Full wwPDB EM Validation Report ⓘ

Feb 5, 2025 – 05:16 PM JST

PDB ID	:	7XNX
EMDB ID	:	EMD-33329
Title	:	High resolution cry-EM structure of the human 80S ribosome from SNORD127+/+ Kasumi-1 cells
Authors	:	Cheng, J.; Beckmann, R.
Deposited on	:	2022-04-30
Resolution	:	2.70 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:

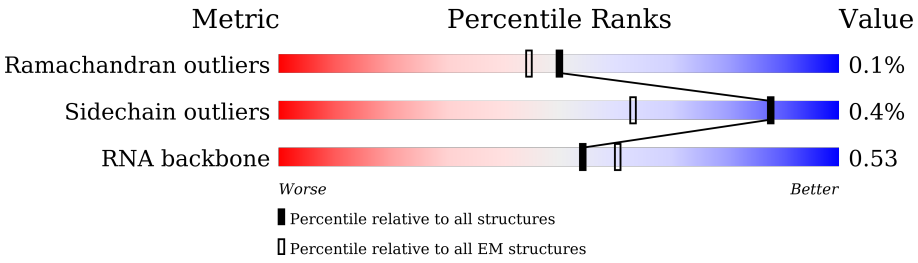
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.70 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	L1	5070	7% 56% 17% 26%
2	L2	121	88% 11%
3	L3	157	75% 24%
4	LA	257	96%
5	LB	403	100%
6	LC	427	85% 15%
7	LD	297	99%
8	LE	288	76% 24%

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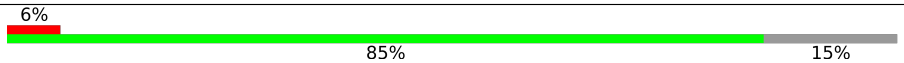
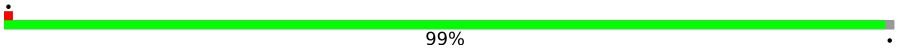
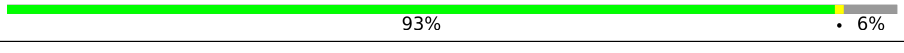
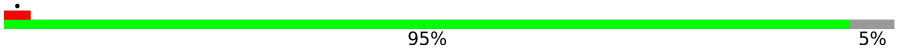
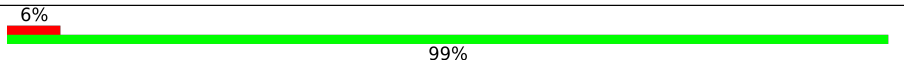
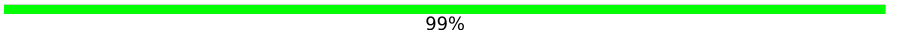
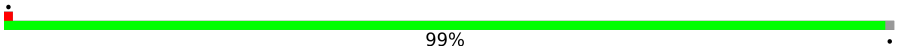
Mol	Chain	Length	Quality of chain
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
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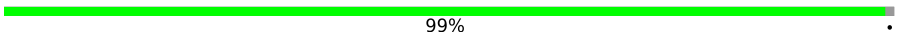
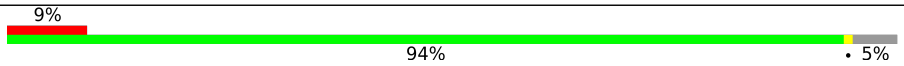
19	LQ	188	
20	LR	196	
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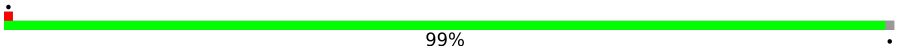
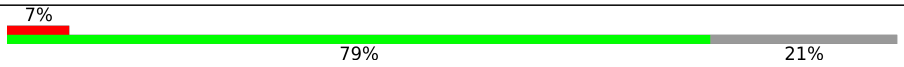
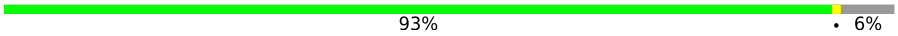
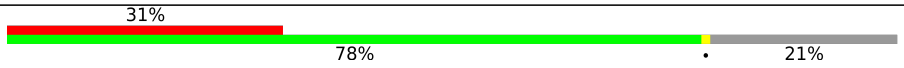
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
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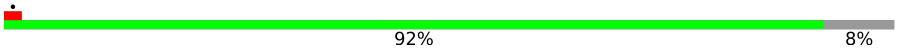
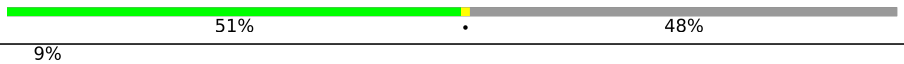
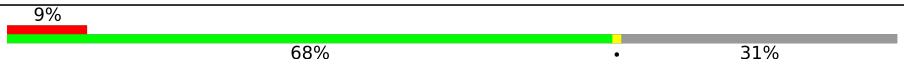
27	LY	145	
28	LZ	282	
28	La	282	
29	Lb	159	
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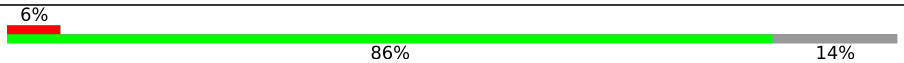
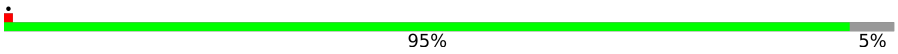
31	Ld	125	
32	Le	135	

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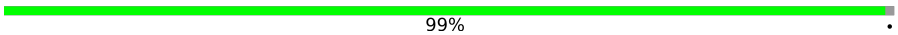
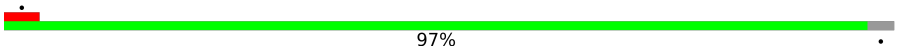
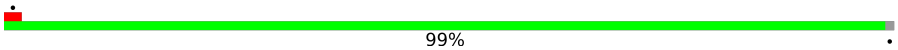
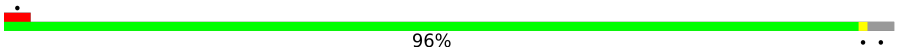
Mol	Chain	Length	Quality of chain
33	Lf	110	
34	Lg	117	
35	Lh	123	
36	Li	105	
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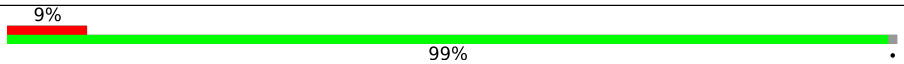
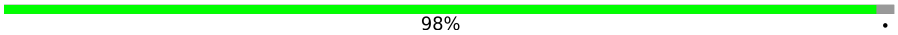
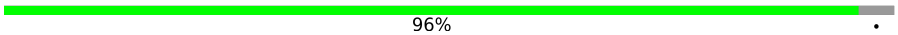
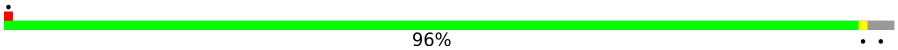
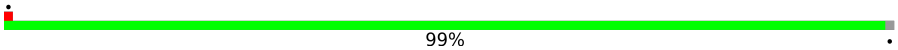
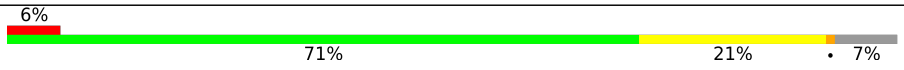
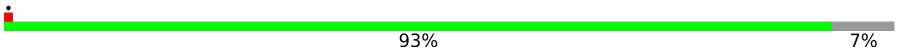
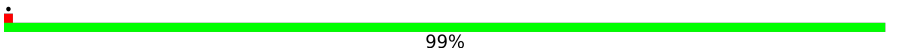
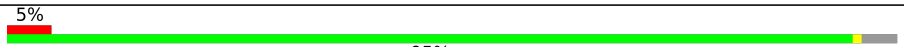
38	Lk	70	
39	Ll	51	
40	Lm	128	
41	Ln	25	
42	Lo	106	
43	Lp	92	
44	Lr	137	
45	S2	1869	
46	SA	295	
47	SB	264	
48	SD	243	
49	SE	263	
50	SF	204	
51	SH	194	
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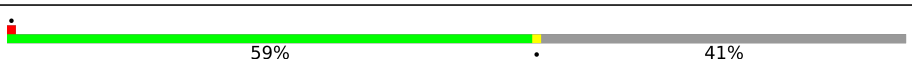
53	SK	165	
54	SL	158	
55	SP	145	
56	SQ	146	
57	SR	135	

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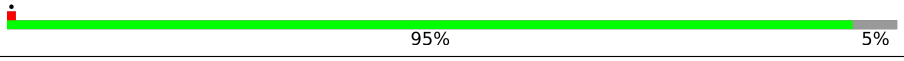
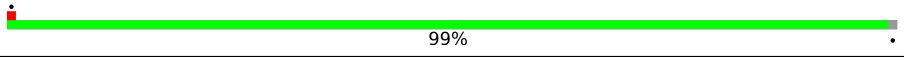
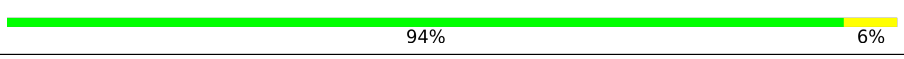
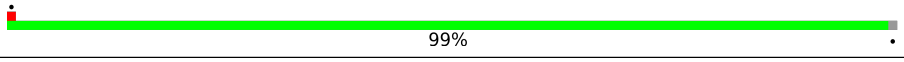
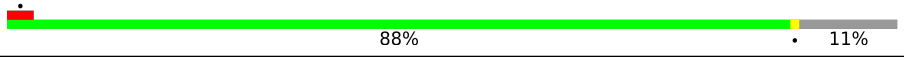
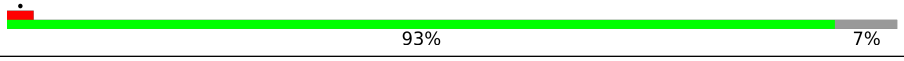
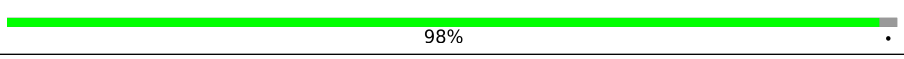
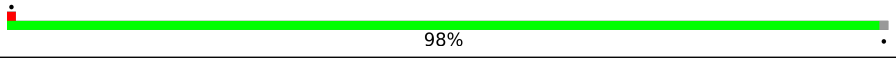
Mol	Chain	Length	Quality of chain
58	SS	152	
59	ST	145	
60	SU	119	
61	SV	83	
62	SX	143	
63	Sa	115	
64	Sc	69	
65	Sd	56	
66	Sg	317	
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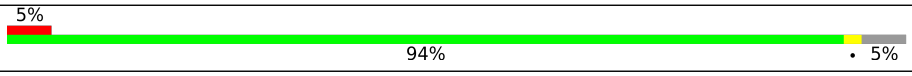
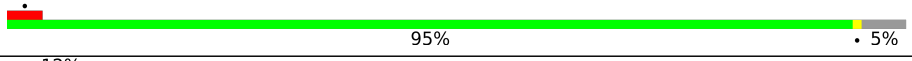
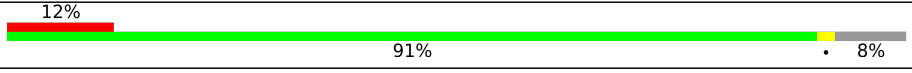
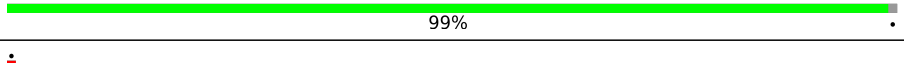
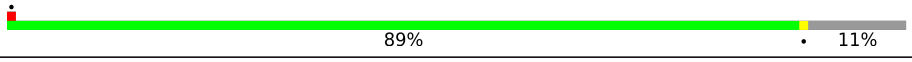
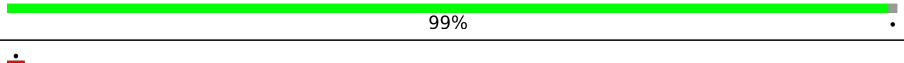
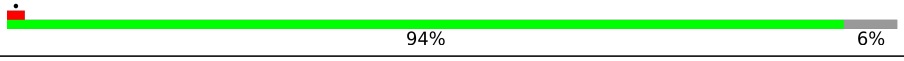
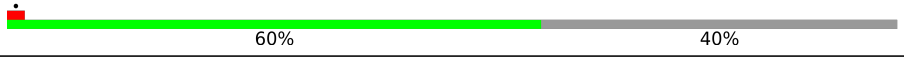
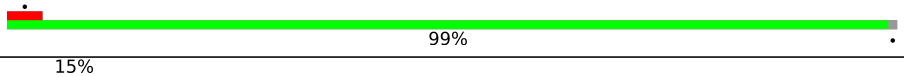
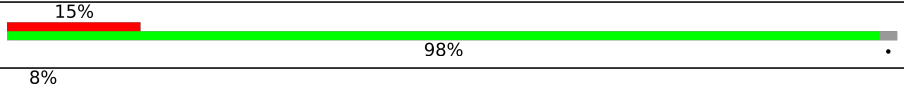
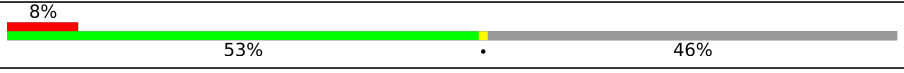
68	SG	249	
69	SJ	194	
70	SM	132	
71	SN	151	
72	SO	151	
73	SW	130	
74	SY	133	
75	SZ	125	
76	Sb	84	
77	Se	59	
78	CE	133	
78	Sf	133	
79	CC	75	

2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 218434 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L1	3773	80211	35727	14590	26122	3772	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L2	120	2558	1141	456	842	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L3	156	3316	1482	585	1094	155	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LC	365	2908	1829	580	486	13	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	220	Total	C	N	O	S	0	0
			1765	1136	334	291	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	227	Total	C	N	O	S	0	0
			1835	1171	353	307	4		

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

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

- Molecule 12 is a protein called Ribosomal protein L10 isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	202	Total	C	N	O	S	0	0
			1639	1041	316	269	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	169	Total	C	N	O	S	0	0
			1353	856	253	238	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	0	0
			1106	714	208	181	3		
28	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 29 is a protein called 60S ribosomal protein L29.

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

- Molecule 30 is a protein called 60S ribosomal protein L30.

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

- Molecule 31 is a protein called 60S ribosomal protein L31.

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

- Molecule 32 is a protein called 60S ribosomal protein L32.

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

- Molecule 33 is a protein called 60S ribosomal protein L35a.

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

- Molecule 34 is a protein called 60S ribosomal protein L34.

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

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

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

- Molecule 36 is a protein called 60S ribosomal protein L36.

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

- Molecule 37 is a protein called 60S ribosomal protein L37.

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

- Molecule 38 is a protein called 60S ribosomal protein L38.

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

- Molecule 39 is a protein called 60S ribosomal protein L39.

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

- Molecule 40 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 41 is a protein called 60S ribosomal protein L41.

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

- Molecule 42 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lo	103	Total	C	N	O	S	0	0
			843	529	172	136	6		

- Molecule 43 is a protein called 60S ribosomal protein L37a.

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

- Molecule 44 is a protein called 60S ribosomal protein L28.

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

- Molecule 45 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	S2	1740	Total	C	N	O	P	0	0
			36959	16515	6600	12105	1739		

- Molecule 46 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SA	222	Total	C	N	O	S	0	0
			1747	1109	306	324	8		

- Molecule 47 is a protein called 40S ribosomal protein S3a.

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

- Molecule 48 is a protein called 40S ribosomal protein S3.

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

- Molecule 49 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 50 is a protein called 40S ribosomal protein S5.

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

- Molecule 51 is a protein called 40S ribosomal protein S7.

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

- Molecule 52 is a protein called 40S ribosomal protein S8.

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

- Molecule 53 is a protein called 40S ribosomal protein S10.

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

- Molecule 54 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SL	144	Total	C	N	O	S	0	0
			1182	752	224	200	6		

- Molecule 55 is a protein called 40S ribosomal protein S15.

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

- Molecule 56 is a protein called 40S ribosomal protein S16.

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

- Molecule 57 is a protein called 40S ribosomal protein S17.

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

- Molecule 58 is a protein called 40S ribosomal protein S18.

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

- Molecule 59 is a protein called 40S ribosomal protein S19.

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

- Molecule 60 is a protein called 40S ribosomal protein S20.

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

- Molecule 61 is a protein called 40S ribosomal protein S21.

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

- Molecule 62 is a protein called 40S ribosomal protein S23.

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

- Molecule 63 is a protein called 40S ribosomal protein S26.

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

- Molecule 64 is a protein called 40S ribosomal protein S28.

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

- Molecule 65 is a protein called 40S ribosomal protein S29.

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

- Molecule 66 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 67 is a protein called 40S ribosomal protein S2.

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

- Molecule 68 is a protein called 40S ribosomal protein S6.

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

- Molecule 69 is a protein called 40S ribosomal protein S9.

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

- Molecule 70 is a protein called 40S ribosomal protein S12.

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

- Molecule 71 is a protein called 40S ribosomal protein S13.

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

- Molecule 72 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 73 is a protein called 40S ribosomal protein S15a.

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

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SY	125	Total	C	N	O	S	0	0
			1022	645	200	172	5		

- Molecule 75 is a protein called 40S ribosomal protein S25.

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

- Molecule 76 is a protein called 40S ribosomal protein S27.

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

- Molecule 77 is a protein called 40S ribosomal protein S30.

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

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sf	61	Total	C	N	O	S	0	0
			497	312	94	84	7		
78	CE	72	Total	C	N	O		0	0
			603	395	105	103			

- Molecule 79 is a RNA chain called tRNA.

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

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	L1	264	Total	Mg	0
			264	264	
80	L2	3	Total	Mg	0
			3	3	
80	L3	5	Total	Mg	0
			5	5	
80	LA	1	Total	Mg	0
			1	1	
80	LC	2	Total	Mg	0
			2	2	
80	LI	1	Total	Mg	0
			1	1	
80	LN	1	Total	Mg	0
			1	1	
80	LP	1	Total	Mg	0
			1	1	
80	LV	1	Total	Mg	0
			1	1	
80	Le	1	Total	Mg	0
			1	1	
80	Lf	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
80	Lg	1	Total Mg 1 1	0
80	S2	135	Total Mg 135 135	0
80	Sd	1	Total Mg 1 1	0
80	SG	1	Total Mg 1 1	0
80	SJ	1	Total Mg 1 1	0
80	CC	1	Total Mg 1 1	0

- Molecule 81 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
81	L1	12	Total K 12 12	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 83 is water.

Mol	Chain	Residues	Atoms	AltConf
83	L1	762	Total O 762 762	0
83	L2	3	Total O 3 3	0
83	L3	6	Total O 6 6	0
83	LA	6	Total O 6 6	0
83	LB	3	Total O 3 3	0
83	LC	13	Total O 13 13	0
83	LD	1	Total O 1 1	0
83	LI	2	Total O 2 2	0
83	LL	1	Total O 1 1	0
83	LN	1	Total O 1 1	0
83	LP	1	Total O 1 1	0
83	LR	1	Total O 1 1	0
83	LX	2	Total O 2 2	0
83	LY	2	Total O 2 2	0
83	La	8	Total O 8 8	0
83	Lb	1	Total O 1 1	0
83	Le	2	Total O 2 2	0
83	Lg	2	Total O 2 2	0
83	Lj	4	Total O 4 4	0
83	Ll	2	Total O 2 2	0
83	Lo	1	Total O 1 1	0
83	S2	10	Total O 10 10	0

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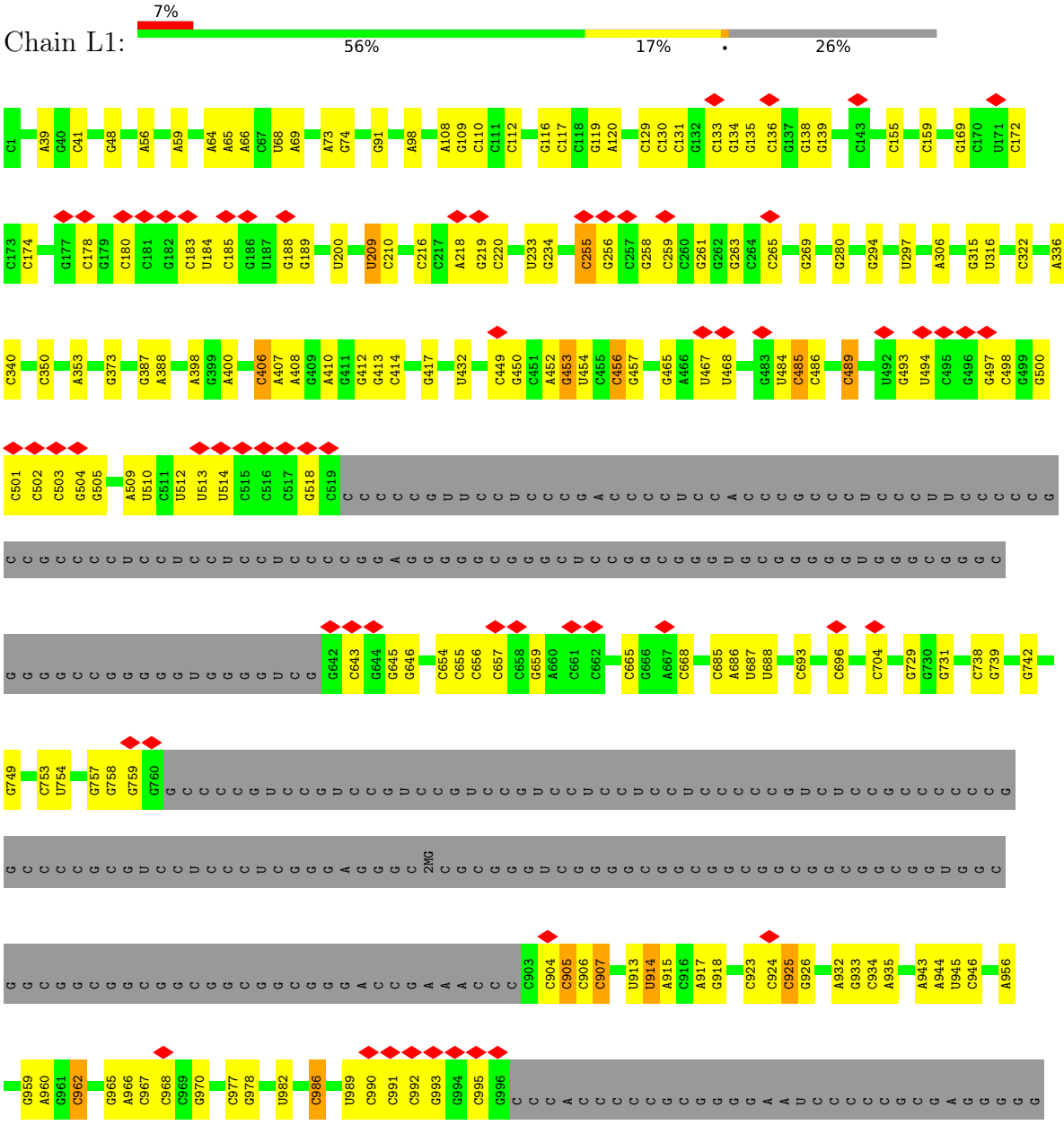
Mol	Chain	Residues	Atoms	AltConf
83	SX	1	Total O 1 1	0
83	CE	1	Total O 1 1	0

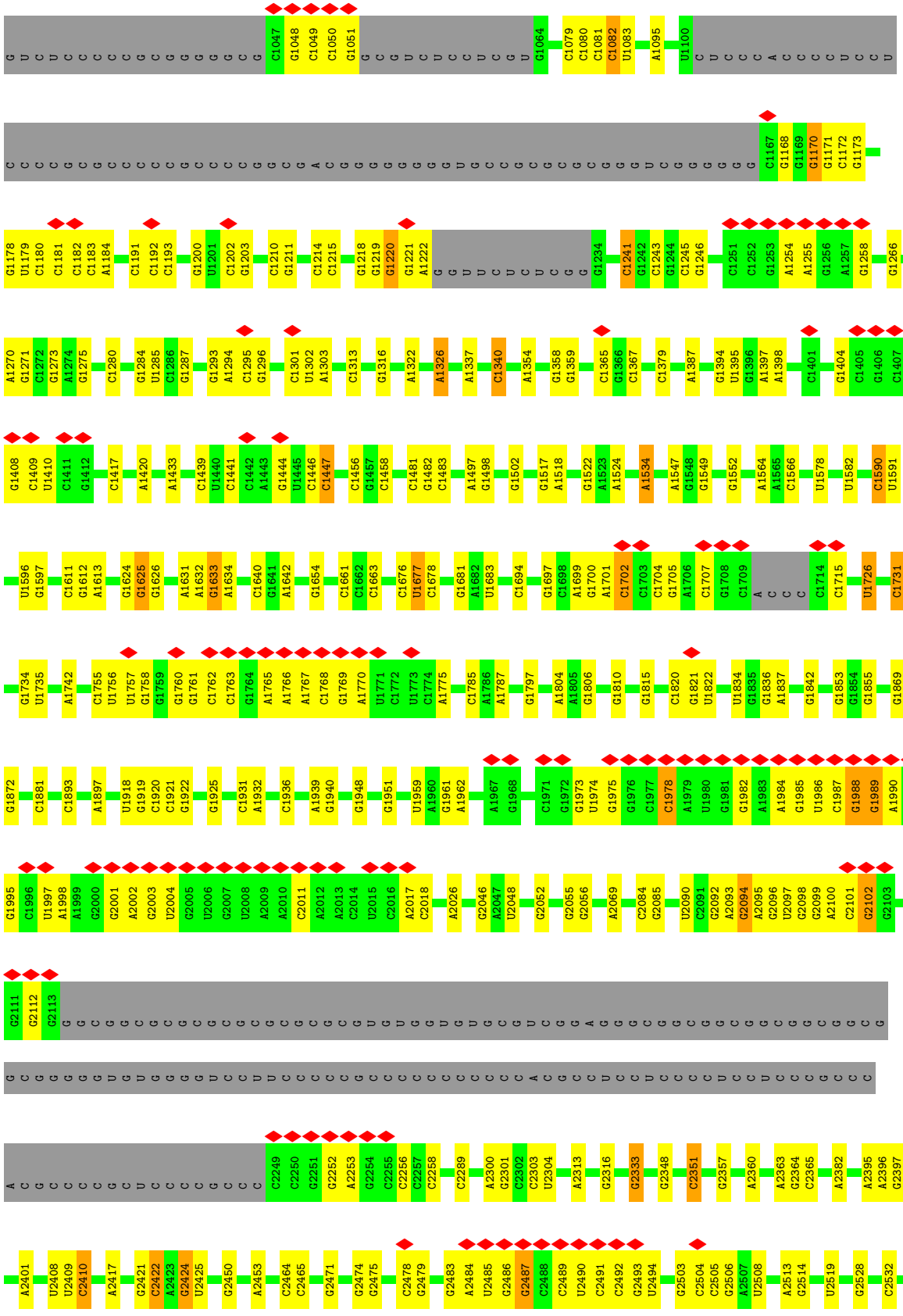
3 Residue-property plots (i)

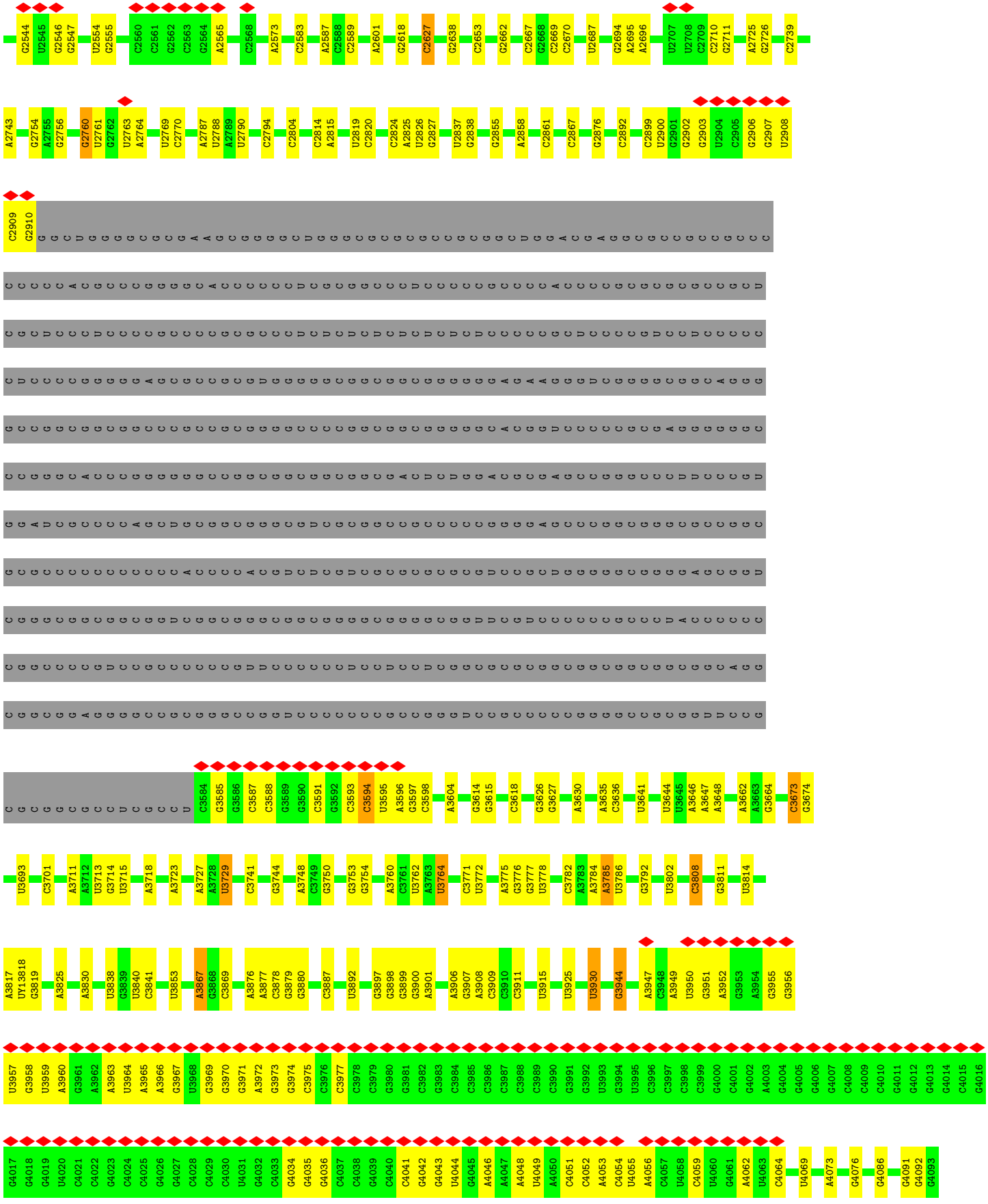
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

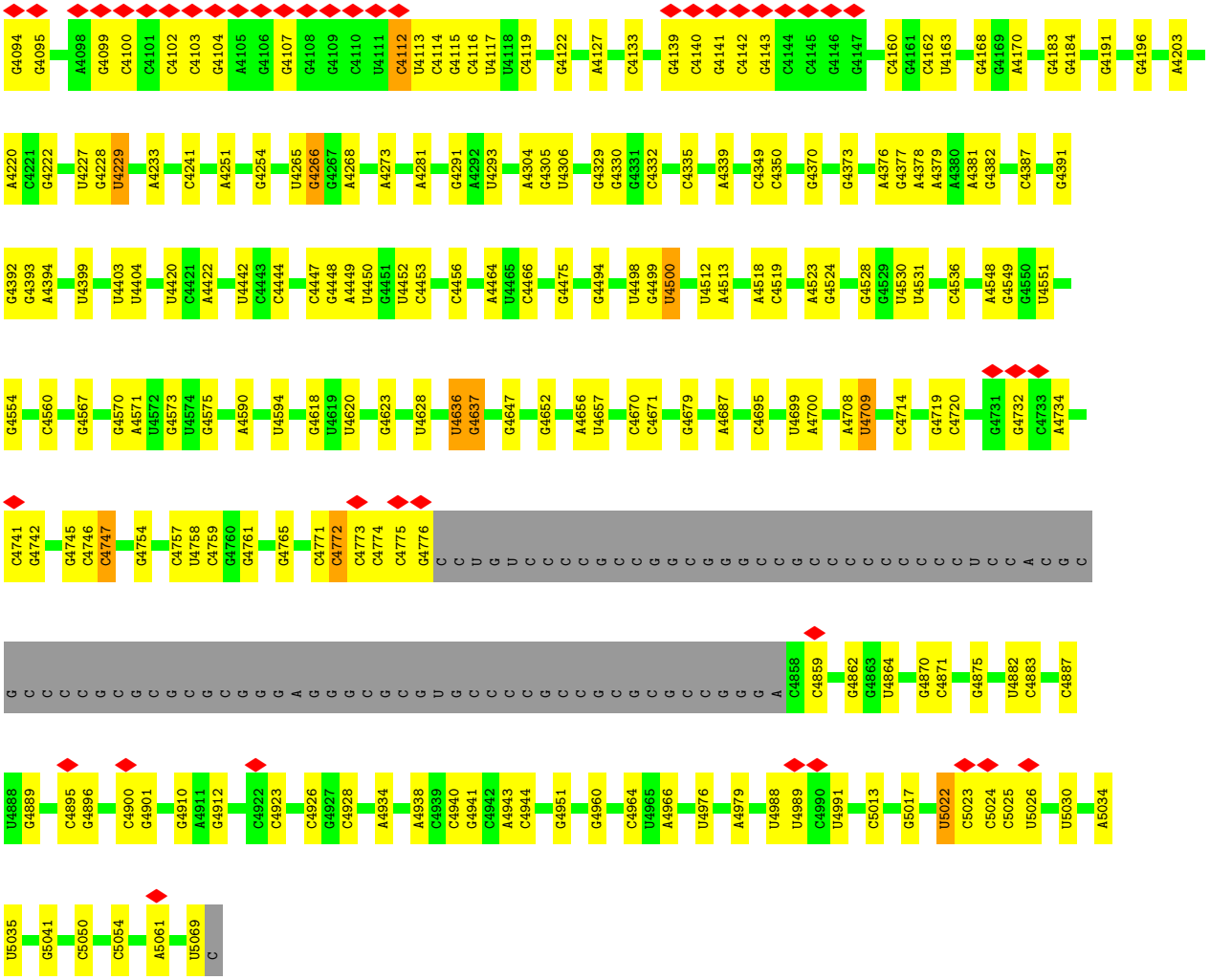
- Molecule 1: 28S rRNA

Chain L1:



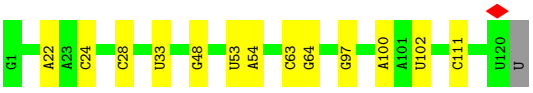






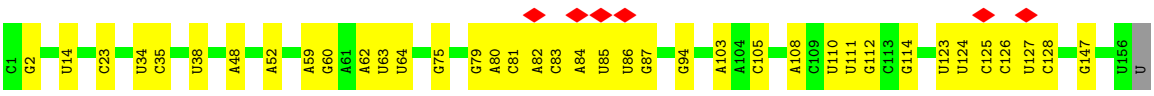
• Molecule 2: 5S rRNA

Chain L2:



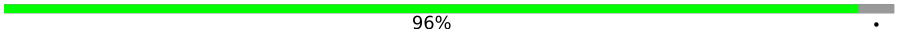
• Molecule 3: 5.8S rRNA

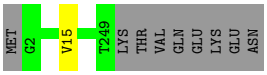
Chain L3:



• Molecule 4: 60S ribosomal protein L8

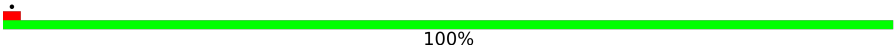
Chain LA:

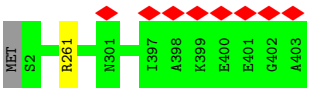




• Molecule 5: 60S ribosomal protein L3

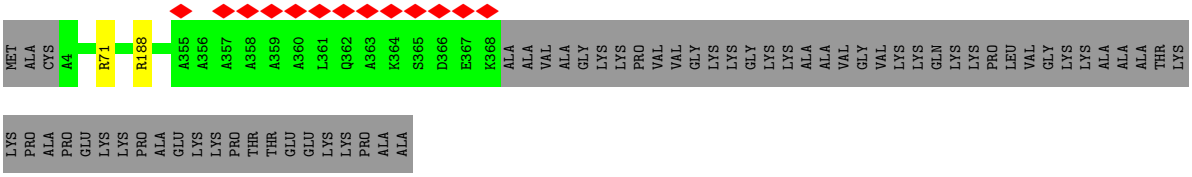
Chain LB:





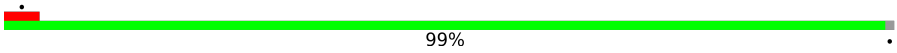
• Molecule 6: 60S ribosomal protein L4

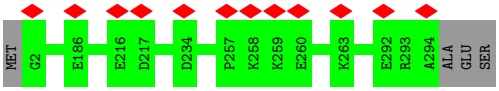
Chain LC:



• Molecule 7: 60S ribosomal protein L5

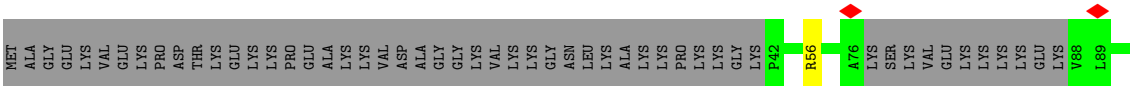
Chain LD:

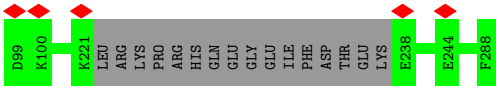




• Molecule 8: 60S ribosomal protein L6

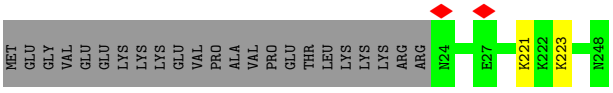
Chain LE:





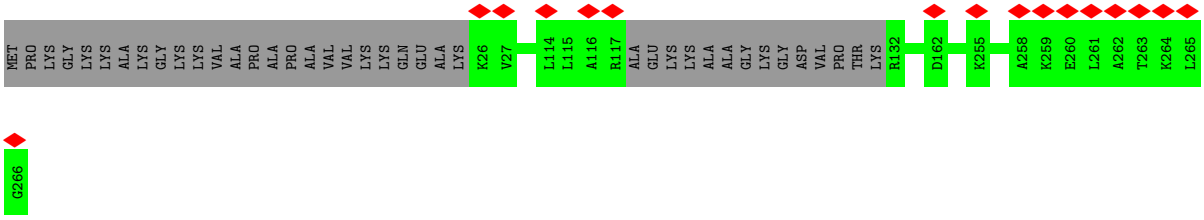
• Molecule 9: 60S ribosomal protein L7

Chain LF:



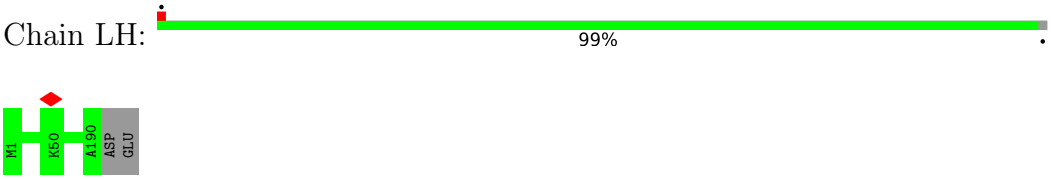
• Molecule 10: 60S ribosomal protein L7a

Chain LG:



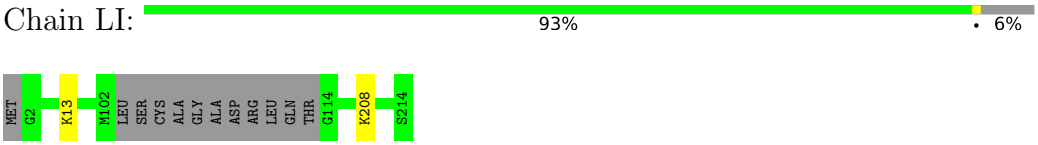
• Molecule 11: 60S ribosomal protein L9

Chain LH:



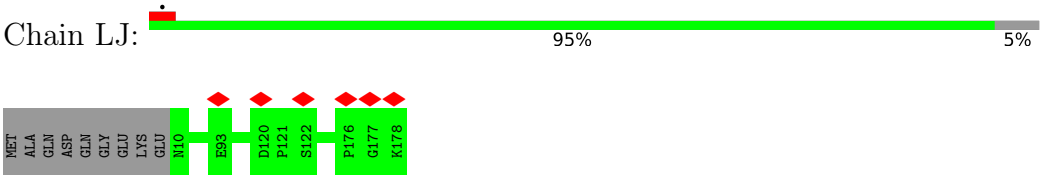
• Molecule 12: Ribosomal protein L10 isoform A

Chain LI:



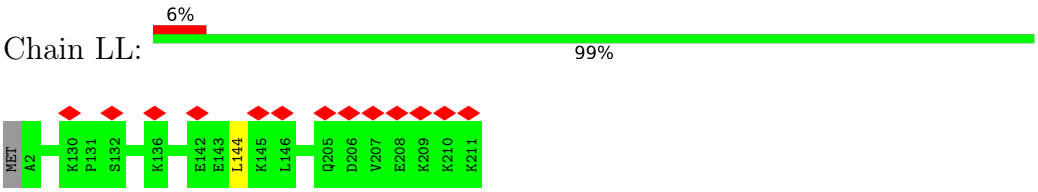
• Molecule 13: 60S ribosomal protein L11

Chain LJ:



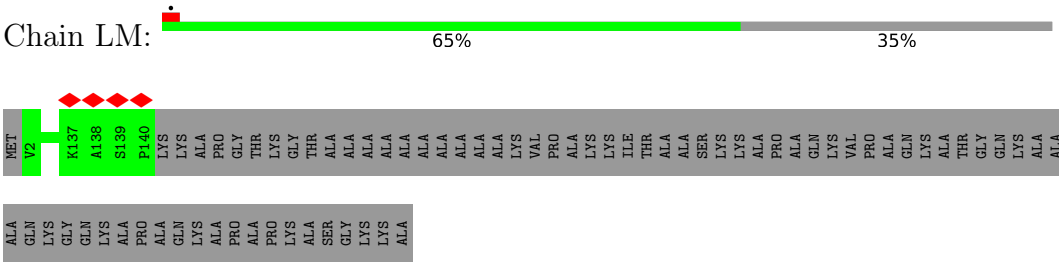
• Molecule 14: 60S ribosomal protein L13

Chain LL:



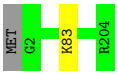
• Molecule 15: 60S ribosomal protein L14

Chain LM:



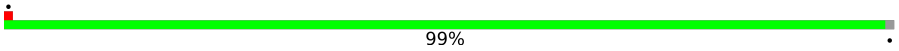
• Molecule 16: 60S ribosomal protein L15

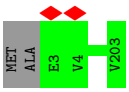
Chain LN:



• Molecule 17: 60S ribosomal protein L13a

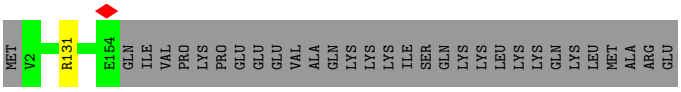
Chain LO:





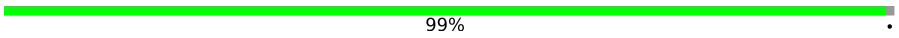
• Molecule 18: 60S ribosomal protein L17

Chain LP:



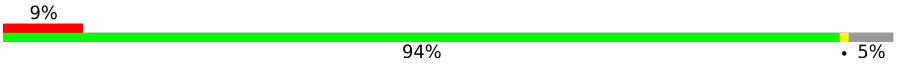
• Molecule 19: 60S ribosomal protein L18

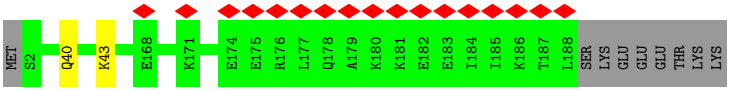
Chain LQ:



• Molecule 20: 60S ribosomal protein L19

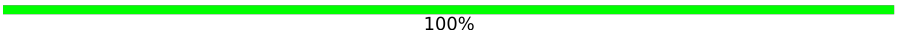
Chain LR:





• Molecule 21: 60S ribosomal protein L18a

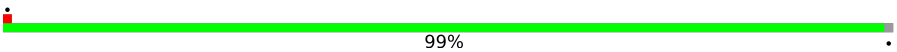
Chain LS:



There are no outlier residues recorded for this chain.

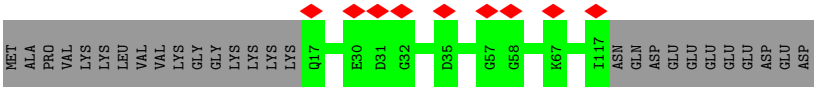
• Molecule 22: 60S ribosomal protein L21

Chain LT:



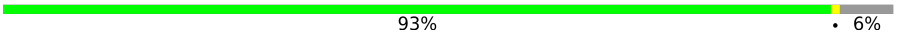
• Molecule 23: 60S ribosomal protein L22

Chain LU:



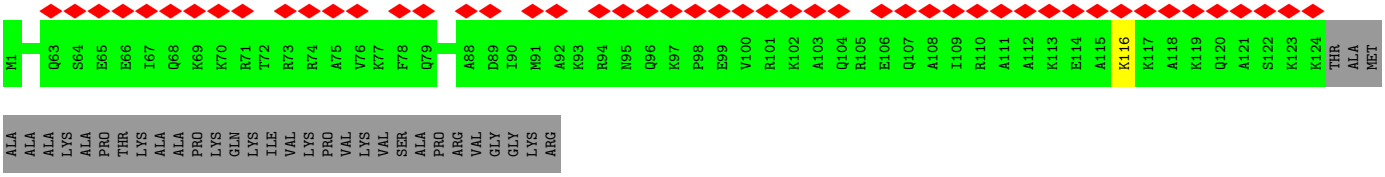
• Molecule 24: 60S ribosomal protein L23

Chain LV:



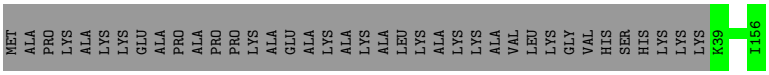
• Molecule 25: 60S ribosomal protein L24

Chain LW:



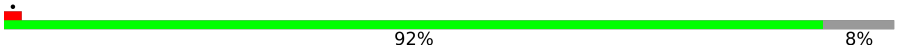
• Molecule 26: 60S ribosomal protein L23a

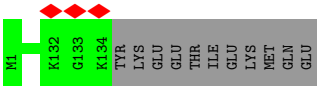
Chain LX:



• Molecule 27: 60S ribosomal protein L26

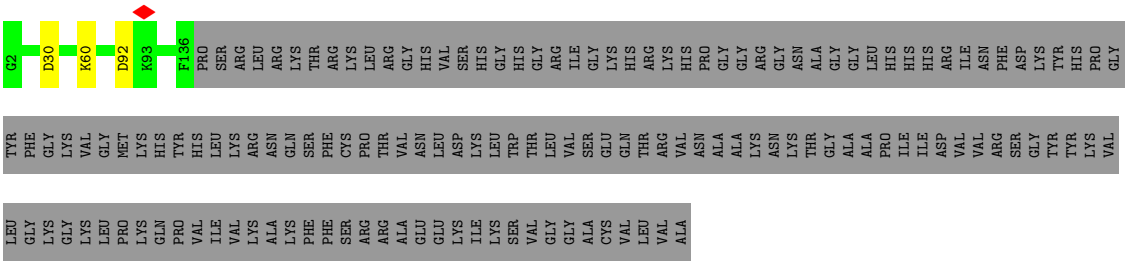
Chain LY:





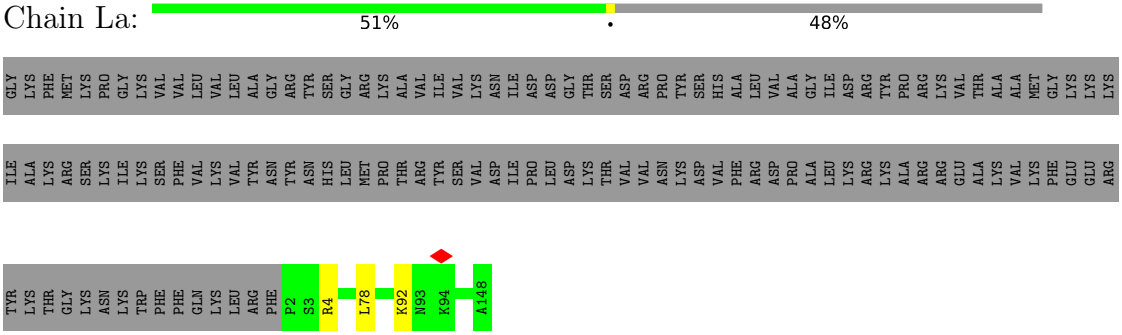
• Molecule 28: 60S ribosomal protein L27

Chain LZ:



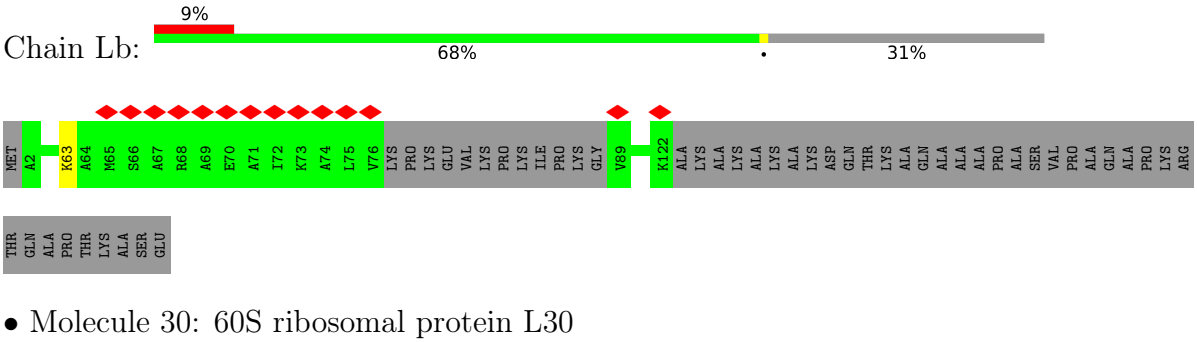
• Molecule 28: 60S ribosomal protein L27

Chain La:



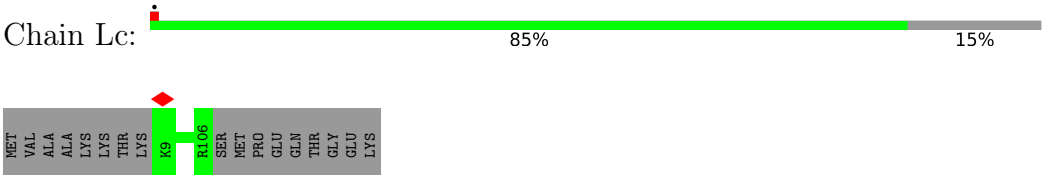
• Molecule 29: 60S ribosomal protein L29

Chain Lb:



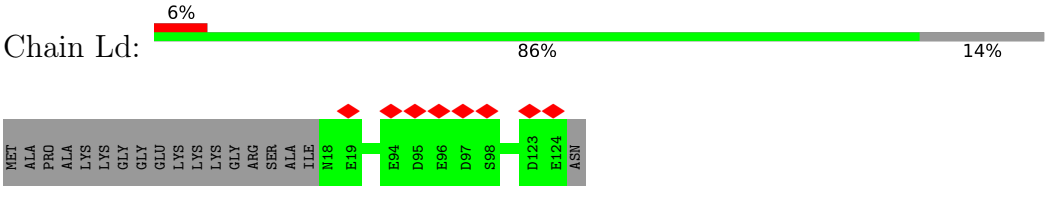
• Molecule 30: 60S ribosomal protein L30

Chain Lc:



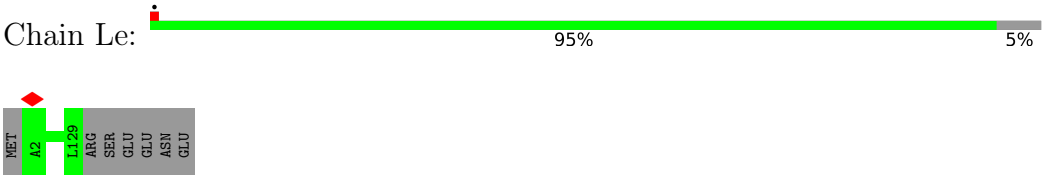
• Molecule 31: 60S ribosomal protein L31

Chain Ld:



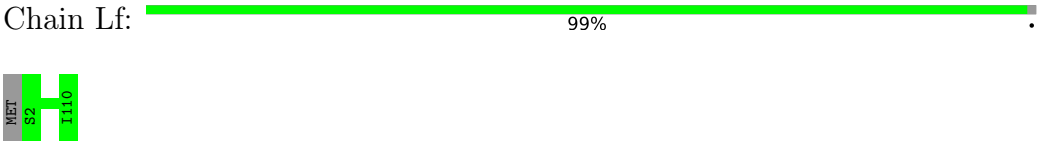
• Molecule 32: 60S ribosomal protein L32

Chain Le:



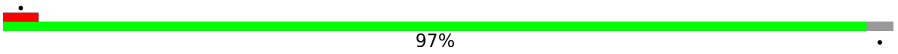
• Molecule 33: 60S ribosomal protein L35a

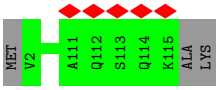
Chain Lf:



• Molecule 34: 60S ribosomal protein L34

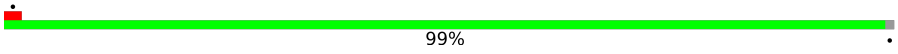
Chain Lg:





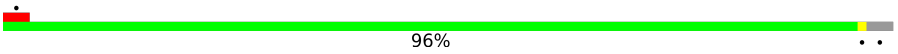
• Molecule 35: 60S ribosomal protein L35

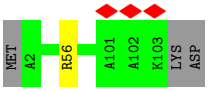
Chain Lh:



• Molecule 36: 60S ribosomal protein L36

Chain Li:



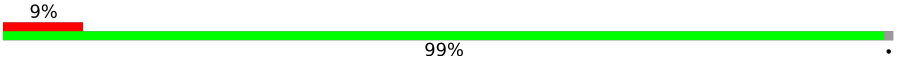


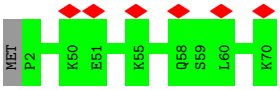
• Molecule 37: 60S ribosomal protein L37

Chain Lj:

• Molecule 38: 60S ribosomal protein L38

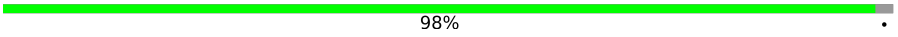
Chain Lk:





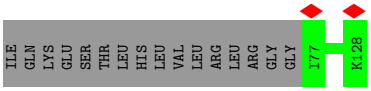
• Molecule 39: 60S ribosomal protein L39

Chain Ll:



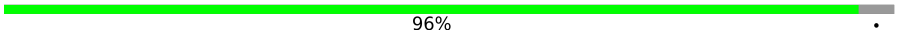
• Molecule 40: Ubiquitin-60S ribosomal protein L40

Chain Lm:



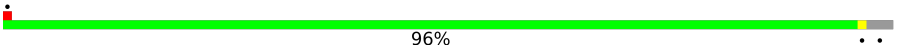
• Molecule 41: 60S ribosomal protein L41

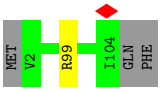
Chain Ln:



• Molecule 42: 60S ribosomal protein L36a

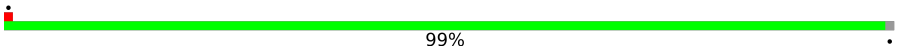
Chain Lo:

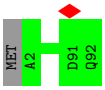




• Molecule 43: 60S ribosomal protein L37a

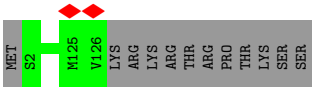
Chain Lp:





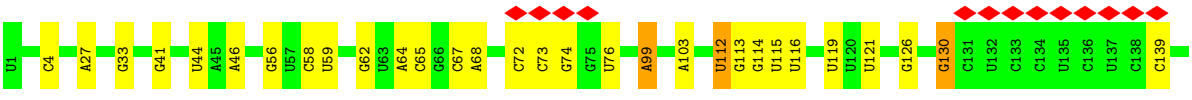
• Molecule 44: 60S ribosomal protein L28

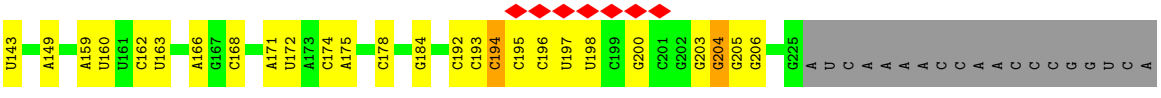
Chain Lr:

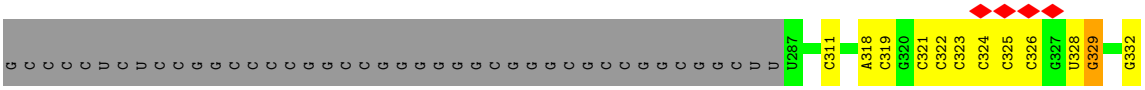


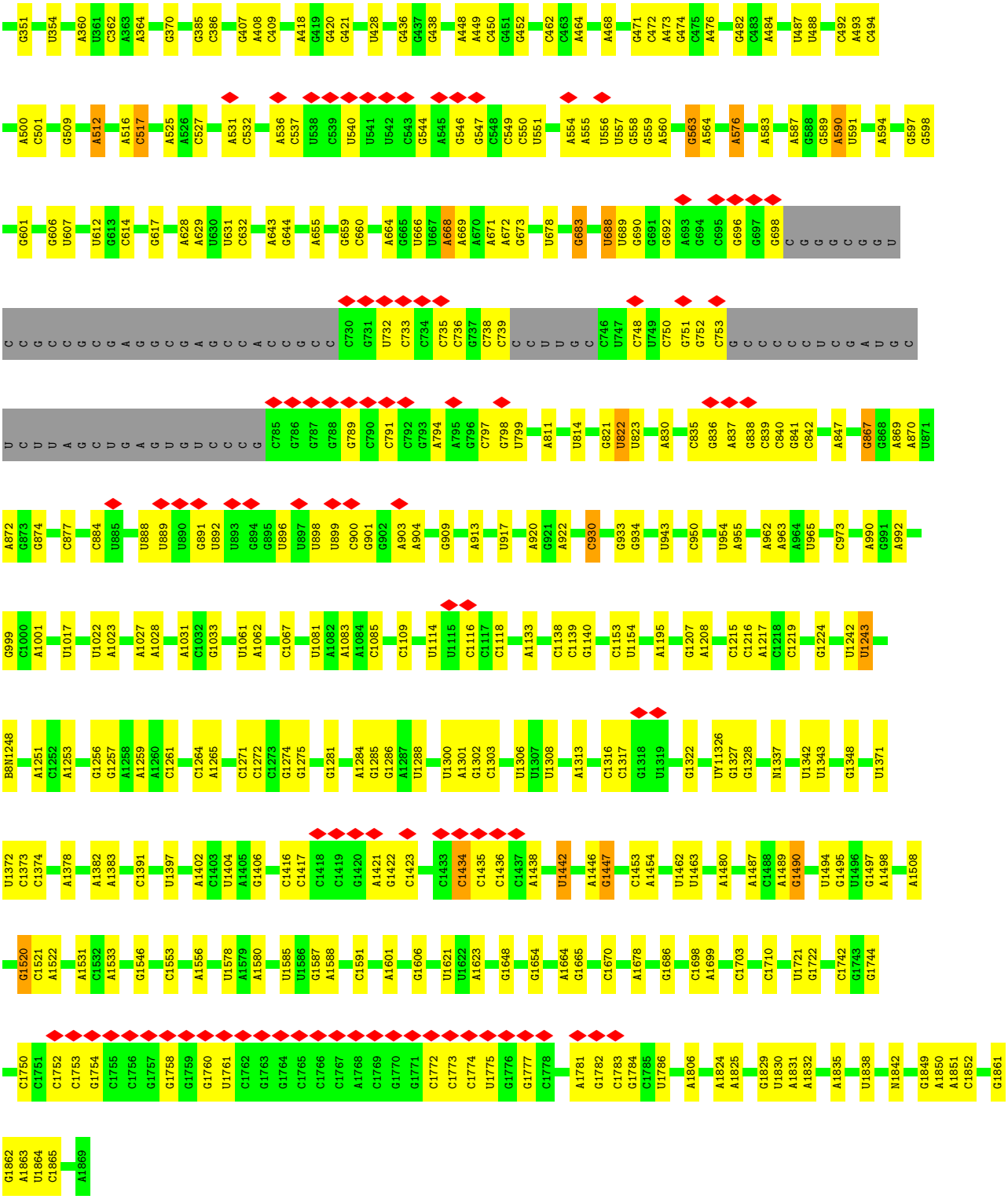
• Molecule 45: 18S rRNA

Chain S2:



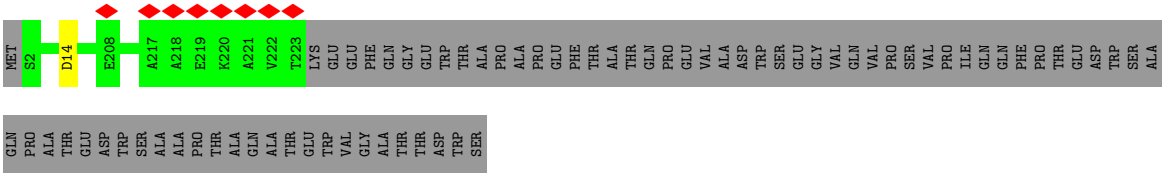






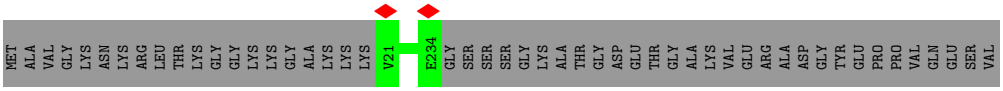
• Molecule 46: 40S ribosomal protein SA

Chain SA:



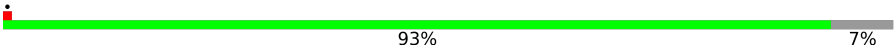
• Molecule 47: 40S ribosomal protein S3a

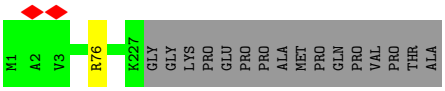
Chain SB:



• Molecule 48: 40S ribosomal protein S3

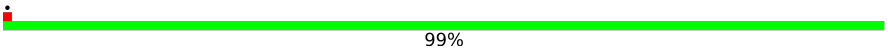
Chain SD:

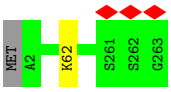




• Molecule 49: 40S ribosomal protein S4, X isoform

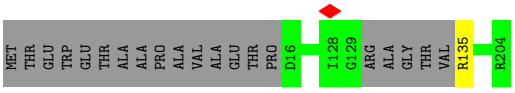
Chain SE:





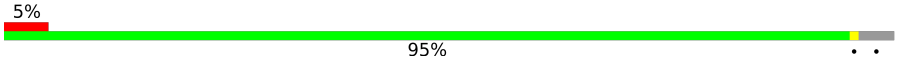
• Molecule 50: 40S ribosomal protein S5

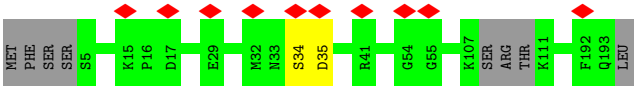
Chain SF:



• Molecule 51: 40S ribosomal protein S7

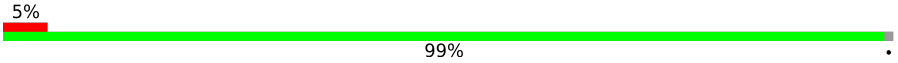
Chain SH:

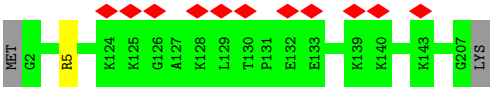




• Molecule 52: 40S ribosomal protein S8

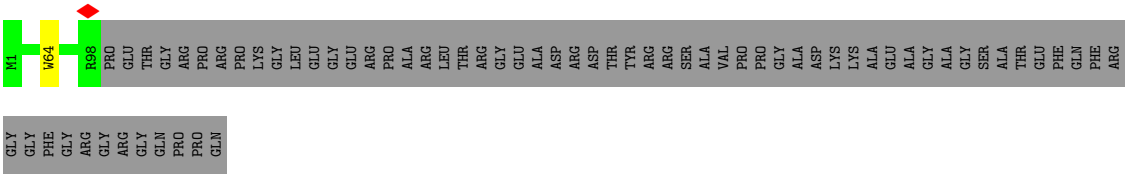
Chain SI:





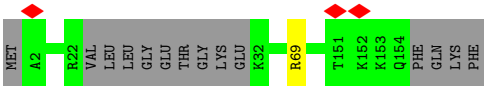
• Molecule 53: 40S ribosomal protein S10

Chain SK:



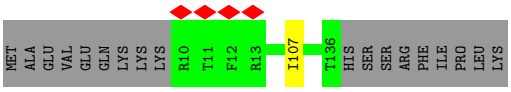
• Molecule 54: 40S ribosomal protein S11

Chain SL:



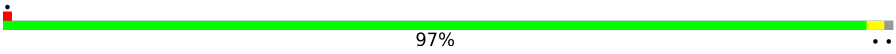
• Molecule 55: 40S ribosomal protein S15

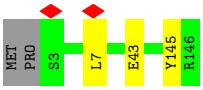
Chain SP:



• Molecule 56: 40S ribosomal protein S16

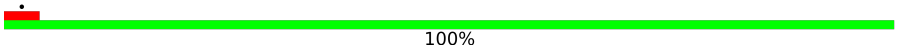
Chain SQ:

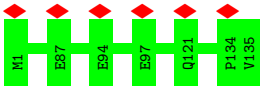




• Molecule 57: 40S ribosomal protein S17

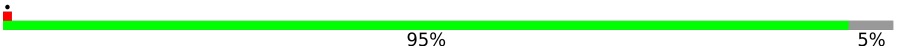
Chain SR:

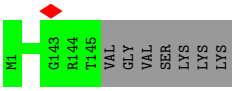




• Molecule 58: 40S ribosomal protein S18

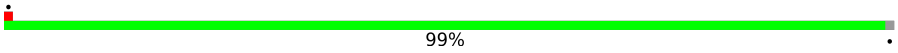
Chain SS:

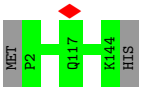




• Molecule 59: 40S ribosomal protein S19

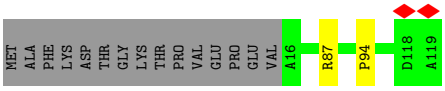
Chain ST:





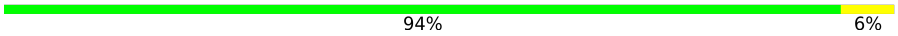
• Molecule 60: 40S ribosomal protein S20

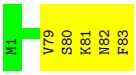
Chain SU:



• Molecule 61: 40S ribosomal protein S21

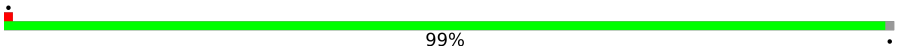
Chain SV:

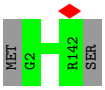




• Molecule 62: 40S ribosomal protein S23

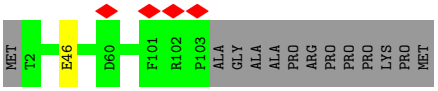
Chain SX:





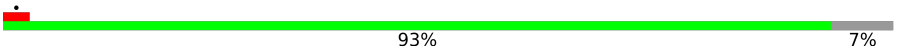
• Molecule 63: 40S ribosomal protein S26

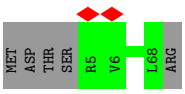
Chain Sa:



• Molecule 64: 40S ribosomal protein S28

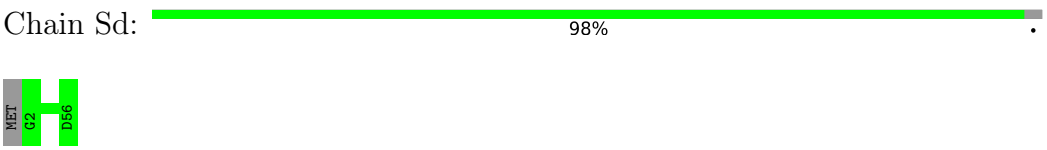
Chain Sc:





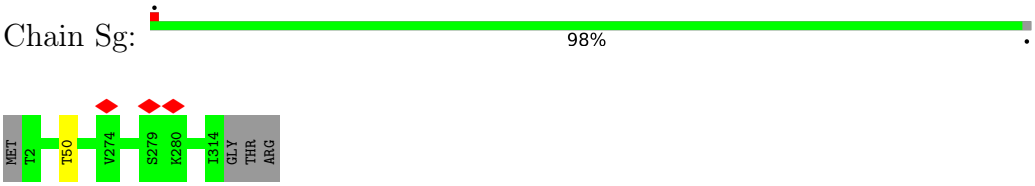
• Molecule 65: 40S ribosomal protein S29

Chain Sd:



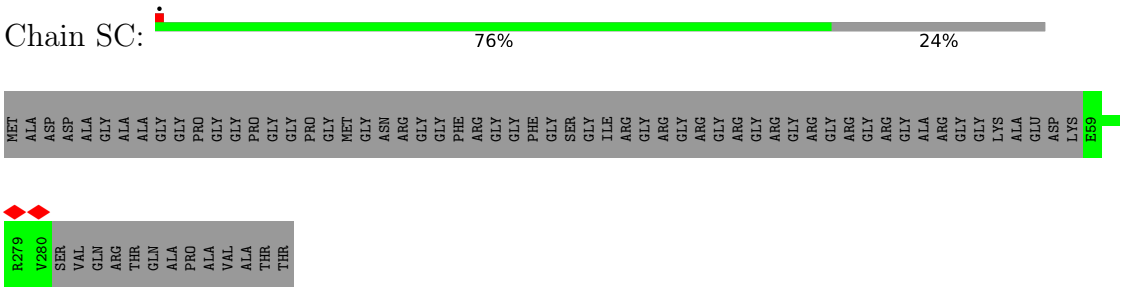
• Molecule 66: Receptor of activated protein C kinase 1

Chain Sg:



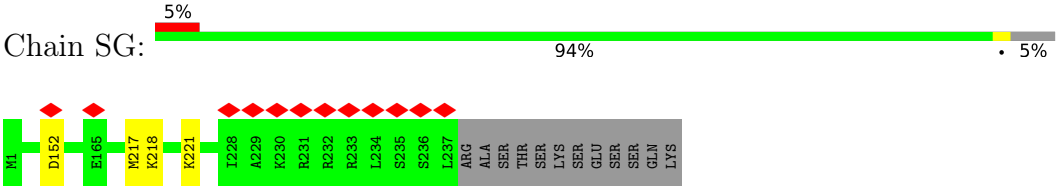
• Molecule 67: 40S ribosomal protein S2

Chain SC:



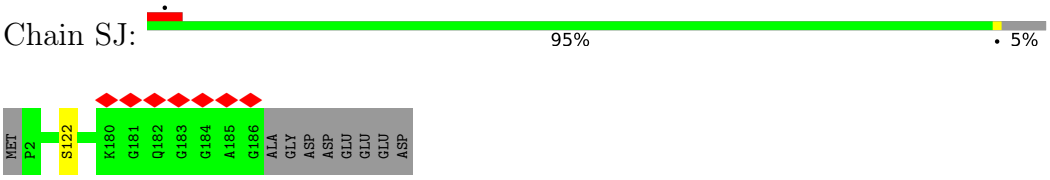
• Molecule 68: 40S ribosomal protein S6

Chain SG:



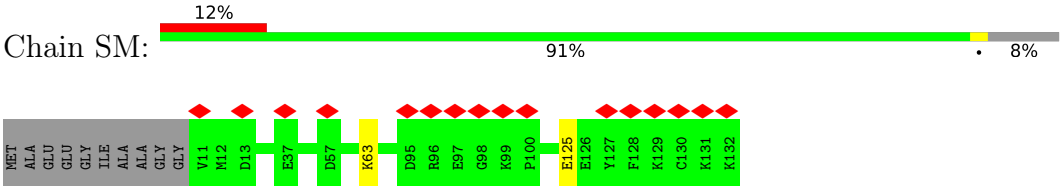
• Molecule 69: 40S ribosomal protein S9

Chain SJ:



• Molecule 70: 40S ribosomal protein S12

Chain SM:

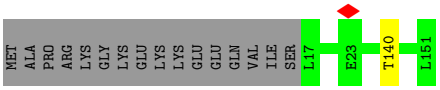


• Molecule 71: 40S ribosomal protein S13

Chain SN:

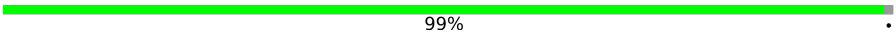
• Molecule 72: 40S ribosomal protein S14

Chain SO:



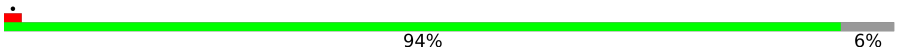
• Molecule 73: 40S ribosomal protein S15a

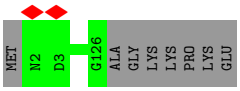
Chain SW:



• Molecule 74: 40S ribosomal protein S24

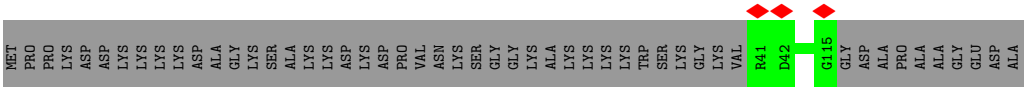
Chain SY:





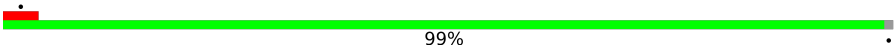
• Molecule 75: 40S ribosomal protein S25

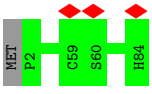
Chain SZ:



• Molecule 76: 40S ribosomal protein S27

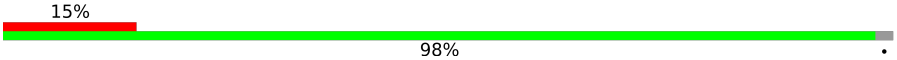
Chain Sb:

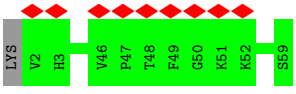




• Molecule 77: 40S ribosomal protein S30

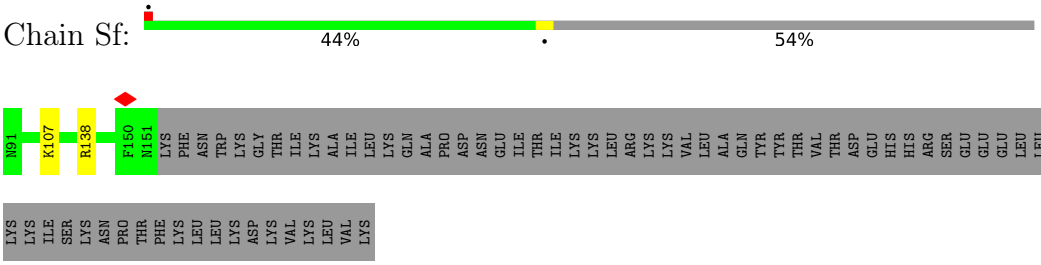
Chain Se:





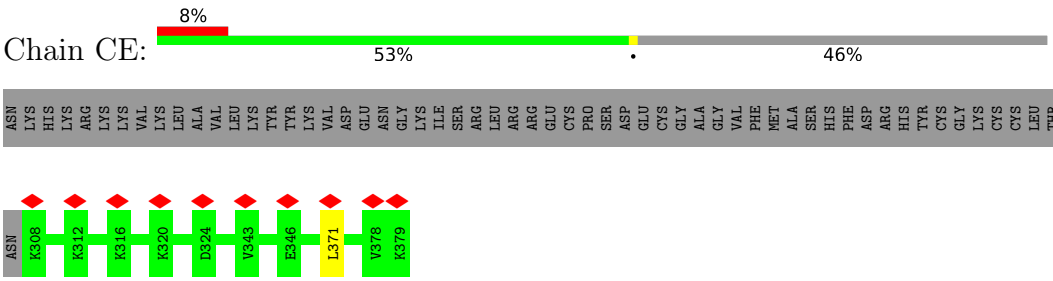
• Molecule 78: Ubiquitin-40S ribosomal protein S27a

Chain Sf:



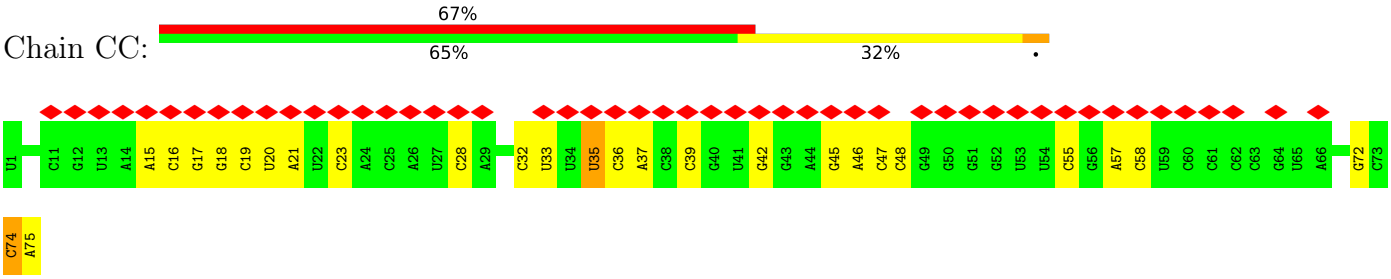
• Molecule 78: Ubiquitin-40S ribosomal protein S27a

Chain CE:



• Molecule 79: tRNA

Chain CC:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49713	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	48.809	Depositor
Minimum map value	-19.709	Depositor
Average map value	0.030	Depositor
Map value standard deviation	1.171	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	444.78, 444.78, 444.78	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M7A, MG, OMU, JMH, K, MA6, B8H, 5MU, UY1, B8N, PSU, B8T, 5MC, A2M, ZN, 2MG, 6MZ, OMG, 1MA, MLZ, UR3, 4AC, OMC

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	0.52	0/87525	1.00	271/136449 (0.2%)
2	L2	0.46	0/2858	0.92	3/4455 (0.1%)
3	L3	0.48	0/3653	0.92	5/5691 (0.1%)
4	LA	0.38	0/1936	0.69	0/2596
5	LB	0.32	0/3306	0.60	0/4424
6	LC	0.32	0/2962	0.62	0/3977
7	LD	0.30	0/2428	0.54	0/3252
8	LE	0.28	0/1799	0.62	0/2414
9	LF	0.34	0/1905	0.60	0/2539
10	LG	0.30	0/1866	0.60	0/2511
11	LH	0.30	0/1537	0.57	0/2066
12	LI	0.35	0/1677	0.59	0/2237
13	LJ	0.28	0/1376	0.60	0/1840
14	LL	0.30	0/1732	0.64	1/2315 (0.0%)
15	LM	0.31	0/1161	0.61	0/1554
16	LN	0.35	0/1746	0.64	0/2338
17	LO	0.32	0/1682	0.58	0/2250
18	LP	0.31	0/1268	0.58	0/1701
19	LQ	0.33	0/1537	0.64	0/2052
20	LR	0.31	0/1582	0.59	0/2091
21	LS	0.34	0/1501	0.60	0/2013
22	LT	0.32	0/1326	0.57	0/1770
23	LU	0.33	0/839	0.67	0/1126
24	LV	0.32	0/993	0.60	0/1332
25	LW	0.31	0/1030	0.62	0/1364
26	LX	0.29	0/984	0.56	0/1323
27	LY	0.29	0/1132	0.59	0/1504
28	LZ	0.35	0/1129	0.65	2/1507 (0.1%)
28	La	0.34	0/1191	0.65	1/1591 (0.1%)
29	Lb	0.29	0/889	0.59	0/1175
30	Lc	0.36	0/774	0.60	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	Ld	0.29	0/903	0.60	0/1216
32	Le	0.32	0/1071	0.63	0/1429
33	Lf	0.35	0/895	0.64	0/1198
34	Lg	0.34	0/916	0.63	0/1220
35	Lh	0.29	0/1023	0.56	0/1351
36	Li	0.28	0/843	0.60	0/1115
37	Lj	0.35	0/720	0.69	0/952
38	Lk	0.33	0/575	0.63	0/761
39	Ll	0.29	0/454	0.64	0/599
40	Lm	0.29	0/435	0.59	0/575
41	Ln	0.30	0/231	0.74	0/294
42	Lo	0.31	0/845	0.56	0/1113
43	Lp	0.32	0/718	0.59	0/953
44	Lr	0.29	0/1017	0.59	0/1364
45	S2	0.41	0/39961	0.96	99/62247 (0.2%)
46	SA	0.30	0/1784	0.56	1/2424 (0.0%)
47	SB	0.30	0/1765	0.59	0/2362
48	SD	0.28	0/1793	0.56	0/2414
49	SE	0.29	0/2118	0.59	0/2849
50	SF	0.26	0/1481	0.57	0/1988
51	SH	0.42	0/1519	0.59	0/2033
52	SI	0.31	0/1715	0.62	0/2287
53	SK	0.28	0/851	0.58	0/1147
54	SL	0.31	0/1202	0.57	0/1606
55	SP	0.29	0/1065	0.65	1/1423 (0.1%)
56	SQ	0.31	0/1160	0.72	1/1553 (0.1%)
57	SR	0.30	0/1105	0.57	0/1484
58	SS	0.28	0/1216	0.68	0/1628
59	ST	0.27	0/1131	0.60	0/1515
60	SU	0.35	0/831	0.60	0/1115
61	SV	0.33	0/643	0.55	0/860
62	SX	0.29	0/1116	0.59	0/1490
63	Sa	0.33	0/836	0.66	0/1121
64	Sc	0.31	0/508	0.70	0/680
65	Sd	0.28	0/470	0.67	0/623
66	Sg	0.26	0/2493	0.59	0/3394
67	SC	0.32	0/1762	0.57	0/2381
68	SG	0.30	0/1946	0.62	1/2590 (0.0%)
69	SJ	0.31	0/1550	0.60	0/2069
70	SM	0.35	0/950	0.70	2/1275 (0.2%)
71	SN	0.29	0/1232	0.54	0/1656
72	SO	0.31	0/1023	0.59	0/1372
73	SW	0.31	0/1051	0.61	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	SY	0.28	0/1039	0.57	0/1381
75	SZ	0.25	0/604	0.65	0/810
76	Sb	0.28	0/665	0.57	0/891
77	Se	0.26	0/465	0.57	0/612
78	CE	0.26	0/613	0.57	1/819 (0.1%)
78	Sf	0.27	0/507	0.63	0/673
79	CC	0.27	0/1773	0.94	6/2759 (0.2%)
All	All	0.42	0/229913	0.86	395/337572 (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
18	LP	0	1
56	SQ	0	2
All	All	0	3

There are no bond length outliers.

All (395) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	S2	1772	C	N1-C2-O2	13.69	127.11	118.90
45	S2	1772	C	N3-C2-O2	-13.01	112.79	121.90
45	S2	194	C	N3-C2-O2	-12.59	113.09	121.90
1	L1	906	C	N3-C2-O2	-12.41	113.21	121.90
45	S2	501	C	N1-C2-O2	11.81	125.98	118.90
45	S2	501	C	C2-N1-C1'	11.73	131.71	118.80
1	L1	1191	C	N3-C2-O2	-11.65	113.74	121.90
45	S2	195	C	N3-C2-O2	-11.39	113.93	121.90
1	L1	4771	C	N1-C2-O2	11.34	125.70	118.90
1	L1	130	C	N3-C2-O2	-11.30	113.99	121.90
1	L1	129	C	N3-C2-O2	-11.06	114.16	121.90
45	S2	193	C	N3-C2-O2	-10.93	114.25	121.90
45	S2	322	C	N3-C2-O2	-10.73	114.39	121.90
1	L1	485	C	C2-N1-C1'	10.70	130.56	118.80
1	L1	3594	C	N1-C2-O2	10.26	125.06	118.90
45	S2	194	C	N1-C2-O2	10.22	125.03	118.90
1	L1	907	C	N3-C2-O2	-10.17	114.78	121.90
1	L1	1082	C	O4'-C1'-N1	10.04	116.24	108.20
45	S2	1772	C	C2-N1-C1'	9.86	129.65	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	1447	C	N3-C2-O2	-9.75	115.08	121.90
45	S2	1317	C	N3-C2-O2	-9.67	115.13	121.90
1	L1	1978	C	N3-C2-O2	-9.64	115.16	121.90
1	L1	1994	C	N3-C2-O2	-9.59	115.19	121.90
1	L1	4771	C	N3-C2-O2	-9.56	115.20	121.90
1	L1	131	C	N3-C2-O2	-9.49	115.26	121.90
1	L1	906	C	N1-C2-O2	9.47	124.58	118.90
1	L1	417	G	O4'-C1'-N9	9.13	115.51	108.20
1	L1	456	C	O4'-C1'-N1	9.12	115.50	108.20
1	L1	4862	G	N3-C2-N2	9.09	126.26	119.90
1	L1	1192	C	N3-C2-O2	-9.07	115.55	121.90
45	S2	1453	C	C2-N1-C1'	9.02	128.72	118.80
45	S2	501	C	N3-C2-O2	-9.01	115.60	121.90
45	S2	1453	C	N1-C2-O2	8.93	124.25	118.90
1	L1	655	C	N3-C2-O2	-8.86	115.70	121.90
1	L1	3594	C	N3-C2-O2	-8.76	115.77	121.90
1	L1	4862	G	N3-C4-N9	8.76	131.26	126.00
45	S2	1772	C	C6-N1-C2	-8.74	116.81	120.30
1	L1	456	C	N3-C2-O2	-8.58	115.90	121.90
1	L1	2409	U	C2-N1-C1'	8.47	127.87	117.70
1	L1	4771	C	C6-N1-C2	-8.47	116.91	120.30
45	S2	501	C	C6-N1-C1'	-8.46	110.64	120.80
45	S2	1520	G	N3-C4-C5	-8.40	124.40	128.60
1	L1	4420	U	N1-C2-O2	8.38	128.66	122.80
1	L1	2409	U	N3-C2-O2	-8.33	116.37	122.20
1	L1	1079	C	N3-C2-O2	-8.31	116.08	121.90
1	L1	2409	U	N1-C2-O2	8.23	128.56	122.80
45	S2	322	C	N1-C2-O2	8.18	123.81	118.90
1	L1	4709	U	C2-N1-C1'	8.05	127.36	117.70
1	L1	4420	U	C2-N1-C1'	8.04	127.34	117.70
56	SQ	7	LEU	CA-CB-CG	7.98	133.65	115.30
1	L1	4420	U	N3-C2-O2	-7.96	116.63	122.20
1	L1	485	C	C6-N1-C1'	-7.92	111.29	120.80
45	S2	1520	G	C2-N3-C4	7.85	115.83	111.90
1	L1	925	C	N3-C2-O2	-7.83	116.42	121.90
1	L1	4771	C	C5-C6-N1	7.82	124.91	121.00
1	L1	2303	C	C6-N1-C1'	7.81	130.17	120.80
1	L1	3594	C	C2-N1-C1'	7.78	127.35	118.80
1	L1	1082	C	N3-C2-O2	-7.77	116.46	121.90
1	L1	336	A	C2-N3-C4	7.76	114.48	110.60
1	L1	3741	C	N3-C2-O2	-7.70	116.51	121.90
1	L1	1988	G	N3-C4-N9	7.68	130.61	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	2627	C	C2-N1-C1'	7.52	127.07	118.80
28	LZ	30	ASP	CB-CG-OD2	7.50	125.05	118.30
45	S2	1139	C	N3-C2-O2	-7.48	116.67	121.90
1	L1	1241	C	C2-N1-C1'	7.47	127.02	118.80
1	L1	2333	G	C5-C6-O6	7.44	133.06	128.60
1	L1	1080	C	N3-C2-O2	-7.42	116.70	121.90
45	S2	195	C	N1-C2-O2	7.42	123.35	118.90
1	L1	2303	C	C2-N1-C1'	-7.41	110.65	118.80
45	S2	1546	G	N3-C2-N2	7.41	125.09	119.90
1	L1	4771	C	C2-N1-C1'	7.40	126.94	118.80
1	L1	1079	C	N1-C2-O2	7.38	123.33	118.90
1	L1	3778	U	N1-C2-O2	7.28	127.90	122.80
1	L1	4229	U	N3-C2-O2	-7.26	117.12	122.20
45	S2	1139	C	N1-C2-O2	7.23	123.24	118.90
1	L1	180	C	N1-C2-O2	7.20	123.22	118.90
1	L1	485	C	N1-C2-O2	7.20	123.22	118.90
1	L1	174	C	N3-C2-O2	-7.19	116.87	121.90
1	L1	3647	A	C5-C6-N1	7.16	121.28	117.70
1	L1	1191	C	C6-N1-C2	-7.16	117.44	120.30
1	L1	1978	C	N1-C2-O2	7.14	123.18	118.90
1	L1	2102	G	O4'-C1'-N9	7.13	113.90	108.20
1	L1	4758	U	C2-N1-C1'	7.12	126.25	117.70
1	L1	4862	G	N1-C2-N2	-7.08	109.82	116.20
45	S2	1139	C	C2-N1-C1'	7.06	126.57	118.80
45	S2	1022	U	C2-N1-C1'	7.03	126.14	117.70
45	S2	1453	C	N3-C2-O2	-7.00	117.00	121.90
1	L1	1241	C	C6-N1-C2	-6.93	117.53	120.30
45	S2	168	C	N1-C2-O2	6.92	123.05	118.90
1	L1	1191	C	N1-C2-O2	6.90	123.04	118.90
1	L1	2303	C	C5-C4-N4	6.89	125.02	120.20
79	CC	23	C	N1-C2-O2	6.84	123.00	118.90
1	L1	1447	C	N1-C2-O2	6.84	123.00	118.90
1	L1	2303	C	N3-C4-N4	-6.80	113.24	118.00
1	L1	757	G	N1-C6-O6	-6.80	115.82	119.90
79	CC	55	C	N3-C2-O2	-6.75	117.17	121.90
45	S2	205	G	N1-C2-N2	-6.75	110.13	116.20
1	L1	906	C	C6-N1-C2	-6.72	117.61	120.30
45	S2	329	G	N3-C2-N2	6.71	124.60	119.90
45	S2	501	C	C6-N1-C2	-6.71	117.62	120.30
45	S2	195	C	C6-N1-C2	-6.68	117.63	120.30
1	L1	1552	G	O4'-C1'-N9	6.68	113.54	108.20
1	L1	1632	A	C2-N3-C4	6.66	113.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	1241	C	N1-C2-O2	6.66	122.89	118.90
1	L1	2627	C	N1-C2-O2	6.66	122.89	118.90
1	L1	4758	U	N1-C2-O2	6.62	127.44	122.80
1	L1	1241	C	N3-C2-O2	-6.62	117.27	121.90
1	L1	2304	U	N1-C2-O2	6.62	127.43	122.80
1	L1	1994	C	N1-C2-O2	6.61	122.86	118.90
1	L1	4774	C	N3-C2-O2	-6.61	117.28	121.90
79	CC	23	C	N3-C2-O2	-6.60	117.28	121.90
1	L1	2410	C	C2-N1-C1'	6.60	126.06	118.80
1	L1	3741	C	N1-C2-O2	6.60	122.86	118.90
1	L1	1988	G	C4-N9-C1'	6.59	135.07	126.50
45	S2	329	G	N1-C2-N2	-6.59	110.27	116.20
1	L1	2514	G	N9-C4-C5	-6.57	102.77	105.40
1	L1	655	C	C6-N1-C2	-6.50	117.70	120.30
1	L1	4746	C	C2-N1-C1'	6.50	125.95	118.80
1	L1	907	C	C6-N1-C2	-6.50	117.70	120.30
45	S2	192	C	N1-C2-O2	6.49	122.79	118.90
1	L1	2528	G	N3-C4-C5	-6.48	125.36	128.60
45	S2	1139	C	C6-N1-C2	-6.48	117.71	120.30
1	L1	129	C	C6-N1-C2	-6.43	117.73	120.30
1	L1	1597	G	O4'-C1'-N9	6.43	113.34	108.20
1	L1	907	C	N1-C2-O2	6.40	122.74	118.90
45	S2	321	C	N1-C2-O2	6.39	122.73	118.90
55	SP	107	ILE	C-N-CA	6.39	137.67	121.70
1	L1	3594	C	C6-N1-C2	-6.38	117.75	120.30
79	CC	55	C	N1-C2-O2	6.38	122.73	118.90
1	L1	2528	G	C4-N9-C1'	6.33	134.72	126.50
1	L1	1988	G	C8-N9-C1'	-6.32	118.78	127.00
1	L1	4709	U	C5-C4-O4	-6.31	122.11	125.90
1	L1	1590	C	P-O3'-C3'	6.31	127.27	119.70
1	L1	4774	C	N1-C2-O2	6.30	122.68	118.90
3	L3	64	U	N3-C2-O2	-6.27	117.81	122.20
45	S2	527	C	N3-C2-O2	-6.26	117.52	121.90
1	L1	2760	G	P-O3'-C3'	6.26	127.21	119.70
1	L1	209	U	C2-N1-C1'	6.26	125.21	117.70
1	L1	914	U	P-O3'-C3'	6.26	127.21	119.70
1	L1	1192	C	C6-N1-C2	-6.26	117.80	120.30
45	S2	1316	C	N1-C2-O2	6.25	122.65	118.90
1	L1	3778	U	N3-C2-O2	-6.23	117.84	122.20
1	L1	4266	G	N3-C4-C5	-6.23	125.48	128.60
1	L1	4862	G	C4-N9-C1'	6.23	134.60	126.50
1	L1	3772	U	N3-C2-O2	-6.22	117.84	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	La	78	LEU	CA-CB-CG	6.22	129.61	115.30
1	L1	4092	G	C6-C5-N7	-6.20	126.68	130.40
45	S2	1453	C	C6-N1-C1'	-6.20	113.36	120.80
1	L1	453	G	N3-C4-C5	-6.20	125.50	128.60
1	L1	453	G	C4-N9-C1'	6.20	134.55	126.50
1	L1	4862	G	C8-N9-C1'	-6.19	118.95	127.00
1	L1	3892	U	N3-C2-O2	-6.17	117.88	122.20
1	L1	1080	C	C6-N1-C2	-6.17	117.83	120.30
1	L1	4758	U	N3-C2-O2	-6.17	117.88	122.20
45	S2	1317	C	N1-C2-O2	6.17	122.60	118.90
45	S2	550	C	N3-C2-O2	-6.16	117.59	121.90
1	L1	2627	C	C6-N1-C2	-6.13	117.85	120.30
1	L1	2333	G	N9-C4-C5	6.12	107.85	105.40
1	L1	263	G	C5-C6-O6	6.11	132.27	128.60
45	S2	1772	C	C6-N1-C1'	-6.09	113.49	120.80
1	L1	129	C	N1-C2-O2	6.09	122.55	118.90
3	L3	128	C	N1-C2-O2	6.08	122.55	118.90
45	S2	659	G	C4-N9-C1'	6.06	134.38	126.50
1	L1	3598	C	C2-N1-C1'	6.05	125.46	118.80
1	L1	4112	C	N1-C2-O2	6.04	122.52	118.90
45	S2	1317	C	C6-N1-C2	-6.03	117.89	120.30
1	L1	1170	G	N1-C2-N2	-6.03	110.77	116.20
1	L1	757	G	N1-C2-N2	-6.03	110.77	116.20
1	L1	2333	G	N1-C6-O6	-6.01	116.30	119.90
1	L1	3909	C	C6-N1-C2	-6.01	117.90	120.30
45	S2	1261	C	C2-N1-C1'	6.01	125.41	118.80
45	S2	1520	G	C4-N9-C1'	6.00	134.30	126.50
45	S2	193	C	N1-C2-O2	6.00	122.50	118.90
45	S2	1271	C	N1-C2-O2	5.99	122.49	118.90
45	S2	1453	C	C6-N1-C2	-5.96	117.92	120.30
1	L1	3647	A	C6-N1-C2	-5.96	115.03	118.60
45	S2	194	C	C6-N1-C2	-5.95	117.92	120.30
1	L1	130	C	N1-C2-O2	5.93	122.46	118.90
79	CC	74	C	C6-N1-C2	-5.92	117.93	120.30
1	L1	4092	G	N7-C8-N9	5.92	116.06	113.10
1	L1	5022	U	N1-C2-O2	5.92	126.94	122.80
45	S2	1520	G	N3-C4-N9	5.92	129.55	126.00
1	L1	5022	U	N3-C2-O2	-5.91	118.06	122.20
45	S2	1520	G	C8-N9-C4	-5.89	104.04	106.40
1	L1	753	C	N1-C2-O2	5.89	122.43	118.90
1	L1	4714	C	N1-C2-O2	5.88	122.43	118.90
1	L1	1973	G	N1-C2-N2	-5.88	110.91	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L3	128	C	C2-N1-C1'	5.88	125.26	118.80
1	L1	3772	U	C2-N1-C1'	5.88	124.75	117.70
1	L1	4229	U	N1-C2-O2	5.87	126.91	122.80
1	L1	4862	G	N3-C4-C5	-5.87	125.66	128.60
45	S2	550	C	C6-N1-C2	-5.87	117.95	120.30
1	L1	1663	C	C6-N1-C2	-5.86	117.96	120.30
1	L1	485	C	C5-C6-N1	5.85	123.93	121.00
1	L1	3636	C	N3-C2-O2	-5.85	117.80	121.90
1	L1	2820	C	N1-C2-O2	5.85	122.41	118.90
45	S2	206	G	N1-C2-N2	-5.84	110.94	116.20
1	L1	4862	G	N9-C4-C5	-5.84	103.06	105.40
1	L1	1245	C	C2-N1-C1'	5.83	125.22	118.80
45	S2	130	G	N3-C4-N9	5.82	129.49	126.00
45	S2	130	G	C4-N9-C1'	5.82	134.06	126.50
1	L1	2858	A	N1-C6-N6	-5.82	115.11	118.60
45	S2	930	C	N1-C2-O2	5.80	122.38	118.90
79	CC	35	U	P-O3'-C3'	5.80	126.66	119.70
1	L1	130	C	C6-N1-C2	-5.80	117.98	120.30
1	L1	1993	C	N1-C2-O2	5.79	122.37	118.90
1	L1	654	C	N1-C2-O2	5.79	122.37	118.90
1	L1	1633	G	P-O3'-C3'	5.79	126.64	119.70
28	LZ	92	ASP	CB-CG-OD2	5.79	123.51	118.30
1	L1	3693	U	N3-C2-O2	-5.78	118.16	122.20
1	L1	3647	A	N1-C6-N6	-5.77	115.14	118.60
1	L1	255	C	N3-C2-O2	-5.76	117.87	121.90
1	L1	485	C	C6-N1-C2	-5.76	118.00	120.30
1	L1	2099	G	N1-C2-N2	-5.75	111.02	116.20
45	S2	130	G	N3-C4-C5	-5.75	125.72	128.60
1	L1	180	C	N3-C2-O2	-5.73	117.89	121.90
1	L1	2333	G	C4-C5-N7	-5.73	108.51	110.80
1	L1	1995	G	C6-C5-N7	-5.72	126.97	130.40
1	L1	3911	C	C5-C6-N1	5.72	123.86	121.00
45	S2	494	C	N1-C2-O2	5.71	122.33	118.90
1	L1	456	C	N1-C2-O2	5.71	122.32	118.90
46	SA	14	ASP	CB-CG-OD1	5.70	123.43	118.30
1	L1	453	G	N3-C4-N9	5.69	129.41	126.00
1	L1	986	C	C2-N1-C1'	5.69	125.06	118.80
1	L1	758	G	N1-C2-N2	-5.69	111.08	116.20
1	L1	1872	G	C5-C6-O6	5.68	132.01	128.60
1	L1	1994	C	C6-N1-C2	-5.66	118.04	120.30
45	S2	1261	C	C6-N1-C2	-5.65	118.04	120.30
1	L1	4241	C	C2-N1-C1'	5.64	125.01	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	1243	C	C2-N1-C1'	5.63	125.00	118.80
45	S2	1591	C	N1-C2-O2	5.63	122.28	118.90
1	L1	757	G	C5-C6-O6	5.63	131.98	128.60
45	S2	632	C	C2-N1-C1'	5.63	125.00	118.80
1	L1	1995	G	N3-C4-N9	5.63	129.38	126.00
1	L1	263	G	N1-C6-O6	-5.61	116.53	119.90
1	L1	1853	G	C4-N9-C1'	5.61	133.79	126.50
1	L1	2667	C	N1-C2-O2	5.61	122.27	118.90
1	L1	1447	C	C6-N1-C2	-5.60	118.06	120.30
45	S2	688	U	P-O3'-C3'	5.60	126.42	119.70
1	L1	753	C	C2-N1-C1'	5.60	124.96	118.80
1	L1	2410	C	C5-C6-N1	5.59	123.79	121.00
1	L1	3880	G	N1-C6-O6	-5.58	116.56	119.90
1	L1	3641	U	C4-C5-C6	5.57	123.04	119.70
1	L1	4266	G	N3-C4-N9	5.55	129.33	126.00
1	L1	2494	U	N1-C2-O2	5.55	126.68	122.80
45	S2	501	C	C5-C6-N1	5.54	123.77	121.00
1	L1	294	G	N3-C4-C5	-5.54	125.83	128.60
14	LL	144	LEU	CA-CB-CG	5.54	128.03	115.30
1	L1	693	C	C2-N1-C1'	5.53	124.89	118.80
1	L1	2096	G	C4-N9-C1'	5.53	133.69	126.50
1	L1	977	C	C2-N1-C1'	5.53	124.88	118.80
1	L1	1995	G	C4-N9-C1'	5.53	133.69	126.50
1	L1	2409	U	C6-N1-C1'	-5.53	113.46	121.20
45	S2	549	C	N1-C2-O2	5.52	122.21	118.90
1	L1	4404	U	C2-N1-C1'	5.52	124.33	117.70
1	L1	3693	U	N1-C2-O2	5.51	126.65	122.80
1	L1	1715	C	N1-C2-O2	5.50	122.20	118.90
1	L1	1893	C	C2-N1-C1'	5.49	124.83	118.80
1	L1	1872	G	N1-C6-O6	-5.48	116.61	119.90
45	S2	666	U	C2-N1-C1'	5.48	124.28	117.70
45	S2	1281	G	N1-C6-O6	-5.48	116.61	119.90
1	L1	923	C	C2-N1-C1'	5.47	124.82	118.80
1	L1	693	C	N1-C2-O2	5.47	122.18	118.90
1	L1	4112	C	C2-N1-C1'	5.47	124.82	118.80
1	L1	2492	C	C6-N1-C2	-5.46	118.12	120.30
1	L1	131	C	N1-C2-O2	5.45	122.17	118.90
1	L1	2094	G	C4-N9-C1'	5.45	133.59	126.50
45	S2	1422	G	C4-N9-C1'	5.45	133.58	126.50
68	SG	152	ASP	CB-CG-OD1	5.45	123.20	118.30
1	L1	406	C	P-O3'-C3'	5.44	126.23	119.70
1	L1	1082	C	P-O3'-C3'	5.44	126.23	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	S2	112	U	P-O3'-C3'	5.44	126.23	119.70
45	S2	1772	C	C5-C6-N1	5.44	123.72	121.00
45	S2	1281	G	C5-C6-O6	5.44	131.86	128.60
1	L1	139	G	C8-N9-C4	-5.43	104.23	106.40
1	L1	2528	G	N3-C4-N9	5.43	129.26	126.00
45	S2	1261	C	N1-C2-O2	5.43	122.16	118.90
1	L1	2819	U	N3-C2-O2	-5.42	118.40	122.20
1	L1	1973	G	N1-C6-O6	-5.42	116.65	119.90
1	L1	4266	G	C4-N9-C1'	5.42	133.54	126.50
1	L1	4709	U	C6-N1-C1'	-5.42	113.62	121.20
1	L1	1170	G	N1-C6-O6	-5.41	116.65	119.90
45	S2	1422	G	N3-C4-C5	-5.41	125.89	128.60
1	L1	2627	C	N3-C2-O2	-5.39	118.13	121.90
1	L1	4594	U	C2-N1-C1'	5.39	124.16	117.70
1	L1	68	U	N3-C2-O2	-5.38	118.43	122.20
1	L1	4399	U	N3-C2-O2	-5.38	118.43	122.20
45	S2	1316	C	N3-C2-O2	-5.38	118.13	121.90
45	S2	1022	U	N1-C2-O2	5.38	126.56	122.80
1	L1	2820	C	N3-C2-O2	-5.37	118.14	121.90
1	L1	220	C	C2-N1-C1'	5.36	124.70	118.80
1	L1	1446	C	N1-C2-O2	5.36	122.11	118.90
1	L1	2528	G	C2-N3-C4	5.35	114.58	111.90
1	L1	4092	G	C4-C5-N7	5.35	112.94	110.80
1	L1	4862	G	C6-C5-N7	-5.35	127.19	130.40
45	S2	329	G	N3-C4-N9	5.35	129.21	126.00
2	L2	102	U	N1-C2-O2	5.33	126.53	122.80
1	L1	925	C	C6-N1-C2	-5.33	118.17	120.30
45	S2	1281	G	N1-C2-N2	-5.33	111.41	116.20
1	L1	1702	C	N1-C2-O2	5.33	122.10	118.90
78	CE	371	LEU	CA-CB-CG	5.32	127.54	115.30
45	S2	1750	C	N1-C2-O2	5.32	122.09	118.90
45	S2	1453	C	C5-C6-N1	5.32	123.66	121.00
1	L1	1995	G	N9-C4-C5	-5.32	103.27	105.40
45	S2	563	G	P-O3'-C3'	5.32	126.08	119.70
1	L1	3930	U	N1-C2-O2	5.31	126.52	122.80
1	L1	1988	G	N3-C4-C5	-5.31	125.94	128.60
1	L1	2532	C	C2-N1-C1'	5.31	124.64	118.80
1	L1	1995	G	C8-N9-C1'	-5.30	120.11	127.00
1	L1	138	G	C8-N9-C4	-5.30	104.28	106.40
1	L1	336	A	C5-C6-N6	-5.29	119.46	123.70
1	L1	2487	G	N1-C6-O6	-5.29	116.72	119.90
1	L1	138	G	N1-C2-N2	-5.29	111.44	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	4709	U	N3-C4-O4	5.28	123.09	119.40
1	L1	4772	C	C6-N1-C2	-5.28	118.19	120.30
1	L1	3673	C	P-O3'-C3'	5.27	126.03	119.70
1	L1	3853	U	N3-C2-O2	-5.27	118.51	122.20
1	L1	1220	G	N1-C2-N2	-5.26	111.46	116.20
45	S2	1434	C	P-O3'-C3'	5.26	126.02	119.70
1	L1	112	C	C2-N1-C1'	5.26	124.59	118.80
45	S2	322	C	C6-N1-C2	-5.26	118.20	120.30
1	L1	3772	U	N1-C2-O2	5.25	126.48	122.80
1	L1	905	C	N1-C2-O2	5.25	122.05	118.90
1	L1	1458	C	N1-C2-O2	5.24	122.04	118.90
45	S2	168	C	C2-N1-C1'	5.24	124.56	118.80
70	SM	125	GLU	N-CA-CB	5.23	120.02	110.60
1	L1	2627	C	C5-C6-N1	5.23	123.61	121.00
45	S2	178	C	N1-C2-O2	5.23	122.04	118.90
1	L1	1989	G	C5-C6-O6	5.22	131.73	128.60
1	L1	1995	G	C4-C5-N7	5.22	112.89	110.80
1	L1	74	G	N3-C4-N9	5.22	129.13	126.00
1	L1	2333	G	N3-C4-N9	-5.21	122.87	126.00
45	S2	1271	C	C2-N1-C1'	5.21	124.53	118.80
1	L1	5035	U	N3-C2-O2	-5.21	118.56	122.20
45	S2	168	C	N3-C2-O2	-5.21	118.26	121.90
45	S2	1261	C	N3-C2-O2	-5.20	118.26	121.90
1	L1	3911	C	C6-N1-C2	-5.19	118.22	120.30
1	L1	655	C	N1-C2-N3	5.19	122.83	119.20
1	L1	2099	G	N1-C6-O6	-5.18	116.79	119.90
1	L1	2102	G	N3-C4-N9	5.18	129.11	126.00
3	L3	128	C	C5-C6-N1	5.18	123.59	121.00
1	L1	962	C	N1-C2-O2	5.18	122.00	118.90
1	L1	1731	C	C2-N1-C1'	5.17	124.49	118.80
1	L1	923	C	N1-C2-O2	5.17	122.00	118.90
1	L1	489	C	C2-N1-C1'	5.16	124.47	118.80
1	L1	4887	C	N1-C2-O2	5.16	121.99	118.90
45	S2	965	U	N3-C2-O2	-5.16	118.59	122.20
1	L1	2304	U	N3-C2-O2	-5.15	118.59	122.20
2	L2	28	C	C6-N1-C2	-5.15	118.24	120.30
1	L1	139	G	N1-C2-N2	-5.15	111.57	116.20
1	L1	1973	G	N3-C2-N2	5.14	123.50	119.90
1	L1	1988	G	C6-C5-N7	-5.14	127.31	130.40
1	L1	4420	U	C6-N1-C1'	-5.14	114.00	121.20
45	S2	205	G	C4-N9-C1'	5.14	133.19	126.50
45	S2	1306	U	C2-N1-C1'	5.14	123.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	2333	G	N1-C2-N3	5.14	126.98	123.90
45	S2	659	G	C8-N9-C1'	-5.13	120.33	127.00
1	L1	4747	C	C2-N1-C1'	5.13	124.44	118.80
45	S2	204	G	N1-C6-O6	-5.13	116.82	119.90
1	L1	3909	C	N3-C2-O2	-5.12	118.31	121.90
45	S2	1417	C	N3-C2-O2	-5.12	118.31	121.90
1	L1	1079	C	C6-N1-C2	-5.12	118.25	120.30
45	S2	1422	G	N3-C4-N9	5.12	129.07	126.00
1	L1	2102	G	N9-C1'-C2'	5.11	120.65	114.00
1	L1	2303	C	N3-C2-O2	-5.11	118.32	121.90
1	L1	1702	C	C2-N1-C1'	5.09	124.40	118.80
3	L3	128	C	C6-N1-C2	-5.09	118.26	120.30
1	L1	1973	G	C5-C6-O6	5.09	131.66	128.60
1	L1	131	C	C6-N1-C2	-5.09	118.27	120.30
1	L1	3930	U	N3-C2-O2	-5.09	118.64	122.20
1	L1	1726	U	N3-C2-O2	-5.09	118.64	122.20
1	L1	1395	U	N3-C2-O2	-5.08	118.64	122.20
45	S2	550	C	C5-C4-N4	5.08	123.76	120.20
70	SM	125	GLU	CA-CB-CG	5.08	124.58	113.40
1	L1	294	G	C2-N3-C4	5.07	114.44	111.90
45	S2	1670	C	N1-C2-O2	5.07	121.94	118.90
2	L2	102	U	N3-C2-O2	-5.06	118.66	122.20
45	S2	1416	C	N1-C2-O2	5.06	121.94	118.90
1	L1	2494	U	N3-C2-O2	-5.05	118.66	122.20
45	S2	973	C	N1-C2-O2	5.05	121.93	118.90
1	L1	512	U	N1-C2-O2	5.05	126.33	122.80
1	L1	4112	C	N3-C2-O2	-5.05	118.37	121.90
1	L1	2303	C	N1-C2-N3	5.04	122.73	119.20
1	L1	914	U	C5-C4-O4	-5.04	122.88	125.90
1	L1	453	G	C8-N9-C1'	-5.04	120.45	127.00
1	L1	1081	C	N1-C2-O2	5.03	121.92	118.90
1	L1	1220	G	N1-C6-O6	-5.03	116.88	119.90
45	S2	193	C	N1-C2-N3	5.03	122.72	119.20
45	S2	192	C	C2-N1-C1'	5.03	124.33	118.80
1	L1	155	C	N3-C2-O2	-5.02	118.38	121.90
1	L1	4864	U	N1-C2-O2	5.02	126.31	122.80
1	L1	4551	U	N3-C2-O2	-5.01	118.69	122.20
1	L1	41	C	C6-N1-C2	-5.01	118.30	120.30
1	L1	138	G	N1-C6-O6	-5.01	116.90	119.90
1	L1	2096	G	N3-C4-C5	-5.01	126.10	128.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	LP	131	ARG	Peptide
56	SQ	145	TYR	Peptide
56	SQ	43	GLU	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	230 (94%)	16 (6%)	0	100	100
5	LB	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
6	LC	363/427 (85%)	354 (98%)	9 (2%)	0	100	100
7	LD	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
8	LE	214/288 (74%)	205 (96%)	9 (4%)	0	100	100
9	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
10	LG	223/266 (84%)	218 (98%)	5 (2%)	0	100	100
11	LH	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
12	LI	198/214 (92%)	190 (96%)	8 (4%)	0	100	100
13	LJ	167/178 (94%)	161 (96%)	6 (4%)	0	100	100
14	LL	208/211 (99%)	196 (94%)	12 (6%)	0	100	100
15	LM	137/215 (64%)	132 (96%)	5 (4%)	0	100	100
16	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
17	LO	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	LQ	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
20	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
21	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
22	LT	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
23	LU	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
24	LV	129/140 (92%)	121 (94%)	8 (6%)	0	100	100
25	LW	122/157 (78%)	118 (97%)	4 (3%)	0	100	100
26	LX	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
27	LY	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
28	LZ	133/282 (47%)	126 (95%)	7 (5%)	0	100	100
28	La	145/282 (51%)	139 (96%)	6 (4%)	0	100	100
29	Lb	105/159 (66%)	99 (94%)	6 (6%)	0	100	100
30	Lc	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
31	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
32	Le	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
33	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
34	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
35	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
36	Li	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
37	Lj	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
38	Lk	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
39	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
40	Lm	50/128 (39%)	50 (100%)	0	0	100	100
41	Ln	22/25 (88%)	22 (100%)	0	0	100	100
42	Lo	100/106 (94%)	97 (97%)	3 (3%)	0	100	100
43	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
44	Lr	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
46	SA	220/295 (75%)	215 (98%)	5 (2%)	0	100	100
47	SB	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
48	SD	225/243 (93%)	220 (98%)	5 (2%)	0	100	100
49	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	SF	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
51	SH	182/194 (94%)	169 (93%)	11 (6%)	2 (1%)	12	30
52	SI	204/208 (98%)	193 (95%)	11 (5%)	0	100	100
53	SK	96/165 (58%)	90 (94%)	5 (5%)	1 (1%)	13	33
54	SL	140/158 (89%)	131 (94%)	9 (6%)	0	100	100
55	SP	125/145 (86%)	120 (96%)	5 (4%)	0	100	100
56	SQ	142/146 (97%)	128 (90%)	14 (10%)	0	100	100
57	SR	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
58	SS	143/152 (94%)	136 (95%)	7 (5%)	0	100	100
59	ST	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
60	SU	102/119 (86%)	95 (93%)	6 (6%)	1 (1%)	13	33
61	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
62	SX	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
63	Sa	100/115 (87%)	94 (94%)	5 (5%)	1 (1%)	13	33
64	Sc	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
65	Sd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
66	Sg	311/317 (98%)	292 (94%)	18 (6%)	1 (0%)	37	61
67	SC	220/293 (75%)	217 (99%)	3 (1%)	0	100	100
68	SG	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
69	SJ	183/194 (94%)	176 (96%)	6 (3%)	1 (0%)	25	49
70	SM	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
71	SN	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
72	SO	133/151 (88%)	126 (95%)	6 (4%)	1 (1%)	16	38
73	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
74	SY	123/133 (92%)	117 (95%)	6 (5%)	0	100	100
75	SZ	73/125 (58%)	69 (94%)	4 (6%)	0	100	100
76	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
77	Se	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
78	CE	70/133 (53%)	67 (96%)	3 (4%)	0	100	100
78	Sf	59/133 (44%)	52 (88%)	7 (12%)	0	100	100
All	All	11319/13078 (86%)	10904 (96%)	407 (4%)	8 (0%)	50	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	SU	94	PRO
51	SH	34	SER
51	SH	35	ASP
66	Sg	50	THR
69	SJ	122	SER
72	SO	140	THR
53	SK	64	TRP
63	Sa	46	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	LA	190/199 (96%)	189 (100%)	1 (0%)	86 95
5	LB	348/349 (100%)	347 (100%)	1 (0%)	91 97
6	LC	304/348 (87%)	302 (99%)	2 (1%)	81 93
7	LD	246/250 (98%)	246 (100%)	0	100 100
8	LE	194/252 (77%)	193 (100%)	1 (0%)	86 95
9	LF	194/215 (90%)	192 (99%)	2 (1%)	73 89
10	LG	196/223 (88%)	196 (100%)	0	100 100
11	LH	169/171 (99%)	169 (100%)	0	100 100
12	LI	172/181 (95%)	170 (99%)	2 (1%)	67 86
13	LJ	142/149 (95%)	142 (100%)	0	100 100
14	LL	176/177 (99%)	176 (100%)	0	100 100
15	LM	118/161 (73%)	118 (100%)	0	100 100
16	LN	171/172 (99%)	170 (99%)	1 (1%)	84 94
17	LO	173/174 (99%)	173 (100%)	0	100 100
18	LP	134/163 (82%)	134 (100%)	0	100 100
19	LQ	164/165 (99%)	164 (100%)	0	100 100
20	LR	166/175 (95%)	164 (99%)	2 (1%)	67 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	LS	157/157 (100%)	157 (100%)	0	100	100
22	LT	139/140 (99%)	139 (100%)	0	100	100
23	LU	91/115 (79%)	91 (100%)	0	100	100
24	LV	101/107 (94%)	100 (99%)	1 (1%)	73	89
25	LW	103/126 (82%)	102 (99%)	1 (1%)	73	89
26	LX	106/133 (80%)	106 (100%)	0	100	100
27	LY	124/135 (92%)	124 (100%)	0	100	100
28	LZ	117/237 (49%)	116 (99%)	1 (1%)	75	90
28	La	120/237 (51%)	118 (98%)	2 (2%)	56	81
29	Lb	88/126 (70%)	87 (99%)	1 (1%)	70	87
30	Lc	83/97 (86%)	83 (100%)	0	100	100
31	Ld	98/110 (89%)	98 (100%)	0	100	100
32	Le	114/121 (94%)	114 (100%)	0	100	100
33	Lf	88/89 (99%)	88 (100%)	0	100	100
34	Lg	98/100 (98%)	98 (100%)	0	100	100
35	Lh	109/110 (99%)	109 (100%)	0	100	100
36	Li	86/89 (97%)	85 (99%)	1 (1%)	67	86
37	Lj	73/80 (91%)	73 (100%)	0	100	100
38	Lk	64/65 (98%)	64 (100%)	0	100	100
39	Ll	47/48 (98%)	47 (100%)	0	100	100
40	Lm	48/116 (41%)	48 (100%)	0	100	100
41	Ln	23/24 (96%)	23 (100%)	0	100	100
42	Lo	90/93 (97%)	89 (99%)	1 (1%)	70	87
43	Lp	74/75 (99%)	74 (100%)	0	100	100
44	Lr	109/121 (90%)	109 (100%)	0	100	100
46	SA	184/243 (76%)	184 (100%)	0	100	100
47	SB	195/231 (84%)	195 (100%)	0	100	100
48	SD	190/202 (94%)	189 (100%)	1 (0%)	86	95
49	SE	224/225 (100%)	223 (100%)	1 (0%)	89	96
50	SF	156/170 (92%)	155 (99%)	1 (1%)	84	94
51	SH	166/174 (95%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	SI	178/180 (99%)	177 (99%)	1 (1%)	84 94
53	SK	89/136 (65%)	89 (100%)	0	100 100
54	SL	130/142 (92%)	129 (99%)	1 (1%)	79 91
55	SP	113/130 (87%)	113 (100%)	0	100 100
56	SQ	119/121 (98%)	119 (100%)	0	100 100
57	SR	122/122 (100%)	122 (100%)	0	100 100
58	SS	126/132 (96%)	126 (100%)	0	100 100
59	ST	113/115 (98%)	113 (100%)	0	100 100
60	SU	94/107 (88%)	93 (99%)	1 (1%)	70 87
61	SV	67/67 (100%)	62 (92%)	5 (8%)	11 28
62	SX	113/115 (98%)	113 (100%)	0	100 100
63	Sa	89/98 (91%)	89 (100%)	0	100 100
64	Sc	57/62 (92%)	57 (100%)	0	100 100
65	Sd	48/49 (98%)	48 (100%)	0	100 100
66	Sg	272/275 (99%)	272 (100%)	0	100 100
67	SC	188/225 (84%)	188 (100%)	0	100 100
68	SG	207/218 (95%)	204 (99%)	3 (1%)	62 84
69	SJ	161/168 (96%)	161 (100%)	0	100 100
70	SM	102/108 (94%)	101 (99%)	1 (1%)	73 89
71	SN	130/131 (99%)	130 (100%)	0	100 100
72	SO	105/119 (88%)	105 (100%)	0	100 100
73	SW	112/113 (99%)	112 (100%)	0	100 100
74	SY	109/115 (95%)	109 (100%)	0	100 100
75	SZ	66/103 (64%)	66 (100%)	0	100 100
76	Sb	75/76 (99%)	75 (100%)	0	100 100
77	Se	47/48 (98%)	47 (100%)	0	100 100
78	CE	68/122 (56%)	68 (100%)	0	100 100
78	Sf	54/122 (44%)	52 (96%)	2 (4%)	29 58
All	All	9876/11139 (89%)	9839 (100%)	37 (0%)	88 96

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	15	VAL
5	LB	261	ARG
6	LC	71	ARG
6	LC	188	ARG
8	LE	56	ARG
9	LF	221	LYS
9	LF	223	LYS
12	LI	13	LYS
12	LI	208	LYS
16	LN	83	LYS
20	LR	40	GLN
20	LR	43	LYS
24	LV	48	ARG
25	LW	116	LYS
28	LZ	60	LYS
28	La	4	ARG
28	La	92	LYS
29	Lb	63	LYS
36	Li	56	ARG
42	Lo	99	ARG
48	SD	76	ARG
49	SE	62	LYS
50	SF	135	ARG
52	SI	5	ARG
54	SL	69	ARG
60	SU	87	ARG
61	SV	79	VAL
61	SV	80	SER
61	SV	81	LYS
61	SV	82	ASN
61	SV	83	PHE
68	SG	217	MET
68	SG	218	LYS
68	SG	221	LYS
70	SM	63	LYS
78	Sf	107	LYS
78	Sf	138	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	194	ASN
11	LH	39	ASN

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Mol	Chain	Res	Type
15	LM	20	HIS
15	LM	48	GLN
30	Lc	40	GLN
32	Le	92	ASN
34	Lg	110	GLN
38	Lk	58	GLN
47	SB	186	ASN
53	SK	50	GLN
59	ST	142	ASN
60	SU	28	ASN
72	SO	113	GLN
77	Se	15	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	3701/5070 (72%)	743 (20%)	12 (0%)
2	L2	119/121 (98%)	11 (9%)	0
3	L3	155/157 (98%)	34 (21%)	0
45	S2	1708/1869 (91%)	334 (19%)	9 (0%)
79	CC	74/75 (98%)	23 (31%)	2 (2%)
All	All	5757/7292 (78%)	1145 (19%)	23 (0%)

All (1145) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	39	A
1	L1	48	G
1	L1	56	A
1	L1	59	A
1	L1	64	A
1	L1	65	A
1	L1	66	A
1	L1	69	A
1	L1	73	A
1	L1	91	G
1	L1	98	A
1	L1	108	A
1	L1	109	G
1	L1	110	C
1	L1	116	G

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Mol	Chain	Res	Type
1	L1	117	C
1	L1	119	G
1	L1	120	A
1	L1	133	C
1	L1	134	G
1	L1	135	G
1	L1	136	C
1	L1	159	C
1	L1	169	G
1	L1	172	C
1	L1	178	C
1	L1	183	C
1	L1	184	U
1	L1	185	C
1	L1	188	G
1	L1	189	G
1	L1	200	U
1	L1	209	U
1	L1	210	C
1	L1	216	C
1	L1	218	A
1	L1	219	G
1	L1	233	U
1	L1	234	G
1	L1	255	C
1	L1	256	G
1	L1	258	G
1	L1	259	C
1	L1	261	G
1	L1	265	C
1	L1	269	G
1	L1	280	G
1	L1	297	U
1	L1	306	A
1	L1	315	G
1	L1	316	U
1	L1	322	C
1	L1	340	C
1	L1	350	C
1	L1	353	A
1	L1	373	G
1	L1	387	G

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Mol	Chain	Res	Type
1	L1	388	A
1	L1	407	A
1	L1	408	A
1	L1	410	A
1	L1	412	G
1	L1	413	G
1	L1	414	C
1	L1	432	U
1	L1	449	C
1	L1	450	G
1	L1	452	A
1	L1	453	G
1	L1	454	U
1	L1	456	C
1	L1	457	G
1	L1	465	G
1	L1	467	U
1	L1	468	U
1	L1	484	U
1	L1	485	C
1	L1	486	C
1	L1	489	C
1	L1	493	G
1	L1	494	U
1	L1	497	G
1	L1	498	C
1	L1	500	G
1	L1	501	C
1	L1	502	C
1	L1	503	C
1	L1	504	G
1	L1	505	G
1	L1	509	A
1	L1	510	U
1	L1	513	U
1	L1	514	U
1	L1	518	G
1	L1	643	C
1	L1	645	G
1	L1	646	G
1	L1	656	C
1	L1	657	C

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Mol	Chain	Res	Type
1	L1	659	G
1	L1	665	C
1	L1	668	C
1	L1	685	C
1	L1	686	A
1	L1	687	U
1	L1	688	U
1	L1	696	C
1	L1	704	C
1	L1	731	G
1	L1	738	C
1	L1	739	G
1	L1	742	G
1	L1	749	G
1	L1	754	U
1	L1	759	G
1	L1	904	C
1	L1	905	C
1	L1	907	C
1	L1	913	U
1	L1	914	U
1	L1	915	A
1	L1	917	A
1	L1	918	G
1	L1	924	C
1	L1	925	C
1	L1	926	G
1	L1	932	A
1	L1	933	G
1	L1	934	C
1	L1	935	A
1	L1	943	A
1	L1	944	A
1	L1	945	U
1	L1	946	C
1	L1	956	A
1	L1	959	G
1	L1	960	A
1	L1	962	C
1	L1	965	G
1	L1	966	A
1	L1	967	C

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Mol	Chain	Res	Type
1	L1	968	C
1	L1	970	G
1	L1	982	U
1	L1	986	C
1	L1	989	U
1	L1	990	C
1	L1	991	C
1	L1	992	C
1	L1	993	G
1	L1	995	C
1	L1	1048	G
1	L1	1049	C
1	L1	1050	C
1	L1	1051	G
1	L1	1082	C
1	L1	1083	U
1	L1	1095	A
1	L1	1168	G
1	L1	1170	G
1	L1	1171	G
1	L1	1172	C
1	L1	1173	G
1	L1	1178	G
1	L1	1179	U
1	L1	1180	C
1	L1	1181	C
1	L1	1182	C
1	L1	1183	C
1	L1	1184	A
1	L1	1193	C
1	L1	1200	G
1	L1	1202	C
1	L1	1203	G
1	L1	1210	C
1	L1	1211	G
1	L1	1214	C
1	L1	1215	C
1	L1	1218	G
1	L1	1219	G
1	L1	1220	G
1	L1	1221	G
1	L1	1222	A

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Mol	Chain	Res	Type
1	L1	1241	C
1	L1	1246	G
1	L1	1254	A
1	L1	1255	A
1	L1	1258	G
1	L1	1266	G
1	L1	1269	G
1	L1	1270	A
1	L1	1271	G
1	L1	1273	G
1	L1	1275	G
1	L1	1280	C
1	L1	1284	G
1	L1	1285	U
1	L1	1287	G
1	L1	1293	G
1	L1	1294	A
1	L1	1295	C
1	L1	1296	G
1	L1	1301	C
1	L1	1302	U
1	L1	1303	A
1	L1	1313	C
1	L1	1326	A2M
1	L1	1337	A
1	L1	1340	OMC
1	L1	1354	A
1	L1	1358	G
1	L1	1359	G
1	L1	1365	C
1	L1	1367	C
1	L1	1379	C
1	L1	1387	A
1	L1	1394	G
1	L1	1397	A
1	L1	1398	A
1	L1	1404	G
1	L1	1408	G
1	L1	1409	C
1	L1	1410	U
1	L1	1417	C
1	L1	1420	A

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Mol	Chain	Res	Type
1	L1	1433	A
1	L1	1439	C
1	L1	1441	C
1	L1	1444	G
1	L1	1447	C
1	L1	1481	C
1	L1	1482	G
1	L1	1483	C
1	L1	1497	A
1	L1	1498	G
1	L1	1502	G
1	L1	1518	A
1	L1	1534	A2M
1	L1	1547	A
1	L1	1549	G
1	L1	1564	A
1	L1	1566	C
1	L1	1578	U
1	L1	1591	U
1	L1	1596	U
1	L1	1611	C
1	L1	1612	G
1	L1	1624	G
1	L1	1625	OMG
1	L1	1626	G
1	L1	1631	A
1	L1	1633	G
1	L1	1634	A
1	L1	1640	C
1	L1	1642	A
1	L1	1654	G
1	L1	1661	C
1	L1	1676	C
1	L1	1677	PSU
1	L1	1678	C
1	L1	1681	G
1	L1	1694	C
1	L1	1697	G
1	L1	1699	A
1	L1	1700	G
1	L1	1701	A
1	L1	1702	C

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Mol	Chain	Res	Type
1	L1	1704	C
1	L1	1705	G
1	L1	1707	C
1	L1	1726	U
1	L1	1731	C
1	L1	1734	G
1	L1	1735	U
1	L1	1742	A
1	L1	1755	C
1	L1	1756	U
1	L1	1757	U
1	L1	1758	G
1	L1	1760	G
1	L1	1761	G
1	L1	1762	C
1	L1	1763	C
1	L1	1765	A
1	L1	1766	A
1	L1	1767	A
1	L1	1768	C
1	L1	1769	G
1	L1	1770	A
1	L1	1775	A
1	L1	1785	C
1	L1	1787	A
1	L1	1797	G
1	L1	1804	A
1	L1	1806	G
1	L1	1810	G
1	L1	1815	G
1	L1	1820	C
1	L1	1821	G
1	L1	1822	U
1	L1	1834	U
1	L1	1836	G
1	L1	1837	A
1	L1	1842	G
1	L1	1855	G
1	L1	1869	G
1	L1	1897	A
1	L1	1918	U
1	L1	1919	G

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Mol	Chain	Res	Type
1	L1	1920	C
1	L1	1921	C
1	L1	1922	G
1	L1	1925	G
1	L1	1931	C
1	L1	1932	A
1	L1	1936	C
1	L1	1939	A
1	L1	1940	G
1	L1	1948	G
1	L1	1951	G
1	L1	1959	U
1	L1	1961	G
1	L1	1962	A
1	L1	1974	U
1	L1	1975	G
1	L1	1978	C
1	L1	1982	G
1	L1	1984	A
1	L1	1985	G
1	L1	1986	U
1	L1	1987	C
1	L1	1988	G
1	L1	1989	G
1	L1	1990	A
1	L1	1993	C
1	L1	1997	U
1	L1	1998	A
1	L1	2001	G
1	L1	2002	A
1	L1	2003	G
1	L1	2004	U
1	L1	2011	C
1	L1	2017	A
1	L1	2018	C
1	L1	2026	A
1	L1	2046	G
1	L1	2048	U
1	L1	2052	G
1	L1	2055	G
1	L1	2056	G
1	L1	2069	A

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Mol	Chain	Res	Type
1	L1	2084	C
1	L1	2085	G
1	L1	2090	U
1	L1	2092	G
1	L1	2093	A
1	L1	2094	G
1	L1	2095	A
1	L1	2097	U
1	L1	2098	G
1	L1	2100	A
1	L1	2101	C
1	L1	2102	G
1	L1	2110	C
1	L1	2112	G
1	L1	2252	G
1	L1	2253	A
1	L1	2256	C
1	L1	2258	C
1	L1	2289	C
1	L1	2300	A
1	L1	2301	G
1	L1	2313	A
1	L1	2316	G
1	L1	2333	G
1	L1	2348	G
1	L1	2351	OMC
1	L1	2357	G
1	L1	2360	A
1	L1	2382	A
1	L1	2395	A
1	L1	2396	A
1	L1	2397	G
1	L1	2408	U
1	L1	2410	C
1	L1	2417	A
1	L1	2421	G
1	L1	2422	OMC
1	L1	2424	OMG
1	L1	2425	U
1	L1	2450	G
1	L1	2453	A
1	L1	2464	C

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Mol	Chain	Res	Type
1	L1	2465	C
1	L1	2471	G
1	L1	2474	G
1	L1	2475	G
1	L1	2478	C
1	L1	2479	G
1	L1	2483	G
1	L1	2484	A
1	L1	2485	U
1	L1	2486	G
1	L1	2487	G
1	L1	2489	C
1	L1	2490	U
1	L1	2491	C
1	L1	2493	G
1	L1	2503	G
1	L1	2504	C
1	L1	2505	C
1	L1	2506	G
1	L1	2513	A
1	L1	2519	U
1	L1	2537	A
1	L1	2544	G
1	L1	2546	G
1	L1	2547	G
1	L1	2554	U
1	L1	2555	G
1	L1	2565	A
1	L1	2573	A
1	L1	2583	C
1	L1	2587	A
1	L1	2589	C
1	L1	2601	A
1	L1	2618	G
1	L1	2627	C
1	L1	2638	G
1	L1	2653	C
1	L1	2662	G
1	L1	2669	C
1	L1	2670	C
1	L1	2687	U
1	L1	2694	G

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Mol	Chain	Res	Type
1	L1	2695	A
1	L1	2696	A
1	L1	2710	C
1	L1	2711	G
1	L1	2725	A
1	L1	2726	G
1	L1	2739	C
1	L1	2743	A
1	L1	2754	G
1	L1	2756	G
1	L1	2761	U
1	L1	2763	U
1	L1	2764	A
1	L1	2769	U
1	L1	2770	C
1	L1	2788	U
1	L1	2790	U
1	L1	2794	C
1	L1	2814	C
1	L1	2825	A
1	L1	2826	U
1	L1	2827	G
1	L1	2838	G
1	L1	2855	G
1	L1	2867	C
1	L1	2892	C
1	L1	2899	C
1	L1	2900	U
1	L1	2902	G
1	L1	2903	G
1	L1	2906	G
1	L1	2907	G
1	L1	2908	U
1	L1	2909	C
1	L1	2910	G
1	L1	3585	G
1	L1	3587	C
1	L1	3588	C
1	L1	3591	C
1	L1	3593	C
1	L1	3594	C
1	L1	3595	U

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Mol	Chain	Res	Type
1	L1	3596	A
1	L1	3597	G
1	L1	3604	A
1	L1	3615	G
1	L1	3618	C
1	L1	3626	G
1	L1	3630	A
1	L1	3635	A
1	L1	3644	U
1	L1	3646	A
1	L1	3648	A
1	L1	3662	A
1	L1	3664	G
1	L1	3673	C
1	L1	3674	G
1	L1	3711	A
1	L1	3713	U
1	L1	3714	G
1	L1	3727	A
1	L1	3729	PSU
1	L1	3748	A
1	L1	3750	G
1	L1	3753	G
1	L1	3754	G
1	L1	3760	A
1	L1	3764	PSU
1	L1	3771	C
1	L1	3775	A
1	L1	3776	G
1	L1	3777	G
1	L1	3784	A
1	L1	3785	A2M
1	L1	3786	U
1	L1	3802	U
1	L1	3808	OMC
1	L1	3811	G
1	L1	3814	U
1	L1	3817	A
1	L1	3819	G
1	L1	3838	U
1	L1	3840	U
1	L1	3867	A2M

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Mol	Chain	Res	Type
1	L1	3876	A
1	L1	3877	A
1	L1	3878	C
1	L1	3879	G
1	L1	3897	G
1	L1	3898	G
1	L1	3900	G
1	L1	3901	A
1	L1	3906	A
1	L1	3907	G
1	L1	3908	A
1	L1	3915	U
1	L1	3930	U
1	L1	3944	OMG
1	L1	3947	A
1	L1	3949	A
1	L1	3950	U
1	L1	3951	G
1	L1	3952	A
1	L1	3955	G
1	L1	3956	G
1	L1	3957	U
1	L1	3958	G
1	L1	3959	U
1	L1	3960	A
1	L1	3963	A
1	L1	3964	U
1	L1	3965	A
1	L1	3966	A
1	L1	3967	G
1	L1	3969	G
1	L1	3970	G
1	L1	3971	G
1	L1	3972	A
1	L1	3973	G
1	L1	3974	G
1	L1	3975	C
1	L1	3977	C
1	L1	4034	G
1	L1	4035	G
1	L1	4036	G
1	L1	4041	C

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Mol	Chain	Res	Type
1	L1	4042	G
1	L1	4043	G
1	L1	4044	U
1	L1	4046	A
1	L1	4048	A
1	L1	4049	U
1	L1	4051	C
1	L1	4052	C
1	L1	4053	A
1	L1	4054	C
1	L1	4055	U
1	L1	4056	A
1	L1	4059	C
1	L1	4062	A
1	L1	4064	C
1	L1	4069	U
1	L1	4073	A
1	L1	4076	G
1	L1	4086	G
1	L1	4091	G
1	L1	4094	G
1	L1	4095	G
1	L1	4099	G
1	L1	4100	C
1	L1	4102	C
1	L1	4103	C
1	L1	4104	G
1	L1	4107	G
1	L1	4112	C
1	L1	4113	U
1	L1	4114	C
1	L1	4115	G
1	L1	4116	C
1	L1	4117	U
1	L1	4119	C
1	L1	4122	G
1	L1	4127	A
1	L1	4133	C
1	L1	4139	G
1	L1	4140	C
1	L1	4141	G
1	L1	4142	C

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Mol	Chain	Res	Type
1	L1	4143	G
1	L1	4160	C
1	L1	4162	C
1	L1	4163	U
1	L1	4168	G
1	L1	4170	A
1	L1	4183	G
1	L1	4184	G
1	L1	4191	G
1	L1	4203	A
1	L1	4222	G
1	L1	4229	U
1	L1	4233	A
1	L1	4251	A
1	L1	4254	G
1	L1	4265	U
1	L1	4266	G
1	L1	4268	A
1	L1	4273	A
1	L1	4281	A
1	L1	4291	G
1	L1	4304	A
1	L1	4305	G
1	L1	4329	G
1	L1	4330	G
1	L1	4332	C
1	L1	4339	A
1	L1	4349	C
1	L1	4350	C
1	L1	4373	G
1	L1	4376	A
1	L1	4377	G
1	L1	4378	A
1	L1	4379	A
1	L1	4381	A
1	L1	4382	G
1	L1	4387	C
1	L1	4391	G
1	L1	4393	G
1	L1	4394	A
1	L1	4422	A
1	L1	4444	C

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Mol	Chain	Res	Type
1	L1	4448	G
1	L1	4449	A
1	L1	4452	U
1	L1	4453	C
1	L1	4464	A
1	L1	4466	C
1	L1	4475	G
1	L1	4500	PSU
1	L1	4512	U
1	L1	4513	A
1	L1	4518	A
1	L1	4519	C
1	L1	4524	G
1	L1	4528	G
1	L1	4548	A
1	L1	4549	G
1	L1	4554	G
1	L1	4560	C
1	L1	4567	G
1	L1	4570	G
1	L1	4573	G
1	L1	4575	G
1	L1	4590	A
1	L1	4636	PSU
1	L1	4637	OMG
1	L1	4647	G
1	L1	4652	G
1	L1	4656	A
1	L1	4657	U
1	L1	4670	C
1	L1	4679	G
1	L1	4687	A
1	L1	4695	C
1	L1	4700	A
1	L1	4708	A
1	L1	4709	U
1	L1	4719	G
1	L1	4720	C
1	L1	4732	G
1	L1	4734	A
1	L1	4741	C
1	L1	4742	G

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Mol	Chain	Res	Type
1	L1	4745	G
1	L1	4747	C
1	L1	4754	G
1	L1	4757	C
1	L1	4759	C
1	L1	4761	G
1	L1	4765	G
1	L1	4772	C
1	L1	4773	C
1	L1	4775	C
1	L1	4776	G
1	L1	4859	C
1	L1	4870	G
1	L1	4871	C
1	L1	4875	G
1	L1	4882	U
1	L1	4883	C
1	L1	4889	G
1	L1	4895	C
1	L1	4896	G
1	L1	4900	C
1	L1	4901	G
1	L1	4910	G
1	L1	4912	G
1	L1	4923	C
1	L1	4926	C
1	L1	4928	C
1	L1	4934	A
1	L1	4938	A
1	L1	4940	C
1	L1	4941	G
1	L1	4943	A
1	L1	4944	C
1	L1	4951	G
1	L1	4960	G
1	L1	4964	C
1	L1	4966	A
1	L1	4976	U
1	L1	4979	A
1	L1	4988	U
1	L1	4989	U
1	L1	4991	U

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Mol	Chain	Res	Type
1	L1	5013	C
1	L1	5017	G
1	L1	5022	U
1	L1	5023	C
1	L1	5024	C
1	L1	5025	C
1	L1	5026	U
1	L1	5030	U
1	L1	5034	A
1	L1	5041	G
1	L1	5050	C
1	L1	5054	C
1	L1	5061	A
1	L1	5069	U
2	L2	22	A
2	L2	24	C
2	L2	33	U
2	L2	48	G
2	L2	53	U
2	L2	54	A
2	L2	63	C
2	L2	64	G
2	L2	97	G
2	L2	100	A
2	L2	111	C
3	L3	2	G
3	L3	23	C
3	L3	34	U
3	L3	35	C
3	L3	38	U
3	L3	48	A
3	L3	52	A
3	L3	59	A
3	L3	60	G
3	L3	62	A
3	L3	63	U
3	L3	79	G
3	L3	80	A
3	L3	81	C
3	L3	82	A
3	L3	83	C
3	L3	84	A

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Mol	Chain	Res	Type
3	L3	85	U
3	L3	86	U
3	L3	87	G
3	L3	94	G
3	L3	103	A
3	L3	105	C
3	L3	108	A
3	L3	110	U
3	L3	111	U
3	L3	112	G
3	L3	114	G
3	L3	123	U
3	L3	124	U
3	L3	125	C
3	L3	126	C
3	L3	127	U
3	L3	147	G
45	S2	4	C
45	S2	33	G
45	S2	41	G
45	S2	44	U
45	S2	46	A
45	S2	56	G
45	S2	58	C
45	S2	59	U
45	S2	62	G
45	S2	64	A
45	S2	65	C
45	S2	67	C
45	S2	68	A
45	S2	72	C
45	S2	73	C
45	S2	74	G
45	S2	76	U
45	S2	99	A2M
45	S2	103	A
45	S2	113	G
45	S2	114	G
45	S2	115	U
45	S2	126	G
45	S2	130	G
45	S2	139	C

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Mol	Chain	Res	Type
45	S2	143	U
45	S2	149	A
45	S2	160	U
45	S2	162	C
45	S2	163	U
45	S2	171	A
45	S2	175	A
45	S2	184	G
45	S2	194	C
45	S2	196	C
45	S2	197	U
45	S2	198	U
45	S2	200	G
45	S2	203	G
45	S2	204	G
45	S2	311	C
45	S2	318	A
45	S2	319	C
45	S2	323	C
45	S2	324	C
45	S2	325	C
45	S2	326	C
45	S2	328	U
45	S2	329	G
45	S2	332	G
45	S2	351	G
45	S2	360	A
45	S2	362	C
45	S2	364	A
45	S2	370	G
45	S2	385	G
45	S2	386	C
45	S2	407	G
45	S2	408	A
45	S2	409	C
45	S2	418	A
45	S2	420	G
45	S2	421	G
45	S2	438	G
45	S2	448	A
45	S2	449	A
45	S2	450	C

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Mol	Chain	Res	Type
45	S2	452	G
45	S2	464	A
45	S2	471	G
45	S2	472	C
45	S2	473	A
45	S2	474	G
45	S2	476	A
45	S2	482	G
45	S2	487	U
45	S2	488	U
45	S2	492	C
45	S2	493	A
45	S2	500	A
45	S2	512	A2M
45	S2	516	A
45	S2	517	OMC
45	S2	525	A
45	S2	531	A
45	S2	532	C
45	S2	536	A
45	S2	537	C
45	S2	540	U
45	S2	544	G
45	S2	546	G
45	S2	547	G
45	S2	551	U
45	S2	554	A
45	S2	555	A
45	S2	556	U
45	S2	557	U
45	S2	558	G
45	S2	559	G
45	S2	560	A
45	S2	563	G
45	S2	564	A
45	S2	576	A2M
45	S2	583	A
45	S2	587	A
45	S2	589	G
45	S2	590	A2M
45	S2	591	U
45	S2	594	A

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Mol	Chain	Res	Type
45	S2	597	G
45	S2	598	G
45	S2	606	G
45	S2	607	U
45	S2	614	C
45	S2	617	G
45	S2	628	A
45	S2	629	A
45	S2	631	U
45	S2	643	A
45	S2	655	A
45	S2	660	C
45	S2	664	A
45	S2	668	A2M
45	S2	669	A
45	S2	671	A
45	S2	672	A
45	S2	673	G
45	S2	678	U
45	S2	683	OMG
45	S2	688	U
45	S2	689	U
45	S2	690	G
45	S2	692	G
45	S2	696	G
45	S2	698	G
45	S2	732	U
45	S2	733	C
45	S2	735	C
45	S2	736	C
45	S2	738	C
45	S2	739	C
45	S2	748	C
45	S2	750	C
45	S2	751	G
45	S2	752	G
45	S2	753	C
45	S2	789	G
45	S2	791	C
45	S2	794	A
45	S2	797	C
45	S2	798	G

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Mol	Chain	Res	Type
45	S2	799	U
45	S2	811	A
45	S2	821	G
45	S2	822	PSU
45	S2	830	A
45	S2	835	C
45	S2	836	G
45	S2	837	A
45	S2	838	G
45	S2	839	C
45	S2	840	C
45	S2	841	G
45	S2	842	C
45	S2	847	A
45	S2	867	OMG
45	S2	869	A
45	S2	870	A
45	S2	872	A
45	S2	874	G
45	S2	877	C
45	S2	884	C
45	S2	888	U
45	S2	889	U
45	S2	891	G
45	S2	892	U
45	S2	896	U
45	S2	898	U
45	S2	899	U
45	S2	900	C
45	S2	901	G
45	S2	903	A
45	S2	904	A
45	S2	909	G
45	S2	913	A
45	S2	917	U
45	S2	920	A
45	S2	922	A
45	S2	930	C
45	S2	933	G
45	S2	934	G
45	S2	943	U
45	S2	950	C

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Mol	Chain	Res	Type
45	S2	955	A
45	S2	962	A
45	S2	963	A
45	S2	990	A
45	S2	992	A
45	S2	999	G
45	S2	1001	A
45	S2	1017	U
45	S2	1023	A
45	S2	1027	A
45	S2	1028	A
45	S2	1033	G
45	S2	1061	U
45	S2	1062	A
45	S2	1067	C
45	S2	1083	A
45	S2	1085	C
45	S2	1109	C
45	S2	1114	U
45	S2	1116	C
45	S2	1118	C
45	S2	1133	A
45	S2	1138	C
45	S2	1140	G
45	S2	1153	C
45	S2	1154	U
45	S2	1195	A
45	S2	1207	G
45	S2	1208	A
45	S2	1215	C
45	S2	1216	C
45	S2	1217	A
45	S2	1224	G
45	S2	1242	U
45	S2	1243	PSU
45	S2	1251	A
45	S2	1253	A
45	S2	1256	G
45	S2	1257	G
45	S2	1259	A
45	S2	1264	C
45	S2	1265	A

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Mol	Chain	Res	Type
45	S2	1274	G
45	S2	1275	G
45	S2	1284	A
45	S2	1285	G
45	S2	1286	G
45	S2	1300	U
45	S2	1301	A
45	S2	1302	G
45	S2	1303	C
45	S2	1308	U
45	S2	1313	A
45	S2	1322	G
45	S2	1327	G
45	S2	1342	U
45	S2	1343	U
45	S2	1348	G
45	S2	1371	U
45	S2	1372	U
45	S2	1373	C
45	S2	1378	A
45	S2	1382	A
45	S2	1397	U
45	S2	1402	A
45	S2	1404	U
45	S2	1406	G
45	S2	1421	A
45	S2	1423	C
45	S2	1434	C
45	S2	1435	C
45	S2	1436	C
45	S2	1438	A
45	S2	1442	OMU
45	S2	1447	OMG
45	S2	1454	A
45	S2	1462	U
45	S2	1463	U
45	S2	1480	A
45	S2	1487	A
45	S2	1489	A
45	S2	1490	OMG
45	S2	1494	U
45	S2	1495	G

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Mol	Chain	Res	Type
45	S2	1497	G
45	S2	1498	A
45	S2	1508	A
45	S2	1521	C
45	S2	1522	A
45	S2	1531	A
45	S2	1533	A
45	S2	1553	C
45	S2	1556	A
45	S2	1578	U
45	S2	1580	A
45	S2	1585	U
45	S2	1587	G
45	S2	1588	A
45	S2	1601	A
45	S2	1606	G
45	S2	1621	U
45	S2	1623	A
45	S2	1648	G
45	S2	1654	G
45	S2	1664	A
45	S2	1665	G
45	S2	1686	G
45	S2	1698	C
45	S2	1699	A
45	S2	1721	U
45	S2	1722	G
45	S2	1742	C
45	S2	1744	G
45	S2	1752	C
45	S2	1753	C
45	S2	1754	G
45	S2	1758	G
45	S2	1760	G
45	S2	1761	U
45	S2	1773	C
45	S2	1774	C
45	S2	1775	U
45	S2	1777	G
45	S2	1781	A
45	S2	1782	G
45	S2	1783	C

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Mol	Chain	Res	Type
45	S2	1784	G
45	S2	1786	U
45	S2	1824	A
45	S2	1825	A
45	S2	1829	G
45	S2	1831	A
45	S2	1835	A
45	S2	1838	U
45	S2	1849	G
45	S2	1852	C
45	S2	1861	G
45	S2	1862	G
45	S2	1863	A
45	S2	1864	U
45	S2	1865	C
79	CC	15	A
79	CC	16	C
79	CC	17	G
79	CC	18	G
79	CC	19	C
79	CC	20	U
79	CC	21	A
79	CC	28	C
79	CC	32	C
79	CC	33	U
79	CC	35	U
79	CC	36	C
79	CC	37	A
79	CC	39	C
79	CC	42	G
79	CC	45	G
79	CC	46	A
79	CC	47	C
79	CC	48	C
79	CC	57	A
79	CC	58	C
79	CC	72	G
79	CC	75	A

All (23) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type

Mol	Chain	Res	Type
1	L1	406	C
1	L1	914	U
1	L1	1082	C
1	L1	1590	C
1	L1	1613	A
1	L1	1625	OMG
1	L1	1633	G
1	L1	2760	G
1	L1	3614	G
1	L1	3673	C
1	L1	3878	C
1	L1	4699	U
45	S2	112	U
45	S2	563	G
45	S2	628	A
45	S2	688	U
45	S2	867	OMG
45	S2	954	U
45	S2	1434	C
45	S2	1446	A
45	S2	1520	G
79	CC	35	U
79	CC	74	C

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

144 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	$\#\|Z\| > 2$
45	A2M	S2	590	45	18,25,26	4.24	7 (38%)	18,36,39	3.38	3 (16%)
1	5MC	L1	4447	1,80	18,22,23	3.41	7 (38%)	26,32,35	1.15	2 (7%)
1	2MG	L1	729	1	18,26,27	2.17	7 (38%)	16,38,41	1.37	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	A2M	L1	3785	1	18,25,26	3.95	7 (38%)	18,36,39	3.52	3 (16%)
1	A2M	L1	2401	1	18,25,26	4.22	7 (38%)	18,36,39	3.48	3 (16%)
1	OMG	L1	3744	1	18,26,27	2.46	8 (44%)	19,38,41	1.47	4 (21%)
1	OMC	L1	1340	1	19,22,23	2.89	8 (42%)	26,31,34	0.85	0
1	OMC	L1	3887	1	19,22,23	2.92	8 (42%)	26,31,34	0.86	0
3	OMG	L3	75	3	18,26,27	2.54	8 (44%)	19,38,41	1.52	4 (21%)
45	M7A	S2	1806	45	20,25,26	1.86	5 (25%)	28,37,40	3.94	8 (28%)
45	A2M	S2	468	45	18,25,26	4.21	7 (38%)	18,36,39	3.44	3 (16%)
1	6MZ	L1	4220	1	18,25,26	1.89	3 (16%)	16,36,39	2.31	3 (18%)
1	5MC	L1	4335	1	18,22,23	3.51	7 (38%)	26,32,35	0.99	2 (7%)
1	OMC	L1	2365	1,80	19,22,23	2.90	8 (42%)	26,31,34	0.62	0
45	MA6	S2	1850	45	18,26,27	1.07	1 (5%)	19,38,41	4.60	3 (15%)
1	OMC	L1	2351	1	19,22,23	2.87	8 (42%)	26,31,34	1.25	3 (11%)
45	A2M	S2	1383	45	18,25,26	4.25	6 (33%)	18,36,39	3.44	3 (16%)
45	OMC	S2	1703	45	19,22,23	2.97	8 (42%)	26,31,34	0.74	0
1	OMU	L1	4227	1	19,22,23	2.82	7 (36%)	26,31,34	1.72	4 (15%)
1	OMG	L1	4196	1	18,26,27	2.46	8 (44%)	19,38,41	1.44	4 (21%)
1	PSU	L1	3764	1	18,21,22	1.02	1 (5%)	22,30,33	1.65	4 (18%)
1	A2M	L1	2815	1	18,25,26	4.20	7 (38%)	18,36,39	3.45	3 (16%)
1	OMG	L1	4618	1	18,26,27	2.51	8 (44%)	19,38,41	1.53	4 (21%)
45	OMG	S2	509	80,45	18,26,27	2.47	8 (44%)	19,38,41	1.41	4 (21%)
1	OMG	L1	2876	1	18,26,27	2.54	8 (44%)	19,38,41	1.57	4 (21%)
45	PSU	S2	119	45	18,21,22	0.97	1 (5%)	22,30,33	1.63	4 (18%)
1	OMC	L1	1881	1,80	19,22,23	2.93	8 (42%)	26,31,34	0.95	0
1	PSU	L1	3715	1	18,21,22	1.10	1 (5%)	22,30,33	1.84	5 (22%)
1	OMC	L1	2422	1,80	19,22,23	2.89	8 (42%)	26,31,34	0.73	0
1	PSU	L1	2508	1	18,21,22	1.04	1 (5%)	22,30,33	1.70	3 (13%)
45	A2M	S2	1678	45	18,25,26	4.27	7 (38%)	18,36,39	3.44	3 (16%)
45	OMG	S2	683	45	18,26,27	2.55	8 (44%)	19,38,41	1.60	4 (21%)
45	PSU	S2	1081	45	18,21,22	1.05	1 (5%)	22,30,33	1.78	5 (22%)
1	OMG	L1	4228	1	18,26,27	2.47	8 (44%)	19,38,41	1.47	3 (15%)
1	OMG	L1	1316	1,80	18,26,27	2.49	8 (44%)	19,38,41	1.49	4 (21%)
45	PSU	S2	822	45	18,21,22	1.05	1 (5%)	22,30,33	1.77	5 (22%)
1	PSU	L1	4403	1	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
1	PSU	L1	4293	1	18,21,22	1.00	1 (5%)	22,30,33	1.68	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	A2M	S2	166	45	18,25,26	4.25	7 (38%)	18,36,39	3.48	3 (16%)
1	A2M	L1	400	1	18,25,26	4.25	6 (33%)	18,36,39	3.48	3 (16%)
1	A2M	L1	3718	1	18,25,26	4.24	6 (33%)	18,36,39	3.36	3 (16%)
45	5MU	S2	814	45	19,22,23	7.26	8 (42%)	28,32,35	3.30	12 (42%)
1	OMC	L1	4456	1	19,22,23	2.88	8 (42%)	26,31,34	0.86	0
45	OMU	S2	116	45	19,22,23	2.83	6 (31%)	26,31,34	1.71	5 (19%)
1	2MG	L1	1517	1	18,26,27	2.30	8 (44%)	16,38,41	1.52	3 (18%)
1	A2M	L1	2363	1,80	18,25,26	4.20	6 (33%)	18,36,39	3.50	3 (16%)
1	PSU	L1	4442	1	18,21,22	1.09	1 (5%)	22,30,33	1.78	5 (22%)
45	A2M	S2	668	80,45	18,25,26	4.13	7 (38%)	18,36,39	3.54	4 (22%)
1	PSU	L1	4500	1	18,21,22	0.98	1 (5%)	22,30,33	1.76	4 (18%)
45	5MC	S2	1374	45	18,22,23	3.53	7 (38%)	26,32,35	1.02	2 (7%)
1	PSU	L1	1677	81,1	18,21,22	1.16	2 (11%)	22,30,33	1.94	5 (22%)
45	OMC	S2	1391	45	19,22,23	3.02	8 (42%)	26,31,34	0.85	1 (3%)
1	1MA	L1	1322	1,80	16,25,26	3.57	4 (25%)	18,37,40	1.84	3 (16%)
45	PSU	S2	612	45	18,21,22	1.02	1 (5%)	22,30,33	1.81	5 (22%)
45	OMC	S2	1272	45	19,22,23	3.06	8 (42%)	26,31,34	0.81	0
1	A2M	L1	398	1	18,25,26	4.29	7 (38%)	18,36,39	3.40	3 (16%)
1	OMG	L1	4637	1	18,26,27	2.46	8 (44%)	19,38,41	1.47	3 (15%)
45	OMU	S2	172	45	19,22,23	2.88	6 (31%)	26,31,34	1.76	5 (19%)
45	A2M	S2	159	45	18,25,26	4.23	7 (38%)	18,36,39	3.47	3 (16%)
1	A2M	L1	4523	1,80	18,25,26	4.22	7 (38%)	18,36,39	3.24	3 (16%)
45	OMG	S2	601	45	18,26,27	2.51	8 (44%)	19,38,41	1.53	4 (21%)
45	OMG	S2	1490	80,45	18,26,27	2.53	8 (44%)	19,38,41	1.37	4 (21%)
1	B8H	L1	3762	1	19,22,23	6.72	6 (31%)	22,32,35	2.39	5 (22%)
45	A2M	S2	576	45	18,25,26	4.24	6 (33%)	18,36,39	3.42	3 (16%)
45	PSU	S2	1243	45	18,21,22	1.09	1 (5%)	22,30,33	1.70	4 (18%)
1	OMG	L1	4370	1	18,26,27	2.46	8 (44%)	19,38,41	1.44	4 (21%)
1	A2M	L1	3825	1	18,25,26	4.21	6 (33%)	18,36,39	3.48	3 (16%)
1	OMG	L1	4392	1	18,26,27	2.48	8 (44%)	19,38,41	1.47	3 (15%)
1	OMU	L1	4306	1	19,22,23	2.79	6 (31%)	26,31,34	1.66	4 (15%)
1	A2M	L1	1326	1	18,25,26	4.05	6 (33%)	18,36,39	3.34	3 (16%)
3	OMU	L3	14	3,1	19,22,23	2.88	6 (31%)	26,31,34	1.71	5 (19%)
45	OMG	S2	436	45	18,26,27	2.53	8 (44%)	19,38,41	1.51	4 (21%)
1	OMC	L1	3841	1	19,22,23	2.94	8 (42%)	26,31,34	0.91	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	MLZ	Lo	53	42	8,9,10	0.68	0	4,9,11	0.58	0
1	OMC	L1	2861	1	19,22,23	2.93	8 (42%)	26,31,34	0.72	0
45	A2M	S2	27	80,45	18,25,26	4.22	7 (38%)	18,36,39	3.44	3 (16%)
45	A2M	S2	512	45	18,25,26	4.25	6 (33%)	18,36,39	3.59	3 (16%)
45	OMU	S2	1442	80,45	19,22,23	2.94	7 (36%)	26,31,34	1.66	4 (15%)
45	OMG	S2	1447	45	18,26,27	1.08	2 (11%)	19,38,41	1.36	3 (15%)
1	OMU	L1	2837	1	19,22,23	2.84	6 (31%)	26,31,34	1.73	5 (19%)
45	A2M	S2	484	45	18,25,26	4.22	7 (38%)	18,36,39	3.41	3 (16%)
45	UY1	S2	1326	80,45	19,22,23	4.33	10 (52%)	22,31,34	1.84	3 (13%)
1	2MG	L1	978	1	18,26,27	2.26	8 (44%)	16,38,41	1.49	4 (25%)
1	OMC	L1	2824	1	19,22,23	2.93	8 (42%)	26,31,34	0.99	2 (7%)
45	4AC	S2	1842	45	21,24,25	3.40	10 (47%)	29,34,37	1.09	2 (6%)
1	UR3	L1	4530	1	19,22,23	2.75	8 (42%)	26,32,35	1.44	3 (11%)
45	OMC	S2	1710	45	19,22,23	3.04	8 (42%)	26,31,34	0.83	1 (3%)
1	A2M	L1	3723	1	18,25,26	4.24	7 (38%)	18,36,39	3.35	3 (16%)
1	PSU	L1	1683	81,1	18,21,22	1.10	1 (5%)	22,30,33	1.67	3 (13%)
1	OMG	L1	2424	1	18,26,27	2.50	8 (44%)	19,38,41	1.52	5 (26%)
1	OMG	L1	1522	1	18,26,27	2.53	8 (44%)	19,38,41	1.50	3 (15%)
45	OMG	S2	1328	45	18,26,27	2.58	8 (44%)	19,38,41	1.47	4 (21%)
1	OMG	L1	3627	1	18,26,27	2.54	8 (44%)	19,38,41	1.56	4 (21%)
1	JMH	L1	1456	1	18,22,23	2.64	5 (27%)	21,32,35	0.91	1 (4%)
1	OMU	L1	4498	1	19,22,23	2.85	7 (36%)	26,31,34	1.78	4 (15%)
1	OMC	L1	3869	1	19,22,23	2.94	8 (42%)	26,31,34	0.74	0
1	B8T	L1	4671	1	19,22,23	3.21	8 (42%)	26,31,34	0.98	1 (3%)
45	OMU	S2	121	45	19,22,23	2.84	6 (31%)	26,31,34	1.58	4 (15%)
1	OMC	L1	2804	1	19,22,23	2.89	7 (36%)	26,31,34	0.90	0
1	PSU	L1	4531	1	18,21,22	1.00	1 (5%)	22,30,33	1.70	4 (18%)
1	OMG	L1	2364	1,80	18,26,27	2.45	8 (44%)	19,38,41	1.54	5 (26%)
1	5MC	L1	3782	1,80	18,22,23	3.37	7 (38%)	26,32,35	1.21	3 (11%)
45	JMH	S2	1219	80,45	18,22,23	2.84	5 (27%)	21,32,35	1.74	4 (19%)
45	B8N	S2	1248	45	24,29,30	3.11	7 (29%)	29,42,45	1.75	6 (20%)
45	6MZ	S2	1832	80,45	18,25,26	2.07	3 (16%)	16,36,39	2.18	4 (25%)
1	OMC	L1	3808	1,80	19,22,23	2.94	8 (42%)	26,31,34	1.04	1 (3%)
1	OMU	L1	3925	1	19,22,23	2.85	6 (31%)	26,31,34	1.92	5 (19%)
45	OMC	S2	174	80,45	19,22,23	3.01	8 (42%)	26,31,34	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	A2M	L1	2787	1	18,25,26	4.24	6 (33%)	18,36,39	3.32	3 (16%)
1	OMG	L1	1625	1	18,26,27	1.18	2 (11%)	19,38,41	1.08	2 (10%)
45	A2M	S2	1031	45	18,25,26	4.18	7 (38%)	18,36,39	3.38	3 (16%)
1	A2M	L1	1534	1,80	18,25,26	4.24	7 (38%)	18,36,39	3.59	3 (16%)
1	PSU	L1	3729	1	18,21,22	1.05	1 (5%)	22,30,33	1.63	4 (18%)
1	PSU	L1	4636	1	18,21,22	1.09	1 (5%)	22,30,33	1.93	5 (22%)
45	OMC	S2	517	45	19,22,23	2.98	8 (42%)	26,31,34	0.78	0
45	OMU	S2	428	45	19,22,23	2.92	7 (36%)	26,31,34	1.71	4 (15%)
45	A2M	S2	99	80,45	18,25,26	4.23	7 (38%)	18,36,39	3.31	3 (16%)
1	UY1	L1	3818	81,1,80	19,22,23	4.44	12 (63%)	22,31,34	2.02	4 (18%)
45	PSU	S2	823	45	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
45	4AC	S2	1337	45	21,24,25	3.51	10 (47%)	29,34,37	1.07	2 (6%)
1	PSU	L1	1582	1	18,21,22	1.07	1 (5%)	22,30,33	1.57	4 (18%)
1	A2M	L1	4571	1	18,25,26	4.25	7 (38%)	18,36,39	3.42	3 (16%)
45	OMU	S2	1288	45	19,22,23	2.94	8 (42%)	26,31,34	1.64	4 (15%)
1	OMG	L1	3792	1	18,26,27	2.50	8 (44%)	19,38,41	1.48	4 (21%)
1	A2M	L1	1524	1	18,25,26	4.20	8 (44%)	18,36,39	3.30	3 (16%)
1	OMC	L1	3701	1,80	19,22,23	2.88	8 (42%)	26,31,34	0.84	0
1	OMG	L1	3899	1,80	18,26,27	2.50	8 (44%)	19,38,41	1.59	4 (21%)
1	OMG	L1	3944	1	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)
45	OMC	S2	462	45	19,22,23	2.97	8 (42%)	26,31,34	0.75	0
45	UR3	S2	1830	45	19,22,23	2.76	7 (36%)	26,32,35	1.61	4 (15%)
1	OMG	L1	4623	1	18,26,27	2.49	8 (44%)	19,38,41	1.54	4 (21%)
45	OMG	S2	867	45	18,26,27	2.55	8 (44%)	19,38,41	1.47	4 (21%)
1	A2M	L1	3867	1	18,25,26	4.08	7 (38%)	18,36,39	3.49	3 (16%)
1	PSU	L1	4628	1	18,21,22	0.92	1 (5%)	22,30,33	1.69	3 (13%)
1	OMG	L1	4499	1	18,26,27	2.52	8 (44%)	19,38,41	1.53	4 (21%)
1	PSU	L1	4450	1,80	18,21,22	1.11	1 (5%)	22,30,33	1.83	3 (13%)
45	OMG	S2	644	45	18,26,27	2.52	8 (44%)	19,38,41	1.46	4 (21%)
1	A2M	L1	3830	1	18,25,26	4.21	7 (38%)	18,36,39	3.52	3 (16%)
1	OMC	L1	4536	1	19,22,23	2.91	8 (42%)	26,31,34	0.75	0
1	OMG	L1	4494	1	18,26,27	2.46	8 (44%)	19,38,41	1.53	4 (21%)
1	OMU	L1	4620	1	19,22,23	2.80	7 (36%)	26,31,34	1.65	4 (15%)
45	OMU	S2	354	45	19,22,23	2.89	7 (36%)	26,31,34	1.80	5 (19%)
45	MA6	S2	1851	45	18,26,27	0.95	1 (5%)	19,38,41	4.99	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	A2M	L1	1871	1,80	18,25,26	4.26	7 (38%)	18,36,39	3.60	3 (16%)

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
45	A2M	S2	590	45	-	3/5/27/28	0/3/3/3
1	5MC	L1	4447	1,80	-	4/7/25/26	0/2/2/2
1	2MG	L1	729	1	-	1/5/27/28	0/3/3/3
1	A2M	L1	3785	1	-	2/5/27/28	0/3/3/3
1	A2M	L1	2401	1	-	1/5/27/28	0/3/3/3
1	OMG	L1	3744	1	-	0/5/27/28	0/3/3/3
1	OMC	L1	1340	1	-	2/9/27/28	0/2/2/2
1	OMC	L1	3887	1	-	0/9/27/28	0/2/2/2
3	OMG	L3	75	3	-	0/5/27/28	0/3/3/3
45	M7A	S2	1806	45	-	0/7/37/38	0/3/3/3
45	A2M	S2	468	45	-	0/5/27/28	0/3/3/3
1	6MZ	L1	4220	1	-	0/5/27/28	0/3/3/3
1	5MC	L1	4335	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	2365	1,80	-	0/9/27/28	0/2/2/2
45	MA6	S2	1850	45	-	3/7/29/30	0/3/3/3
1	OMC	L1	2351	1	-	3/9/27/28	0/2/2/2
45	A2M	S2	1383	45	-	0/5/27/28	0/3/3/3
45	OMC	S2	1703	45	-	0/9/27/28	0/2/2/2
1	OMU	L1	4227	1	-	0/9/27/28	0/2/2/2
1	OMG	L1	4196	1	-	1/5/27/28	0/3/3/3
1	PSU	L1	3764	1	-	2/7/25/26	0/2/2/2
1	A2M	L1	2815	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	4618	1	-	0/5/27/28	0/3/3/3
45	OMG	S2	509	80,45	-	0/5/27/28	0/3/3/3
1	OMG	L1	2876	1	-	0/5/27/28	0/3/3/3
45	PSU	S2	119	45	-	0/7/25/26	0/2/2/2
1	OMC	L1	1881	1,80	-	0/9/27/28	0/2/2/2
1	PSU	L1	3715	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	2422	1,80	-	1/9/27/28	0/2/2/2
1	PSU	L1	2508	1	-	0/7/25/26	0/2/2/2
45	A2M	S2	1678	45	-	1/5/27/28	0/3/3/3
45	OMG	S2	683	45	-	2/5/27/28	0/3/3/3
45	PSU	S2	1081	45	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	L1	4228	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	1316	1,80	-	0/5/27/28	0/3/3/3
45	PSU	S2	822	45	-	1/7/25/26	0/2/2/2
1	PSU	L1	4403	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	4293	1	-	1/7/25/26	0/2/2/2
45	A2M	S2	166	45	-	0/5/27/28	0/3/3/3
1	A2M	L1	400	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	3718	1	-	0/5/27/28	0/3/3/3
45	5MU	S2	814	45	-	0/7/25/26	0/2/2/2
1	OMC	L1	4456	1	-	0/9/27/28	0/2/2/2
45	OMU	S2	116	45	-	0/9/27/28	0/2/2/2
1	2MG	L1	1517	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	2363	1,80	-	1/5/27/28	0/3/3/3
1	PSU	L1	4442	1	-	0/7/25/26	0/2/2/2
45	A2M	S2	668	80,45	-	2/5/27/28	0/3/3/3
1	PSU	L1	4500	1	-	3/7/25/26	0/2/2/2
45	5MC	S2	1374	45	-	0/7/25/26	0/2/2/2
1	PSU	L1	1677	81,1	-	4/7/25/26	0/2/2/2
45	OMC	S2	1391	45	-	2/9/27/28	0/2/2/2
1	1MA	L1	1322	1,80	-	0/3/25/26	0/3/3/3
45	PSU	S2	612	45	-	0/7/25/26	0/2/2/2
45	OMC	S2	1272	45	-	0/9/27/28	0/2/2/2
1	A2M	L1	398	1	-	2/5/27/28	0/3/3/3
1	OMG	L1	4637	1	-	1/5/27/28	0/3/3/3
45	OMU	S2	172	45	-	0/9/27/28	0/2/2/2
45	A2M	S2	159	45	-	2/5/27/28	0/3/3/3
1	A2M	L1	4523	1,80	-	0/5/27/28	0/3/3/3
45	OMG	S2	601	45	-	1/5/27/28	0/3/3/3
45	OMG	S2	1490	80,45	-	1/5/27/28	0/3/3/3
1	B8H	L1	3762	1	-	0/7/25/26	0/2/2/2
45	A2M	S2	576	45	-	3/5/27/28	0/3/3/3
45	PSU	S2	1243	45	-	2/7/25/26	0/2/2/2
1	OMG	L1	4370	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	3825	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	4392	1	-	0/5/27/28	0/3/3/3
1	OMU	L1	4306	1	-	0/9/27/28	0/2/2/2
1	A2M	L1	1326	1	-	1/5/27/28	0/3/3/3
3	OMU	L3	14	3,1	-	1/9/27/28	0/2/2/2
45	OMG	S2	436	45	-	0/5/27/28	0/3/3/3
1	OMC	L1	3841	1	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	MLZ	Lo	53	42	-	2/7/8/10	-
1	OMC	L1	2861	1	-	0/9/27/28	0/2/2/2
45	A2M	S2	27	80,45	-	0/5/27/28	0/3/3/3
45	A2M	S2	512	45	-	2/5/27/28	0/3/3/3
45	OMU	S2	1442	80,45	-	3/9/27/28	0/2/2/2
45	OMG	S2	1447	45	-	1/5/27/28	0/3/3/3
1	OMU	L1	2837	1	-	0/9/27/28	0/2/2/2
45	A2M	S2	484	45	-	0/5/27/28	0/3/3/3
45	UY1	S2	1326	80,45	-	1/9/27/28	0/2/2/2
1	2MG	L1	978	1	-	0/5/27/28	0/3/3/3
1	OMC	L1	2824	1	-	2/9/27/28	0/2/2/2
45	4AC	S2	1842	45	-	0/11/29/30	0/2/2/2
1	UR3	L1	4530	1	-	0/7/25/26	0/2/2/2
45	OMC	S2	1710	45	-	0/9/27/28	0/2/2/2
1	A2M	L1	3723	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	1683	81,1	-	0/7/25/26	0/2/2/2
1	OMG	L1	2424	1	-	2/5/27/28	0/3/3/3
1	OMG	L1	1522	1	-	0/5/27/28	0/3/3/3
45	OMG	S2	1328	45	-	1/5/27/28	0/3/3/3
1	OMG	L1	3627	1	-	0/5/27/28	0/3/3/3
1	JMH	L1	1456	1	-	0/7/25/26	0/2/2/2
1	OMU	L1	4498	1	-	0/9/27/28	0/2/2/2
1	OMC	L1	3869	1	-	1/9/27/28	0/2/2/2
1	B8T	L1	4671	1	-	1/7/27/28	0/2/2/2
45	OMU	S2	121	45	-	0/9/27/28	0/2/2/2
1	OMC	L1	2804	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	4531	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	2364	1,80	-	2/5/27/28	0/3/3/3
1	5MC	L1	3782	1,80	-	0/7/25/26	0/2/2/2
45	JMH	S2	1219	80,45	-	2/7/25/26	0/2/2/2
45	B8N	S2	1248	45	-	3/16/34/35	0/2/2/2
45	6MZ	S2	1832	80,45	-	2/5/27/28	0/3/3/3
1	OMC	L1	3808	1,80	-	2/9/27/28	0/2/2/2
1	OMU	L1	3925	1	-	1/9/27/28	0/2/2/2
45	OMC	S2	174	80,45	-	0/9/27/28	0/2/2/2
1	A2M	L1	2787	1	-	1/5/27/28	0/3/3/3
1	OMG	L1	1625	1	-	0/5/27/28	0/3/3/3
45	A2M	S2	1031	45	-	0/5/27/28	0/3/3/3
1	A2M	L1	1534	1,80	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L1	3729	1	-	2/7/25/26	0/2/2/2
1	PSU	L1	4636	1	-	3/7/25/26	0/2/2/2
45	OMC	S2	517	45	-	2/9/27/28	0/2/2/2
45	OMU	S2	428	45	-	2/9/27/28	0/2/2/2
45	A2M	S2	99	80,45	-	2/5/27/28	0/3/3/3
1	UY1	L1	3818	81,1,80	-	4/9/27/28	0/2/2/2
45	PSU	S2	823	45	-	0/7/25/26	0/2/2/2
45	4AC	S2	1337	45	-	0/11/29/30	0/2/2/2
1	PSU	L1	1582	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	4571	1	-	0/5/27/28	0/3/3/3
45	OMU	S2	1288	45	-	0/9/27/28	0/2/2/2
1	OMG	L1	3792	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	1524	1	-	1/5/27/28	0/3/3/3
1	OMC	L1	3701	1,80	-	4/9/27/28	0/2/2/2
1	OMG	L1	3899	1,80	-	0/5/27/28	0/3/3/3
1	OMG	L1	3944	1	-	2/5/27/28	0/3/3/3
45	OMC	S2	462	45	-	0/9/27/28	0/2/2/2
45	UR3	S2	1830	45	-	2/7/25/26	0/2/2/2
1	OMG	L1	4623	1	-	0/5/27/28	0/3/3/3
45	OMG	S2	867	45	-	3/5/27/28	0/3/3/3
1	A2M	L1	3867	1	-	2/5/27/28	0/3/3/3
1	PSU	L1	4628	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	4499	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	4450	1,80	-	1/7/25/26	0/2/2/2
45	OMG	S2	644	45	-	2/5/27/28	0/3/3/3
1	A2M	L1	3830	1	-	0/5/27/28	0/3/3/3
1	OMC	L1	4536	1	-	0/9/27/28	0/2/2/2
1	OMG	L1	4494	1	-	0/5/27/28	0/3/3/3
1	OMU	L1	4620	1	-	1/9/27/28	0/2/2/2
45	OMU	S2	354	45	-	0/9/27/28	0/2/2/2
45	MA6	S2	1851	45	-	2/7/29/30	0/3/3/3
1	A2M	L1	1871	1,80	-	0/5/27/28	0/3/3/3

All (890) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	814	5MU	C4-C5	20.75	1.79	1.44
45	S2	814	5MU	C6-N1	16.52	1.66	1.38
1	L1	398	A2M	O4'-C1'	15.56	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3762	B8H	C6-C5	-15.50	1.13	1.34
45	S2	512	A2M	O4'-C1'	15.37	1.62	1.41
45	S2	1383	A2M	O4'-C1'	15.37	1.62	1.41
45	S2	576	A2M	O4'-C1'	15.35	1.62	1.41
45	S2	166	A2M	O4'-C1'	15.33	1.62	1.41
1	L1	1871	A2M	O4'-C1'	15.27	1.62	1.41
1	L1	400	A2M	O4'-C1'	15.26	1.62	1.41
1	L1	3723	A2M	O4'-C1'	15.24	1.62	1.41
1	L1	2401	A2M	O4'-C1'	15.23	1.62	1.41
1	L1	4571	A2M	O4'-C1'	15.21	1.62	1.41
1	L1	3718	A2M	O4'-C1'	15.21	1.62	1.41
45	S2	1678	A2M	O4'-C1'	15.20	1.62	1.41
1	L1	3830	A2M	O4'-C1'	15.19	1.62	1.41
45	S2	484	A2M	O4'-C1'	15.16	1.62	1.41
45	S2	159	A2M	O4'-C1'	15.15	1.62	1.41
1	L1	4523	A2M	O4'-C1'	15.15	1.62	1.41
45	S2	590	A2M	O4'-C1'	15.14	1.62	1.41
1	L1	1534	A2M	O4'-C1'	15.14	1.62	1.41
45	S2	99	A2M	O4'-C1'	15.14	1.62	1.41
45	S2	27	A2M	O4'-C1'	15.11	1.62	1.41
1	L1	3825	A2M	O4'-C1'	15.11	1.62	1.41
1	L1	2787	A2M	O4'-C1'	15.09	1.62	1.41
45	S2	468	A2M	O4'-C1'	15.09	1.62	1.41
1	L1	2815	A2M	O4'-C1'	14.95	1.61	1.41
45	S2	1031	A2M	O4'-C1'	14.93	1.61	1.41
1	L1	2363	A2M	O4'-C1'	14.93	1.61	1.41
1	L1	3762	B8H	C4-N3	-14.86	1.11	1.38
1	L1	1524	A2M	O4'-C1'	14.83	1.61	1.41
1	L1	3867	A2M	O4'-C1'	14.52	1.61	1.41
1	L1	1326	A2M	O4'-C1'	14.35	1.61	1.41
45	S2	668	A2M	O4'-C1'	14.35	1.61	1.41
1	L1	3762	B8H	C4-C5	14.15	1.84	1.44
1	L1	3785	A2M	O4'-C1'	13.92	1.60	1.41
1	L1	1322	1MA	C2-N3	12.75	1.44	1.29
1	L1	3762	B8H	C6-N1	12.60	1.67	1.36
1	L1	3818	UY1	O4'-C1'	-11.74	1.27	1.43
45	S2	1326	UY1	O4'-C1'	-11.19	1.28	1.43
45	S2	814	5MU	C4-N3	-11.07	1.18	1.38
45	S2	814	5MU	C6-C5	-10.71	1.17	1.34
1	L1	4335	5MC	C6-C5	9.06	1.49	1.34
1	L1	4447	5MC	C6-C5	8.98	1.49	1.34
45	S2	1374	5MC	C6-C5	8.98	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3782	5MC	C6-C5	8.59	1.48	1.34
45	S2	1219	JMH	C2-N1	8.31	1.50	1.38
45	S2	1248	B8N	C6-N1	7.79	1.55	1.36
45	S2	1832	6MZ	C6-N6	7.77	1.47	1.35
45	S2	1248	B8N	C4-N3	-7.49	1.26	1.40
45	S2	1830	UR3	C2-N1	7.38	1.49	1.38
1	L1	3818	UY1	C3'-C4'	-7.20	1.34	1.53
45	S2	1337	4AC	C4-N3	7.14	1.45	1.32
3	L3	14	OMU	C2-N1	7.13	1.49	1.38
45	S2	428	OMU	C2-N1	7.10	1.49	1.38
45	S2	1288	OMU	C2-N1	7.09	1.49	1.38
45	S2	1442	OMU	C2-N1	7.05	1.49	1.38
1	L1	1456	JMH	C2-N1	7.03	1.48	1.38
1	L1	4530	UR3	C2-N1	7.02	1.48	1.38
45	S2	1326	UY1	C3'-C4'	-7.01	1.35	1.53
1	L1	4671	B8T	C4-N3	7.00	1.45	1.32
45	S2	668	A2M	O4'-C4'	-6.99	1.29	1.45
45	S2	354	OMU	C2-N1	6.98	1.49	1.38
45	S2	172	OMU	C2-N1	6.96	1.49	1.38
1	L1	4498	OMU	C2-N1	6.91	1.49	1.38
1	L1	4220	6MZ	C6-N6	6.91	1.46	1.35
1	L1	2837	OMU	C2-N1	6.90	1.49	1.38
45	S2	1842	4AC	C4-N3	6.83	1.44	1.32
1	L1	4227	OMU	C2-N1	6.81	1.49	1.38
1	L1	3925	OMU	C2-N1	6.74	1.49	1.38
45	S2	121	OMU	C2-N1	6.72	1.49	1.38
45	S2	116	OMU	C2-N1	6.69	1.49	1.38
45	S2	1442	OMU	C2-N3	6.68	1.49	1.38
1	L1	1524	A2M	O4'-C4'	-6.67	1.30	1.45
1	L1	4620	OMU	C2-N1	6.67	1.49	1.38
1	L1	1534	A2M	O4'-C4'	-6.63	1.30	1.45
45	S2	428	OMU	C2-N3	6.60	1.49	1.38
45	S2	1288	OMU	C2-N3	6.60	1.49	1.38
45	S2	1678	A2M	O4'-C4'	-6.60	1.30	1.45
45	S2	1248	B8N	C6-C5	6.55	1.44	1.34
45	S2	172	OMU	C2-N3	6.53	1.49	1.38
1	L1	4571	A2M	O4'-C4'	-6.52	1.30	1.45
45	S2	590	A2M	O4'-C4'	-6.52	1.30	1.45
1	L1	4306	OMU	C2-N1	6.49	1.48	1.38
45	S2	1248	B8N	C2-N1	6.48	1.58	1.39
45	S2	354	OMU	C2-N3	6.47	1.49	1.38
1	L1	1871	A2M	O4'-C4'	-6.45	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	1272	OMC	C2-N3	6.45	1.49	1.36
1	L1	400	A2M	O4'-C4'	-6.45	1.30	1.45
1	L1	2815	A2M	O4'-C4'	-6.44	1.30	1.45
1	L1	2363	A2M	O4'-C4'	-6.44	1.30	1.45
45	S2	121	OMU	C2-N3	6.43	1.49	1.38
45	S2	1710	OMC	C2-N3	6.43	1.49	1.36
45	S2	1374	5MC	C4-N3	6.42	1.45	1.34
45	S2	174	OMC	C2-N3	6.40	1.49	1.36
1	L1	3723	A2M	O4'-C4'	-6.38	1.30	1.45
45	S2	1391	OMC	C2-N3	6.37	1.49	1.36
1	L1	2787	A2M	O4'-C4'	-6.36	1.30	1.45
45	S2	27	A2M	O4'-C4'	-6.36	1.30	1.45
45	S2	1337	4AC	C6-C5	6.36	1.49	1.35
45	S2	484	A2M	O4'-C4'	-6.35	1.30	1.45
45	S2	116	OMU	C2-N3	6.33	1.49	1.38
1	L1	4335	5MC	C4-N3	6.33	1.44	1.34
1	L1	1881	OMC	C2-N3	6.32	1.49	1.36
3	L3	14	OMU	C2-N3	6.31	1.49	1.38
45	S2	468	A2M	O4'-C4'	-6.31	1.30	1.45
45	S2	517	OMC	C2-N3	6.31	1.49	1.36
45	S2	99	A2M	O4'-C4'	-6.30	1.30	1.45
45	S2	1326	UY1	O4'-C4'	6.29	1.59	1.45
1	L1	2837	OMU	C2-N3	6.28	1.49	1.38
1	L1	4523	A2M	O4'-C4'	-6.27	1.31	1.45
45	S2	159	A2M	O4'-C4'	-6.27	1.31	1.45
45	S2	166	A2M	O4'-C4'	-6.25	1.31	1.45
1	L1	1326	A2M	O4'-C4'	-6.25	1.31	1.45
1	L1	3925	OMU	C2-N3	6.25	1.49	1.38
1	L1	1340	OMC	C2-N3	6.24	1.49	1.36
45	S2	1031	A2M	O4'-C4'	-6.24	1.31	1.45
45	S2	462	OMC	C2-N3	6.24	1.49	1.36
1	L1	3718	A2M	O4'-C4'	-6.24	1.31	1.45
1	L1	3785	A2M	O4'-C4'	-6.21	1.31	1.45
1	L1	3825	A2M	O4'-C4'	-6.18	1.31	1.45
1	L1	3867	A2M	O4'-C4'	-6.18	1.31	1.45
1	L1	4227	OMU	C2-N3	6.18	1.49	1.38
45	S2	576	A2M	O4'-C4'	-6.17	1.31	1.45
45	S2	512	A2M	O4'-C4'	-6.16	1.31	1.45
1	L1	2401	A2M	O4'-C4'	-6.16	1.31	1.45
1	L1	2365	OMC	C2-N3	6.15	1.48	1.36
45	S2	1703	OMC	C2-N3	6.15	1.48	1.36
1	L1	398	A2M	O4'-C4'	-6.13	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4498	OMU	C2-N3	6.12	1.48	1.38
1	L1	4536	OMC	C2-N3	6.12	1.48	1.36
1	L1	4620	OMU	C2-N3	6.12	1.48	1.38
45	S2	1383	A2M	O4'-C4'	-6.12	1.31	1.45
45	S2	1337	4AC	C2-N3	6.11	1.48	1.36
1	L1	4306	OMU	C2-N3	6.11	1.48	1.38
1	L1	4456	OMC	C2-N3	6.10	1.48	1.36
45	S2	1842	4AC	C6-C5	6.09	1.49	1.35
45	S2	1374	5MC	C2-N3	6.09	1.48	1.36
1	L1	2861	OMC	C2-N3	6.08	1.48	1.36
1	L1	3808	OMC	C2-N3	6.08	1.48	1.36
1	L1	3887	OMC	C2-N3	6.08	1.48	1.36
1	L1	2824	OMC	C2-N3	6.03	1.48	1.36
45	S2	1272	OMC	C6-C5	6.01	1.49	1.35
1	L1	3830	A2M	O4'-C4'	-6.01	1.31	1.45
1	L1	4530	UR3	C6-C5	6.00	1.49	1.35
1	L1	4671	B8T	C6-C5	6.00	1.49	1.35
1	L1	4335	5MC	C2-N3	5.99	1.48	1.36
45	S2	1710	OMC	C6-C5	5.99	1.49	1.35
45	S2	174	OMC	C6-C5	5.98	1.49	1.35
45	S2	462	OMC	C6-C5	5.98	1.48	1.35
1	L1	2804	OMC	C2-N3	5.97	1.48	1.36
45	S2	1830	UR3	C6-C5	5.97	1.48	1.35
1	L1	3841	OMC	C2-N3	5.96	1.48	1.36
1	L1	3701	OMC	C6-C5	5.96	1.48	1.35
45	S2	1391	OMC	C6-C5	5.96	1.48	1.35
1	L1	3782	5MC	C4-N3	5.95	1.44	1.34
1	L1	2861	OMC	C6-C5	5.95	1.48	1.35
1	L1	4536	OMC	C6-C5	5.95	1.48	1.35
45	S2	1703	OMC	C6-C5	5.93	1.48	1.35
45	S2	517	OMC	C6-C5	5.92	1.48	1.35
1	L1	2422	OMC	C6-C5	5.91	1.48	1.35
1	L1	3808	OMC	C6-C5	5.90	1.48	1.35
45	S2	1337	4AC	C4-N4	5.90	1.48	1.39
1	L1	3701	OMC	C2-N3	5.89	1.48	1.36
45	S2	1288	OMU	C6-C5	5.89	1.48	1.35
1	L1	3818	UY1	O4'-C4'	5.88	1.58	1.45
1	L1	1456	JMH	C6-C5	5.86	1.48	1.35
1	L1	3869	OMC	C2-N3	5.86	1.48	1.36
45	S2	1842	4AC	C2-N3	5.83	1.48	1.36
1	L1	3869	OMC	C6-C5	5.83	1.48	1.35
45	S2	1442	OMU	C6-C5	5.83	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	2422	OMC	C2-N3	5.82	1.48	1.36
1	L1	2365	OMC	C6-C5	5.81	1.48	1.35
1	L1	2351	OMC	C6-C5	5.80	1.48	1.35
45	S2	1337	4AC	C7-N4	5.79	1.47	1.37
1	L1	3841	OMC	C6-C5	5.76	1.48	1.35
45	S2	1219	JMH	C6-C5	5.76	1.48	1.35
1	L1	3782	5MC	C2-N3	5.75	1.48	1.36
1	L1	3887	OMC	C6-C5	5.74	1.48	1.35
45	S2	428	OMU	C6-C5	5.74	1.48	1.35
1	L1	4447	5MC	C4-N3	5.74	1.43	1.34
45	S2	121	OMU	C6-C5	5.73	1.48	1.35
1	L1	2824	OMC	C6-C5	5.73	1.48	1.35
45	S2	116	OMU	C6-C5	5.72	1.48	1.35
45	S2	172	OMU	C6-C5	5.71	1.48	1.35
1	L1	2804	OMC	C6-C5	5.69	1.48	1.35
1	L1	1881	OMC	C6-C5	5.69	1.48	1.35
1	L1	4620	OMU	C6-C5	5.67	1.48	1.35
1	L1	4671	B8T	C2-N3	5.66	1.47	1.36
1	L1	4498	OMU	C6-C5	5.66	1.48	1.35
1	L1	4456	OMC	C6-C5	5.65	1.48	1.35
45	S2	354	OMU	C6-C5	5.63	1.48	1.35
1	L1	4306	OMU	C6-C5	5.62	1.48	1.35
45	S2	1842	4AC	C7-N4	5.61	1.47	1.37
1	L1	2837	OMU	C6-C5	5.58	1.48	1.35
1	L1	4447	5MC	C2-N3	5.57	1.47	1.36
1	L1	4227	OMU	C6-C5	5.56	1.48	1.35
45	S2	1842	4AC	C4-N4	5.55	1.47	1.39
1	L1	1340	OMC	C6-C5	5.54	1.47	1.35
1	L1	2351	OMC	C2-N3	5.52	1.47	1.36
1	L1	1316	OMG	C2-N3	5.52	1.46	1.33
1	L1	3944	OMG	C2-N3	5.51	1.46	1.33
1	L1	3925	OMU	C6-C5	5.50	1.47	1.35
3	L3	14	OMU	C6-C5	5.48	1.47	1.35
45	S2	1328	OMG	C2-N3	5.47	1.46	1.33
45	S2	683	OMG	C2-N3	5.44	1.46	1.33
1	L1	3818	UY1	O4-C4	-5.43	1.13	1.23
45	S2	867	OMG	C2-N3	5.41	1.46	1.33
1	L1	2876	OMG	C2-N3	5.40	1.46	1.33
1	L1	3627	OMG	C2-N3	5.40	1.46	1.33
1	L1	3818	UY1	O2-C2	-5.40	1.12	1.23
1	L1	1522	OMG	C2-N3	5.39	1.46	1.33
45	S2	509	OMG	C2-N3	5.38	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	75	OMG	C2-N3	5.36	1.46	1.33
45	S2	1490	OMG	C2-N3	5.36	1.46	1.33
1	L1	4618	OMG	C2-N3	5.35	1.46	1.33
1	L1	4392	OMG	C2-N3	5.35	1.46	1.33
45	S2	644	OMG	C2-N3	5.34	1.46	1.33
45	S2	601	OMG	C2-N3	5.34	1.46	1.33
45	S2	436	OMG	C2-N3	5.33	1.46	1.33
1	L1	4637	OMG	C2-N3	5.32	1.46	1.33
45	S2	1326	UY1	O4-C4	-5.31	1.13	1.23
1	L1	4530	UR3	C2-N3	5.31	1.49	1.39
1	L1	4499	OMG	C2-N3	5.30	1.46	1.33
45	S2	1272	OMC	C4-N3	5.26	1.45	1.34
1	L1	978	2MG	C2-N2	5.26	1.45	1.33
1	L1	4370	OMG	C2-N3	5.24	1.45	1.33
1	L1	4623	OMG	C2-N3	5.24	1.45	1.33
1	L1	2424	OMG	C2-N3	5.22	1.45	1.33
1	L1	1517	2MG	C2-N2	5.21	1.45	1.33
1	L1	3792	OMG	C2-N3	5.20	1.45	1.33
1	L1	729	2MG	C2-N2	5.16	1.44	1.33
45	S2	814	5MU	C2-N3	5.16	1.47	1.38
1	L1	4196	OMG	C2-N3	5.14	1.45	1.33
1	L1	4494	OMG	C2-N3	5.13	1.45	1.33
45	S2	174	OMC	C4-N3	5.12	1.44	1.34
1	L1	3744	OMG	C2-N3	5.11	1.45	1.33
45	S2	1710	OMC	C4-N3	5.09	1.44	1.34
45	S2	1391	OMC	C4-N3	5.09	1.44	1.34
45	S2	436	OMG	C4-N3	5.07	1.49	1.37
45	S2	517	OMC	C4-N3	5.06	1.44	1.34
1	L1	3899	OMG	C2-N3	5.05	1.45	1.33
1	L1	3627	OMG	C4-N3	5.05	1.49	1.37
1	L1	1881	OMC	C4-N3	5.05	1.44	1.34
45	S2	683	OMG	C4-N3	5.04	1.49	1.37
1	L1	3944	OMG	C4-N3	5.04	1.49	1.37
1	L1	4228	OMG	C2-N3	5.03	1.45	1.33
45	S2	1272	OMC	C4-N4	5.01	1.45	1.33
1	L1	2876	OMG	C4-N3	5.01	1.49	1.37
45	S2	1328	OMG	C4-N3	5.00	1.49	1.37
1	L1	1340	OMC	C4-N3	5.00	1.44	1.34
1	L1	3841	OMC	C4-N3	4.99	1.44	1.34
1	L1	2351	OMC	C2-N1	4.98	1.50	1.40
1	L1	3792	OMG	C4-N3	4.98	1.49	1.37
45	S2	867	OMG	C4-N3	4.97	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	75	OMG	C4-N3	4.96	1.49	1.37
1	L1	4618	OMG	C4-N3	4.96	1.49	1.37
45	S2	644	OMG	C4-N3	4.96	1.49	1.37
45	S2	1490	OMG	C4-N3	4.95	1.49	1.37
45	S2	462	OMC	C4-N3	4.94	1.44	1.34
45	S2	1710	OMC	C4-N4	4.93	1.45	1.33
1	L1	4392	OMG	C4-N3	4.93	1.49	1.37
1	L1	1522	OMG	C4-N3	4.92	1.49	1.37
1	L1	3762	B8H	C2-N3	4.92	1.46	1.38
45	S2	1703	OMC	C4-N3	4.92	1.44	1.34
45	S2	1326	UY1	O2-C2	-4.91	1.13	1.23
1	L1	1316	OMG	C4-N3	4.91	1.49	1.37
1	L1	3869	OMC	C4-N3	4.91	1.44	1.34
45	S2	601	OMG	C4-N3	4.90	1.49	1.37
1	L1	4499	OMG	C4-N3	4.90	1.49	1.37
1	L1	3899	OMG	C4-N3	4.88	1.49	1.37
45	S2	1391	OMC	C4-N4	4.88	1.45	1.33
45	S2	462	OMC	C4-N4	4.87	1.45	1.33
45	S2	174	OMC	C4-N4	4.87	1.45	1.33
1	L1	3887	OMC	C4-N3	4.86	1.44	1.34
45	S2	509	OMG	C4-N3	4.86	1.49	1.37
1	L1	4671	B8T	C4-N4	4.85	1.45	1.35
1	L1	2804	OMC	C4-N3	4.85	1.44	1.34
45	S2	1326	UY1	C1'-C5	4.84	1.61	1.50
1	L1	2364	OMG	C2-N3	4.84	1.44	1.33
1	L1	4370	OMG	C4-N3	4.84	1.49	1.37
1	L1	2861	OMC	C4-N3	4.83	1.44	1.34
1	L1	4623	OMG	C4-N3	4.82	1.49	1.37
45	S2	1830	UR3	C2-N3	4.82	1.48	1.39
45	S2	1703	OMC	C4-N4	4.82	1.45	1.33
1	L1	3744	OMG	C4-N3	4.81	1.49	1.37
1	L1	4228	OMG	C4-N3	4.81	1.49	1.37
1	L1	4637	OMG	C4-N3	4.80	1.49	1.37
45	S2	1219	JMH	C2-N3	4.80	1.48	1.39
1	L1	3944	OMG	C2-N2	4.78	1.45	1.34
1	L1	2365	OMC	C4-N4	4.78	1.45	1.33
1	L1	2861	OMC	C4-N4	4.77	1.45	1.33
1	L1	1881	OMC	C4-N4	4.77	1.45	1.33
1	L1	2365	OMC	C4-N3	4.77	1.44	1.34
1	L1	2824	OMC	C4-N3	4.77	1.44	1.34
1	L1	2424	OMG	C4-N3	4.76	1.48	1.37
45	S2	1328	OMG	C2-N2	4.76	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	2422	OMC	C4-N4	4.74	1.45	1.33
1	L1	2824	OMC	C4-N4	4.74	1.45	1.33
1	L1	3887	OMC	C4-N4	4.73	1.45	1.33
45	S2	517	OMC	C4-N4	4.73	1.45	1.33
45	S2	1272	OMC	C2-N1	4.72	1.50	1.40
1	L1	4456	OMC	C4-N3	4.71	1.44	1.34
1	L1	3808	OMC	C2-N1	4.71	1.50	1.40
45	S2	1490	OMG	C2-N2	4.71	1.45	1.34
1	L1	1340	OMC	C4-N4	4.70	1.45	1.33
1	L1	2804	OMC	C4-N4	4.69	1.45	1.33
1	L1	3701	OMC	C4-N3	4.69	1.44	1.34
1	L1	4536	OMC	C4-N3	4.68	1.43	1.34
1	L1	3869	OMC	C4-N4	4.68	1.44	1.33
45	S2	1391	OMC	C2-N1	4.68	1.50	1.40
1	L1	2424	OMG	C2-N2	4.67	1.45	1.34
1	L1	4494	OMG	C4-N3	4.67	1.48	1.37
1	L1	4456	OMC	C2-N1	4.67	1.50	1.40
45	S2	1710	OMC	C2-N1	4.66	1.50	1.40
1	L1	4499	OMG	C2-N2	4.66	1.45	1.34
45	S2	867	OMG	C2-N2	4.65	1.45	1.34
3	L3	75	OMG	C2-N2	4.64	1.45	1.34
1	L1	3792	OMG	C2-N2	4.64	1.45	1.34
45	S2	683	OMG	C2-N2	4.64	1.45	1.34
45	S2	436	OMG	C2-N2	4.64	1.45	1.34
1	L1	4196	OMG	C4-N3	4.62	1.48	1.37
1	L1	2422	OMC	C4-N3	4.61	1.43	1.34
45	S2	517	OMC	C2-N1	4.61	1.50	1.40
1	L1	3808	OMC	C4-N3	4.61	1.43	1.34
1	L1	3841	OMC	C2-N1	4.60	1.50	1.40
1	L1	3869	OMC	C2-N1	4.59	1.50	1.40
45	S2	601	OMG	C2-N2	4.59	1.45	1.34
1	L1	3808	OMC	C4-N4	4.58	1.44	1.33
1	L1	2364	OMG	C4-N3	4.58	1.48	1.37
1	L1	3841	OMC	C4-N4	4.58	1.44	1.33
1	L1	2824	OMC	C2-N1	4.57	1.49	1.40
1	L1	4618	OMG	C2-N2	4.56	1.45	1.34
1	L1	4456	OMC	C4-N4	4.55	1.44	1.33
45	S2	644	OMG	C2-N2	4.55	1.45	1.34
1	L1	4370	OMG	C2-N2	4.53	1.45	1.34
1	L1	2364	OMG	C2-N2	4.53	1.45	1.34
1	L1	4536	OMC	C4-N4	4.52	1.44	1.33
1	L1	4196	OMG	C2-N2	4.52	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1316	OMG	C2-N2	4.52	1.44	1.34
45	S2	1806	M7A	C6-N6	4.51	1.45	1.34
1	L1	3701	OMC	C4-N4	4.51	1.44	1.33
1	L1	4671	B8T	C2-N1	4.50	1.49	1.40
45	S2	174	OMC	C2-N1	4.50	1.49	1.40
45	S2	1374	5MC	C6-N1	4.50	1.45	1.38
1	L1	2351	OMC	C4-N4	4.49	1.44	1.33
1	L1	2804	OMC	C2-N1	4.49	1.49	1.40
1	L1	4228	OMG	C2-N2	4.49	1.44	1.34
45	S2	1703	OMC	C2-N1	4.47	1.49	1.40
1	L1	3899	OMG	C2-N2	4.47	1.44	1.34
1	L1	4623	OMG	C2-N2	4.46	1.44	1.34
1	L1	3627	OMG	C2-N2	4.46	1.44	1.34
45	S2	462	OMC	C2-N1	4.45	1.49	1.40
1	L1	1456	JMH	C2-N3	4.45	1.47	1.39
1	L1	4494	OMG	C2-N2	4.44	1.44	1.34
1	L1	2876	OMG	C2-N2	4.43	1.44	1.34
1	L1	4335	5MC	C6-N1	4.43	1.45	1.38
1	L1	3744	OMG	C2-N2	4.42	1.44	1.34
1	L1	3887	OMC	C2-N1	4.41	1.49	1.40
1	L1	3818	UY1	C1'-C5	4.41	1.60	1.50
1	L1	4392	OMG	C2-N2	4.40	1.44	1.34
45	S2	509	OMG	C2-N2	4.38	1.44	1.34
45	S2	1374	5MC	C4-N4	4.36	1.45	1.34
1	L1	4637	OMG	C2-N2	4.36	1.44	1.34
1	L1	2351	OMC	C4-N3	4.36	1.43	1.34
1	L1	1881	OMC	C2-N1	4.33	1.49	1.40
1	L1	2422	OMC	C2-N1	4.32	1.49	1.40
1	L1	4447	5MC	C6-N1	4.31	1.45	1.38
1	L1	4447	5MC	C4-N4	4.30	1.45	1.34
1	L1	1522	OMG	C2-N2	4.30	1.44	1.34
1	L1	2861	OMC	C2-N1	4.29	1.49	1.40
45	S2	1337	4AC	C5-C4	4.28	1.49	1.40
1	L1	4335	5MC	C4-N4	4.27	1.45	1.34
1	L1	3782	5MC	C6-N1	4.26	1.45	1.38
45	S2	1326	UY1	C6-C5	4.22	1.40	1.35
1	L1	4536	OMC	C2-N1	4.20	1.49	1.40
45	S2	1842	4AC	C5-C4	4.19	1.49	1.40
1	L1	1340	OMC	C2-N1	4.17	1.49	1.40
1	L1	3782	5MC	C2-N1	4.13	1.49	1.40
45	S2	814	5MU	C2-N1	4.13	1.45	1.38
45	S2	1374	5MC	C2-N1	4.12	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3701	OMC	C2-N1	4.08	1.48	1.40
45	S2	1337	4AC	C2-N1	4.07	1.48	1.40
1	L1	1322	1MA	C2-N1	4.05	1.43	1.35
1	L1	3782	5MC	C4-N4	4.04	1.44	1.34
1	L1	2365	OMC	C2-N1	3.97	1.48	1.40
1	L1	4335	5MC	C2-N1	3.93	1.48	1.40
1	L1	3818	UY1	C6-C5	3.90	1.39	1.35
45	S2	1842	4AC	C2-N1	3.89	1.48	1.40
1	L1	729	2MG	C4-N3	3.82	1.46	1.37
1	L1	3818	UY1	C2-N3	-3.81	1.31	1.37
1	L1	1517	2MG	C4-N3	3.79	1.46	1.37
1	L1	4447	5MC	C2-N1	3.79	1.48	1.40
1	L1	978	2MG	C4-N3	3.78	1.46	1.37
1	L1	1322	1MA	C4-N3	3.78	1.49	1.37
45	S2	1326	UY1	C2-N3	-3.70	1.31	1.37
45	S2	867	OMG	C6-N1	3.65	1.43	1.37
1	L1	1517	2MG	C6-N1	3.64	1.43	1.37
1	L1	978	2MG	C6-N1	3.60	1.43	1.37
45	S2	1328	OMG	C6-N1	3.60	1.43	1.37
45	S2	1243	PSU	C6-C5	3.59	1.39	1.35
1	L1	3944	OMG	C6-N1	3.55	1.43	1.37
45	S2	1806	M7A	C2-N1	3.53	1.40	1.33
1	L1	3818	UY1	C2-N1	-3.53	1.32	1.36
45	S2	1288	OMU	C4-N3	3.53	1.44	1.38
1	L1	2364	OMG	C6-N1	3.51	1.43	1.37
1	L1	1683	PSU	C6-C5	3.51	1.39	1.35
1	L1	1582	PSU	C6-C5	3.49	1.39	1.35
45	S2	644	OMG	C6-N1	3.47	1.43	1.37
45	S2	1490	OMG	C6-N1	3.47	1.43	1.37
45	S2	1442	OMU	C4-N3	3.46	1.44	1.38
1	L1	4450	PSU	C6-C5	3.46	1.39	1.35
1	L1	2351	OMC	C6-N1	3.45	1.46	1.38
1	L1	978	2MG	C2-N1	3.44	1.42	1.36
3	L3	75	OMG	C6-N1	3.44	1.43	1.37
45	S2	1806	M7A	C71-N7	-3.44	1.40	1.46
1	L1	4442	PSU	C6-C5	3.43	1.39	1.35
45	S2	601	OMG	C6-N1	3.42	1.43	1.37
1	L1	2424	OMG	C6-N1	3.41	1.43	1.37
1	L1	4671	B8T	C5-C4	3.41	1.48	1.40
1	L1	1517	2MG	C2-N1	3.39	1.42	1.36
1	L1	4671	B8T	C6-N1	3.38	1.46	1.38
1	L1	3869	OMC	C6-N1	3.37	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	2365	OMC	C6-N1	3.35	1.46	1.38
45	S2	683	OMG	C6-N1	3.34	1.42	1.37
1	L1	2508	PSU	C6-C5	3.33	1.39	1.35
45	S2	172	OMU	C4-N3	3.33	1.44	1.38
45	S2	436	OMG	C6-N1	3.32	1.42	1.37
1	L1	4499	OMG	C6-N1	3.31	1.42	1.37
45	S2	428	OMU	C4-N3	3.31	1.44	1.38
1	L1	2876	OMG	C6-N1	3.31	1.42	1.37
1	L1	3627	OMG	C6-N1	3.31	1.42	1.37
1	L1	3715	PSU	C6-C5	3.30	1.39	1.35
1	L1	3925	OMU	O2-C2	-3.30	1.17	1.23
1	L1	4671	B8T	O2-C2	-3.30	1.17	1.23
1	L1	4536	OMC	C6-N1	3.30	1.46	1.38
1	L1	4196	OMG	C6-N1	3.30	1.42	1.37
1	L1	2787	A2M	O3'-C3'	-3.29	1.35	1.43
1	L1	2422	OMC	C6-N1	3.29	1.45	1.38
1	L1	3729	PSU	C6-C5	3.29	1.39	1.35
1	L1	1522	OMG	C6-N1	3.28	1.42	1.37
45	S2	1806	M7A	C4-N9	3.28	1.44	1.38
1	L1	3887	OMC	C6-N1	3.27	1.45	1.38
45	S2	822	PSU	C6-C5	3.27	1.39	1.35
45	S2	823	PSU	C6-C5	3.27	1.39	1.35
45	S2	1081	PSU	C6-C5	3.26	1.39	1.35
1	L1	4228	OMG	C6-N1	3.26	1.42	1.37
1	L1	4623	OMG	C6-N1	3.25	1.42	1.37
1	L1	3764	PSU	C6-C5	3.25	1.39	1.35
1	L1	3899	OMG	C6-N1	3.25	1.42	1.37
1	L1	4636	PSU	C6-C5	3.25	1.39	1.35
1	L1	729	2MG	C2-N1	3.24	1.41	1.36
45	S2	1842	4AC	C6-N1	3.24	1.45	1.38
45	S2	1391	OMC	C6-N1	3.24	1.45	1.38
45	S2	1219	JMH	C6-N1	3.23	1.45	1.38
1	L1	1456	JMH	C6-N1	3.22	1.45	1.38
45	S2	1248	B8N	O4-C4	-3.22	1.16	1.23
3	L3	14	OMU	C4-N3	3.21	1.44	1.38
45	S2	1710	OMC	C6-N1	3.21	1.45	1.38
1	L1	3701	OMC	C6-N1	3.21	1.45	1.38
1	L1	4403	PSU	C6-C5	3.21	1.39	1.35
1	L1	3808	OMC	C6-N1	3.21	1.45	1.38
45	S2	1272	OMC	C6-N1	3.20	1.45	1.38
1	L1	3925	OMU	O4-C4	-3.20	1.18	1.24
1	L1	4494	OMG	C6-N1	3.20	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	1703	OMC	C6-N1	3.20	1.45	1.38
45	S2	159	A2M	O3'-C3'	-3.19	1.35	1.43
45	S2	121	OMU	C4-N3	3.19	1.44	1.38
1	L1	2824	OMC	C6-N1	3.19	1.45	1.38
45	S2	116	OMU	C4-N3	3.19	1.44	1.38
1	L1	3792	OMG	C6-N1	3.19	1.42	1.37
45	S2	174	OMC	C6-N1	3.18	1.45	1.38
45	S2	1337	4AC	C6-N1	3.18	1.45	1.38
45	S2	509	OMG	C6-N1	3.18	1.42	1.37
45	S2	462	OMC	C6-N1	3.17	1.45	1.38
1	L1	2815	A2M	O3'-C3'	-3.17	1.35	1.43
1	L1	729	2MG	C6-N1	3.17	1.42	1.37
45	S2	119	PSU	C6-C5	3.17	1.39	1.35
1	L1	4306	OMU	O2-C2	-3.17	1.17	1.23
1	L1	3841	OMC	C6-N1	3.17	1.45	1.38
45	S2	1678	A2M	O3'-C3'	-3.16	1.35	1.43
1	L1	1871	A2M	O3'-C3'	-3.16	1.35	1.43
1	L1	3701	OMC	O2-C2	-3.16	1.17	1.23
1	L1	4498	OMU	C4-N3	3.15	1.44	1.38
45	S2	354	OMU	C4-N3	3.15	1.44	1.38
45	S2	1678	A2M	C6-N6	3.15	1.45	1.34
1	L1	1677	PSU	C6-C5	3.15	1.39	1.35
45	S2	1326	UY1	C2-N1	-3.15	1.32	1.36
45	S2	99	A2M	O3'-C3'	-3.14	1.35	1.43
45	S2	612	PSU	C6-C5	3.14	1.39	1.35
1	L1	2837	OMU	O4-C4	-3.13	1.18	1.24
45	S2	590	A2M	C6-N6	3.13	1.45	1.34
1	L1	2804	OMC	O2-C2	-3.12	1.17	1.23
45	S2	166	A2M	C6-N6	3.12	1.45	1.34
1	L1	4498	OMU	O4-C4	-3.12	1.18	1.24
45	S2	159	A2M	C6-N6	3.12	1.45	1.34
45	S2	468	A2M	O3'-C3'	-3.12	1.35	1.43
1	L1	4293	PSU	C6-C5	3.12	1.39	1.35
45	S2	517	OMC	C6-N1	3.11	1.45	1.38
1	L1	2861	OMC	C6-N1	3.11	1.45	1.38
1	L1	4536	OMC	O2-C2	-3.11	1.18	1.23
45	S2	668	A2M	C6-N6	3.10	1.45	1.34
1	L1	1522	OMG	C5-C6	3.10	1.53	1.47
1	L1	3830	A2M	O3'-C3'	-3.10	1.35	1.43
45	S2	576	A2M	C6-N6	3.09	1.45	1.34
45	S2	468	A2M	C6-N6	3.09	1.45	1.34
1	L1	398	A2M	C6-N6	3.09	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4531	PSU	C6-C5	3.09	1.38	1.35
1	L1	400	A2M	C6-N6	3.09	1.45	1.34
1	L1	4227	OMU	C4-N3	3.08	1.44	1.38
1	L1	1524	A2M	C6-N6	3.08	1.45	1.34
1	L1	4637	OMG	C5-C6	3.08	1.53	1.47
1	L1	3925	OMU	C4-N3	3.08	1.44	1.38
45	S2	27	A2M	C6-N6	3.07	1.45	1.34
45	S2	1842	4AC	O2-C2	-3.07	1.18	1.23
45	S2	166	A2M	O3'-C3'	-3.07	1.35	1.43
1	L1	2861	OMC	O2-C2	-3.06	1.18	1.23
45	S2	484	A2M	C6-N6	3.06	1.45	1.34
1	L1	398	A2M	O3'-C3'	-3.05	1.35	1.43
45	S2	512	A2M	C6-N6	3.05	1.45	1.34
1	L1	3867	A2M	C6-N6	3.05	1.45	1.34
1	L1	2401	A2M	C6-N6	3.05	1.45	1.34
1	L1	3785	A2M	C5-C4	-3.05	1.32	1.40
1	L1	4618	OMG	C6-N1	3.04	1.42	1.37
1	L1	3830	A2M	C5-C4	-3.04	1.32	1.40
1	L1	4370	OMG	C6-N1	3.04	1.42	1.37
3	L3	14	OMU	O4-C4	-3.04	1.18	1.24
45	S2	1383	A2M	O3'-C3'	-3.04	1.35	1.43
45	S2	27	A2M	O3'-C3'	-3.04	1.35	1.43
1	L1	2787	A2M	C5-C4	-3.03	1.32	1.40
1	L1	3723	A2M	C6-N6	3.03	1.45	1.34
1	L1	2364	OMG	C5-C6	3.03	1.53	1.47
1	L1	3718	A2M	C6-N6	3.03	1.45	1.34
1	L1	2837	OMU	C4-N3	3.03	1.44	1.38
45	S2	1383	A2M	C6-N6	3.03	1.45	1.34
45	S2	590	A2M	O3'-C3'	-3.03	1.35	1.43
1	L1	4571	A2M	C6-N6	3.02	1.45	1.34
1	L1	3825	A2M	C5-C4	-3.02	1.32	1.40
1	L1	4392	OMG	C5-C6	3.02	1.53	1.47
1	L1	3744	OMG	C6-N1	3.01	1.42	1.37
1	L1	1326	A2M	O2'-C2'	3.01	1.50	1.42
45	S2	576	A2M	O3'-C3'	-3.01	1.35	1.43
1	L1	4571	A2M	O3'-C3'	-3.01	1.35	1.43
1	L1	2422	OMC	O2-C2	-3.01	1.18	1.23
1	L1	4456	OMC	O2-C2	-3.01	1.18	1.23
1	L1	3944	OMG	C5-C6	3.00	1.53	1.47
45	S2	99	A2M	C6-N6	3.00	1.45	1.34
1	L1	1316	OMG	C6-N1	3.00	1.42	1.37
1	L1	3808	OMC	O2-C2	-3.00	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3841	OMC	O2-C2	-2.99	1.18	1.23
45	S2	354	OMU	O4-C4	-2.99	1.18	1.24
1	L1	4306	OMU	C4-N3	2.98	1.43	1.38
1	L1	3869	OMC	O2-C2	-2.98	1.18	1.23
1	L1	2804	OMC	C6-N1	2.98	1.45	1.38
45	S2	512	A2M	O3'-C3'	-2.98	1.36	1.43
1	L1	1871	A2M	C6-N6	2.98	1.44	1.34
1	L1	3627	OMG	C5-C6	2.98	1.53	1.47
1	L1	1340	OMC	O2-C2	-2.98	1.18	1.23
1	L1	400	A2M	O3'-C3'	-2.98	1.36	1.43
45	S2	1678	A2M	O2'-C2'	2.98	1.50	1.42
1	L1	1534	A2M	C6-N6	2.98	1.44	1.34
45	S2	1328	OMG	C5-C6	2.98	1.53	1.47
1	L1	3744	OMG	C5-C6	2.97	1.53	1.47
1	L1	2815	A2M	O2'-C2'	2.97	1.50	1.42
1	L1	3899	OMG	C5-C4	-2.97	1.35	1.43
1	L1	4523	A2M	C5-C4	-2.97	1.33	1.40
45	S2	509	OMG	C5-C6	2.96	1.53	1.47
3	L3	14	OMU	O2-C2	-2.96	1.17	1.23
1	L1	3718	A2M	O2'-C2'	2.96	1.50	1.42
1	L1	2363	A2M	C5-C4	-2.96	1.33	1.40
1	L1	2876	OMG	C5-C6	2.95	1.53	1.47
45	S2	1031	A2M	C6-N6	2.95	1.44	1.34
45	S2	1703	OMC	O2-C2	-2.94	1.18	1.23
1	L1	3718	A2M	O3'-C3'	-2.94	1.36	1.43
1	L1	4523	A2M	C6-N6	2.94	1.44	1.34
1	L1	4447	5MC	O2-C2	-2.94	1.18	1.23
45	S2	1830	UR3	C6-N1	2.94	1.45	1.38
1	L1	4620	OMU	C4-N3	2.94	1.43	1.38
1	L1	2351	OMC	O2-C2	-2.94	1.18	1.23
1	L1	2365	OMC	O2-C2	-2.93	1.18	1.23
1	L1	2824	OMC	O2-C2	-2.93	1.18	1.23
1	L1	2363	A2M	O3'-C3'	-2.93	1.36	1.43
1	L1	3825	A2M	O3'-C3'	-2.93	1.36	1.43
45	S2	1031	A2M	O2'-C2'	2.93	1.50	1.42
1	L1	3825	A2M	C6-N6	2.92	1.44	1.34
45	S2	1031	A2M	C5-C4	-2.92	1.33	1.40
1	L1	2815	A2M	C6-N6	2.92	1.44	1.34
1	L1	3723	A2M	O3'-C3'	-2.92	1.36	1.43
1	L1	1524	A2M	O3'-C3'	-2.92	1.36	1.43
1	L1	3887	OMC	O2-C2	-2.92	1.18	1.23
1	L1	4227	OMU	O4-C4	-2.91	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3867	A2M	O2'-C2'	2.91	1.50	1.42
1	L1	2787	A2M	C6-N6	2.91	1.44	1.34
1	L1	4306	OMU	O4-C4	-2.91	1.18	1.24
1	L1	3830	A2M	C6-N6	2.91	1.44	1.34
1	L1	1871	A2M	O2'-C2'	2.90	1.50	1.42
1	L1	4623	OMG	C5-C6	2.90	1.53	1.47
1	L1	4456	OMC	C6-N1	2.90	1.45	1.38
1	L1	3782	5MC	O2-C2	-2.89	1.18	1.23
3	L3	75	OMG	C5-C6	2.89	1.53	1.47
1	L1	4227	OMU	O2-C2	-2.89	1.17	1.23
1	L1	4620	OMU	O2-C2	-2.88	1.17	1.23
1	L1	2363	A2M	C6-N6	2.88	1.44	1.34
1	L1	1625	OMG	C6-N1	-2.87	1.33	1.37
1	L1	1322	1MA	C5-C4	-2.87	1.35	1.43
1	L1	4618	OMG	C5-C6	2.87	1.53	1.47
45	S2	159	A2M	O2'-C2'	2.86	1.50	1.42
45	S2	1031	A2M	O3'-C3'	-2.86	1.36	1.43
1	L1	4392	OMG	O6-C6	-2.85	1.17	1.23
45	S2	1337	4AC	O2-C2	-2.85	1.18	1.23
45	S2	436	OMG	C5-C6	2.85	1.53	1.47
45	S2	99	A2M	C5-C4	-2.85	1.33	1.40
45	S2	644	OMG	C5-C6	2.84	1.53	1.47
1	L1	4228	OMG	C5-C6	2.84	1.53	1.47
1	L1	1881	OMC	O2-C2	-2.84	1.18	1.23
45	S2	1490	OMG	C5-C6	2.84	1.53	1.47
1	L1	3792	OMG	C5-C6	2.84	1.53	1.47
1	L1	2364	OMG	C5-C4	-2.83	1.35	1.43
1	L1	3867	A2M	O3'-C3'	-2.82	1.36	1.43
1	L1	2424	OMG	C5-C4	-2.82	1.35	1.43
45	S2	484	A2M	O2'-C2'	2.82	1.49	1.42
45	S2	590	A2M	O2'-C2'	2.82	1.49	1.42
1	L1	2401	A2M	O3'-C3'	-2.82	1.36	1.43
45	S2	683	OMG	C5-C6	2.82	1.53	1.47
1	L1	1340	OMC	C6-N1	2.82	1.44	1.38
1	L1	4620	OMU	O4-C4	-2.82	1.19	1.24
45	S2	27	A2M	O2'-C2'	2.82	1.49	1.42
45	S2	576	A2M	O2'-C2'	2.81	1.49	1.42
1	L1	1524	A2M	O2'-C2'	2.81	1.49	1.42
1	L1	1534	A2M	O3'-C3'	-2.81	1.36	1.43
1	L1	2401	A2M	C5-C4	-2.81	1.33	1.40
1	L1	4335	5MC	O2-C2	-2.81	1.18	1.23
45	S2	116	OMU	O2-C2	-2.81	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1517	2MG	CM2-N2	2.80	1.50	1.45
45	S2	1806	M7A	C5-N7	2.80	1.46	1.39
1	L1	3723	A2M	O2'-C2'	2.80	1.49	1.42
1	L1	4637	OMG	C6-N1	2.80	1.42	1.37
1	L1	4618	OMG	C5-C4	-2.80	1.35	1.43
1	L1	1534	A2M	C5-C4	-2.79	1.33	1.40
1	L1	1881	OMC	C6-N1	2.79	1.44	1.38
1	L1	4494	OMG	C5-C6	2.79	1.53	1.47
45	S2	116	OMU	O4-C4	-2.79	1.19	1.24
45	S2	166	A2M	O2'-C2'	2.79	1.49	1.42
1	L1	4196	OMG	C5-C6	2.79	1.53	1.47
45	S2	1850	MA6	C5-C4	-2.79	1.33	1.40
45	S2	27	A2M	C5-C4	-2.79	1.33	1.40
1	L1	4498	OMU	O2-C2	-2.79	1.17	1.23
1	L1	4499	OMG	C5-C6	2.79	1.53	1.47
45	S2	867	OMG	C5-C6	2.78	1.53	1.47
1	L1	3825	A2M	O2'-C2'	2.78	1.49	1.42
1	L1	4494	OMG	C5-C4	-2.78	1.36	1.43
45	S2	668	A2M	O3'-C3'	-2.78	1.36	1.43
45	S2	668	A2M	C5-C4	-2.78	1.33	1.40
45	S2	517	OMC	O2-C2	-2.78	1.18	1.23
45	S2	1383	A2M	C5-C4	-2.78	1.33	1.40
45	S2	462	OMC	O2-C2	-2.78	1.18	1.23
1	L1	1326	A2M	C6-N6	2.78	1.44	1.34
1	L1	3744	OMG	C5-C4	-2.78	1.36	1.43
1	L1	1326	A2M	O3'-C3'	-2.78	1.36	1.43
45	S2	428	OMU	O4-C4	-2.77	1.19	1.24
45	S2	1383	A2M	O2'-C2'	2.77	1.49	1.42
1	L1	400	A2M	O2'-C2'	2.77	1.49	1.42
1	L1	2401	A2M	O2'-C2'	2.77	1.49	1.42
45	S2	668	A2M	O2'-C2'	2.77	1.49	1.42
1	L1	1522	OMG	C5-C4	-2.77	1.36	1.43
1	L1	4196	OMG	C5-C4	-2.77	1.36	1.43
1	L1	3723	A2M	C5-C4	-2.77	1.33	1.40
45	S2	484	A2M	O3'-C3'	-2.77	1.36	1.43
1	L1	1326	A2M	C5-C4	-2.77	1.33	1.40
45	S2	1710	OMC	O2-C2	-2.76	1.18	1.23
1	L1	3867	A2M	C5-C4	-2.76	1.33	1.40
45	S2	121	OMU	O2-C2	-2.76	1.18	1.23
1	L1	1871	A2M	C5-C4	-2.76	1.33	1.40
1	L1	1316	OMG	C5-C6	2.76	1.53	1.47
1	L1	4530	UR3	C6-N1	2.76	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	601	OMG	C5-C6	2.76	1.53	1.47
1	L1	1524	A2M	C5-C4	-2.76	1.33	1.40
1	L1	3792	OMG	C5-C4	-2.76	1.36	1.43
1	L1	400	A2M	C5-C4	-2.75	1.33	1.40
1	L1	4623	OMG	C5-C4	-2.75	1.36	1.43
1	L1	3718	A2M	C5-C4	-2.75	1.33	1.40
1	L1	4228	OMG	C5-C4	-2.75	1.36	1.43
1	L1	2363	A2M	O2'-C2'	2.74	1.49	1.42
1	L1	2837	OMU	O2-C2	-2.74	1.18	1.23
45	S2	99	A2M	O2'-C2'	2.74	1.49	1.42
1	L1	3627	OMG	C5-C4	-2.74	1.36	1.43
1	L1	3899	OMG	C5-C6	2.74	1.53	1.47
45	S2	1374	5MC	O2-C2	-2.73	1.18	1.23
45	S2	428	OMU	O2-C2	-2.73	1.18	1.23
45	S2	166	A2M	C5-C4	-2.73	1.33	1.40
45	S2	1391	OMC	O2-C2	-2.73	1.18	1.23
1	L1	1522	OMG	O6-C6	-2.73	1.17	1.23
45	S2	468	A2M	C5-C4	-2.72	1.33	1.40
45	S2	1678	A2M	C5-C4	-2.72	1.33	1.40
1	L1	4571	A2M	O2'-C2'	2.72	1.49	1.42
45	S2	354	OMU	O2-C2	-2.72	1.18	1.23
1	L1	3785	A2M	O2'-C2'	2.72	1.49	1.42
45	S2	174	OMC	O2-C2	-2.72	1.18	1.23
1	L1	4571	A2M	C5-C4	-2.72	1.33	1.40
45	S2	121	OMU	O4-C4	-2.72	1.19	1.24
1	L1	398	A2M	O2'-C2'	2.71	1.49	1.42
1	L1	4392	OMG	C6-N1	2.71	1.41	1.37
1	L1	4523	A2M	O3'-C3'	-2.71	1.36	1.43
1	L1	3830	A2M	O2'-C2'	2.71	1.49	1.42
1	L1	3785	A2M	C6-N6	2.71	1.43	1.34
45	S2	1272	OMC	O2-C2	-2.71	1.18	1.23
1	L1	4499	OMG	C2-N1	2.71	1.44	1.37
1	L1	2815	A2M	C5-C4	-2.70	1.33	1.40
45	S2	172	OMU	O4-C4	-2.70	1.19	1.24
1	L1	3627	OMG	O6-C6	-2.70	1.17	1.23
1	L1	4370	OMG	C5-C4	-2.70	1.36	1.43
1	L1	4499	OMG	C5-C4	-2.70	1.36	1.43
1	L1	398	A2M	C5-C4	-2.69	1.33	1.40
1	L1	1517	2MG	O6-C6	-2.69	1.17	1.23
45	S2	512	A2M	C5-C4	-2.69	1.33	1.40
3	L3	75	OMG	C5-C4	-2.69	1.36	1.43
45	S2	159	A2M	C5-C4	-2.69	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	512	A2M	O2'-C2'	2.69	1.49	1.42
45	S2	601	OMG	C5-C4	-2.68	1.36	1.43
45	S2	1851	MA6	C5-C4	-2.68	1.33	1.40
1	L1	3899	OMG	O6-C6	-2.67	1.17	1.23
1	L1	1534	A2M	O2'-C2'	2.67	1.49	1.42
45	S2	1328	OMG	C2-N1	2.67	1.44	1.37
1	L1	1517	2MG	C5-C4	-2.67	1.36	1.43
45	S2	814	5MU	O4-C4	-2.66	1.18	1.23
45	S2	172	OMU	O2-C2	-2.65	1.18	1.23
45	S2	468	A2M	O2'-C2'	2.65	1.49	1.42
1	L1	3944	OMG	C2-N1	2.64	1.44	1.37
1	L1	4628	PSU	C6-C5	2.64	1.38	1.35
45	S2	644	OMG	C5-C4	-2.64	1.36	1.43
45	S2	484	A2M	C5-C4	-2.64	1.33	1.40
45	S2	1442	OMU	O4-C4	-2.64	1.19	1.24
1	L1	4523	A2M	O2'-C2'	2.64	1.49	1.42
1	L1	4500	PSU	C6-C5	2.63	1.38	1.35
45	S2	1288	OMU	O4-C4	-2.63	1.19	1.24
1	L1	2787	A2M	O2'-C2'	2.63	1.49	1.42
45	S2	576	A2M	C5-C4	-2.62	1.34	1.40
45	S2	867	OMG	C2-N1	2.62	1.44	1.37
1	L1	4370	OMG	C5-C6	2.62	1.52	1.47
45	S2	1442	OMU	O2-C2	-2.61	1.18	1.23
45	S2	683	OMG	C5-C4	-2.61	1.36	1.43
45	S2	436	OMG	C5-C4	-2.60	1.36	1.43
45	S2	814	5MU	O2-C2	-2.60	1.18	1.23
1	L1	4494	OMG	O6-C6	-2.60	1.18	1.23
1	L1	4637	OMG	C5-C4	-2.60	1.36	1.43
1	L1	2424	OMG	C2-N1	2.59	1.44	1.37
1	L1	2876	OMG	O6-C6	-2.59	1.18	1.23
45	S2	590	A2M	C5-C4	-2.57	1.34	1.40
1	L1	4637	OMG	O6-C6	-2.57	1.18	1.23
1	L1	2876	OMG	C5-C4	-2.56	1.36	1.43
1	L1	729	2MG	C5-C4	-2.56	1.36	1.43
45	S2	1830	UR3	O2-C2	-2.56	1.17	1.22
45	S2	1703	OMC	C5-C4	2.56	1.48	1.42
3	L3	75	OMG	C2-N1	2.56	1.44	1.37
1	L1	3899	OMG	C2-N1	2.55	1.44	1.37
1	L1	2424	OMG	C5-C6	2.55	1.52	1.47
1	L1	4228	OMG	C2-N1	2.54	1.44	1.37
45	S2	1490	OMG	C5-C4	-2.54	1.36	1.43
45	S2	867	OMG	C5-C4	-2.54	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4530	UR3	O4-C4	-2.53	1.18	1.23
1	L1	4220	6MZ	C5-C4	-2.53	1.34	1.40
45	S2	1328	OMG	C5-C4	-2.53	1.36	1.43
1	L1	2364	OMG	C2-N1	2.51	1.43	1.37
45	S2	1490	OMG	C2-N1	2.51	1.43	1.37
1	L1	978	2MG	CM2-N2	2.51	1.50	1.45
45	S2	601	OMG	C2-N1	2.51	1.43	1.37
45	S2	683	OMG	O6-C6	-2.50	1.18	1.23
1	L1	4618	OMG	O6-C6	-2.50	1.18	1.23
1	L1	978	2MG	C5-C4	-2.50	1.36	1.43
1	L1	4228	OMG	O6-C6	-2.50	1.18	1.23
45	S2	174	OMC	C5-C4	2.50	1.48	1.42
45	S2	1710	OMC	C5-C4	2.50	1.48	1.42
45	S2	436	OMG	C2-N1	2.49	1.43	1.37
45	S2	1288	OMU	O2-C2	-2.49	1.18	1.23
1	L1	3944	OMG	C5-C4	-2.49	1.36	1.43
1	L1	4623	OMG	O6-C6	-2.48	1.18	1.23
1	L1	3701	OMC	C5-C4	2.48	1.48	1.42
1	L1	3744	OMG	O6-C6	-2.48	1.18	1.23
45	S2	509	OMG	C5-C4	-2.48	1.36	1.43
1	L1	1316	OMG	C5-C4	-2.48	1.36	1.43
1	L1	3762	B8H	O2-C2	-2.48	1.18	1.23
1	L1	978	2MG	O6-C6	-2.48	1.18	1.23
1	L1	4370	OMG	O6-C6	-2.47	1.18	1.23
45	S2	1447	OMG	C6-N1	-2.46	1.34	1.37
1	L1	3869	OMC	C5-C4	2.46	1.48	1.42
45	S2	462	OMC	C5-C4	2.45	1.48	1.42
45	S2	644	OMG	C2-N1	2.45	1.43	1.37
1	L1	3744	OMG	C2-N1	2.45	1.43	1.37
1	L1	2876	OMG	C2-N1	2.45	1.43	1.37
1	L1	4494	OMG	C2-N1	2.45	1.43	1.37
45	S2	1272	OMC	C5-C4	2.45	1.48	1.42
1	L1	4196	OMG	O6-C6	-2.45	1.18	1.23
1	L1	4618	OMG	C2-N1	2.45	1.43	1.37
1	L1	3792	OMG	O6-C6	-2.45	1.18	1.23
1	L1	1456	JMH	C5-C4	2.44	1.48	1.42
1	L1	3818	UY1	C4-C5	-2.44	1.37	1.44
45	S2	683	OMG	C2-N1	2.43	1.43	1.37
1	L1	4392	OMG	C2-N1	2.43	1.43	1.37
1	L1	4392	OMG	C5-C4	-2.43	1.36	1.43
1	L1	1316	OMG	O6-C6	-2.41	1.18	1.23
1	L1	2424	OMG	O6-C6	-2.41	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4370	OMG	C2-N1	2.41	1.43	1.37
45	S2	509	OMG	C2-N1	2.41	1.43	1.37
1	L1	4196	OMG	C2-N1	2.40	1.43	1.37
1	L1	4499	OMG	O6-C6	-2.39	1.18	1.23
45	S2	517	OMC	C5-C4	2.39	1.48	1.42
1	L1	4530	UR3	O2-C2	-2.38	1.18	1.22
1	L1	4623	OMG	C2-N1	2.38	1.43	1.37
45	S2	668	A2M	O5'-C5'	-2.38	1.38	1.44
1	L1	2422	OMC	C5-C4	2.37	1.48	1.42
1	L1	2365	OMC	C5-C4	2.37	1.48	1.42
45	S2	1842	4AC	O7-C7	-2.36	1.17	1.23
1	L1	1316	OMG	C2-N1	2.36	1.43	1.37
45	S2	1391	OMC	C5-C4	2.35	1.48	1.42
1	L1	4536	OMC	C5-C4	2.35	1.48	1.42
45	S2	436	OMG	O6-C6	-2.35	1.18	1.23
3	L3	75	OMG	O6-C6	-2.35	1.18	1.23
1	L1	729	2MG	O6-C6	-2.34	1.18	1.23
1	L1	2364	OMG	O6-C6	-2.34	1.18	1.23
45	S2	1832	6MZ	C5-C4	-2.34	1.34	1.40
1	L1	1881	OMC	C5-C4	2.34	1.48	1.42
45	S2	1830	UR3	O4-C4	-2.33	1.18	1.23
1	L1	3808	OMC	C5-C4	2.33	1.48	1.42
1	L1	1677	PSU	O4'-C1'	-2.32	1.40	1.43
1	L1	3944	OMG	O6-C6	-2.32	1.18	1.23
1	L1	3792	OMG	C2-N1	2.31	1.43	1.37
45	S2	601	OMG	O6-C6	-2.31	1.18	1.23
1	L1	2861	OMC	C5-C4	2.30	1.48	1.42
1	L1	3841	OMC	C5-C4	2.30	1.48	1.42
45	S2	1326	UY1	C4-C5	-2.30	1.37	1.44
45	S2	509	OMG	O6-C6	-2.29	1.18	1.23
45	S2	644	OMG	O6-C6	-2.29	1.18	1.23
45	S2	1447	OMG	O4'-C1'	2.28	1.44	1.41
45	S2	1490	OMG	O6-C6	-2.28	1.18	1.23
1	L1	1522	OMG	C2-N1	2.27	1.43	1.37
45	S2	1328	OMG	O6-C6	-2.26	1.18	1.23
1	L1	1625	OMG	O4'-C1'	2.26	1.44	1.41
1	L1	2351	OMC	C5-C4	2.26	1.48	1.42
1	L1	4637	OMG	C2-N1	2.25	1.43	1.37
45	S2	867	OMG	O6-C6	-2.25	1.18	1.23
1	L1	3887	OMC	C5-C4	2.23	1.48	1.42
1	L1	2824	OMC	C5-C4	2.23	1.48	1.42
1	L1	3627	OMG	C2-N1	2.23	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1517	2MG	C5-C6	2.21	1.51	1.47
1	L1	3785	A2M	O3'-C3'	-2.21	1.37	1.43
1	L1	3785	A2M	O5'-C5'	-2.18	1.39	1.44
1	L1	3818	UY1	O2'-C2'	-2.18	1.37	1.42
45	S2	1219	JMH	C5-C4	2.17	1.47	1.42
45	S2	590	A2M	C2-N3	2.16	1.35	1.32
1	L1	2815	A2M	O5'-C5'	-2.15	1.39	1.44
1	L1	3818	UY1	O3'-C3'	2.15	1.48	1.43
1	L1	729	2MG	CM2-N2	2.15	1.49	1.45
45	S2	1678	A2M	C2-N3	2.14	1.35	1.32
1	L1	1524	A2M	O5'-C5'	-2.13	1.39	1.44
1	L1	978	2MG	C5-C6	2.13	1.51	1.47
1	L1	4620	OMU	C6-N1	2.12	1.43	1.38
45	S2	166	A2M	C2-N3	2.12	1.35	1.32
45	S2	1288	OMU	C5-C4	2.12	1.48	1.43
1	L1	4498	OMU	C6-N1	2.11	1.43	1.38
45	S2	1248	B8N	O4'-C1'	-2.11	1.40	1.43
1	L1	1871	A2M	O5'-C5'	-2.11	1.39	1.44
45	S2	1442	OMU	C6-N1	2.10	1.43	1.38
45	S2	1337	4AC	O7-C7	-2.10	1.18	1.23
1	L1	4456	OMC	C5-C4	2.10	1.47	1.42
45	S2	1830	UR3	C5-C4	2.10	1.49	1.43
45	S2	1288	OMU	C6-N1	2.09	1.43	1.38
1	L1	398	A2M	C2-N3	2.09	1.35	1.32
45	S2	468	A2M	O5'-C5'	-2.08	1.39	1.44
1	L1	1340	OMC	C5-C4	2.07	1.47	1.42
45	S2	484	A2M	C2-N3	2.07	1.35	1.32
1	L1	4220	6MZ	C2-N3	2.07	1.35	1.32
45	S2	99	A2M	O5'-C5'	-2.05	1.39	1.44
1	L1	4530	UR3	C5-C4	2.05	1.49	1.43
1	L1	4227	OMU	C6-N1	2.05	1.42	1.38
1	L1	2401	A2M	O5'-C5'	-2.05	1.39	1.44
1	L1	3723	A2M	C2-N3	2.04	1.35	1.32
1	L1	1534	A2M	O5'-C5'	-2.03	1.39	1.44
45	S2	1031	A2M	O5'-C5'	-2.03	1.39	1.44
1	L1	4571	A2M	C2-N3	2.03	1.35	1.32
45	S2	1832	6MZ	C2-N3	2.03	1.35	1.32
1	L1	4523	A2M	O5'-C5'	-2.03	1.39	1.44
45	S2	354	OMU	C5-C4	2.03	1.48	1.43
1	L1	3830	A2M	O5'-C5'	-2.03	1.39	1.44
1	L1	3867	A2M	C2-N3	2.03	1.35	1.32
45	S2	159	A2M	C2-N3	2.02	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	1248	B8N	C32-C33	2.02	1.57	1.53
1	L1	4530	UR3	C4-N3	2.02	1.45	1.40
45	S2	27	A2M	C2-N3	2.02	1.35	1.32
45	S2	428	OMU	C6-N1	2.01	1.42	1.38
1	L1	1524	A2M	C2-N3	2.01	1.35	1.32

All (456) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	S2	1851	MA6	N1-C6-N6	-19.00	97.06	117.06
45	S2	1850	MA6	N1-C6-N6	-16.38	99.82	117.06
45	S2	1806	M7A	C5-C6-N6	13.72	147.18	123.74
45	S2	1806	M7A	N6-C6-N1	-11.74	92.64	118.35
1	L1	1871	A2M	C5-C6-N6	11.57	137.94	120.35
45	S2	512	A2M	C5-C6-N6	11.35	137.60	120.35
1	L1	1534	A2M	C5-C6-N6	11.31	137.55	120.35
45	S2	668	A2M	C5-C6-N6	11.11	137.23	120.35
1	L1	2401	A2M	C5-C6-N6	11.07	137.17	120.35
1	L1	2363	A2M	C5-C6-N6	11.03	137.11	120.35
1	L1	400	A2M	C5-C6-N6	11.01	137.08	120.35
1	L1	3867	A2M	C5-C6-N6	10.97	137.02	120.35
45	S2	166	A2M	C5-C6-N6	10.94	136.98	120.35
1	L1	3825	A2M	C5-C6-N6	10.88	136.89	120.35
1	L1	3830	A2M	C5-C6-N6	10.87	136.87	120.35
45	S2	576	A2M	C5-C6-N6	10.87	136.87	120.35
45	S2	27	A2M	C5-C6-N6	10.87	136.87	120.35
1	L1	3718	A2M	C5-C6-N6	10.86	136.85	120.35
45	S2	468	A2M	C5-C6-N6	10.84	136.83	120.35
45	S2	159	A2M	C5-C6-N6	10.83	136.81	120.35
45	S2	1678	A2M	C5-C6-N6	10.81	136.78	120.35
1	L1	4571	A2M	C5-C6-N6	10.80	136.76	120.35
1	L1	398	A2M	C5-C6-N6	10.79	136.75	120.35
1	L1	2815	A2M	C5-C6-N6	10.79	136.75	120.35
45	S2	484	A2M	C5-C6-N6	10.76	136.71	120.35
1	L1	3785	A2M	C5-C6-N6	10.68	136.58	120.35
45	S2	1031	A2M	C5-C6-N6	10.65	136.54	120.35
45	S2	1383	A2M	C5-C6-N6	10.59	136.45	120.35
1	L1	1326	A2M	C5-C6-N6	10.56	136.40	120.35
1	L1	3723	A2M	C5-C6-N6	10.55	136.38	120.35
45	S2	99	A2M	C5-C6-N6	10.49	136.29	120.35
45	S2	590	A2M	C5-C6-N6	10.48	136.28	120.35
1	L1	1524	A2M	C5-C6-N6	10.19	135.84	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	2787	A2M	C5-C6-N6	10.17	135.80	120.35
1	L1	4523	A2M	C5-C6-N6	10.11	135.72	120.35
45	S2	1850	MA6	C1'-N9-C4	-9.95	109.16	126.64
45	S2	814	5MU	C5-C4-N3	9.82	123.69	115.31
45	S2	1851	MA6	C1'-N9-C4	-8.23	112.17	126.64
45	S2	814	5MU	C5-C6-N1	-7.87	115.24	123.34
1	L1	3785	A2M	N6-C6-N1	-7.85	102.29	118.57
1	L1	1534	A2M	N6-C6-N1	-7.81	102.37	118.57
1	L1	3830	A2M	N6-C6-N1	-7.80	102.39	118.57
1	L1	3867	A2M	N6-C6-N1	-7.70	102.59	118.57
45	S2	512	A2M	N6-C6-N1	-7.68	102.63	118.57
1	L1	2363	A2M	N6-C6-N1	-7.65	102.69	118.57
1	L1	2815	A2M	N6-C6-N1	-7.61	102.78	118.57
1	L1	3825	A2M	N6-C6-N1	-7.58	102.84	118.57
1	L1	1871	A2M	N6-C6-N1	-7.56	102.88	118.57
45	S2	27	A2M	N6-C6-N1	-7.54	102.92	118.57
45	S2	166	A2M	N6-C6-N1	-7.54	102.93	118.57
1	L1	400	A2M	N6-C6-N1	-7.52	102.97	118.57
45	S2	576	A2M	N6-C6-N1	-7.45	103.11	118.57
45	S2	159	A2M	N6-C6-N1	-7.45	103.11	118.57
45	S2	668	A2M	N6-C6-N1	-7.44	103.14	118.57
45	S2	468	A2M	N6-C6-N1	-7.42	103.17	118.57
1	L1	398	A2M	N6-C6-N1	-7.42	103.18	118.57
45	S2	1383	A2M	N6-C6-N1	-7.41	103.20	118.57
1	L1	2401	A2M	N6-C6-N1	-7.40	103.21	118.57
45	S2	484	A2M	N6-C6-N1	-7.38	103.26	118.57
45	S2	1678	A2M	N6-C6-N1	-7.37	103.28	118.57
45	S2	590	A2M	N6-C6-N1	-7.36	103.29	118.57
1	L1	3718	A2M	N6-C6-N1	-7.35	103.32	118.57
1	L1	4571	A2M	N6-C6-N1	-7.30	103.42	118.57
1	L1	3723	A2M	N6-C6-N1	-7.29	103.44	118.57
45	S2	99	A2M	N6-C6-N1	-7.18	103.68	118.57
45	S2	1031	A2M	N6-C6-N1	-7.12	103.79	118.57
1	L1	1326	A2M	N6-C6-N1	-7.12	103.80	118.57
1	L1	2787	A2M	N6-C6-N1	-7.01	104.02	118.57
1	L1	4523	A2M	N6-C6-N1	-6.92	104.21	118.57
1	L1	1524	A2M	N6-C6-N1	-6.90	104.26	118.57
1	L1	3762	B8H	C4-N3-C2	-6.86	118.47	127.35
45	S2	814	5MU	C4-N3-C2	-6.53	118.90	127.35
1	L1	3818	UY1	N1-C2-N3	6.19	122.14	115.13
45	S2	512	A2M	N3-C2-N1	-6.14	119.08	128.68
1	L1	3825	A2M	N3-C2-N1	-6.10	119.14	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	3830	A2M	N3-C2-N1	-6.06	119.20	128.68
45	S2	1031	A2M	N3-C2-N1	-6.02	119.27	128.68
1	L1	4220	6MZ	N3-C2-N1	-6.00	119.30	128.68
45	S2	1851	MA6	N3-C2-N1	-5.97	119.35	128.68
1	L1	3925	OMU	C4-N3-C2	-5.95	118.73	126.58
45	S2	166	A2M	N3-C2-N1	-5.91	119.44	128.68
1	L1	2401	A2M	N3-C2-N1	-5.90	119.46	128.68
1	L1	3762	B8H	N3-C2-N1	5.90	121.51	115.14
1	L1	2363	A2M	N3-C2-N1	-5.86	119.52	128.68
1	L1	2815	A2M	N3-C2-N1	-5.86	119.52	128.68
1	L1	1524	A2M	N3-C2-N1	-5.84	119.54	128.68
1	L1	1871	A2M	N3-C2-N1	-5.84	119.56	128.68
45	S2	468	A2M	N3-C2-N1	-5.81	119.60	128.68
45	S2	1383	A2M	N3-C2-N1	-5.74	119.70	128.68
1	L1	3723	A2M	N3-C2-N1	-5.74	119.70	128.68
1	L1	400	A2M	N3-C2-N1	-5.72	119.74	128.68
1	L1	4571	A2M	N3-C2-N1	-5.72	119.75	128.68
45	S2	1678	A2M	N3-C2-N1	-5.71	119.76	128.68
45	S2	159	A2M	N3-C2-N1	-5.70	119.77	128.68
1	L1	1534	A2M	N3-C2-N1	-5.70	119.78	128.68
1	L1	2787	A2M	N3-C2-N1	-5.68	119.81	128.68
45	S2	590	A2M	N3-C2-N1	-5.67	119.81	128.68
45	S2	27	A2M	N3-C2-N1	-5.67	119.82	128.68
1	L1	4523	A2M	N3-C2-N1	-5.66	119.83	128.68
45	S2	99	A2M	N3-C2-N1	-5.65	119.85	128.68
1	L1	4498	OMU	C4-N3-C2	-5.63	119.15	126.58
45	S2	1832	6MZ	N3-C2-N1	-5.60	119.92	128.68
1	L1	1326	A2M	N3-C2-N1	-5.56	119.99	128.68
45	S2	668	A2M	N3-C2-N1	-5.54	120.01	128.68
1	L1	398	A2M	N3-C2-N1	-5.54	120.02	128.68
45	S2	484	A2M	N3-C2-N1	-5.53	120.04	128.68
45	S2	354	OMU	C4-N3-C2	-5.51	119.31	126.58
45	S2	576	A2M	N3-C2-N1	-5.48	120.12	128.68
1	L1	3785	A2M	N3-C2-N1	-5.43	120.19	128.68
1	L1	1322	1MA	N1-C2-N3	-5.43	119.69	126.02
45	S2	1326	UY1	N1-C2-N3	5.41	121.25	115.13
45	S2	1850	MA6	N3-C2-N1	-5.39	120.25	128.68
45	S2	1832	6MZ	C2-N1-C6	5.34	121.17	116.59
45	S2	172	OMU	C4-N3-C2	-5.33	119.55	126.58
45	S2	1806	M7A	N3-C2-N1	-5.29	120.32	128.60
1	L1	4227	OMU	C4-N3-C2	-5.29	119.60	126.58
45	S2	1219	JMH	C1'-N1-C2	5.28	125.90	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	4220	6MZ	C2-N1-C6	5.27	121.11	116.59
3	L3	14	OMU	C4-N3-C2	-5.21	119.71	126.58
45	S2	428	OMU	C4-N3-C2	-5.19	119.73	126.58
1	L1	2837	OMU	C4-N3-C2	-5.19	119.74	126.58
1	L1	1677	PSU	N1-C2-N3	5.17	120.99	115.13
1	L1	3867	A2M	N3-C2-N1	-5.16	120.61	128.68
1	L1	4530	UR3	C4-N3-C2	-5.16	119.70	124.56
1	L1	3718	A2M	N3-C2-N1	-5.14	120.65	128.68
1	L1	4306	OMU	C4-N3-C2	-5.13	119.81	126.58
45	S2	1442	OMU	C4-N3-C2	-5.08	119.87	126.58
45	S2	1806	M7A	N3-C4-N9	5.06	133.26	126.87
45	S2	1288	OMU	C4-N3-C2	-5.04	119.93	126.58
1	L1	4636	PSU	C4-N3-C2	-5.01	119.12	126.34
45	S2	116	OMU	C4-N3-C2	-5.01	119.97	126.58
45	S2	1248	B8N	C5-C4-N3	4.96	125.36	116.17
1	L1	1677	PSU	C4-N3-C2	-4.86	119.34	126.34
1	L1	4620	OMU	C4-N3-C2	-4.82	120.22	126.58
1	L1	4450	PSU	C4-N3-C2	-4.78	119.45	126.34
1	L1	4636	PSU	N1-C2-N3	4.75	120.52	115.13
1	L1	3715	PSU	N1-C2-N3	4.74	120.50	115.13
1	L1	4450	PSU	N1-C2-N3	4.72	120.48	115.13
1	L1	4403	PSU	C4-N3-C2	-4.71	119.55	126.34
45	S2	814	5MU	N3-C2-N1	4.70	121.12	114.89
45	S2	1081	PSU	C4-N3-C2	-4.66	119.62	126.34
45	S2	612	PSU	N1-C2-N3	4.63	120.38	115.13
45	S2	121	OMU	C4-N3-C2	-4.60	120.51	126.58
45	S2	1081	PSU	N1-C2-N3	4.60	120.34	115.13
1	L1	3715	PSU	C4-N3-C2	-4.59	119.73	126.34
45	S2	823	PSU	C4-N3-C2	-4.58	119.73	126.34
45	S2	822	PSU	N1-C2-N3	4.57	120.31	115.13
1	L1	1683	PSU	N1-C2-N3	4.56	120.30	115.13
1	L1	4442	PSU	C4-N3-C2	-4.55	119.79	126.34
1	L1	4403	PSU	N1-C2-N3	4.54	120.28	115.13
1	L1	3925	OMU	N3-C2-N1	4.51	120.87	114.89
1	L1	4531	PSU	C4-N3-C2	-4.48	119.88	126.34
1	L1	4442	PSU	N1-C2-N3	4.46	120.18	115.13
45	S2	822	PSU	C4-N3-C2	-4.44	119.94	126.34
1	L1	2508	PSU	C4-N3-C2	-4.43	119.95	126.34
1	L1	4293	PSU	C4-N3-C2	-4.43	119.96	126.34
1	L1	4628	PSU	C4-N3-C2	-4.41	119.98	126.34
1	L1	2508	PSU	N1-C2-N3	4.41	120.13	115.13
1	L1	4500	PSU	C4-N3-C2	-4.41	119.98	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	S2	1243	PSU	N1-C2-N3	4.41	120.12	115.13
45	S2	1830	UR3	C4-N3-C2	-4.40	120.42	124.56
45	S2	612	PSU	C4-N3-C2	-4.39	120.02	126.34
45	S2	823	PSU	N1-C2-N3	4.35	120.06	115.13
1	L1	4293	PSU	N1-C2-N3	4.32	120.03	115.13
45	S2	1243	PSU	C4-N3-C2	-4.32	120.12	126.34
1	L1	4500	PSU	N1-C2-N3	4.32	120.02	115.13
45	S2	119	PSU	N1-C2-N3	4.32	120.02	115.13
45	S2	1830	UR3	C1'-N1-C2	4.28	124.22	116.99
1	L1	4531	PSU	N1-C2-N3	4.28	119.98	115.13
45	S2	1248	B8N	C4-N3-C2	-4.27	120.06	125.46
1	L1	3764	PSU	N1-C2-N3	4.26	119.96	115.13
1	L1	3729	PSU	C4-N3-C2	-4.23	120.24	126.34
1	L1	1683	PSU	C4-N3-C2	-4.23	120.25	126.34
1	L1	4628	PSU	N1-C2-N3	4.23	119.92	115.13
45	S2	1806	M7A	C4-N9-C1'	-4.22	116.58	126.60
1	L1	3818	UY1	C4-N3-C2	-4.21	120.27	126.34
45	S2	814	5MU	C5M-C5-C6	-4.20	117.24	122.85
1	L1	3764	PSU	C4-N3-C2	-4.17	120.33	126.34
1	L1	1582	PSU	N1-C2-N3	4.17	119.85	115.13
45	S2	119	PSU	C4-N3-C2	-4.17	120.33	126.34
1	L1	3729	PSU	N1-C2-N3	4.14	119.81	115.13
1	L1	4220	6MZ	C9-N6-C6	-4.03	119.41	122.87
1	L1	2351	OMC	O2-C2-N3	-3.98	115.86	122.33
45	S2	116	OMU	N3-C2-N1	3.98	120.17	114.89
45	S2	1219	JMH	C6-N1-C2	-3.97	118.23	121.79
1	L1	4498	OMU	N3-C2-N1	3.96	120.15	114.89
45	S2	1326	UY1	C4-N3-C2	-3.96	120.63	126.34
45	S2	354	OMU	N3-C2-N1	3.88	120.04	114.89
1	L1	1582	PSU	C4-N3-C2	-3.88	120.75	126.34
1	L1	4447	5MC	C5-C6-N1	-3.86	119.37	123.34
1	L1	4498	OMU	C5-C4-N3	3.83	120.58	114.84
1	L1	4306	OMU	N3-C2-N1	3.81	119.94	114.89
45	S2	172	OMU	N3-C2-N1	3.80	119.93	114.89
45	S2	683	OMG	C5-C6-N1	3.78	120.63	113.95
1	L1	3818	UY1	O2-C2-N1	-3.75	118.66	122.79
1	L1	4620	OMU	N3-C2-N1	3.74	119.86	114.89
45	S2	428	OMU	N3-C2-N1	3.72	119.83	114.89
1	L1	3627	OMG	C5-C6-N1	3.71	120.51	113.95
1	L1	2876	OMG	C5-C6-N1	3.69	120.47	113.95
1	L1	3899	OMG	C5-C6-N1	3.69	120.46	113.95
1	L1	4618	OMG	C5-C6-N1	3.67	120.44	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	1322	1MA	C5-C6-N1	3.67	119.38	113.90
45	S2	601	OMG	C5-C6-N1	3.65	120.40	113.95
1	L1	4227	OMU	C5-C4-N3	3.65	120.30	114.84
45	S2	1442	OMU	N3-C2-N1	3.61	119.69	114.89
1	L1	4227	OMU	N3-C2-N1	3.61	119.68	114.89
1	L1	2424	OMG	C5-C6-N1	3.61	120.32	113.95
3	L3	75	OMG	C5-C6-N1	3.60	120.32	113.95
1	L1	4623	OMG	C5-C6-N1	3.60	120.31	113.95
1	L1	1517	2MG	C5-C6-N1	3.59	120.28	113.95
1	L1	3944	OMG	C5-C6-N1	3.58	120.27	113.95
45	S2	354	OMU	C5-C4-N3	3.57	120.18	114.84
1	L1	2837	OMU	N3-C2-N1	3.56	119.62	114.89
3	L3	14	OMU	C5-C4-N3	3.55	120.16	114.84
45	S2	1288	OMU	N3-C2-N1	3.55	119.60	114.89
45	S2	436	OMG	C5-C6-N1	3.54	120.21	113.95
1	L1	978	2MG	C5-C6-N1	3.54	120.21	113.95
1	L1	2876	OMG	C2-N1-C6	-3.54	118.58	125.10
1	L1	3792	OMG	C5-C6-N1	3.54	120.20	113.95
1	L1	3762	B8H	O2-C2-N1	-3.53	118.90	122.87
1	L1	4499	OMG	C5-C6-N1	3.51	120.15	113.95
3	L3	14	OMU	N3-C2-N1	3.51	119.55	114.89
45	S2	814	5MU	O4-C4-C5	-3.50	120.84	124.90
1	L1	4370	OMG	C5-C6-N1	3.49	120.11	113.95
45	S2	1374	5MC	C5-C6-N1	-3.48	119.75	123.34
45	S2	1328	OMG	C5-C6-N1	3.48	120.09	113.95
45	S2	814	5MU	C6-C5-C4	3.47	120.94	118.03
1	L1	3925	OMU	C5-C4-N3	3.46	120.01	114.84
1	L1	4494	OMG	C5-C6-N1	3.45	120.05	113.95
1	L1	2837	OMU	C5-C4-N3	3.45	120.01	114.84
45	S2	121	OMU	N3-C2-N1	3.45	119.47	114.89
1	L1	4392	OMG	C5-C6-N1	3.41	119.97	113.95
1	L1	4637	OMG	C5-C6-N1	3.40	119.96	113.95
1	L1	3744	OMG	C5-C6-N1	3.38	119.93	113.95
45	S2	867	OMG	C5-C6-N1	3.38	119.93	113.95
1	L1	3762	B8H	C5-C4-N3	3.38	124.23	116.58
1	L1	1522	OMG	C5-C6-N1	3.37	119.90	113.95
45	S2	644	OMG	C5-C6-N1	3.37	119.89	113.95
45	S2	509	OMG	C5-C6-N1	3.36	119.89	113.95
1	L1	4196	OMG	C5-C6-N1	3.36	119.88	113.95
1	L1	1316	OMG	C5-C6-N1	3.35	119.87	113.95
1	L1	4335	5MC	C5-C6-N1	-3.34	119.90	123.34
45	S2	172	OMU	C5-C4-N3	3.34	119.84	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	S2	683	OMG	C2-N1-C6	-3.34	118.95	125.10
45	S2	1442	OMU	C5-C4-N3	3.33	119.82	114.84
1	L1	729	2MG	C5-C6-N1	3.32	119.81	113.95
45	S2	428	OMU	C5-C4-N3	3.31	119.79	114.84
1	L1	2364	OMG	C5-C6-N1	3.30	119.79	113.95
1	L1	4392	OMG	C2-N1-C6	-3.30	119.02	125.10
1	L1	4620	OMU	C5-C4-N3	3.30	119.78	114.84
45	S2	1288	OMU	C5-C4-N3	3.29	119.75	114.84
1	L1	4306	OMU	C5-C4-N3	3.28	119.75	114.84
45	S2	1248	B8N	N3-C2-N1	3.27	121.38	116.76
1	L1	4228	OMG	C5-C6-N1	3.26	119.71	113.95
45	S2	1806	M7A	C2-N3-C4	3.26	119.45	111.75
1	L1	4494	OMG	C2-N1-C6	-3.25	119.11	125.10
45	S2	116	OMU	C5-C4-N3	3.24	119.69	114.84
45	S2	1326	UY1	O2-C2-N1	-3.23	119.24	122.79
1	L1	3782	5MC	C5-C6-N1	-3.21	120.04	123.34
45	S2	1490	OMG	C5-C6-N1	3.20	119.60	113.95
45	S2	1219	JMH	O2-C2-N3	-3.18	116.86	121.34
45	S2	601	OMG	C2-N1-C6	-3.18	119.24	125.10
45	S2	1832	6MZ	C9-N6-C6	3.16	125.59	122.87
45	S2	509	OMG	C2-N1-C6	-3.16	119.28	125.10
1	L1	4637	OMG	C2-N1-C6	-3.14	119.31	125.10
45	S2	121	OMU	C5-C4-N3	3.14	119.53	114.84
1	L1	3899	OMG	C2-N1-C6	-3.11	119.37	125.10
1	L1	4499	OMG	C2-N1-C6	-3.10	119.38	125.10
45	S2	436	OMG	C2-N1-C6	-3.10	119.39	125.10
45	S2	644	OMG	C2-N1-C6	-3.10	119.39	125.10
1	L1	3944	OMG	C2-N1-C6	-3.09	119.41	125.10
45	S2	1806	M7A	C71-N7-C5	-3.08	112.18	124.01
3	L3	75	OMG	C2-N1-C6	-3.06	119.46	125.10
45	S2	1328	OMG	C2-N1-C6	-3.06	119.47	125.10
1	L1	1517	2MG	C8-N7-C5	3.05	108.80	102.99
1	L1	2424	OMG	C2-N1-C6	-3.04	119.50	125.10
1	L1	2351	OMC	O2-C2-N1	3.03	125.14	118.89
1	L1	3792	OMG	C2-N1-C6	-3.03	119.53	125.10
1	L1	4628	PSU	O2-C2-N1	-3.03	119.46	122.79
1	L1	4370	OMG	C2-N1-C6	-3.02	119.54	125.10
1	L1	4500	PSU	O2-C2-N1	-3.01	119.48	122.79
1	L1	4618	OMG	C2-N1-C6	-3.01	119.56	125.10
1	L1	4671	B8T	C6-C5-C4	2.99	120.62	116.96
1	L1	4196	OMG	C2-N1-C6	-2.98	119.60	125.10
1	L1	4227	OMU	O4-C4-C5	-2.97	119.93	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	4623	OMG	C2-N1-C6	-2.96	119.65	125.10
1	L1	3744	OMG	C2-N1-C6	-2.96	119.65	125.10
1	L1	1677	PSU	C6-C5-C4	2.96	120.27	118.20
1	L1	1316	OMG	C2-N1-C6	-2.96	119.65	125.10
45	S2	867	OMG	C2-N1-C6	-2.95	119.67	125.10
1	L1	3627	OMG	C2-N1-C6	-2.95	119.67	125.10
1	L1	3782	5MC	CM5-C5-C6	-2.94	118.92	122.85
1	L1	3925	OMU	O4-C4-C5	-2.94	119.99	125.16
45	S2	428	OMU	O4-C4-C5	-2.93	120.00	125.16
45	S2	1442	OMU	O4-C4-C5	-2.88	120.09	125.16
1	L1	3715	PSU	O2-C2-N1	-2.87	119.64	122.79
45	S2	354	OMU	O4-C4-C5	-2.86	120.12	125.16
45	S2	116	OMU	O4-C4-C5	-2.85	120.15	125.16
1	L1	978	2MG	C8-N7-C5	2.85	108.41	102.99
45	S2	612	PSU	O2-C2-N1	-2.84	119.66	122.79
45	S2	1830	UR3	C6-N1-C2	-2.84	119.25	121.79
1	L1	729	2MG	C8-N7-C5	2.82	108.36	102.99
45	S2	814	5MU	O2-C2-N3	-2.81	116.26	121.50
45	S2	1288	OMU	O4-C4-C5	-2.81	120.21	125.16
1	L1	2364	OMG	C2-N1-C6	-2.81	119.92	125.10
1	L1	3808	OMC	O2-C2-N3	-2.80	117.77	122.33
45	S2	1842	4AC	C6-C5-C4	2.80	120.39	116.96
1	L1	4228	OMG	C2-N1-C6	-2.80	119.95	125.10
45	S2	172	OMU	O4-C4-C5	-2.78	120.27	125.16
1	L1	2364	OMG	C8-N7-C5	2.78	108.28	102.99
45	S2	814	5MU	C5M-C5-C4	2.78	121.82	118.77
45	S2	814	5MU	C1'-N1-C2	2.77	122.59	117.57
1	L1	1522	OMG	C2-N1-C6	-2.75	120.04	125.10
1	L1	1522	OMG	C8-N7-C5	2.73	108.19	102.99
45	S2	121	OMU	O4-C4-C5	-2.73	120.37	125.16
45	S2	1490	OMG	C2-N1-C6	-2.71	120.10	125.10
45	S2	1337	4AC	C6-C5-C4	2.70	120.27	116.96
1	L1	2876	OMG	C8-N7-C5	2.69	108.11	102.99
1	L1	4228	OMG	C8-N7-C5	2.68	108.11	102.99
1	L1	3744	OMG	C8-N7-C5	2.68	108.10	102.99
1	L1	3762	B8H	O4-C4-N3	-2.68	114.98	120.12
1	L1	1677	PSU	O2-C2-N1	-2.68	119.84	122.79
1	L1	3899	OMG	C8-N7-C5	2.68	108.09	102.99
1	L1	4450	PSU	C6-C5-C4	2.67	120.07	118.20
1	L1	4531	PSU	O2-C2-N1	-2.67	119.85	122.79
1	L1	3627	OMG	C8-N7-C5	2.66	108.06	102.99
1	L1	4392	OMG	C8-N7-C5	2.65	108.04	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	2837	OMU	O4-C4-C5	-2.65	120.50	125.16
45	S2	822	PSU	O2-C2-N1	-2.64	119.89	122.79
1	L1	1316	OMG	C8-N7-C5	2.64	108.01	102.99
1	L1	4636	PSU	C6-C5-C4	2.64	120.04	118.20
45	S2	436	OMG	C8-N7-C5	2.63	107.99	102.99
1	L1	4637	OMG	C8-N7-C5	2.63	107.99	102.99
1	L1	4498	OMU	O4-C4-C5	-2.62	120.55	125.16
1	L1	4618	OMG	C8-N7-C5	2.62	107.98	102.99
1	L1	4403	PSU	O2-C2-N1	-2.61	119.91	122.79
1	L1	3764	PSU	O2-C2-N1	-2.60	119.93	122.79
45	S2	644	OMG	C8-N7-C5	2.60	107.94	102.99
3	L3	14	OMU	O4-C4-C5	-2.59	120.60	125.16
45	S2	1806	M7A	C5-C4-N3	-2.58	120.56	126.62
1	L1	3944	OMG	C8-N7-C5	2.58	107.91	102.99
1	L1	4499	OMG	C8-N7-C5	2.58	107.90	102.99
1	L1	4623	OMG	C8-N7-C5	2.58	107.90	102.99
1	L1	4196	OMG	C8-N7-C5	2.57	107.89	102.99
1	L1	3792	OMG	C8-N7-C5	2.57	107.88	102.99
45	S2	1328	OMG	C8-N7-C5	2.57	107.88	102.99
45	S2	683	OMG	C8-N7-C5	2.57	107.88	102.99
3	L3	75	OMG	C8-N7-C5	2.56	107.87	102.99
45	S2	601	OMG	C8-N7-C5	2.56	107.86	102.99
45	S2	1243	PSU	O2-C2-N1	-2.55	119.98	122.79
45	S2	612	PSU	C6-N1-C2	-2.53	120.09	122.68
1	L1	2424	OMG	O6-C6-C5	-2.53	119.43	124.37
1	L1	4500	PSU	C6-N1-C2	-2.53	120.09	122.68
1	L1	4530	UR3	C1'-N1-C2	2.52	121.25	116.99
1	L1	2824	OMC	O2-C2-N3	-2.52	118.23	122.33
1	L1	1456	JMH	C6-N1-C2	-2.51	119.54	121.79
45	S2	823	PSU	O2-C2-N1	-2.51	120.03	122.79
1	L1	3841	OMC	O2-C2-N3	-2.50	118.27	122.33
1	L1	4306	OMU	O4-C4-C5	-2.49	120.78	125.16
1	L1	2364	OMG	N2-C2-N1	2.49	122.01	116.71
1	L1	4499	OMG	O6-C6-C5	-2.49	119.51	124.37
1	L1	1322	1MA	C8-N7-C5	2.46	107.68	102.99
45	S2	1337	4AC	C5-C4-N3	-2.46	118.64	122.59
45	S2	814	5MU	O4-C4-N3	-2.46	115.41	120.12
45	S2	119	PSU	O2-C2-N1	-2.45	120.09	122.79
45	S2	683	OMG	O6-C6-C5	-2.45	119.59	124.37
1	L1	4494	OMG	O6-C6-C5	-2.44	119.60	124.37
1	L1	4293	PSU	O2-C2-N1	-2.44	120.10	122.79
1	L1	3764	PSU	C6-N1-C2	-2.43	120.19	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	3729	PSU	O2-C2-N1	-2.43	120.11	122.79
3	L3	14	OMU	C1'-N1-C2	2.43	121.96	117.57
45	S2	867	OMG	C8-N7-C5	2.42	107.61	102.99
45	S2	1830	UR3	O2-C2-N3	-2.42	117.93	121.34
45	S2	601	OMG	O6-C6-C5	-2.42	119.65	124.37
1	L1	3925	OMU	O2-C2-N1	-2.41	119.58	122.79
1	L1	4370	OMG	C8-N7-C5	2.41	107.58	102.99
1	L1	4494	OMG	C8-N7-C5	2.41	107.58	102.99
45	S2	1490	OMG	C8-N7-C5	2.41	107.58	102.99
1	L1	4620	OMU	O4-C4-C5	-2.41	120.93	125.16
1	L1	1582	PSU	O2-C2-N1	-2.41	120.14	122.79
45	S2	1243	PSU	C6-N1-C2	-2.40	120.23	122.68
45	S2	668	A2M	C3'-C2'-C1'	2.39	107.38	102.89
45	S2	509	OMG	C8-N7-C5	2.39	107.54	102.99
45	S2	822	PSU	C6-N1-C2	-2.38	120.25	122.68
1	L1	978	2MG	CM2-N2-C2	-2.38	118.61	123.86
1	L1	1683	PSU	C6-N1-C2	-2.38	120.25	122.68
1	L1	1677	PSU	C6-N1-C2	-2.37	120.26	122.68
3	L3	75	OMG	O6-C6-C5	-2.37	119.74	124.37
1	L1	4636	PSU	O2-C2-N1	-2.36	120.19	122.79
45	S2	116	OMU	O2-C2-N1	-2.35	119.67	122.79
1	L1	3715	PSU	C6-N1-C2	-2.35	120.28	122.68
1	L1	3899	OMG	O6-C6-C5	-2.34	119.79	124.37
45	S2	1842	4AC	C5-C4-N3	-2.34	118.82	122.59
45	S2	867	OMG	O6-C6-C5	-2.33	119.83	124.37
1	L1	4530	UR3	C6-N1-C2	-2.31	119.72	121.79
45	S2	1248	B8N	O4'-C1'-C2'	2.31	108.41	105.14
45	S2	1447	OMG	C5-C6-N1	2.31	118.03	113.95
45	S2	1219	JMH	C1'-N1-C6	-2.29	115.86	120.84
1	L1	3944	OMG	O6-C6-C5	-2.28	119.91	124.37
45	S2	814	5MU	C1'-N1-C6	-2.28	117.32	121.12
1	L1	1625	OMG	C5-C6-N1	2.28	117.98	113.95
1	L1	1316	OMG	O6-C6-C5	-2.27	119.94	124.37
45	S2	612	PSU	O4'-C1'-C2'	2.27	108.34	105.14
45	S2	1328	OMG	O6-C6-C5	-2.27	119.95	124.37
45	S2	1447	OMG	C8-N7-C5	2.26	107.31	102.99
45	S2	1248	B8N	C31-N3-C4	2.26	120.64	117.31
45	S2	436	OMG	O6-C6-C5	-2.26	119.97	124.37
1	L1	3792	OMG	O6-C6-C5	-2.24	120.00	124.37
1	L1	2876	OMG	O6-C6-C5	-2.23	120.01	124.37
1	L1	4618	OMG	O6-C6-C5	-2.23	120.01	124.37
1	L1	4447	5MC	C5-C4-N3	-2.23	119.27	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	2824	OMC	C1'-N1-C2	2.23	123.39	118.42
45	S2	1447	OMG	O4'-C4'-C3'	-2.22	100.71	105.11
45	S2	822	PSU	O4'-C1'-C2'	2.22	108.28	105.14
1	L1	3818	UY1	C5-C6-N1	-2.22	118.78	122.11
1	L1	4442	PSU	C6-C5-C4	2.22	119.75	118.20
1	L1	4442	PSU	O4'-C1'-C2'	2.22	108.27	105.14
45	S2	119	PSU	C6-N1-C2	-2.22	120.42	122.68
1	L1	4531	PSU	C6-N1-C2	-2.22	120.42	122.68
1	L1	4636	PSU	O4'-C1'-C2'	2.19	108.23	105.14
1	L1	978	2MG	O6-C6-C5	-2.18	120.11	124.37
1	L1	2424	OMG	C8-N7-C5	2.17	107.13	102.99
45	S2	644	OMG	O6-C6-C5	-2.17	120.13	124.37
45	S2	1248	B8N	O4-C4-N3	-2.17	116.29	119.98
1	L1	1517	2MG	O6-C6-C5	-2.17	120.14	124.37
1	L1	2351	OMC	C1'-N1-C2	2.17	123.26	118.42
1	L1	2508	PSU	O2-C2-N1	-2.17	120.41	122.79
45	S2	1490	OMG	O6-C6-C5	-2.16	120.16	124.37
1	L1	2837	OMU	C2'-C1'-N1	-2.15	110.04	114.22
1	L1	3729	PSU	C6-N1-C2	-2.15	120.49	122.68
1	L1	4370	OMG	O6-C6-C5	-2.14	120.20	124.37
45	S2	1081	PSU	O2-C2-N1	-2.13	120.44	122.79
45	S2	1081	PSU	O4'-C1'-C2'	2.13	108.15	105.14
1	L1	4623	OMG	O6-C6-C5	-2.13	120.22	124.37
45	S2	1710	OMC	O2-C2-N3	-2.13	118.88	122.33
1	L1	1582	PSU	C6-N1-C2	-2.12	120.51	122.68
1	L1	3782	5MC	O2-C2-N3	-2.12	118.88	122.33
45	S2	509	OMG	O6-C6-C5	-2.09	120.28	124.37
1	L1	4442	PSU	O2-C2-N1	-2.08	120.50	122.79
1	L1	2364	OMG	N1-C2-N3	-2.08	119.43	123.32
45	S2	172	OMU	O2-C2-N1	-2.08	120.03	122.79
45	S2	1391	OMC	O2-C2-N3	-2.07	118.97	122.33
1	L1	4403	PSU	O4'-C1'-C2'	2.05	108.04	105.14
1	L1	4196	OMG	O6-C6-C5	-2.05	120.36	124.37
1	L1	3627	OMG	O6-C6-C5	-2.05	120.37	124.37
45	S2	354	OMU	O2-C2-N1	-2.05	120.06	122.79
45	S2	1832	6MZ	C4-C5-N7	-2.04	107.27	109.40
45	S2	1374	5MC	CM5-C5-C6	-2.04	120.12	122.85
45	S2	1081	PSU	C6-N1-C2	-2.04	120.60	122.68
1	L1	3744	OMG	O6-C6-C5	-2.03	120.40	124.37
1	L1	3715	PSU	C6-C5-C4	2.03	119.62	118.20
1	L1	2424	OMG	N2-C2-N1	2.03	121.03	116.71
45	S2	823	PSU	C6-N1-C2	-2.02	120.61	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	1625	OMG	C8-N7-C5	2.01	106.83	102.99
1	L1	4335	5MC	CM5-C5-C6	-2.01	120.17	122.85
1	L1	729	2MG	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L1	1340	OMC	C3'-C4'-C5'-O5'
1	L1	1340	OMC	O4'-C4'-C5'-O5'
1	L1	1677	PSU	C2'-C1'-C5-C6
1	L1	2424	OMG	O4'-C4'-C5'-O5'
1	L1	2424	OMG	C3'-C4'-C5'-O5'
1	L1	3701	OMC	C2'-C1'-N1-C6
1	L1	3764	PSU	C3'-C4'-C5'-O5'
1	L1	3764	PSU	O4'-C4'-C5'-O5'
1	L1	3808	OMC	C3'-C4'-C5'-O5'
1	L1	3818	UY1	O4'-C4'-C5'-O5'
1	L1	3841	OMC	C3'-C4'-C5'-O5'
1	L1	3867	A2M	C3'-C4'-C5'-O5'
1	L1	3925	OMU	C1'-C2'-O2'-CM2
1	L1	3944	OMG	C3'-C4'-C5'-O5'
1	L1	4196	OMG	C1'-C2'-O2'-CM2
1	L1	4500	PSU	C3'-C4'-C5'-O5'
1	L1	4636	PSU	C3'-C4'-C5'-O5'
1	L1	4637	OMG	C1'-C2'-O2'-CM2
3	L3	14	OMU	C1'-C2'-O2'-CM2
45	S2	512	A2M	O4'-C4'-C5'-O5'
45	S2	576	A2M	O4'-C4'-C5'-O5'
45	S2	576	A2M	C3'-C4'-C5'-O5'
45	S2	590	A2M	O4'-C4'-C5'-O5'
45	S2	601	OMG	C1'-C2'-O2'-CM2
45	S2	644	OMG	C1'-C2'-O2'-CM2
45	S2	668	A2M	O4'-C4'-C5'-O5'
45	S2	668	A2M	C3'-C4'-C5'-O5'
45	S2	867	OMG	C3'-C4'-C5'-O5'
45	S2	867	OMG	C1'-C2'-O2'-CM2
45	S2	1248	B8N	O4'-C4'-C5'-O5'
45	S2	1248	B8N	C3'-C4'-C5'-O5'
45	S2	1328	OMG	C1'-C2'-O2'-CM2
45	S2	1391	OMC	C3'-C4'-C5'-O5'
45	S2	1442	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
45	S2	1442	OMU	O4'-C4'-C5'-O5'
45	S2	1447	OMG	C1'-C2'-O2'-CM2
45	S2	1678	A2M	C1'-C2'-O2'-CM'
45	S2	1830	UR3	O4'-C1'-N1-C2
45	S2	1832	6MZ	N1-C6-N6-C9
1	L1	3701	OMC	C2'-C1'-N1-C2
1	L1	3729	PSU	O4'-C4'-C5'-O5'
1	L1	3785	A2M	O4'-C4'-C5'-O5'
1	L1	3785	A2M	C3'-C4'-C5'-O5'
1	L1	3841	OMC	O4'-C4'-C5'-O5'
1	L1	3867	A2M	O4'-C4'-C5'-O5'
1	L1	4500	PSU	O4'-C4'-C5'-O5'
45	S2	512	A2M	C3'-C4'-C5'-O5'
45	S2	590	A2M	C3'-C4'-C5'-O5'
45	S2	683	OMG	O4'-C4'-C5'-O5'
45	S2	683	OMG	C3'-C4'-C5'-O5'
45	S2	1243	PSU	O4'-C4'-C5'-O5'
45	S2	1391	OMC	O4'-C4'-C5'-O5'
45	S2	1851	MA6	O4'-C4'-C5'-O5'
1	L1	3808	OMC	O4'-C4'-C5'-O5'
1	L1	3818	UY1	C3'-C4'-C5'-O5'
1	L1	3944	OMG	O4'-C4'-C5'-O5'
1	L1	4636	PSU	O4'-C4'-C5'-O5'
45	S2	99	A2M	O4'-C4'-C5'-O5'
45	S2	867	OMG	O4'-C4'-C5'-O5'
45	S2	1442	OMU	C3'-C4'-C5'-O5'
45	S2	1851	MA6	C3'-C4'-C5'-O5'
45	S2	1830	UR3	O4'-C1'-N1-C6
1	L1	1534	A2M	C3'-C2'-O2'-CM'
1	L1	4447	5MC	C2'-C1'-N1-C6
1	L1	3729	PSU	C3'-C4'-C5'-O5'
45	S2	1243	PSU	C3'-C4'-C5'-O5'
42	Lo	53	MLZ	CE-CD-CG-CB
1	L1	398	A2M	O4'-C4'-C5'-O5'
1	L1	1677	PSU	O4'-C4'-C5'-O5'
1	L1	2364	OMG	O4'-C4'-C5'-O5'
45	S2	159	A2M	C3'-C4'-C5'-O5'
45	S2	1850	MA6	C5-C6-N6-C10
1	L1	1677	PSU	C3'-C4'-C5'-O5'
1	L1	4447	5MC	O4'-C1'-N1-C6
45	S2	517	OMC	O4'-C4'-C5'-O5'
1	L1	4620	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
1	L1	4447	5MC	C2'-C1'-N1-C2
1	L1	1534	A2M	C4'-C5'-O5'-P
1	L1	3818	UY1	C4'-C5'-O5'-P
45	S2	517	OMC	C3'-C4'-C5'-O5'
1	L1	4500	PSU	C4'-C5'-O5'-P
1	L1	2824	OMC	C3'-C4'-C5'-O5'
45	S2	1248	B8N	N3-C31-C32-C33
1	L1	3701	OMC	O4'-C1'-N1-C6
1	L1	4447	5MC	O4'-C1'-N1-C2
45	S2	590	A2M	C4'-C5'-O5'-P
45	S2	1490	OMG	C4'-C5'-O5'-P
45	S2	159	A2M	O4'-C4'-C5'-O5'
1	L1	3701	OMC	O4'-C1'-N1-C2
1	L1	1524	A2M	C3'-C2'-O2'-CM'
1	L1	2364	OMG	C3'-C4'-C5'-O5'
42	Lo	53	MLZ	CG-CD-CE-NZ
45	S2	1219	JMH	C2'-C1'-N1-C6
1	L1	3818	UY1	O4'-C1'-C5-C4
1	L1	4450	PSU	O4'-C1'-C5-C4
45	S2	1326	UY1	O4'-C1'-C5-C4
1	L1	2351	OMC	C3'-C2'-O2'-CM2
1	L1	2363	A2M	C3'-C2'-O2'-CM'
1	L1	2401	A2M	C3'-C2'-O2'-CM'
45	S2	644	OMG	C4'-C5'-O5'-P
45	S2	428	OMU	C2'-C1'-N1-C6
1	L1	4293	PSU	O4'-C4'-C5'-O5'
45	S2	1832	6MZ	C5-C6-N6-C9
1	L1	2824	OMC	O4'-C4'-C5'-O5'
45	S2	99	A2M	C3'-C4'-C5'-O5'
45	S2	428	OMU	O4'-C1'-N1-C6
1	L1	1534	A2M	O4'-C4'-C5'-O5'
1	L1	2787	A2M	C3'-C4'-C5'-O5'
45	S2	1850	MA6	O4'-C4'-C5'-O5'
45	S2	1850	MA6	C3'-C4'-C5'-O5'
1	L1	1677	PSU	O4'-C1'-C5-C6
1	L1	4636	PSU	O4'-C1'-C5-C6
1	L1	2351	OMC	C2'-C1'-N1-C2
45	S2	1219	JMH	C2'-C1'-N1-C2
1	L1	729	2MG	O4'-C4'-C5'-O5'
1	L1	2351	OMC	O4'-C4'-C5'-O5'
1	L1	2422	OMC	O4'-C4'-C5'-O5'
45	S2	822	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L1	3869	OMC	C3'-C2'-O2'-CM2
1	L1	398	A2M	C3'-C4'-C5'-O5'
1	L1	1326	A2M	C4'-C5'-O5'-P
1	L1	4671	B8T	C4'-C5'-O5'-P
45	S2	576	A2M	C4'-C5'-O5'-P
45	S2	1081	PSU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 442 ligands modelled in this entry, 442 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

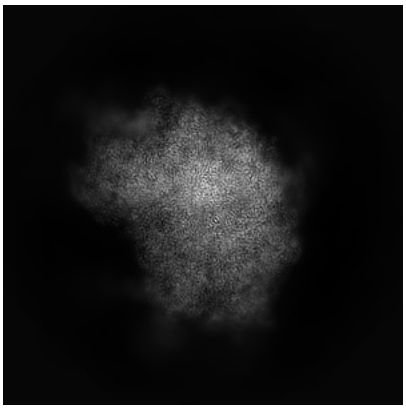
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33329. These allow visual inspection of the internal detail of the map and identification of artifacts.

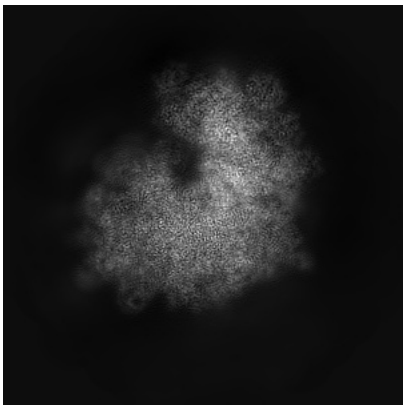
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

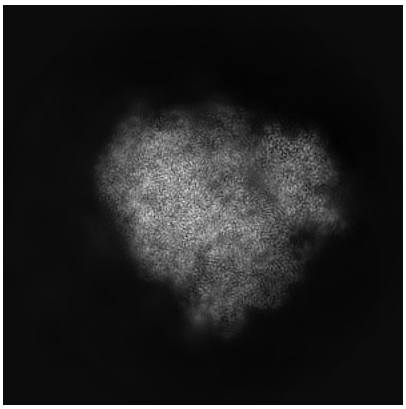
6.1.1 Primary map



X

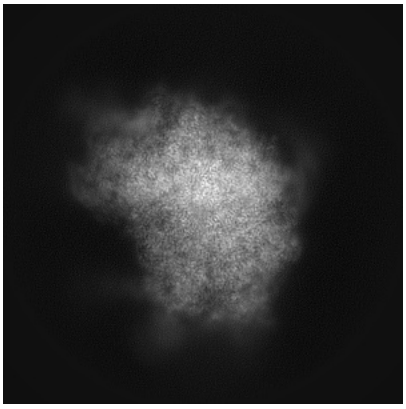


Y

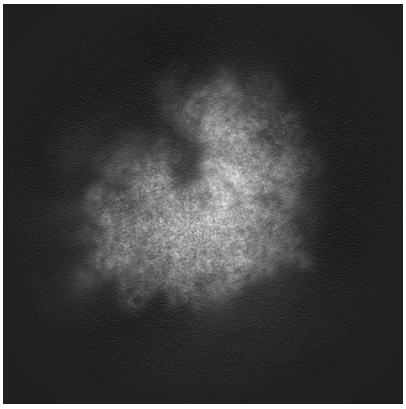


Z

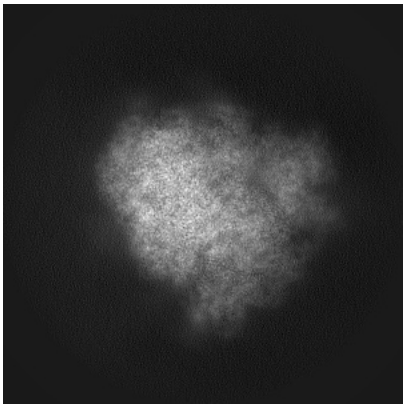
6.1.2 Raw map



X



Y

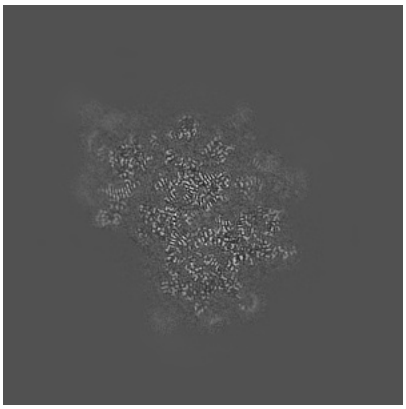


Z

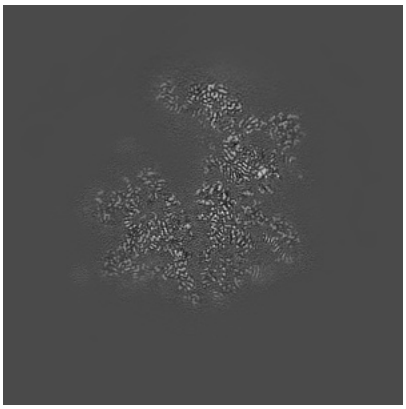
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

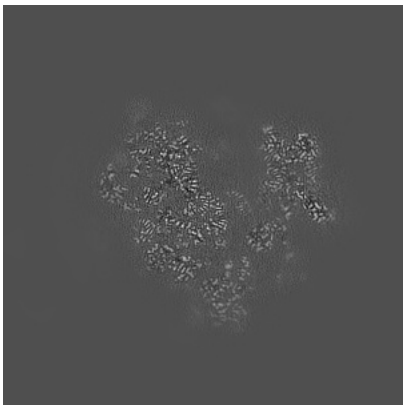
6.2.1 Primary map



X Index: 210

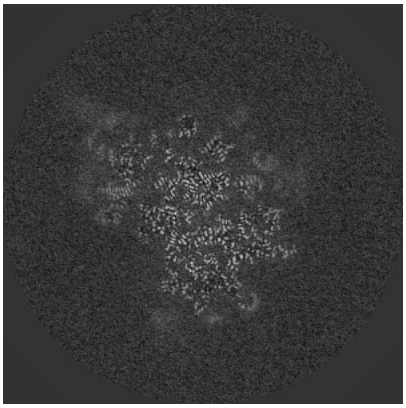


Y Index: 210

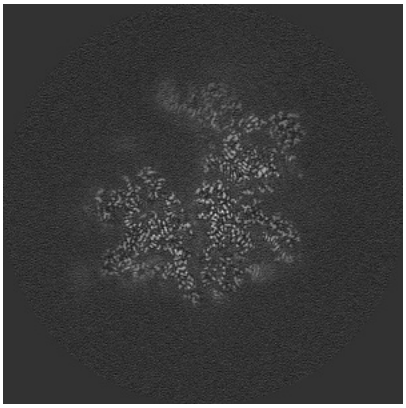


Z Index: 210

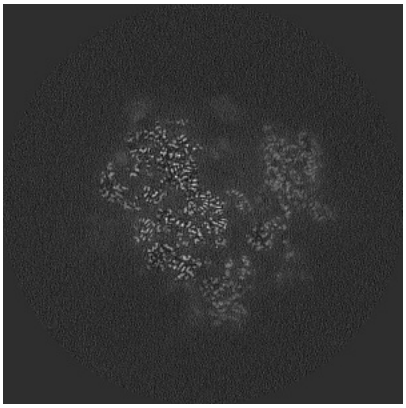
6.2.2 Raw map



X Index: 210



Y Index: 210

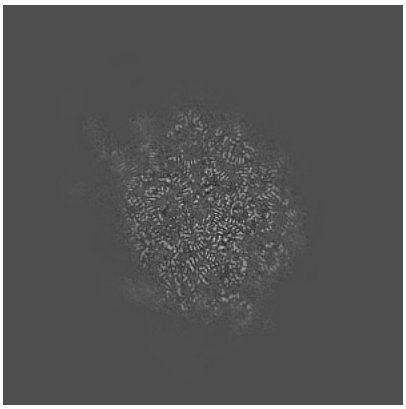


Z Index: 210

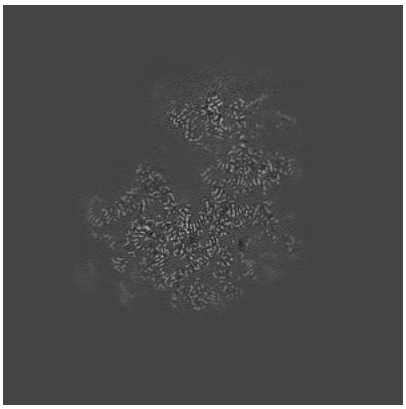
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



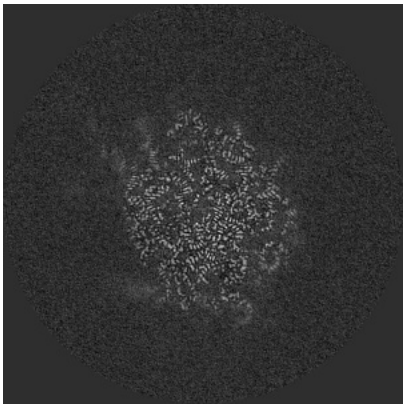
X Index: 188



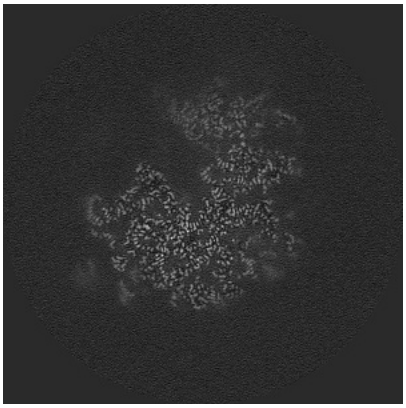
Y Index: 223

Z Index: 231

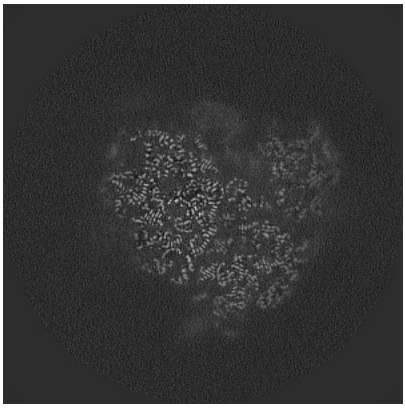
6.3.2 Raw map



X Index: 188



Y Index: 223

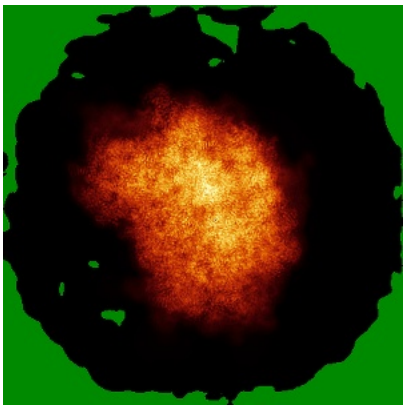


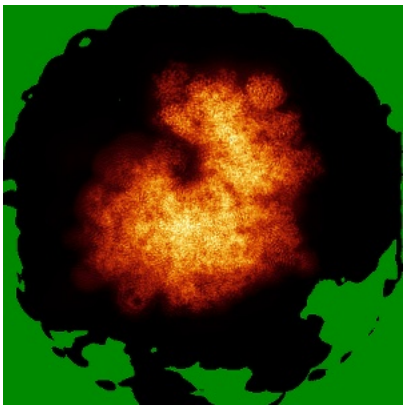
Z Index: 231

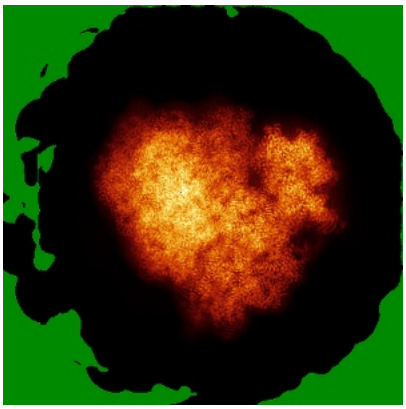
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

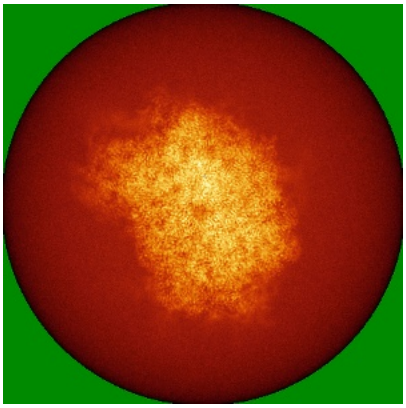
6.4.1 Primary map

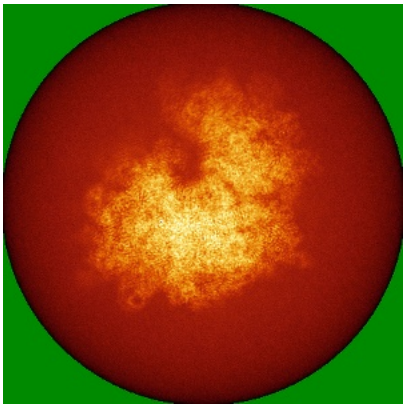

X

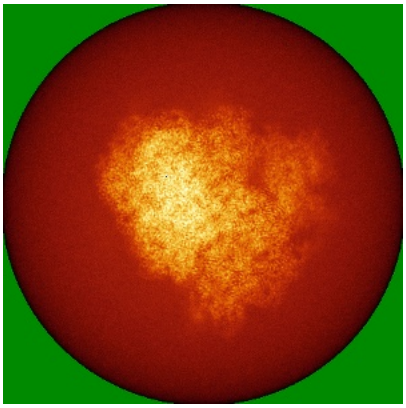

Y


Z

6.4.2 Raw map


X

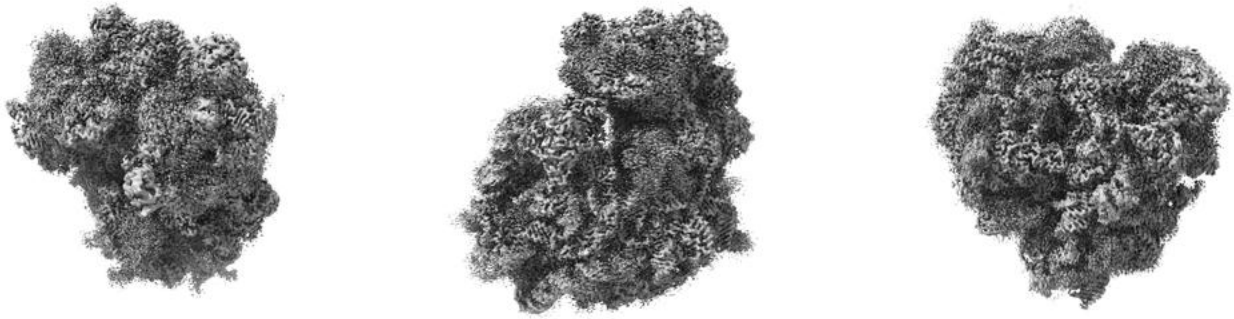

Y


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)

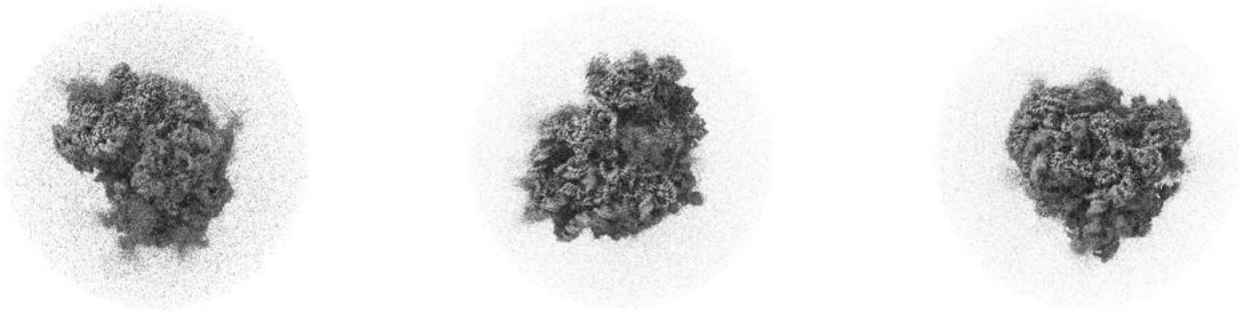
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. 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



X Y Z

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.

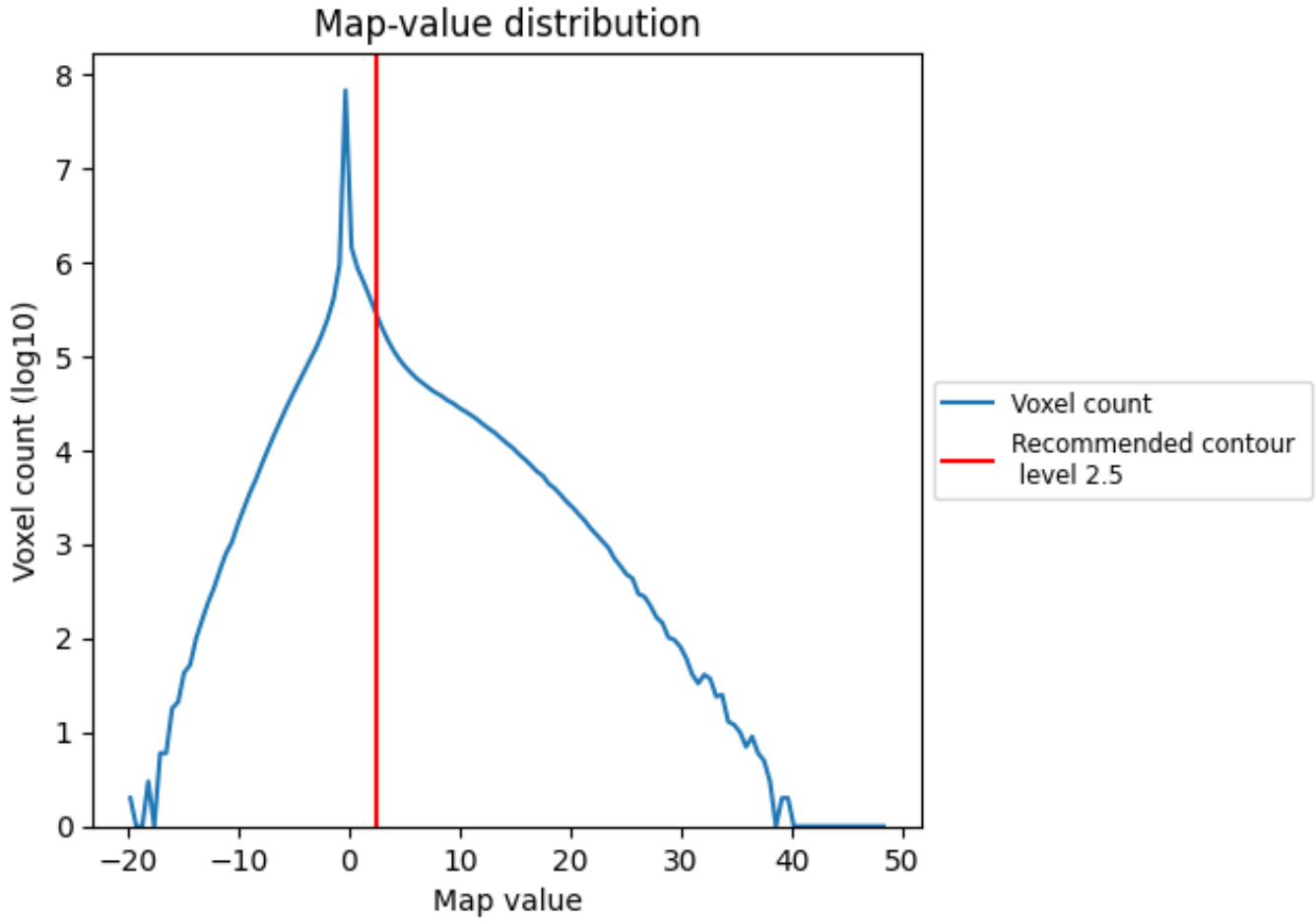
6.6 Mask visualisation (i)

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

7 Map analysis

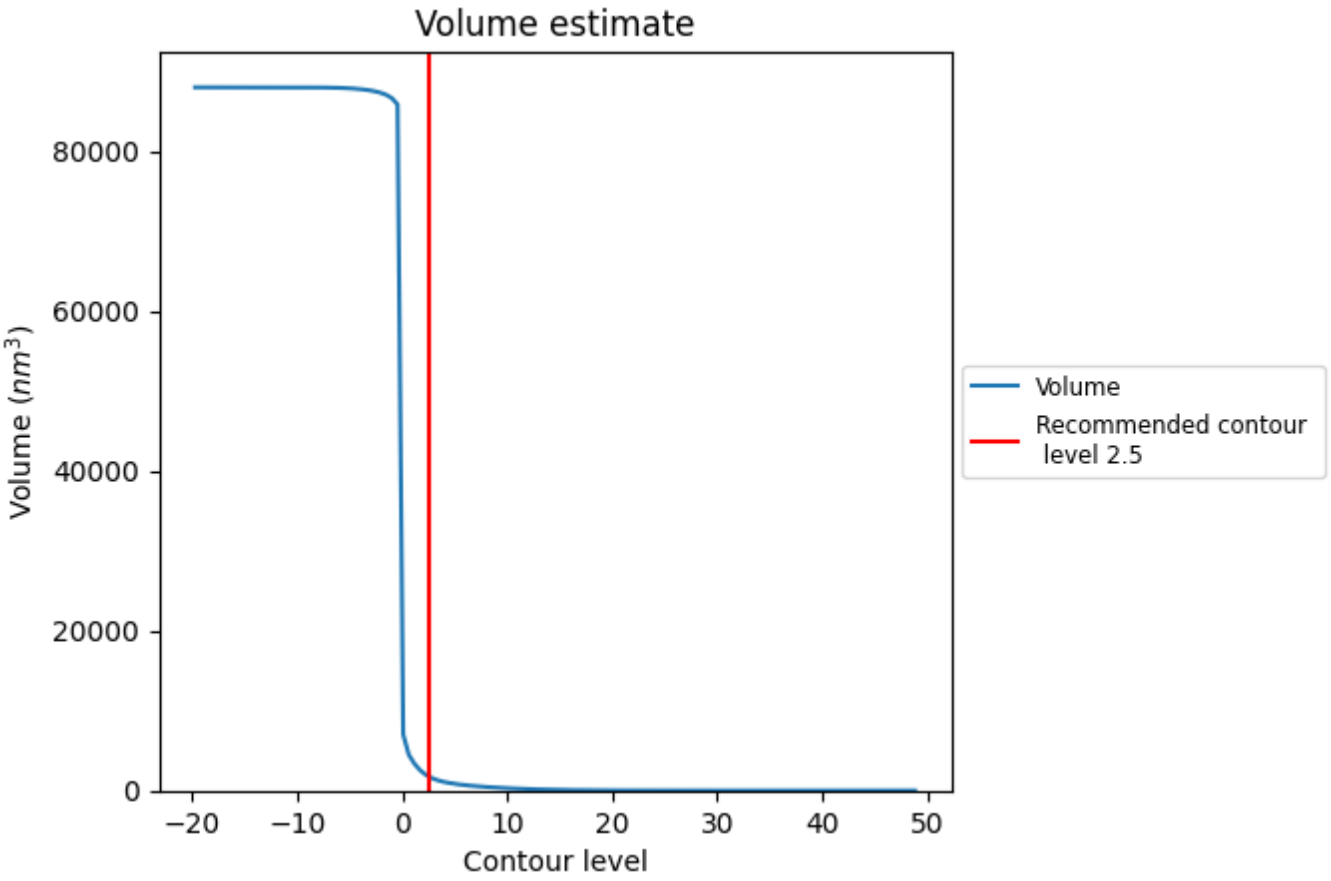
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

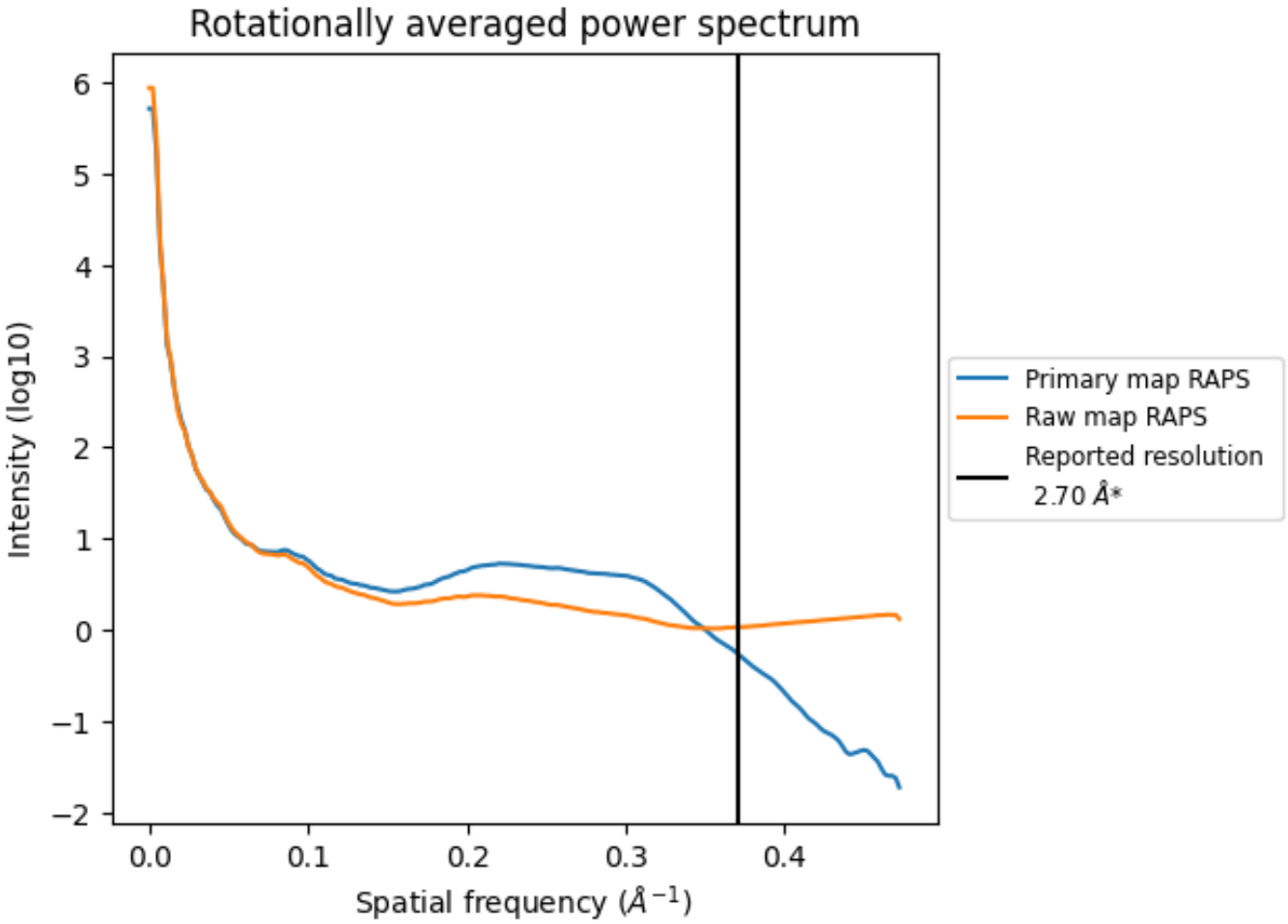
7.2 Volume estimate



The volume at the recommended contour level is 1791 nm^3; this corresponds to an approximate mass of 1617 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)

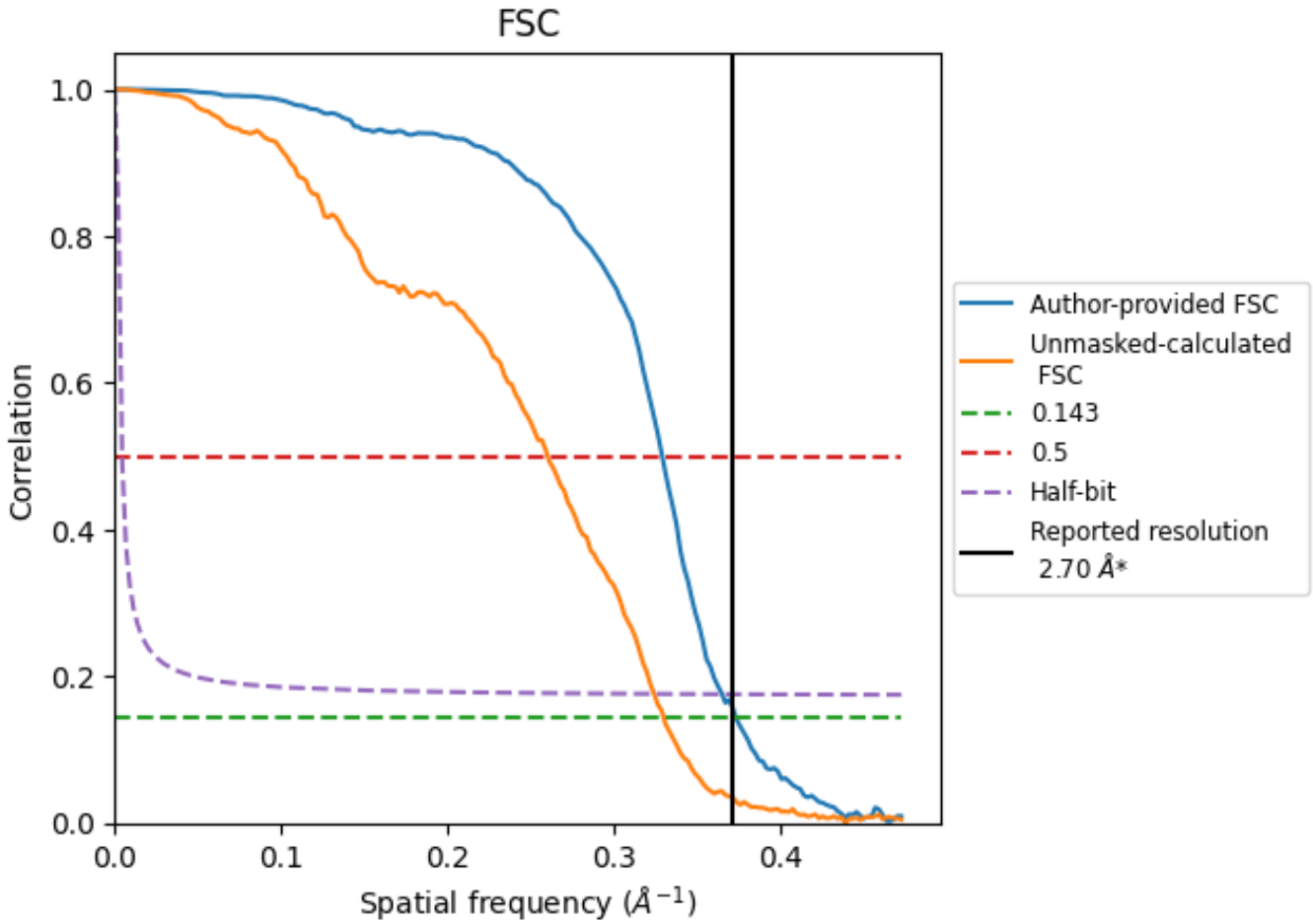


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

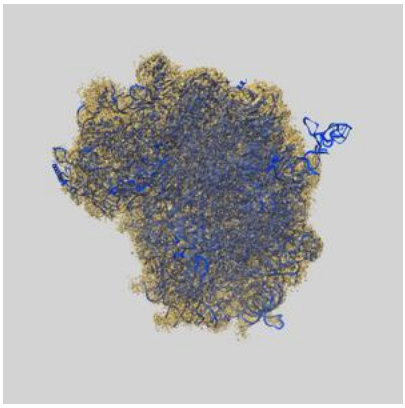
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.04	2.74
Unmasked-calculated*	3.03	3.85	3.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.03 differs from the reported value 2.7 by more than 10 %

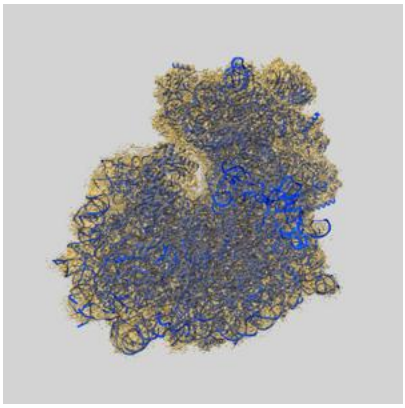
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33329 and PDB model 7XNX. Per-residue inclusion information can be found in section 3 on page 21.

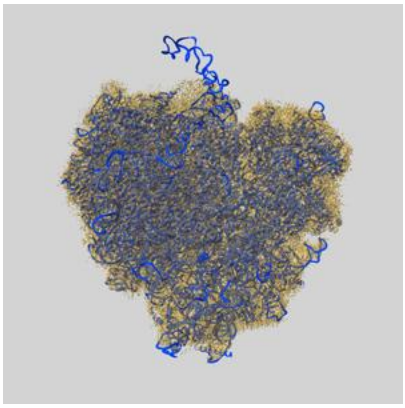
9.1 Map-model overlay



X



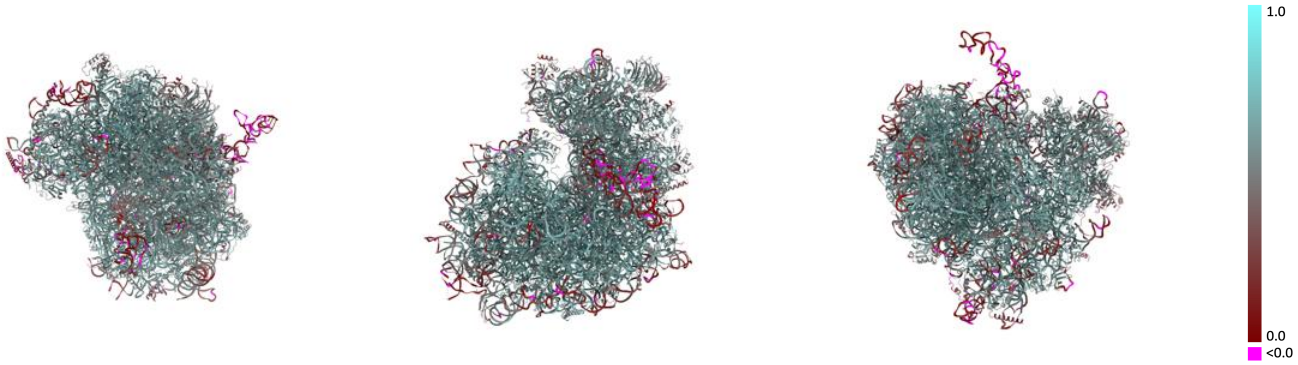
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

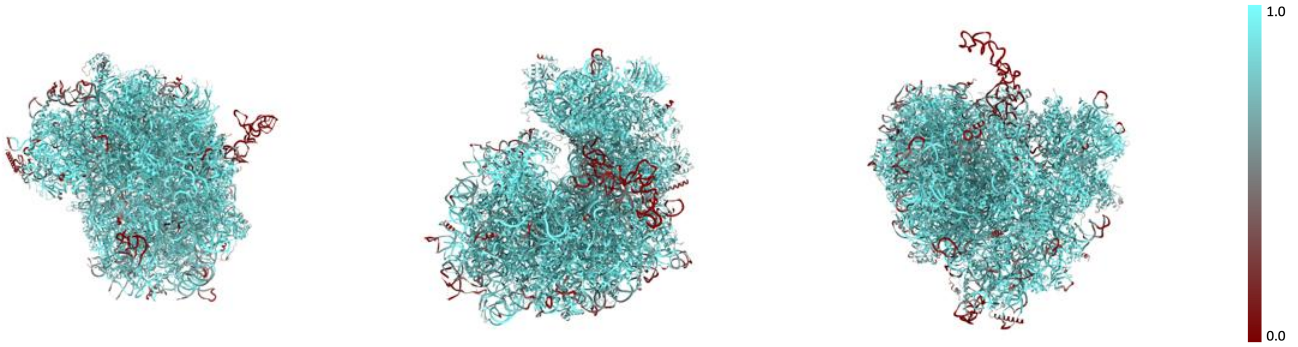
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

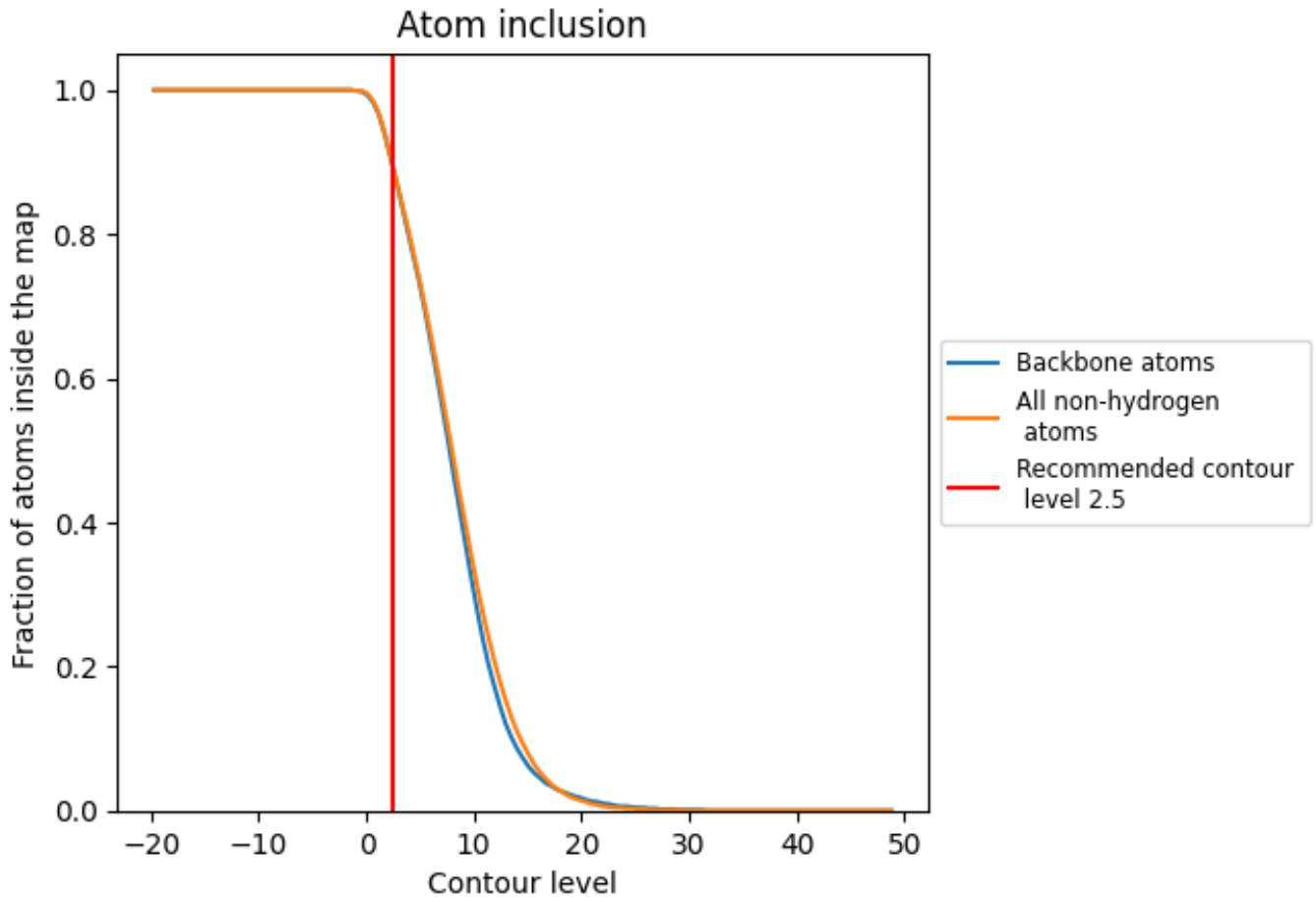
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.5800
CC	0.3530	0.3020
CE	0.7000	0.5000
L1	0.8790	0.5720
L2	0.9870	0.6430
L3	0.9340	0.6070
LA	0.9810	0.6740
LB	0.9310	0.6390
LC	0.9360	0.6380
LD	0.8840	0.6010
LE	0.8790	0.5910
LF	0.9550	0.6530
LG	0.8360	0.5730
LH	0.9080	0.6100
LI	0.9420	0.6350
LJ	0.8190	0.5520
LL	0.8790	0.5920
LM	0.9120	0.6020
LN	0.9890	0.6800
LO	0.9470	0.6490
LP	0.9380	0.6510
LQ	0.9700	0.6660
LR	0.8510	0.6000
LS	0.9670	0.6540
LT	0.9200	0.6230
LU	0.7080	0.5060
LV	0.9570	0.6520
LW	0.5960	0.4410
LX	0.9300	0.6350
LY	0.8990	0.6060
LZ	0.9040	0.6110
La	0.9530	0.6540
Lb	0.7910	0.5400
Lc	0.9370	0.6250
Ld	0.8950	0.6190

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Chain	Atom inclusion	Q-score
Le	0.9620	0.6530
Lf	0.9700	0.6590
Lg	0.9140	0.6220
Lh	0.8900	0.5990
Li	0.9070	0.5990
Lj	0.9720	0.6580
Lk	0.7500	0.5510
Ll	0.9480	0.6340
Lm	0.9280	0.6340
Ln	0.9620	0.6230
Lo	0.9350	0.6420
Lp	0.9650	0.6600
Lr	0.9410	0.6320
S2	0.9120	0.5780
SA	0.9090	0.5950
SB	0.9140	0.5880
SC	0.9630	0.6240
SD	0.9350	0.5380
SE	0.9460	0.5990
SF	0.9370	0.5560
SG	0.8420	0.5110
SH	0.8060	0.4950
SI	0.8870	0.5720
SJ	0.9030	0.5730
SK	0.9080	0.5160
SL	0.9360	0.6330
SM	0.6560	0.2980
SN	0.9570	0.6340
SO	0.9470	0.6090
SP	0.8680	0.4790
SQ	0.9150	0.5290
SR	0.7960	0.5340
SS	0.8830	0.4890
ST	0.9140	0.5330
SU	0.8790	0.4870
SV	0.9260	0.6000
SW	0.9720	0.6430
SX	0.9580	0.6240
SY	0.9080	0.5570
SZ	0.8830	0.5120
Sa	0.9250	0.6030
Sb	0.8980	0.5840

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Chain	Atom inclusion	Q-score
Sc	0.8890	0.5170
Sd	0.9500	0.5660
Se	0.7810	0.5200
Sf	0.8140	0.4610
Sg	0.9100	0.5050