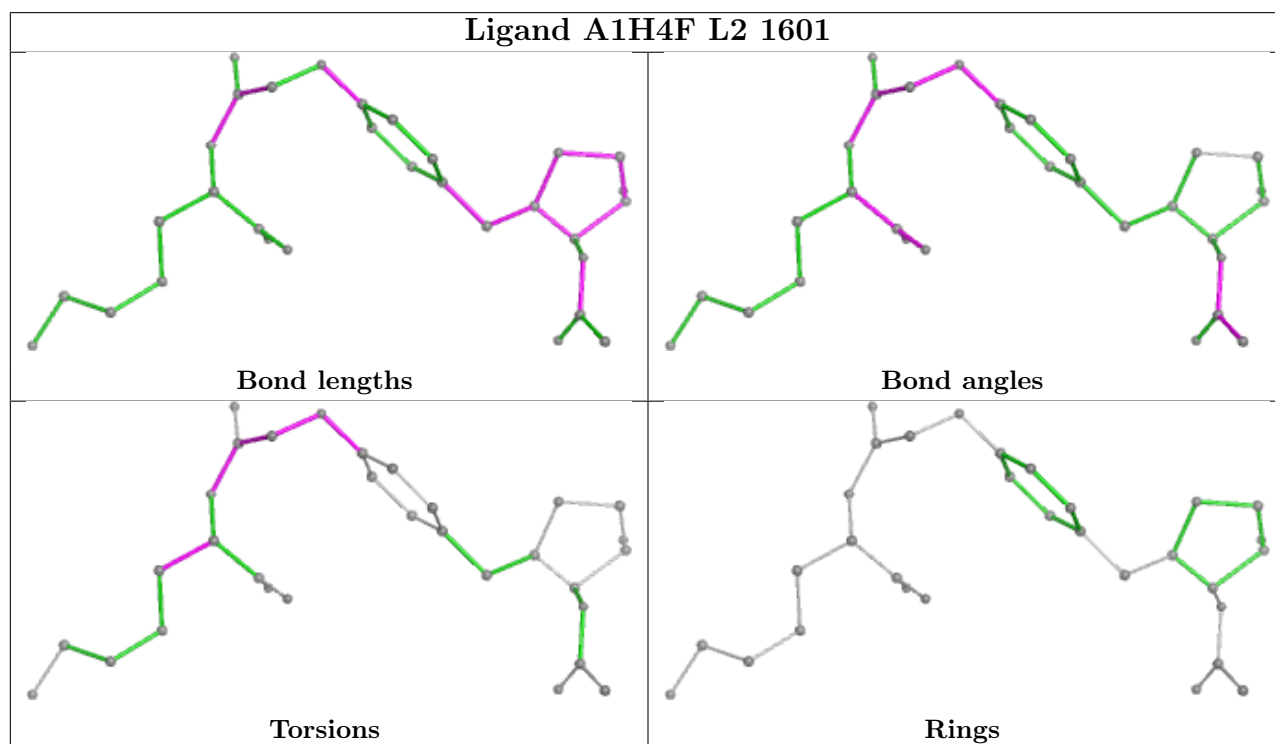
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
93	L2	1601	A1H4F	C12-C13-N14-C15
93	L2	1601	A1H4F	O24-C13-N14-C15
93	L2	1601	A1H4F	C09-C10-O11-C12
93	L2	1601	A1H4F	C25-C10-O11-C12
93	L2	1601	A1H4F	N14-C15-C16-C17
93	L2	1601	A1H4F	C21-C15-C16-C17
93	L2	1601	A1H4F	O11-C12-C13-N14
93	L2	1601	A1H4F	O11-C12-C13-O24
93	L2	1601	A1H4F	C13-C12-O11-C10

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	3.54
1	S1	1542:C	O3'	1543:B8N	P	2.98

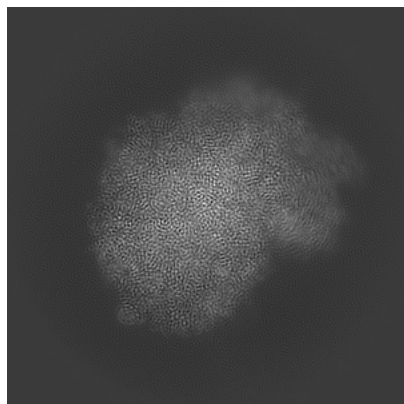
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19576. These allow visual inspection of the internal detail of the map and identification of artifacts.

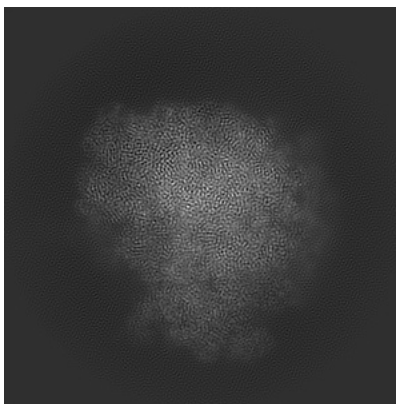
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

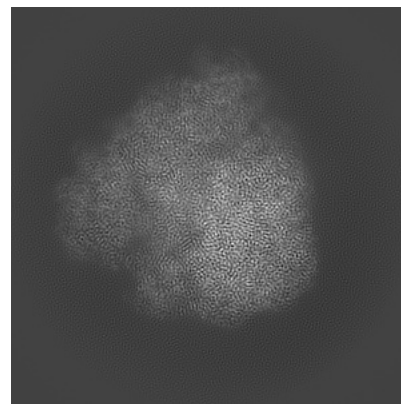
6.1.1 Primary map



X

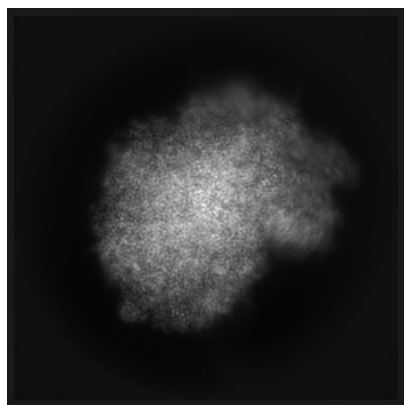


Y

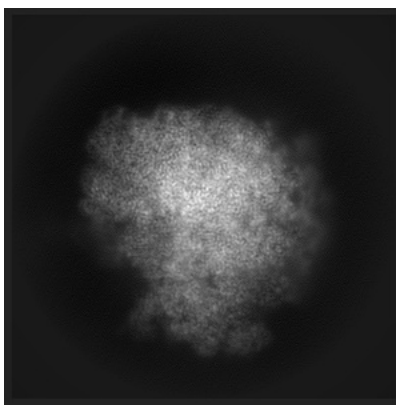


Z

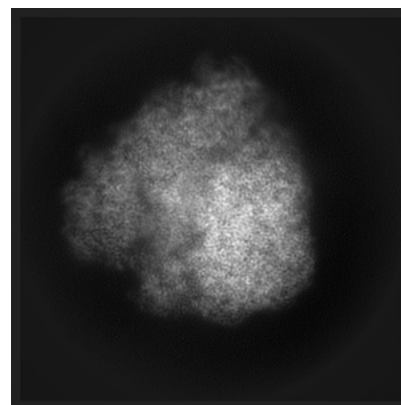
6.1.2 Raw map



X



Y

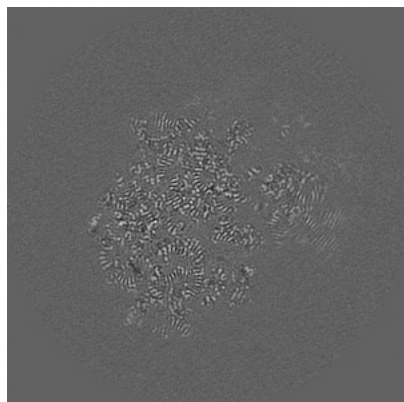


Z

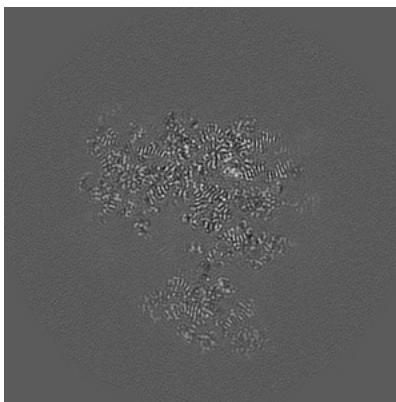
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

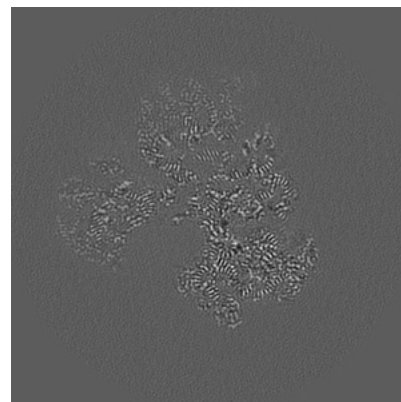
6.2.1 Primary map



X Index: 240

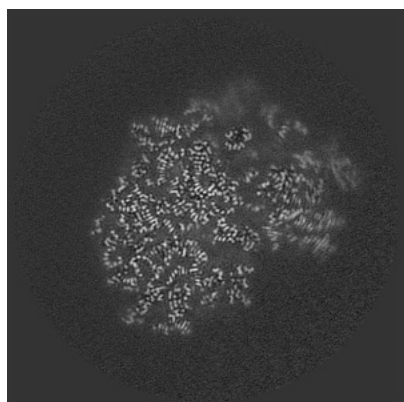


Y Index: 240

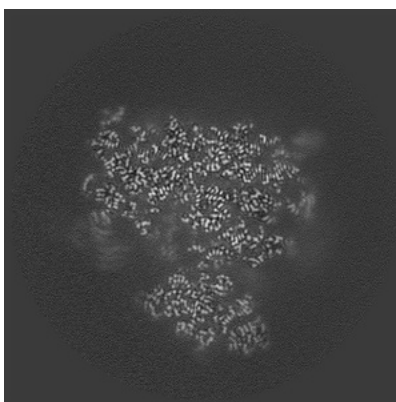


Z Index: 240

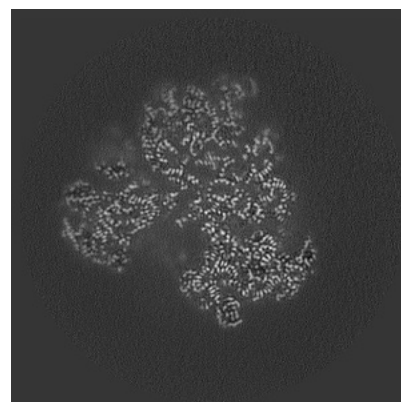
6.2.2 Raw map



X Index: 240



Y Index: 240

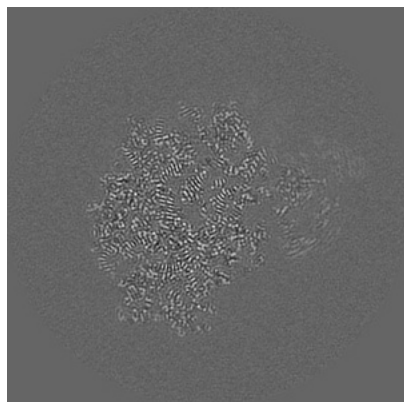


Z Index: 240

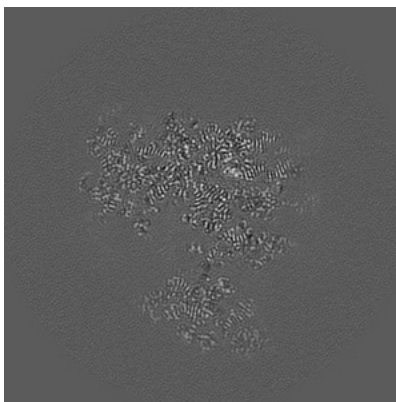
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

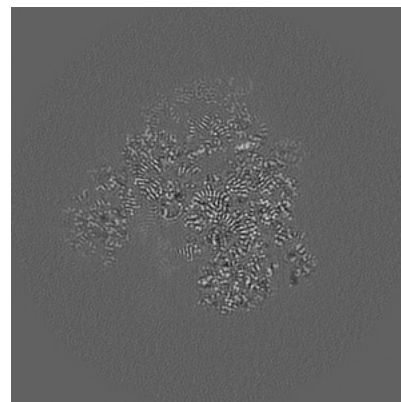
6.3.1 Primary map



X Index: 270

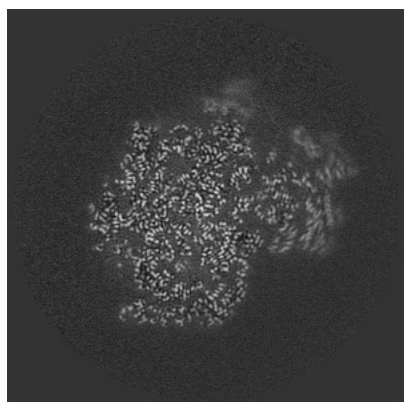


Y Index: 240

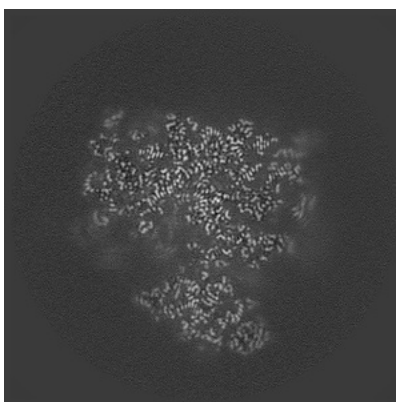


Z Index: 259

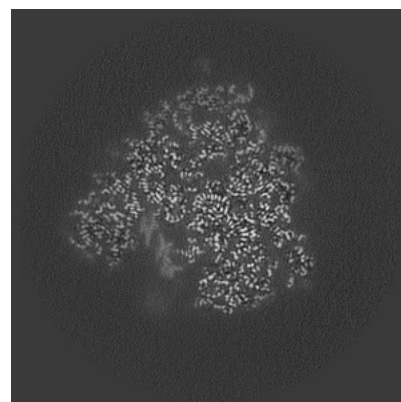
6.3.2 Raw map



X Index: 255



Y Index: 236

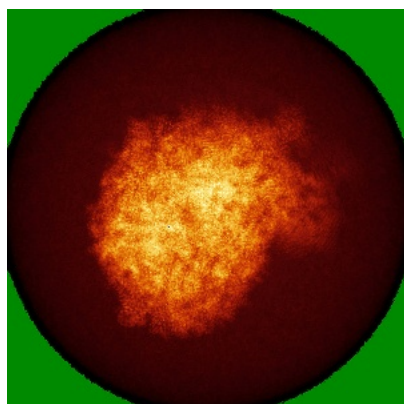


Z Index: 259

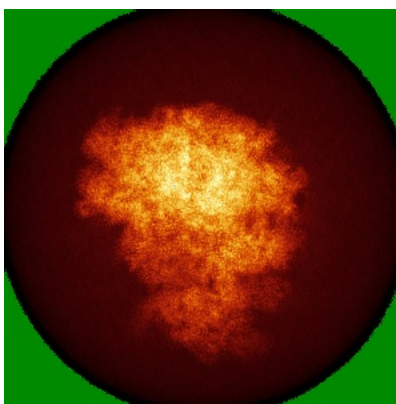
The images above show the largest variance slices of the map in three orthogonal directions.

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

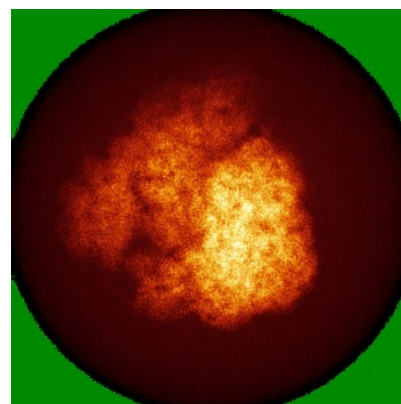
6.4.1 Primary map



X

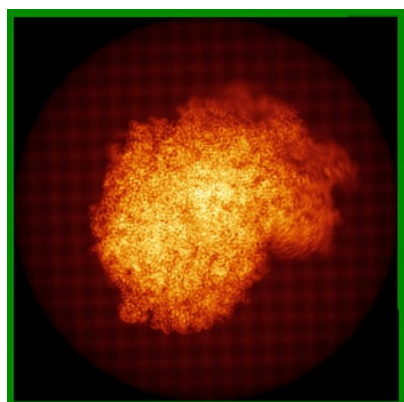


Y

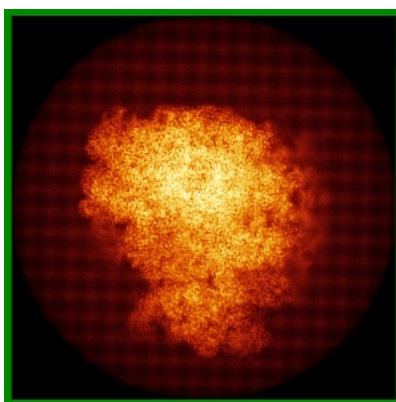


Z

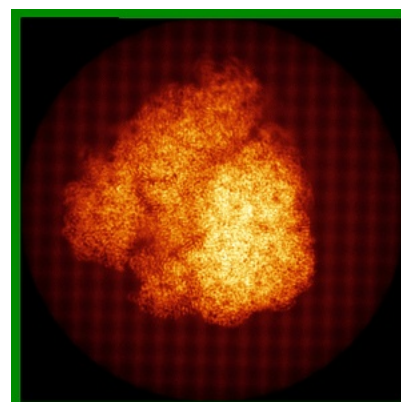
6.4.2 Raw map



X



Y

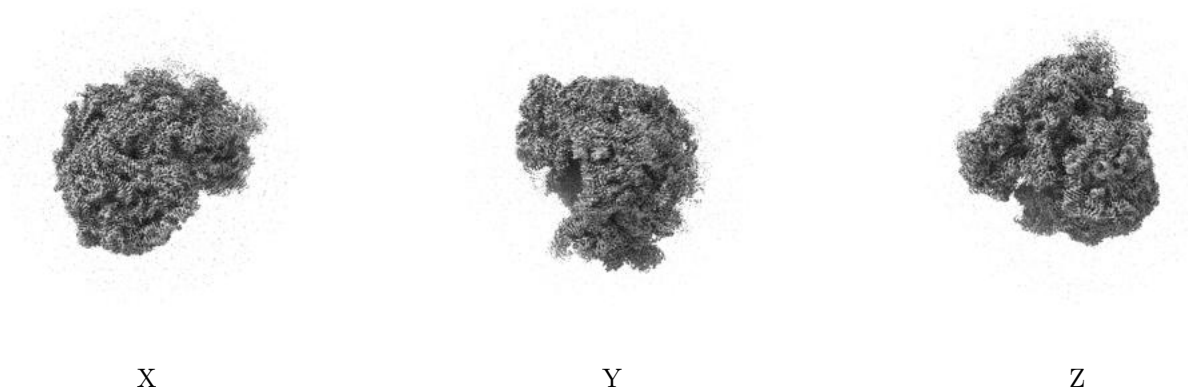


Z

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 0.015. 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.

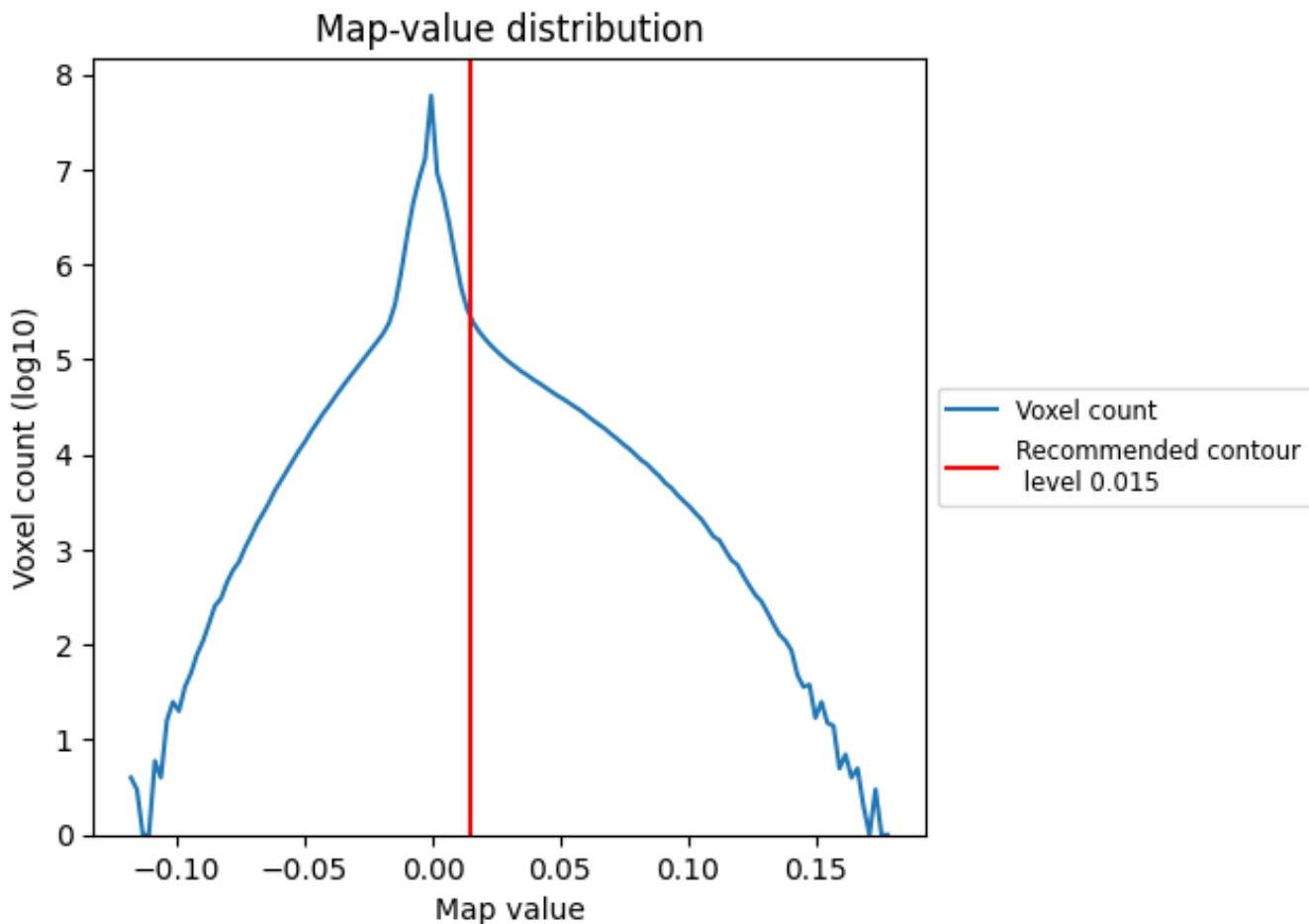
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

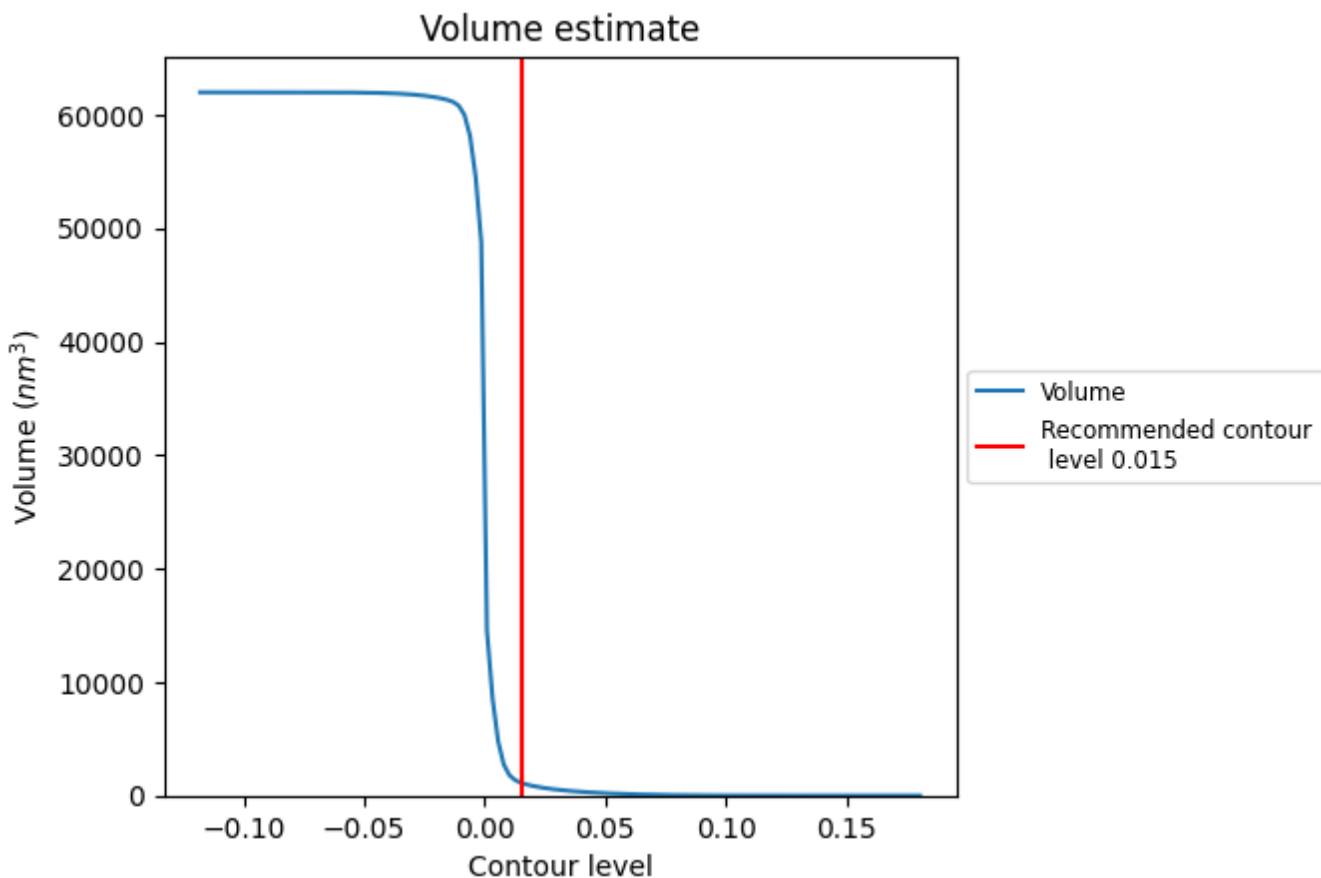
This section contains the results of statistical analysis of the map.

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.

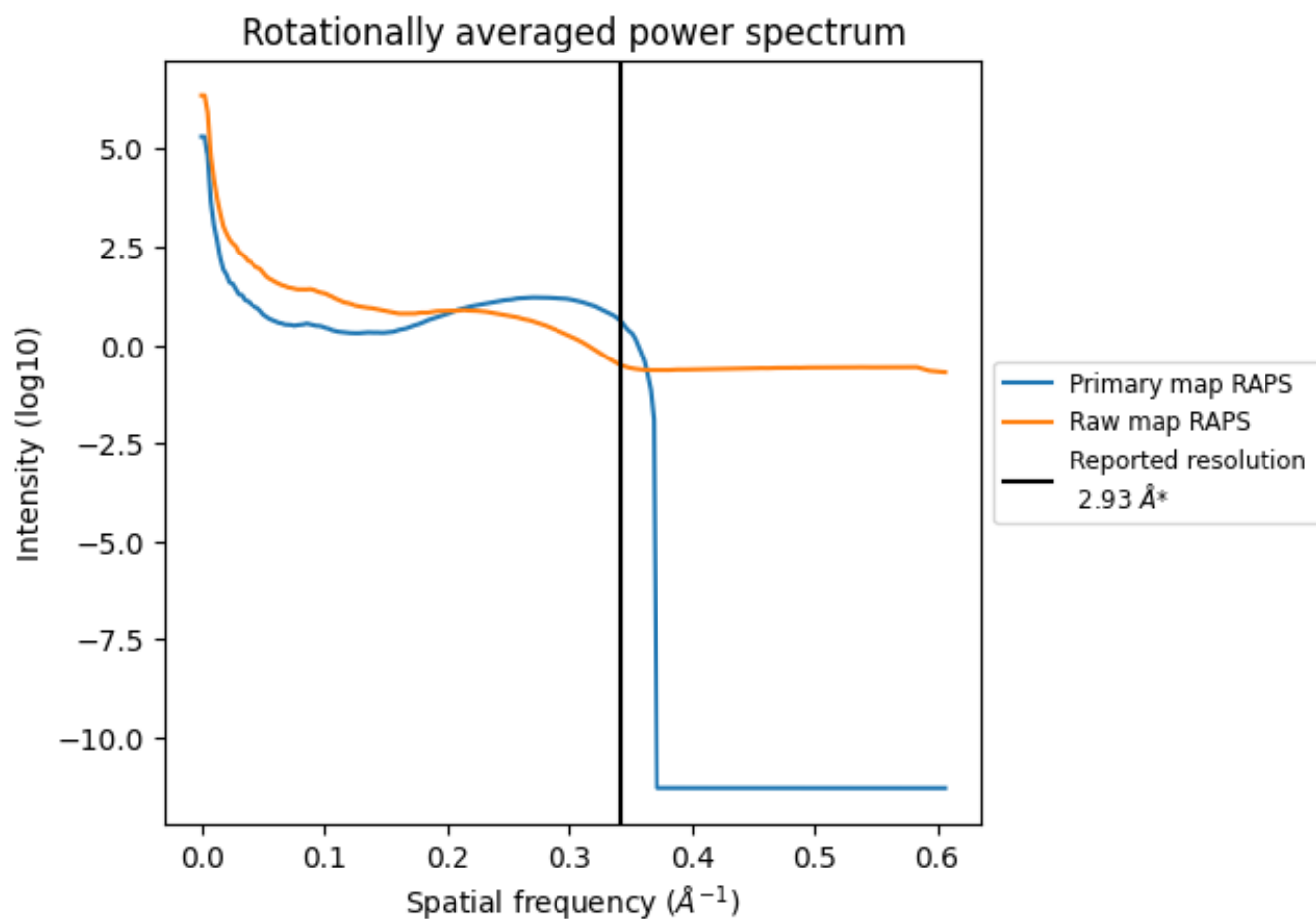
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1131 nm^3 ; this corresponds to an approximate mass of 1022 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](#)

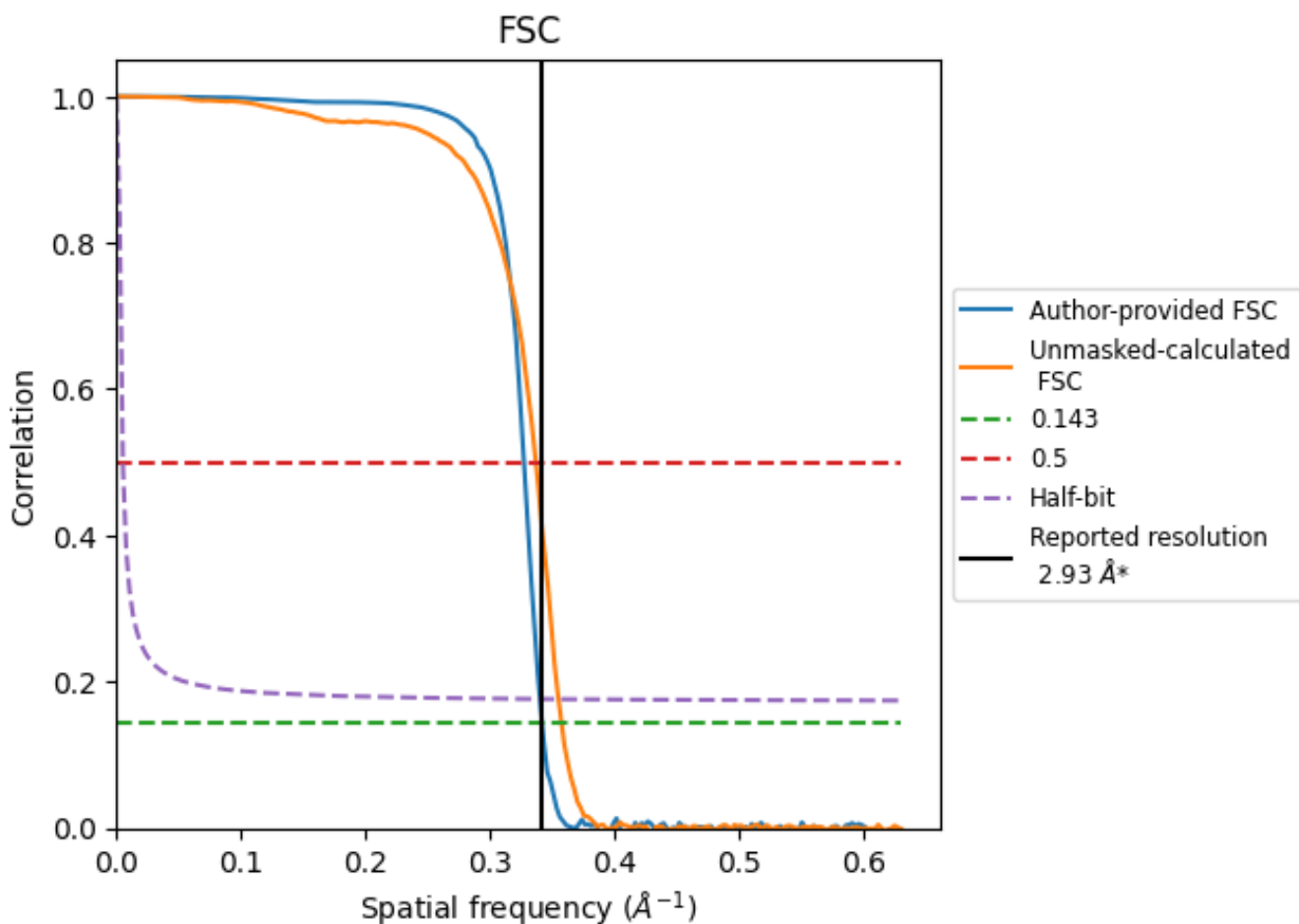


*Reported resolution corresponds to spatial frequency of 0.341 Å⁻¹

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 0.341 Å⁻¹

8.2 Resolution estimates [i](#)

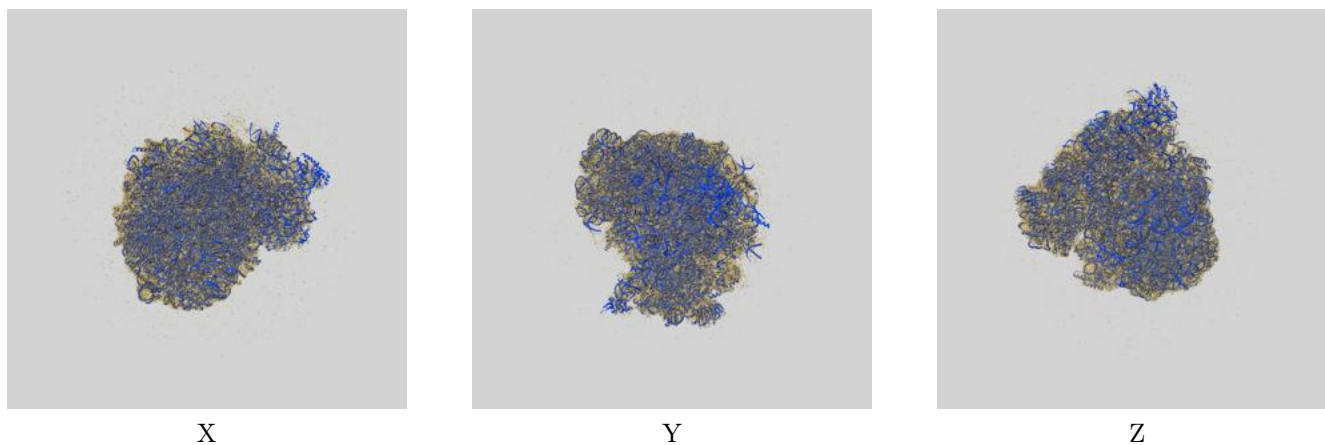
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.92	3.05	2.94
Unmasked-calculated*	2.80	2.97	2.82

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

9 Map-model fit [i](#)

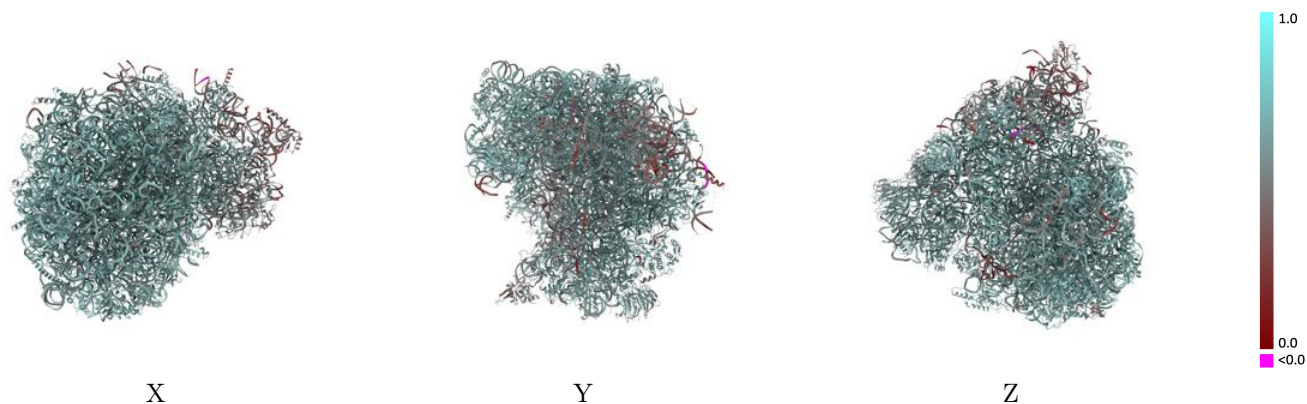
This section contains information regarding the fit between EMDB map EMD-19576 and PDB model 8RXH. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



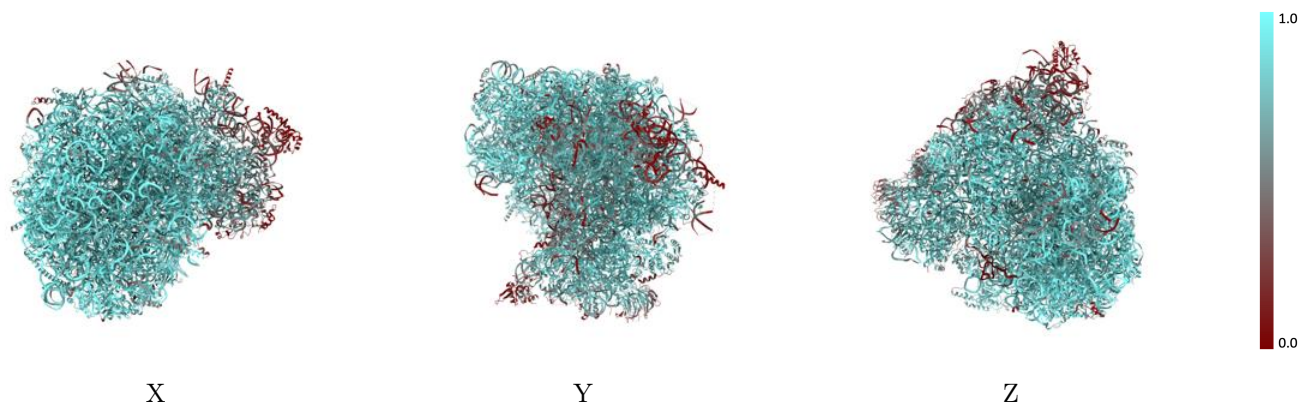
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



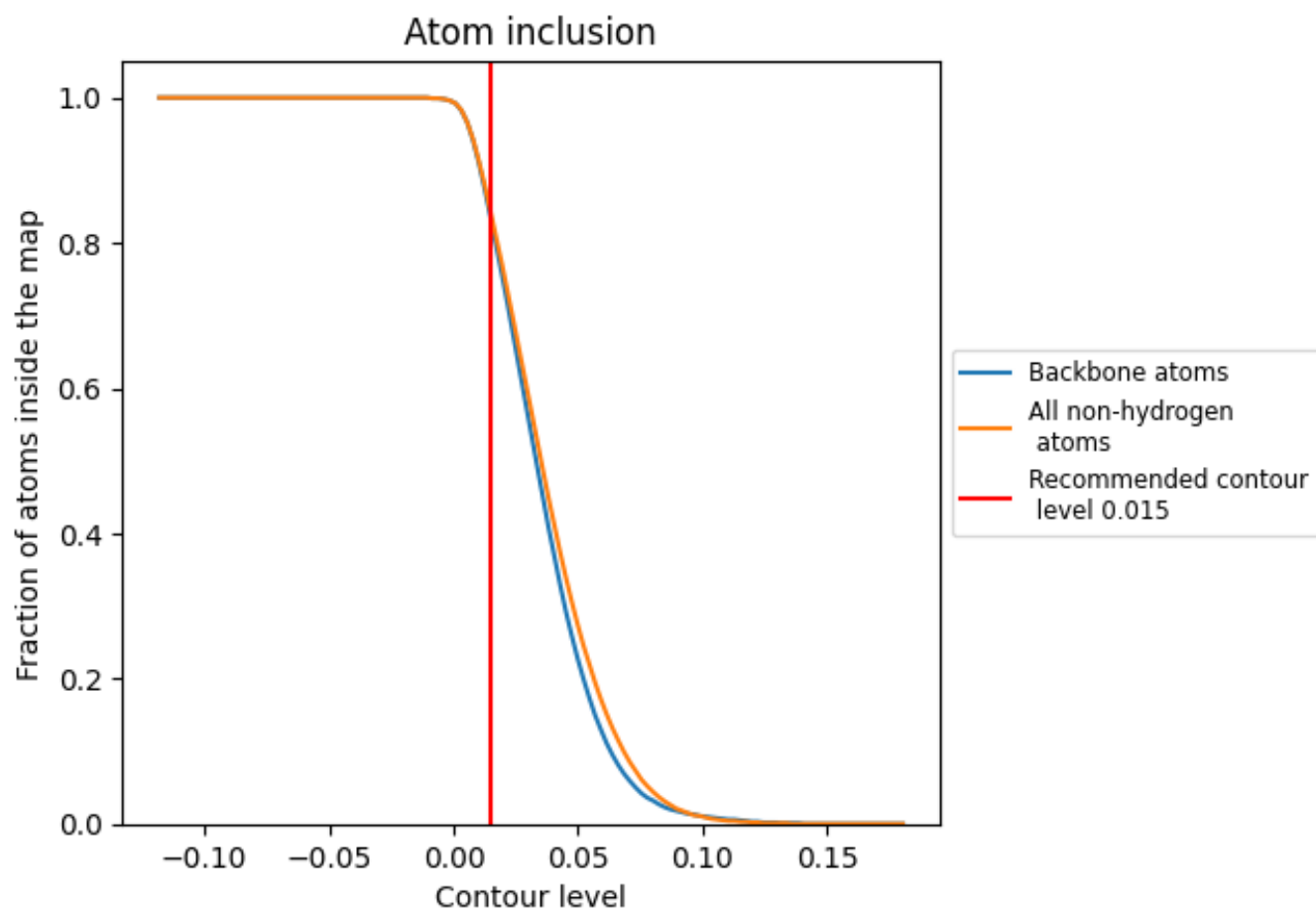
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.6030
L1	 0.9320	 0.6220
L2	 0.9180	 0.6170
L3	 0.8960	 0.6070
L4	 0.9590	 0.6350
L5	 0.8820	 0.6040
L6	 0.8930	 0.6060
L7	 0.9420	 0.6280
L8	 0.9610	 0.6320
LA	 0.9610	 0.6540
LB	 0.9350	 0.6480
LC	 0.9460	 0.6480
LD	 0.7950	 0.6200
LE	 0.9070	 0.6430
LF	 0.8420	 0.6220
LG	 0.8390	 0.6190
LH	 0.9400	 0.6510
LI	 0.8920	 0.6400
LJ	 0.9370	 0.6450
LK	 0.8420	 0.6300
LL	 0.9530	 0.6560
LM	 0.9800	 0.6600
LN	 0.8920	 0.6370
LO	 0.8180	 0.6190
LP	 0.9580	 0.6520
LQ	 0.7810	 0.6070
LR	 0.9520	 0.6510
LS	 0.9180	 0.6380
LT	 0.9700	 0.6580
LU	 0.6830	 0.6010
LV	 0.9440	 0.6490
LW	 0.9420	 0.6530
LX	 0.7440	 0.5880
LY	 0.8830	 0.6370
LZ	 0.9170	 0.6470





























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Chain	Atom inclusion	Q-score
La	 0.9080	 0.6420
Lb	 0.9470	 0.6470
Lc	 0.9490	 0.6530
Ld	 0.8790	 0.6220
Le	 0.8420	 0.6300
Lf	 0.9300	 0.6430
Lg	 0.9470	 0.6540
Lh	 0.8720	 0.6250
Li	 0.8480	 0.6220
Lj	 0.9760	 0.6570
Lk	 0.8260	 0.6310
Ll	 0.9600	 0.6520
Lm	 0.9080	 0.6390
Ln	 0.9080	 0.6330
Lo	 0.9340	 0.6380
Lp	 0.9490	 0.6520
S1	 0.7820	 0.5580
S2	 0.2470	 0.3850
S3	 0.6870	 0.5430
S4	 0.3680	 0.3940
S5	 0.8180	 0.5790
SA	 0.8530	 0.6310
SB	 0.8440	 0.6220
SC	 0.7350	 0.6070
SD	 0.5680	 0.5300
SE	 0.5580	 0.5210
SF	 0.8710	 0.6360
SG	 0.4640	 0.5130
SH	 0.8320	 0.6220
SI	 0.8130	 0.6140
SJ	 0.9330	 0.6430
SK	 0.7710	 0.5930
SL	 0.8580	 0.6210
SM	 0.6760	 0.5900
SN	 0.6840	 0.5830
SO	 0.9080	 0.6360
SP	 0.7980	 0.5820
SQ	 0.1990	 0.4560
SR	 0.7420	 0.6060
SS	 0.8920	 0.6250
ST	 0.9080	 0.6310
SU	 0.8270	 0.6090

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Chain	Atom inclusion	Q-score
SV	 0.6950	 0.6010
SW	 0.7130	 0.6020
SX	 0.8310	 0.6170
SY	 0.8420	 0.6210
SZ	 0.3880	 0.4940
Sa	 0.6330	 0.5710
Sb	 0.9210	 0.6410
Sc	 0.8460	 0.6120
Sd	 0.7370	 0.6000
Se	 0.5230	 0.4940
Sf	 0.2880	 0.4960
Sg	 0.5490	 0.5650
Sh	 0.0860	 0.4150