



Full wwPDB EM Validation Report ⓘ

Mar 29, 2023 – 09:43 PM JST

PDB ID : 7XNY
EMDB ID : EMD-33330
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 : 2.50 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:

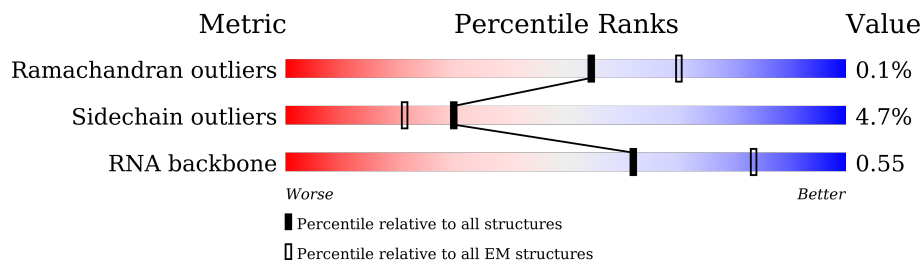
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	L1	5070	
2	L2	120	
3	L3	156	
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	

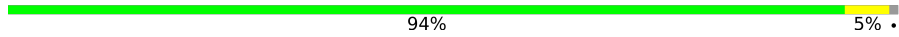
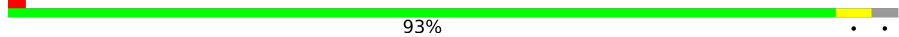
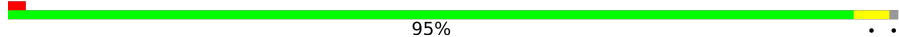
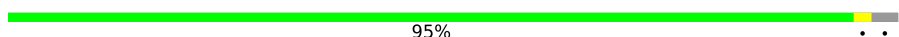






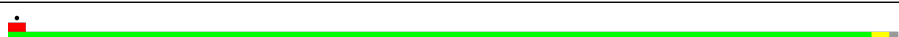


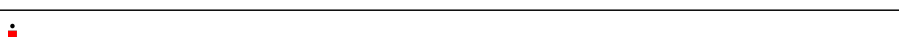
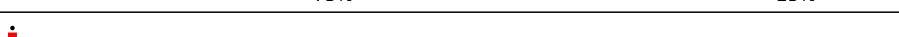
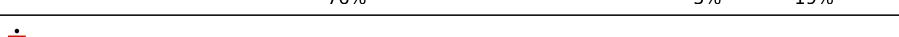

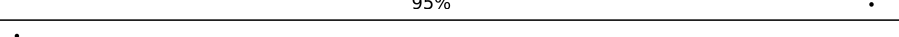

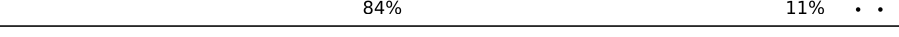
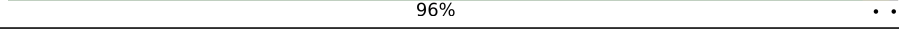




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Mol	Chain	Length	Quality of chain
9	LF	248	89% 9%
10	LG	266	83% 15%
11	LH	192	94% 5%
12	LI	214	93% 6%
13	LJ	178	92% 5%
14	LL	211	95% 5%
15	LM	215	62% 35%
16	LN	204	97%
17	LO	203	97%
18	LP	184	82% 17%
19	LQ	188	98%
20	LR	196	91% 5%
21	LS	176	97%
22	LT	160	95%
23	LU	128	73% 5% 21%
24	LV	140	91% 6%
25	LW	157	15% 76% 21%
26	LX	156	74% 24%
27	LY	145	89% 8%
28	LZ	135	97%
29	La	148	95%
30	Lb	159	6% 64% 5% 31%
31	Lc	115	83% 15%
32	Ld	125	82% 14%
33	Le	135	94% 5%


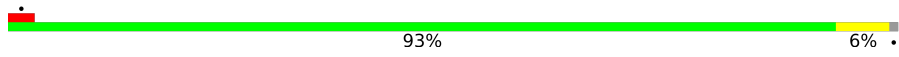

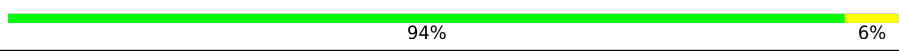
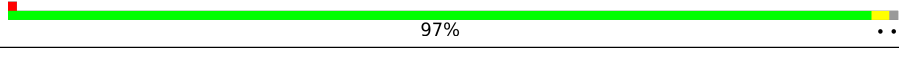


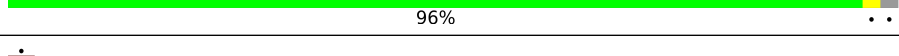
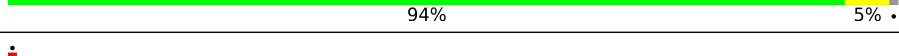
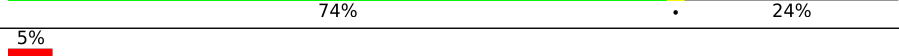

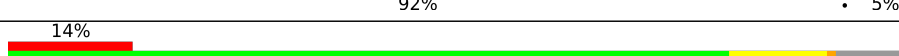

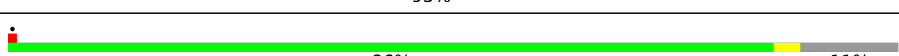
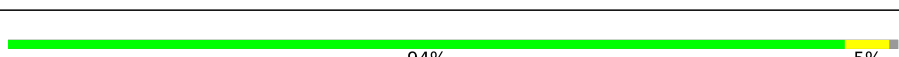
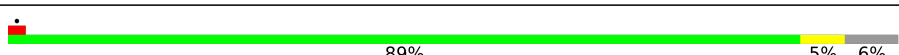

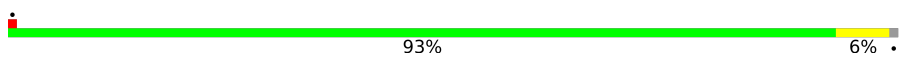
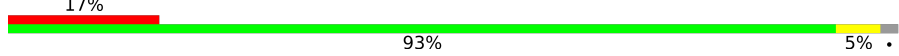


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Mol	Chain	Length	Quality of chain
34	Lf	110	 94% 5%
35	Lg	117	 93%
36	Lh	123	 95%
37	Li	105	 95%
38	Lj	97	 86% 11%
39	Lk	70	 90% 9%
40	Ll	51	 92% 6%
41	Lm	128	 41% 59%
42	Ln	25	 88% 8%
43	Lo	106	 93%
44	Lp	92	 97%
45	Lr	137	 87% 9%
46	S2	1869	 71% 21% 5% 7%
47	SA	295	 73% 25%
48	SB	264	 76% 5% 19%
49	SD	243	 88% 5% 7%
50	SE	263	 95%
51	SF	204	 86% 10%
52	SH	194	 84% 11%
53	SI	208	 96%
54	SK	165	 54% 5% 41%
55	SL	158	 86% 5% 9%
56	SP	145	 81% 6% 12% 8%
57	SQ	146	 90% 8%
58	SR	135	 96%

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Mol	Chain	Length	Quality of chain
59	SS	152	 89% 5% 5%
60	ST	145	 93% 6%
61	SU	119	 78% 9% 13%
62	SV	83	 94% 6%
63	SX	143	 97% ..
64	Sa	115	 87% 6% 11%
65	Sc	69	 88% 6% 7%
66	Sd	56	 96% ..
67	Sg	317	 94% 5%
68	SC	293	 74% 24%
69	SG	249	 89% 5% 6% 5%
70	SJ	194	 92% 5%
71	SM	132	 81% 14% 11% 8%
72	SN	151	 95% ..
73	SO	151	 86% 11%
74	SW	130	 94% 5%
75	SY	133	 89% 5% 6%
76	SZ	125	 57% 40%
77	Sb	84	 93% 6%
78	Se	59	 93% 17% 5%
79	Sf	156	 35% 61%

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 216242 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
			Total	C	N	O	S		
7	LD	293	2382	1507	434	427	14	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
21	LS	176	1461	930	284	236	11	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 42 is a protein called 60S ribosomal protein L41.

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

- Molecule 43 is a protein called 60S ribosomal protein L36a.

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

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

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

- Molecule 46 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S2	1740	Total	C	N	O	P	0	0
			36958	16514	6600	12105	1739		

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

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

- Molecule 48 is a protein called 40S ribosomal protein S3a.

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

- Molecule 49 is a protein called 40S ribosomal protein S3.

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

- Molecule 50 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S7.

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

- Molecule 53 is a protein called 40S ribosomal protein S8.

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

- Molecule 54 is a protein called 40S ribosomal protein S10.

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

- Molecule 55 is a protein called 40S ribosomal protein S11.

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

- Molecule 56 is a protein called 40S ribosomal protein S15.

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

- Molecule 57 is a protein called 40S ribosomal protein S16.

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

- Molecule 58 is a protein called 40S ribosomal protein S17.

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

- Molecule 59 is a protein called 40S ribosomal protein S18.

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

- Molecule 60 is a protein called 40S ribosomal protein S19.

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

- Molecule 61 is a protein called 40S ribosomal protein S20.

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

- Molecule 62 is a protein called 40S ribosomal protein S21.

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

- Molecule 63 is a protein called 40S ribosomal protein S23.

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

- Molecule 64 is a protein called 40S ribosomal protein S26.

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

- Molecule 65 is a protein called 40S ribosomal protein S28.

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

- Molecule 66 is a protein called 40S ribosomal protein S29.

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

- Molecule 67 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 68 is a protein called 40S ribosomal protein S2.

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

- Molecule 69 is a protein called 40S ribosomal protein S6.

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

- Molecule 70 is a protein called 40S ribosomal protein S9.

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

- Molecule 71 is a protein called 40S ribosomal protein S12.

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

- Molecule 72 is a protein called 40S ribosomal protein S13.

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

- Molecule 73 is a protein called 40S ribosomal protein S14.

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

- Molecule 74 is a protein called 40S ribosomal protein S15a.

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

- Molecule 75 is a protein called 40S ribosomal protein S24.

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

- Molecule 76 is a protein called 40S ribosomal protein S25.

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

- Molecule 77 is a protein called 40S ribosomal protein S27.

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

- Molecule 78 is a protein called 40S ribosomal protein S30.

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

- Molecule 79 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sf	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- 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	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	2	Total	Mg	0
			2	2	
80	Lf	1	Total	Mg	0
			1	1	
80	Lg	1	Total	Mg	0
			1	1	
80	Lo	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
80	S2	134	Total 134	Mg 134	0
80	ST	1	Total 1	Mg 1	0
80	Sd	1	Total 1	Mg 1	0
80	SG	1	Total 1	Mg 1	0
80	SJ	1	Total 1	Mg 1	0

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

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

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

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

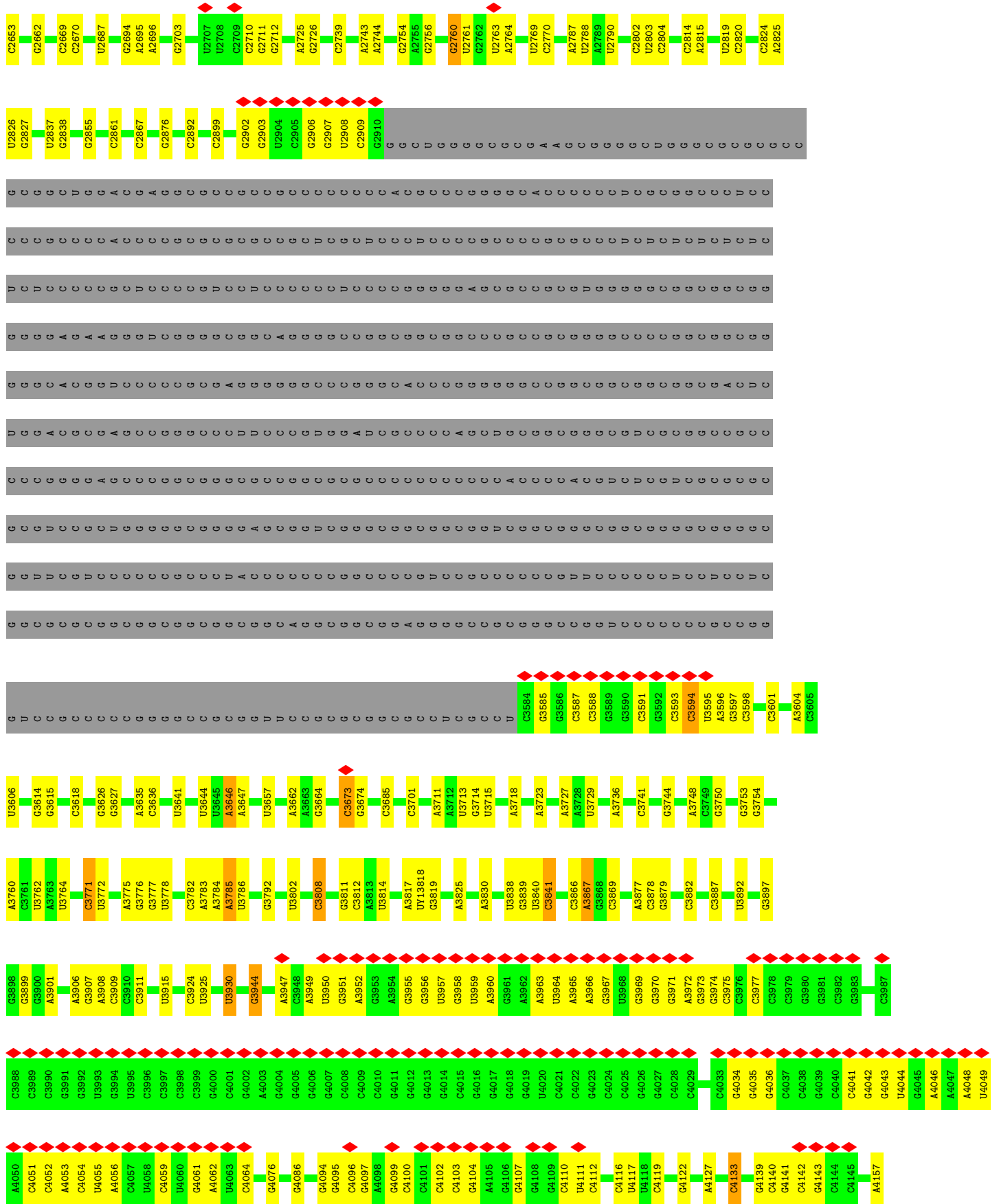
- Molecule 83 is water.

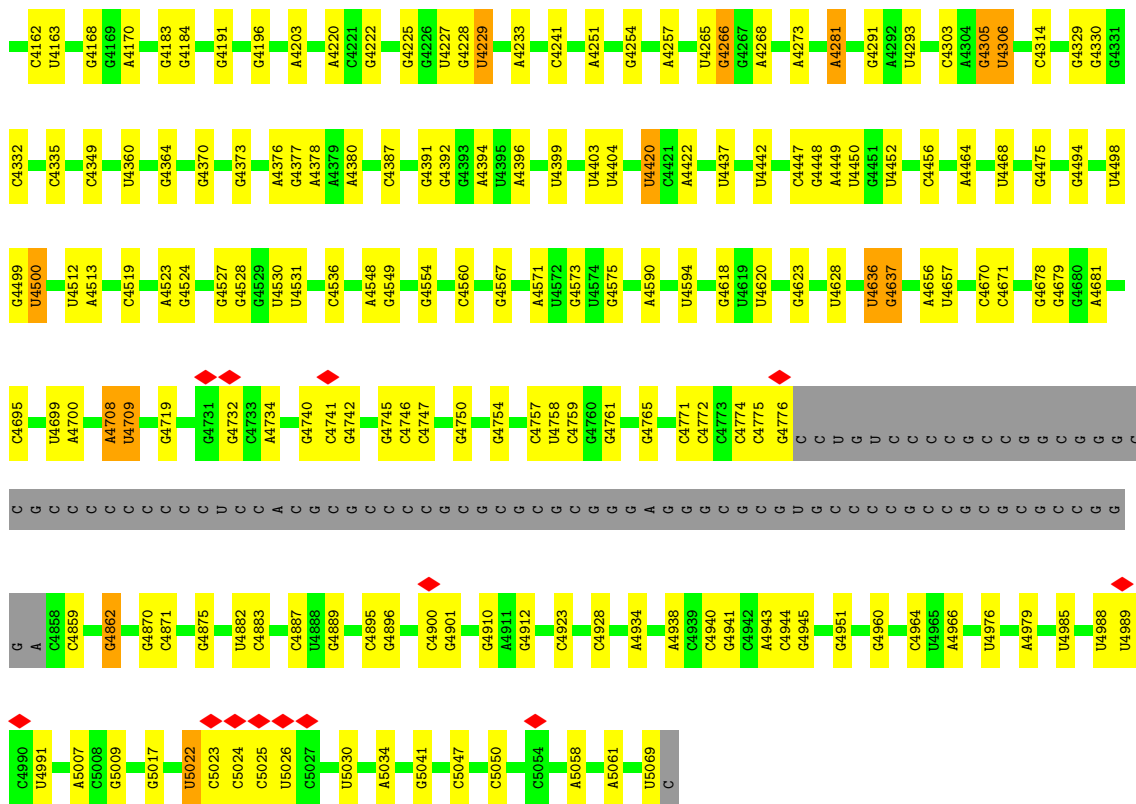
Mol	Chain	Residues	Atoms		AltConf
83	L1	767	Total 767	O 767	0
83	L2	3	Total 3	O 3	0
83	L3	6	Total 6	O 6	0
83	LA	8	Total 8	O 8	0
83	LB	2	Total 2	O 2	0
83	LC	8	Total 8	O 8	0
83	LD	1	Total 1	O 1	0
83	LF	2	Total 2	O 2	0
83	LI	1	Total 1	O 1	0
83	LL	1	Total 1	O 1	0
83	LN	2	Total 2	O 2	0
83	LP	1	Total 1	O 1	0
83	LR	1	Total 1	O 1	0
83	LX	1	Total 1	O 1	0
83	LY	1	Total 1	O 1	0
83	La	5	Total 5	O 5	0
83	Lb	1	Total 1	O 1	0
83	Le	4	Total 4	O 4	0
83	Lg	1	Total 1	O 1	0
83	Lj	4	Total 4	O 4	0
83	Ll	1	Total 1	O 1	0
83	Lo	3	Total 3	O 3	0

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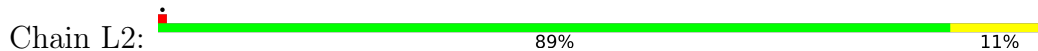
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Mol	Chain	Residues	Atoms		AltConf
83	S2	9	Total 9	O 9	0
83	SQ	1	Total 1	O 1	0
83	SX	1	Total 1	O 1	0
83	Sd	1	Total 1	O 1	0

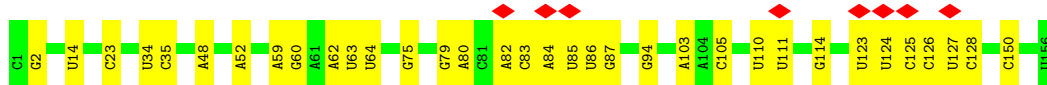
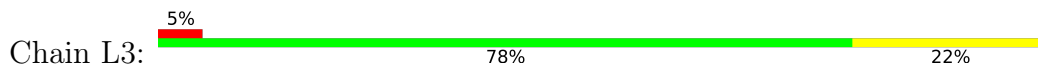




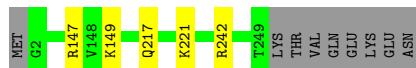
• Molecule 2: 5S rRNA



• Molecule 3: 5.8S rRNA

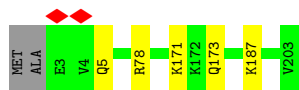


• Molecule 4: 60S ribosomal protein L8

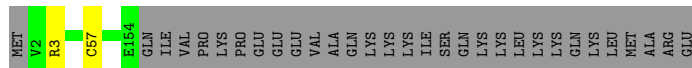
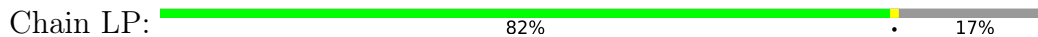


• Molecule 5: 60S ribosomal protein L3





• Molecule 18: 60S ribosomal protein L17



• Molecule 19: 60S ribosomal protein L18



• Molecule 20: 60S ribosomal protein L19



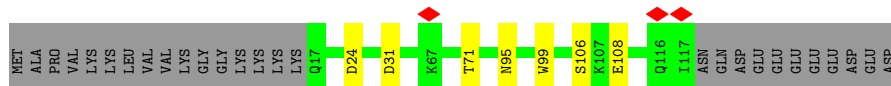
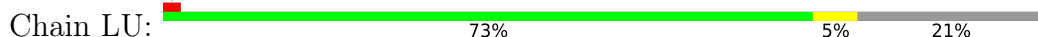
• Molecule 21: 60S ribosomal protein L18a



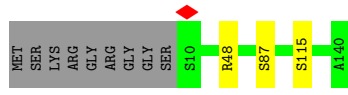
• Molecule 22: 60S ribosomal protein L21



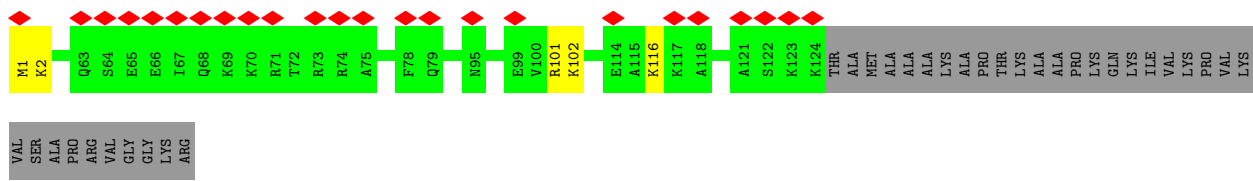
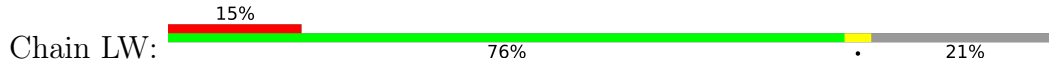
• Molecule 23: 60S ribosomal protein L22



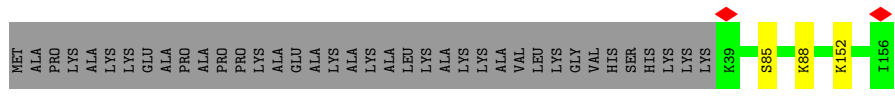
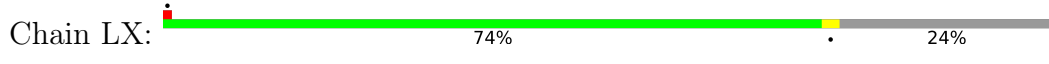
• Molecule 24: 60S ribosomal protein L23



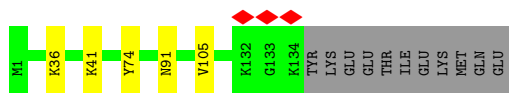
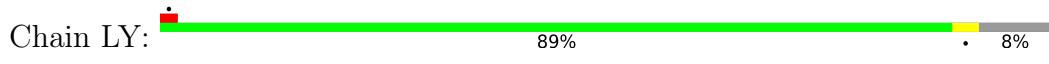
• Molecule 25: 60S ribosomal protein L24



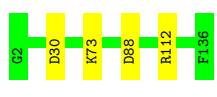
• Molecule 26: 60S ribosomal protein L23a



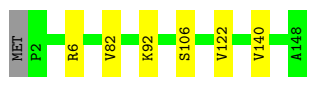
• Molecule 27: 60S ribosomal protein L26



• Molecule 28: 60S ribosomal protein L27

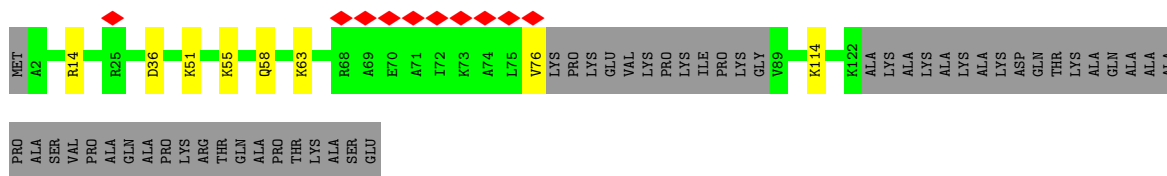


• Molecule 29: 60S ribosomal protein L27a

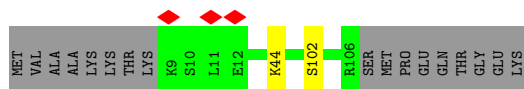
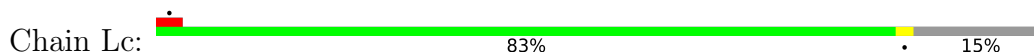


• Molecule 30: 60S ribosomal protein L29

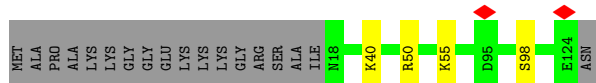
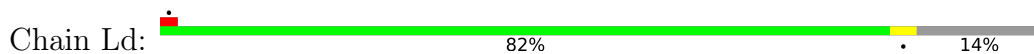




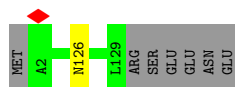
• Molecule 31: 60S ribosomal protein L30



• Molecule 32: 60S ribosomal protein L31



• Molecule 33: 60S ribosomal protein L32



• Molecule 34: 60S ribosomal protein L35a



• Molecule 35: 60S ribosomal protein L34

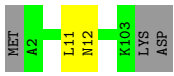


• Molecule 36: 60S ribosomal protein L35




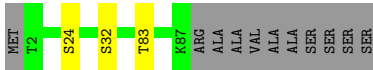
- Molecule 37: 60S ribosomal protein L36

Chain Li:  95%



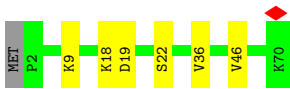
- Molecule 38: 60S ribosomal protein L37

Chain Lj:  86%



- Molecule 39: 60S ribosomal protein L38

Chain Lk:  90%



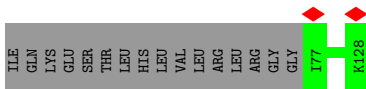
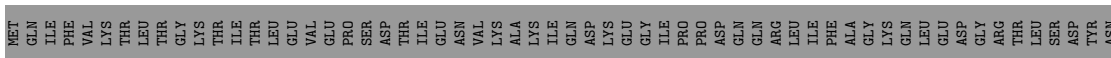
- Molecule 40: 60S ribosomal protein L39

Chain Ll:  92%




- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:  41%

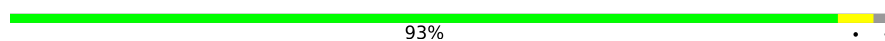


- Molecule 42: 60S ribosomal protein L41

Chain Ln:  88%



- Molecule 43: 60S ribosomal protein L36a

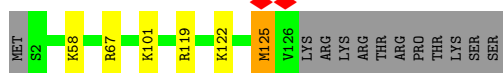
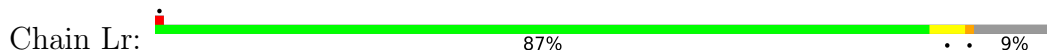
Chain Lo:  93%



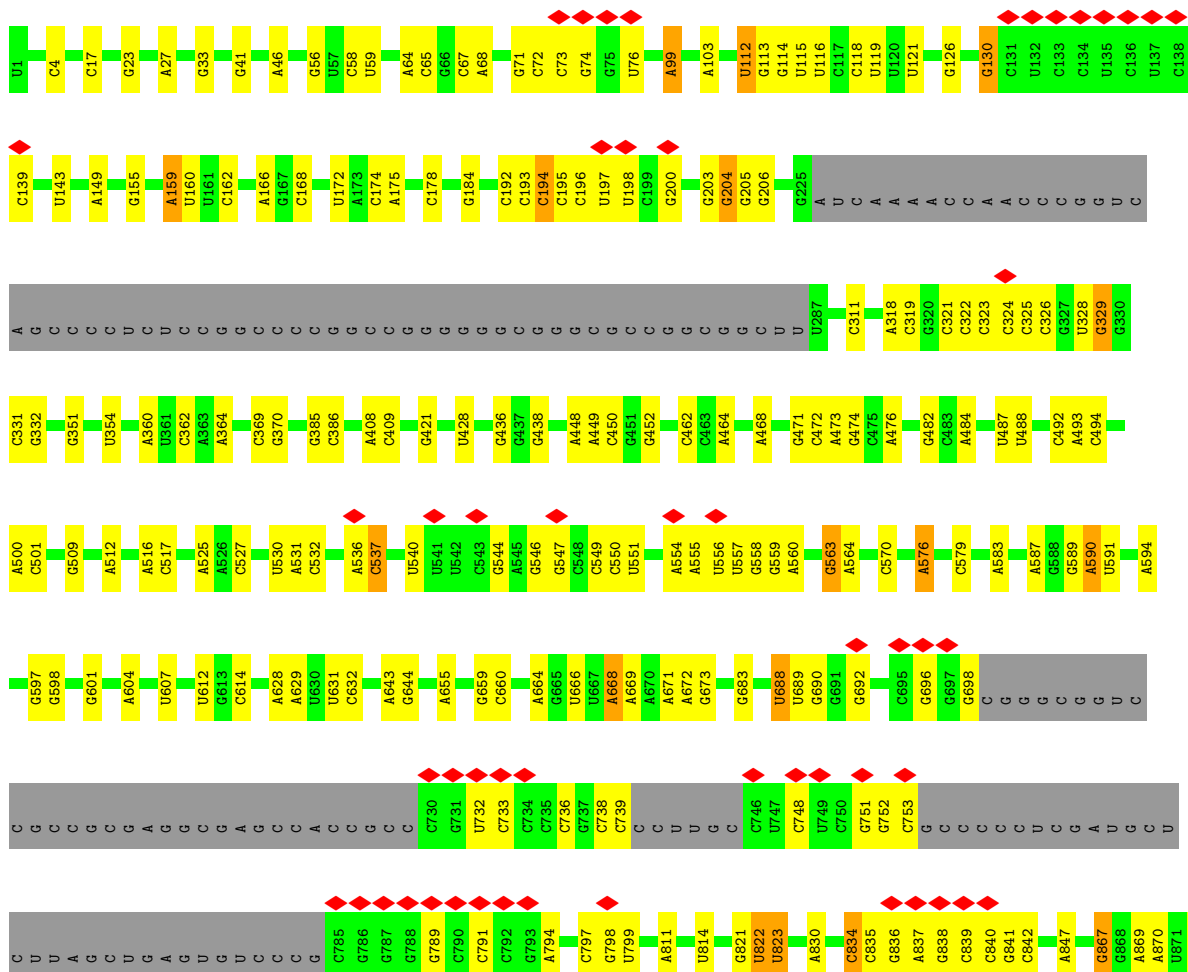
• Molecule 44: 60S ribosomal protein L37a

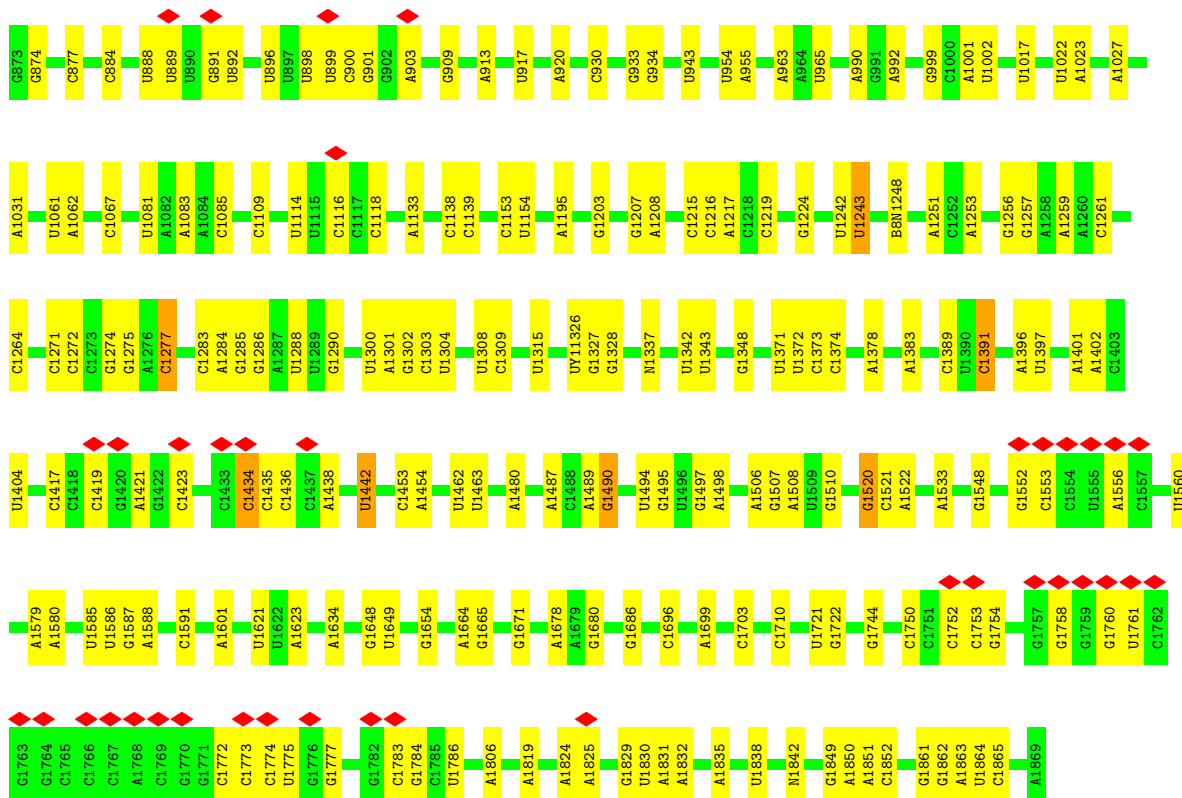


• Molecule 45: 60S ribosomal protein L28

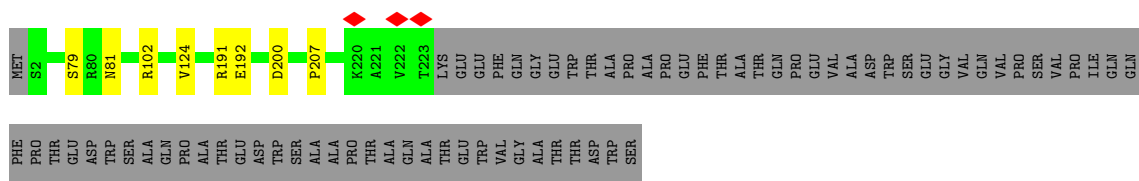
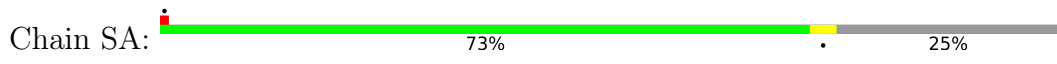


• Molecule 46: 18S rRNA

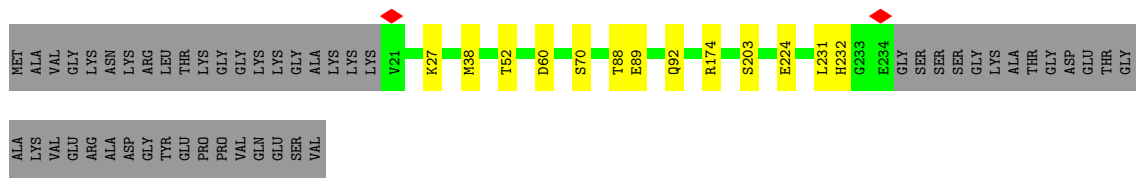
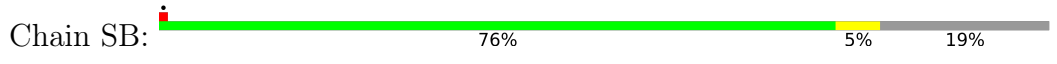




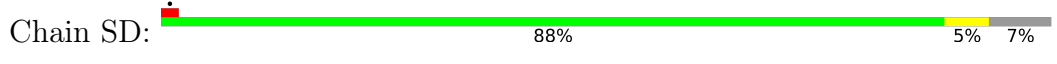
• Molecule 47: 40S ribosomal protein SA



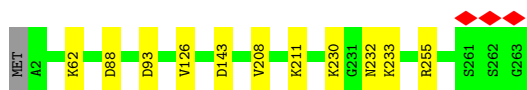
• Molecule 48: 40S ribosomal protein S3a



• Molecule 49: 40S ribosomal protein S3



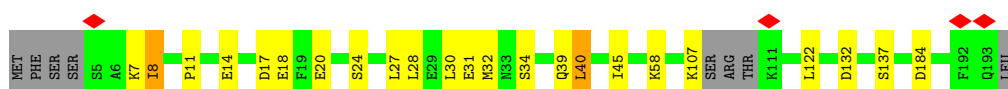
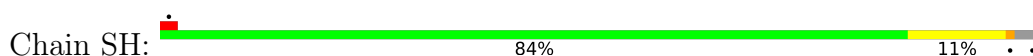
- Molecule 50: 40S ribosomal protein S4, X isoform



- Molecule 51: 40S ribosomal protein S5



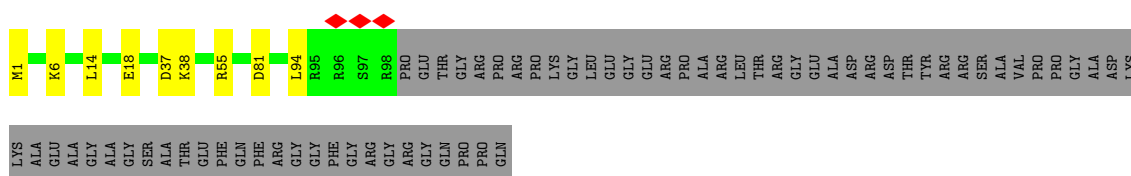
- Molecule 52: 40S ribosomal protein S7



- Molecule 53: 40S ribosomal protein S8



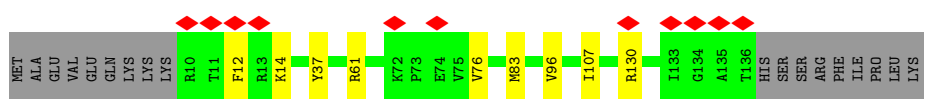
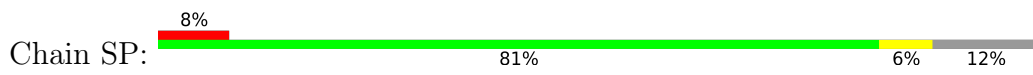
- Molecule 54: 40S ribosomal protein S10



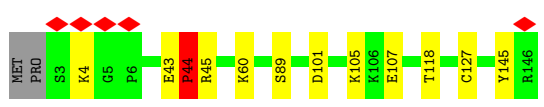
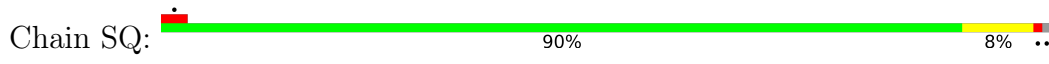
- Molecule 55: 40S ribosomal protein S11



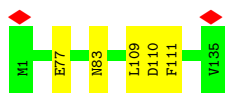
- Molecule 56: 40S ribosomal protein S15



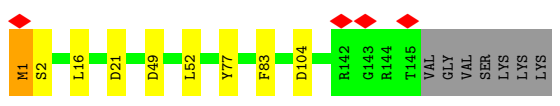
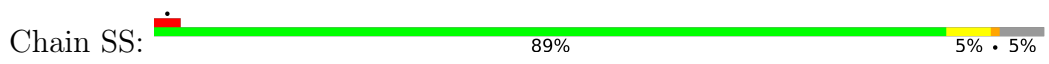
• Molecule 57: 40S ribosomal protein S16



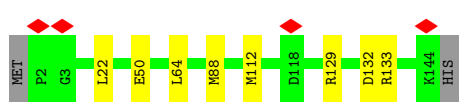
• Molecule 58: 40S ribosomal protein S17



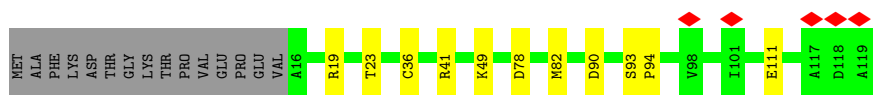
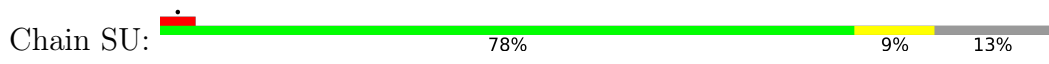
• Molecule 59: 40S ribosomal protein S18



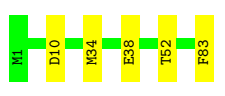
• Molecule 60: 40S ribosomal protein S19

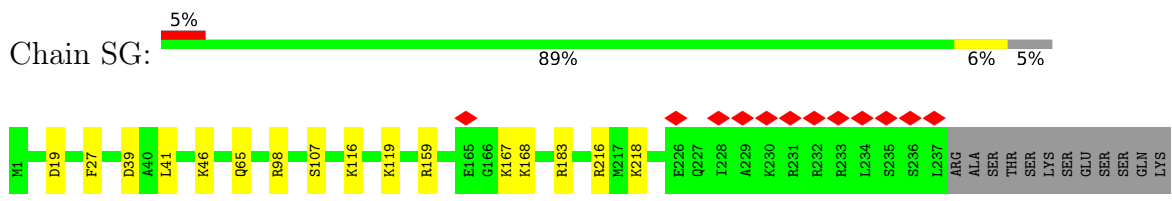


• Molecule 61: 40S ribosomal protein S20

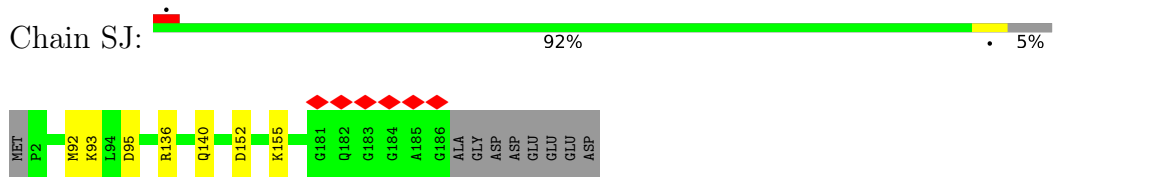


• Molecule 62: 40S ribosomal protein S21

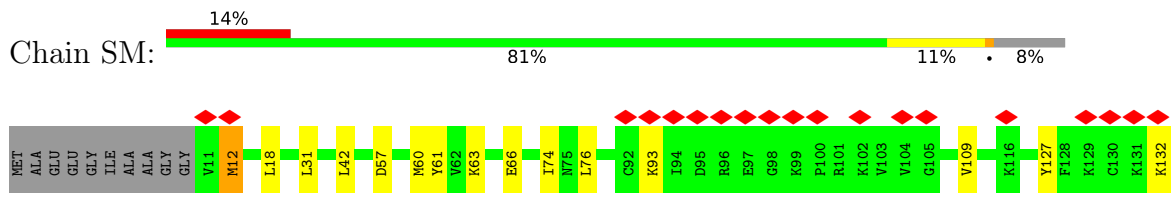




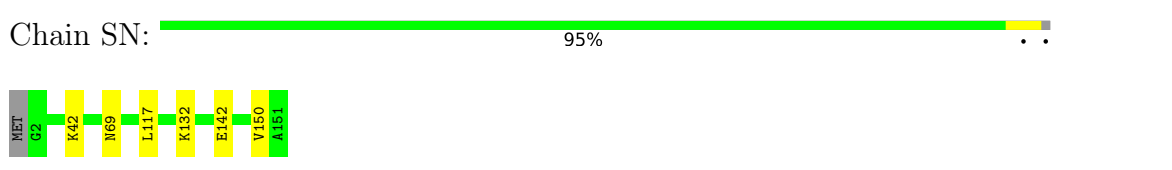
• Molecule 70: 40S ribosomal protein S9



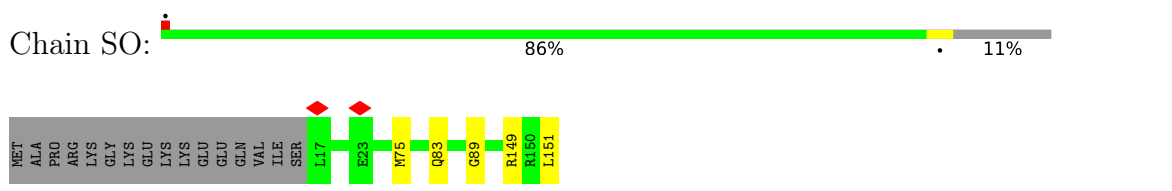
• Molecule 71: 40S ribosomal protein S12



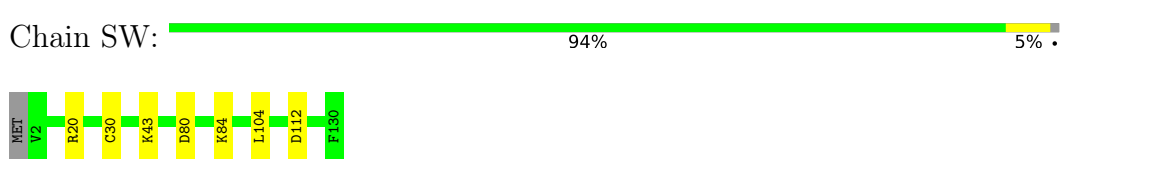
• Molecule 72: 40S ribosomal protein S13



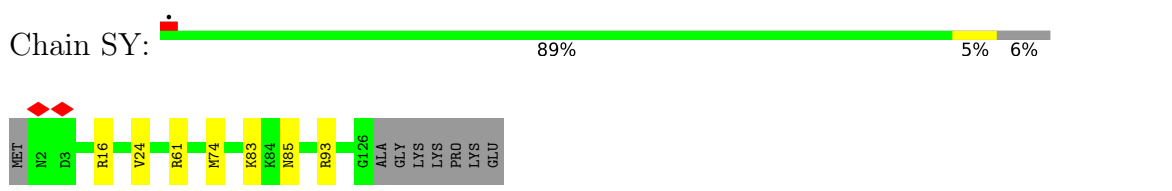
• Molecule 73: 40S ribosomal protein S14



• Molecule 74: 40S ribosomal protein S15a



• Molecule 75: 40S ribosomal protein S24



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114446	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 ($e^-/\text{\AA}^2$)	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	2.785	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	444.78, 444.78, 444.78	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: UR3, 5MC, UY1, OMU, MG, M7A, OMG, K, ZN, 4AC, 1MA, 6MZ, PSU, 5MU, B8H, B8T, OMC, MA6, MLZ, B8N, 2MG, A2M, JMH

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	1/87525 (0.0%)	1.01	275/136449 (0.2%)
2	L2	0.46	0/2858	0.92	2/4455 (0.0%)
3	L3	0.50	0/3653	0.93	1/5691 (0.0%)
4	LA	0.37	0/1936	0.69	0/2596
5	LB	0.32	0/3306	0.60	0/4424
6	LC	0.31	0/2962	0.63	2/3977 (0.1%)
7	LD	0.30	0/2428	0.56	0/3252
8	LE	0.30	0/1799	0.64	0/2414
9	LF	0.33	0/1905	0.60	0/2539
10	LG	0.29	0/1866	0.58	0/2511
11	LH	0.31	0/1537	0.59	1/2066 (0.0%)
12	LI	0.33	0/1677	0.60	0/2237
13	LJ	0.30	0/1376	0.61	0/1840
14	LL	0.30	0/1732	0.62	0/2315
15	LM	0.31	0/1161	0.58	0/1554
16	LN	0.34	0/1746	0.68	2/2338 (0.1%)
17	LO	0.32	0/1682	0.59	0/2250
18	LP	0.30	0/1268	0.59	0/1701
19	LQ	0.32	0/1537	0.65	0/2052
20	LR	0.30	0/1582	0.61	1/2091 (0.0%)
21	LS	0.33	0/1501	0.59	0/2013
22	LT	0.31	0/1326	0.56	0/1770
23	LU	0.36	0/839	0.70	1/1126 (0.1%)
24	LV	0.32	0/993	0.60	0/1332
25	LW	0.31	0/1030	0.60	0/1364
26	LX	0.28	0/984	0.56	0/1323
27	LY	0.30	0/1132	0.61	0/1504
28	LZ	0.33	0/1130	0.63	2/1507 (0.1%)
29	La	0.31	0/1191	0.61	0/1591
30	Lb	0.29	0/889	0.64	1/1175 (0.1%)
31	Lc	0.33	0/774	0.55	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.30	0/903	0.61	0/1216
33	Le	0.32	0/1071	0.65	0/1429
34	Lf	0.35	0/895	0.67	0/1198
35	Lg	0.32	0/916	0.63	0/1220
36	Lh	0.30	0/1023	0.58	0/1351
37	Li	0.28	0/843	0.61	0/1115
38	Lj	0.34	0/720	0.68	0/952
39	Lk	0.29	0/575	0.59	0/761
40	Ll	0.31	0/454	0.69	0/599
41	Lm	0.27	0/435	0.60	0/575
42	Ln	0.31	0/231	0.74	0/294
43	Lo	0.28	0/845	0.59	0/1113
44	Lp	0.32	0/718	0.58	0/953
45	Lr	0.31	0/1017	0.64	1/1364 (0.1%)
46	S2	0.42	0/39987	0.97	102/62288 (0.2%)
47	SA	0.30	0/1784	0.56	1/2424 (0.0%)
48	SB	0.28	0/1765	0.58	1/2362 (0.0%)
49	SD	0.32	0/1793	0.64	3/2414 (0.1%)
50	SE	0.29	0/2118	0.59	0/2849
51	SF	0.30	0/1481	0.56	0/1988
52	SH	0.37	0/1519	0.63	1/2033 (0.0%)
53	SI	0.31	0/1715	0.62	0/2287
54	SK	0.35	0/851	0.65	0/1147
55	SL	0.31	0/1202	0.60	0/1606
56	SP	0.30	0/1065	0.67	1/1423 (0.1%)
57	SQ	0.31	0/1160	0.72	3/1553 (0.2%)
58	SR	0.30	0/1105	0.72	2/1484 (0.1%)
59	SS	0.28	0/1216	0.73	5/1628 (0.3%)
60	ST	0.29	0/1131	0.62	1/1515 (0.1%)
61	SU	0.31	0/831	0.67	0/1115
62	SV	0.28	0/643	0.52	0/860
63	SX	0.30	0/1116	0.59	0/1490
64	Sa	0.30	0/836	0.61	0/1121
65	Sc	0.28	0/508	0.66	0/680
66	Sd	0.31	0/470	0.75	0/623
67	Sg	0.27	0/2493	0.61	1/3394 (0.0%)
68	SC	0.31	0/1762	0.57	1/2381 (0.0%)
69	SG	0.30	0/1946	0.62	1/2590 (0.0%)
70	SJ	0.32	0/1550	0.63	0/2069
71	SM	0.32	0/950	0.77	5/1275 (0.4%)
72	SN	0.31	0/1232	0.56	0/1656
73	SO	0.29	0/1023	0.65	0/1372
74	SW	0.31	0/1051	0.60	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SY	0.31	0/1039	0.58	0/1381
76	SZ	0.26	0/604	0.60	0/810
77	Sb	0.29	0/665	0.59	0/891
78	Se	0.28	0/465	0.61	0/612
79	Sf	0.27	0/507	0.61	0/673
All	All	0.42	1/227554 (0.0%)	0.87	417/334035 (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
61	SU	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3646	A	N7-C5	-5.42	1.36	1.39

All (417) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1772	C	N1-C2-O2	13.79	127.17	118.90
46	S2	501	C	N1-C2-O2	13.05	126.73	118.90
46	S2	1772	C	N3-C2-O2	-12.99	112.81	121.90
46	S2	501	C	C2-N1-C1'	12.71	132.78	118.80
1	L1	906	C	N3-C2-O2	-12.46	113.18	121.90
46	S2	194	C	N3-C2-O2	-12.40	113.22	121.90
1	L1	1191	C	N3-C2-O2	-11.45	113.89	121.90
1	L1	3594	C	N1-C2-O2	11.40	125.74	118.90
46	S2	195	C	N3-C2-O2	-11.24	114.03	121.90
1	L1	485	C	C2-N1-C1'	11.16	131.08	118.80
46	S2	193	C	N3-C2-O2	-10.83	114.32	121.90
1	L1	129	C	N3-C2-O2	-10.80	114.34	121.90
46	S2	322	C	N3-C2-O2	-10.74	114.38	121.90
1	L1	130	C	N3-C2-O2	-10.55	114.51	121.90
46	S2	501	C	N3-C2-O2	-10.35	114.66	121.90
1	L1	1082	C	O4'-C1'-N1	10.20	116.36	108.20
1	L1	4771	C	N1-C2-O2	9.99	124.89	118.90
1	L1	907	C	N3-C2-O2	-9.93	114.95	121.90
46	S2	194	C	N1-C2-O2	9.93	124.86	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1772	C	C2-N1-C1'	9.76	129.54	118.80
1	L1	417	G	O4'-C1'-N9	9.73	115.99	108.20
1	L1	456	C	O4'-C1'-N1	9.68	115.94	108.20
1	L1	3594	C	N3-C2-O2	-9.63	115.16	121.90
1	L1	1994	C	N3-C2-O2	-9.62	115.17	121.90
1	L1	1978	C	N3-C2-O2	-9.57	115.20	121.90
1	L1	1447	C	N3-C2-O2	-9.41	115.31	121.90
46	S2	501	C	C6-N1-C1'	-9.35	109.58	120.80
1	L1	906	C	N1-C2-O2	9.31	124.49	118.90
1	L1	3594	C	C2-N1-C1'	9.19	128.91	118.80
1	L1	131	C	N3-C2-O2	-9.18	115.48	121.90
46	S2	1139	C	N3-C2-O2	-9.17	115.48	121.90
1	L1	1192	C	N3-C2-O2	-9.02	115.59	121.90
1	L1	655	C	N3-C2-O2	-9.01	115.59	121.90
1	L1	456	C	N3-C2-O2	-8.96	115.63	121.90
46	S2	1453	C	N1-C2-O2	8.89	124.23	118.90
1	L1	4862	G	N3-C4-N9	8.83	131.30	126.00
1	L1	4771	C	N3-C2-O2	-8.82	115.72	121.90
1	L1	4862	G	N3-C2-N2	8.80	126.06	119.90
1	L1	2409	U	N3-C2-O2	-8.79	116.05	122.20
46	S2	1453	C	C2-N1-C1'	8.62	128.28	118.80
46	S2	1772	C	C6-N1-C2	-8.61	116.86	120.30
46	S2	1277	C	C2-N1-C1'	8.42	128.06	118.80
1	L1	2409	U	N1-C2-O2	8.39	128.67	122.80
1	L1	925	C	N3-C2-O2	-8.30	116.09	121.90
1	L1	485	C	C6-N1-C1'	-8.30	110.84	120.80
1	L1	2303	C	C2-N1-C1'	-8.28	109.70	118.80
1	L1	4709	U	C2-N1-C1'	8.23	127.58	117.70
1	L1	1079	C	N3-C2-O2	-8.16	116.19	121.90
58	SR	110	ASP	CB-CG-OD1	8.09	125.58	118.30
46	S2	1139	C	N1-C2-O2	8.08	123.75	118.90
1	L1	2627	C	C2-N1-C1'	8.06	127.67	118.80
46	S2	1139	C	C2-N1-C1'	8.01	127.61	118.80
1	L1	1988	G	N3-C4-N9	8.01	130.80	126.00
1	L1	2409	U	C2-N1-C1'	7.99	127.29	117.70
46	S2	1139	C	C6-N1-C2	-7.99	117.10	120.30
1	L1	2303	C	C6-N1-C1'	7.94	130.33	120.80
1	L1	1082	C	N3-C2-O2	-7.92	116.35	121.90
1	L1	336	A	C2-N3-C4	7.88	114.54	110.60
46	S2	322	C	N1-C2-O2	7.87	123.62	118.90
57	SQ	44	PRO	CA-N-CD	-7.86	100.49	111.50
1	L1	1241	C	C2-N1-C1'	7.78	127.35	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4771	C	C6-N1-C2	-7.75	117.20	120.30
28	LZ	88	ASP	CB-CG-OD2	7.69	125.22	118.30
49	SD	219	PRO	CA-N-CD	-7.68	100.75	111.50
1	L1	1079	C	N1-C2-O2	7.67	123.50	118.90
1	L1	2303	C	N3-C4-N4	-7.51	112.74	118.00
71	SM	57	ASP	CB-CG-OD2	7.32	124.89	118.30
1	L1	1080	C	C6-N1-C2	-7.29	117.39	120.30
1	L1	1080	C	N3-C2-O2	-7.27	116.81	121.90
46	S2	1261	C	N1-C2-O2	7.27	123.26	118.90
1	L1	485	C	N1-C2-O2	7.26	123.25	118.90
57	SQ	44	PRO	N-CA-CB	-7.25	94.60	103.30
1	L1	3924	C	C6-N1-C2	-7.24	117.41	120.30
1	L1	1344	C	C6-N1-C2	-7.22	117.41	120.30
1	L1	4420	U	C2-N1-C1'	7.19	126.33	117.70
46	S2	168	C	N1-C2-O2	7.17	123.20	118.90
1	L1	1241	C	N1-C2-O2	7.16	123.20	118.90
1	L1	3892	U	N3-C2-O2	-7.16	117.19	122.20
1	L1	4229	U	N3-C2-O2	-7.15	117.20	122.20
59	SS	16	LEU	CA-CB-CG	7.14	131.71	115.30
1	L1	174	C	N3-C2-O2	-7.13	116.91	121.90
46	S2	195	C	N1-C2-O2	7.09	123.16	118.90
1	L1	4758	U	C2-N1-C1'	7.08	126.19	117.70
1	L1	1978	C	N1-C2-O2	7.07	123.14	118.90
1	L1	1552	G	O4'-C1'-N9	7.05	113.84	108.20
1	L1	3909	C	C6-N1-C2	-7.04	117.48	120.30
1	L1	1988	G	C4-N9-C1'	7.02	135.62	126.50
1	L1	3647	A	C5-C6-N1	7.02	121.21	117.70
1	L1	4862	G	N1-C2-N2	-7.02	109.89	116.20
1	L1	4420	U	N1-C2-O2	6.98	127.69	122.80
1	L1	3641	U	C4-C5-C6	6.97	123.88	119.70
1	L1	2304	U	N1-C2-O2	6.96	127.67	122.80
1	L1	3594	C	C6-N1-C2	-6.94	117.52	120.30
1	L1	4758	U	N1-C2-O2	6.94	127.66	122.80
1	L1	1191	C	C6-N1-C2	-6.93	117.53	120.30
46	S2	570	C	N1-C2-O2	6.90	123.04	118.90
46	S2	195	C	C6-N1-C2	-6.89	117.54	120.30
1	L1	1338	G	C5-C6-O6	6.89	132.73	128.60
46	S2	1453	C	N3-C2-O2	-6.83	117.12	121.90
1	L1	655	C	C6-N1-C2	-6.83	117.57	120.30
1	L1	2627	C	N1-C2-O2	6.82	122.99	118.90
1	L1	2514	G	N9-C4-C5	-6.80	102.68	105.40
1	L1	4771	C	C5-C6-N1	6.79	124.40	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	180	C	N1-C2-O2	6.79	122.97	118.90
1	L1	3741	C	N3-C2-O2	-6.78	117.15	121.90
46	S2	205	G	N1-C2-N2	-6.76	110.11	116.20
1	L1	4758	U	N3-C2-O2	-6.76	117.47	122.20
1	L1	2333	G	C5-C6-O6	6.75	132.65	128.60
1	L1	1988	G	C8-N9-C1'	-6.72	118.26	127.00
46	S2	1417	C	N3-C2-O2	-6.72	117.19	121.90
1	L1	2410	C	C2-N1-C1'	6.70	126.17	118.80
1	L1	2303	C	C5-C4-N4	6.69	124.88	120.20
46	S2	501	C	C6-N1-C2	-6.67	117.63	120.30
1	L1	1241	C	N3-C2-O2	-6.67	117.23	121.90
1	L1	1994	C	N1-C2-O2	6.67	122.90	118.90
46	S2	321	C	N1-C2-O2	6.67	122.90	118.90
1	L1	757	G	N1-C6-O6	-6.65	115.91	119.90
1	L1	907	C	N1-C2-O2	6.65	122.89	118.90
1	L1	906	C	C6-N1-C2	-6.62	117.65	120.30
1	L1	3911	C	C6-N1-C2	-6.62	117.65	120.30
1	L1	1241	C	C6-N1-C2	-6.60	117.66	120.30
46	S2	527	C	N3-C2-O2	-6.60	117.28	121.90
1	L1	4420	U	N3-C2-O2	-6.60	117.58	122.20
46	S2	1022	U	C2-N1-C1'	6.60	125.62	117.70
48	SB	231	LEU	CA-CB-CG	6.59	130.46	115.30
1	L1	2802	C	C6-N1-C2	-6.58	117.67	120.30
1	L1	453	G	N3-C4-C5	-6.56	125.32	128.60
46	S2	1261	C	N3-C2-O2	-6.56	117.31	121.90
1	L1	2528	G	C4-N9-C1'	6.54	135.00	126.50
1	L1	4862	G	C4-N9-C1'	6.52	134.98	126.50
1	L1	4396	A	C6-N1-C2	6.52	122.51	118.60
46	S2	329	G	N1-C2-N2	-6.51	110.34	116.20
1	L1	2102	G	O4'-C1'-N9	6.51	113.41	108.20
1	L1	3911	C	C5-C6-N1	6.49	124.25	121.00
1	L1	4774	C	N3-C2-O2	-6.47	117.37	121.90
1	L1	4862	G	N3-C4-C5	-6.45	125.37	128.60
1	L1	3778	U	N1-C2-O2	6.45	127.31	122.80
1	L1	453	G	C4-N9-C1'	6.42	134.85	126.50
46	S2	1315	U	N1-C2-O2	6.42	127.29	122.80
46	S2	329	G	N3-C2-N2	6.41	124.39	119.90
1	L1	4709	U	C5-C4-O4	-6.41	122.05	125.90
1	L1	4266	G	N3-C4-C5	-6.40	125.40	128.60
28	LZ	30	ASP	CB-CG-OD1	6.39	124.06	118.30
1	L1	4774	C	N1-C2-O2	6.38	122.73	118.90
1	L1	3741	C	N1-C2-O2	6.38	122.73	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4862	G	C8-N9-C1'	-6.37	118.72	127.00
1	L1	757	G	N1-C2-N2	-6.36	110.47	116.20
46	S2	331	C	C2-N1-C1'	6.36	125.79	118.80
46	S2	1277	C	C6-N1-C1'	-6.36	113.17	120.80
1	L1	2492	C	C6-N1-C2	-6.32	117.77	120.30
1	L1	1191	C	N1-C2-O2	6.31	122.69	118.90
1	L1	4746	C	C2-N1-C1'	6.29	125.72	118.80
1	L1	1447	C	N1-C2-O2	6.26	122.66	118.90
1	L1	1192	C	C6-N1-C2	-6.26	117.80	120.30
1	L1	209	U	C2-N1-C1'	6.25	125.20	117.70
1	L1	2760	G	P-O3'-C3'	6.25	127.20	119.70
30	Lb	36	ASP	CB-CG-OD2	6.24	123.92	118.30
1	L1	4771	C	C2-N1-C1'	6.24	125.67	118.80
56	SP	107	ILE	C-N-CA	6.23	137.26	121.70
58	SR	109	LEU	CA-CB-CG	6.21	129.58	115.30
46	S2	494	C	N1-C2-O2	6.20	122.62	118.90
1	L1	130	C	C6-N1-C2	-6.19	117.82	120.30
1	L1	4527	G	O4'-C1'-N9	6.19	113.15	108.20
1	L1	914	U	P-O3'-C3'	6.16	127.10	119.70
1	L1	2627	C	C6-N1-C2	-6.15	117.84	120.30
46	S2	659	G	C4-N9-C1'	6.12	134.45	126.50
46	S2	1453	C	C6-N1-C1'	-6.10	113.48	120.80
46	S2	4	C	C2-N1-C1'	6.09	125.50	118.80
1	L1	2096	G	C4-N9-C1'	6.09	134.42	126.50
1	L1	2820	C	N1-C2-O2	6.09	122.56	118.90
1	L1	3594	C	C6-N1-C1'	-6.09	113.50	120.80
1	L1	3772	U	N3-C2-O2	-6.08	117.94	122.20
46	S2	1591	C	N1-C2-O2	6.08	122.55	118.90
1	L1	129	C	C6-N1-C2	-6.08	117.87	120.30
47	SA	207	PRO	CA-N-CD	-6.07	103.00	111.50
71	SM	74	ILE	CG1-CB-CG2	-6.07	98.05	111.40
1	L1	485	C	C5-C6-N1	6.06	124.03	121.00
46	S2	1389	C	C2-N1-C1'	6.06	125.47	118.80
67	Sg	5	MET	CB-CG-SD	6.06	130.58	112.40
46	S2	1315	U	C2-N1-C1'	6.05	124.96	117.70
71	SM	18	LEU	CA-CB-CG	6.05	129.21	115.30
46	S2	1772	C	C6-N1-C1'	-6.04	113.55	120.80
46	S2	130	G	N3-C4-C5	-6.04	125.58	128.60
1	L1	456	C	N1-C2-O2	6.03	122.52	118.90
1	L1	2528	G	N3-C4-C5	-6.02	125.59	128.60
1	L1	3673	C	P-O3'-C3'	6.02	126.92	119.70
1	L1	5022	U	N3-C2-O2	-6.00	118.00	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	SQ	101	ASP	CB-CG-OD1	6.00	123.70	118.30
11	LH	142	ASP	CB-CG-OD1	5.98	123.69	118.30
1	L1	1973	G	N1-C2-N2	-5.98	110.82	116.20
1	L1	3598	C	C2-N1-C1'	5.96	125.35	118.80
1	L1	485	C	C6-N1-C2	-5.96	117.92	120.30
1	L1	1417	C	C2-N1-C1'	5.95	125.35	118.80
1	L1	1447	C	C6-N1-C2	-5.95	117.92	120.30
46	S2	1750	C	N1-C2-O2	5.95	122.47	118.90
1	L1	3647	A	C6-N1-C2	-5.93	115.04	118.60
1	L1	753	C	C2-N1-C1'	5.93	125.32	118.80
1	L1	1170	G	N1-C2-N2	-5.93	110.87	116.20
1	L1	1590	C	P-O3'-C3'	5.92	126.81	119.70
1	L1	4396	A	N1-C2-N3	-5.92	126.34	129.30
1	L1	5022	U	N1-C2-O2	5.90	126.93	122.80
1	L1	986	C	C2-N1-C1'	5.89	125.28	118.80
46	S2	1261	C	C2-N1-C1'	5.89	125.28	118.80
1	L1	1243	C	C2-N1-C1'	5.88	125.27	118.80
46	S2	194	C	C6-N1-C2	-5.88	117.95	120.30
46	S2	570	C	C2-N1-C1'	5.88	125.27	118.80
46	S2	130	G	C4-N9-C1'	5.87	134.13	126.50
1	L1	1245	C	C2-N1-C1'	5.86	125.25	118.80
1	L1	282	C	N1-C2-O2	5.85	122.41	118.90
1	L1	1884	C	C6-N1-C2	-5.83	117.97	120.30
1	L1	1995	G	C6-C5-N7	-5.82	126.91	130.40
1	L1	3772	U	C2-N1-C1'	5.82	124.68	117.70
1	L1	3673	C	OP2-P-O3'	5.82	118.00	105.20
1	L1	516	C	C2-N1-C1'	5.82	125.20	118.80
46	S2	130	G	N3-C4-N9	5.82	129.49	126.00
1	L1	453	G	N3-C4-N9	5.81	129.49	126.00
1	L1	907	C	C6-N1-C2	-5.81	117.97	120.30
1	L1	3641	U	C2-N1-C1'	5.81	124.67	117.70
1	L1	753	C	N1-C2-O2	5.80	122.38	118.90
1	L1	1993	C	N1-C2-O2	5.78	122.37	118.90
1	L1	1995	G	N3-C4-N9	5.78	129.47	126.00
3	L3	64	U	N3-C2-O2	-5.78	118.15	122.20
46	S2	1271	C	N1-C2-O2	5.77	122.36	118.90
46	S2	537	C	C2-N1-C1'	5.76	125.14	118.80
1	L1	4229	U	N1-C2-O2	5.76	126.83	122.80
46	S2	1396	A	O4'-C1'-N9	5.75	112.80	108.20
1	L1	4709	U	C6-N1-C1'	-5.75	113.15	121.20
1	L1	3866	C	C5-C6-N1	5.75	123.87	121.00
59	SS	49	ASP	CB-CG-OD2	5.73	123.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	550	C	N3-C2-O2	-5.73	117.89	121.90
1	L1	2627	C	N3-C2-O2	-5.72	117.89	121.90
46	S2	193	C	N1-C2-O2	5.72	122.33	118.90
1	L1	2409	U	C6-N1-C1'	-5.72	113.19	121.20
46	S2	1315	U	N3-C2-O2	-5.72	118.20	122.20
46	S2	550	C	C6-N1-C2	-5.71	118.01	120.30
1	L1	74	G	N3-C4-N9	5.71	129.43	126.00
46	S2	192	C	N1-C2-O2	5.71	122.33	118.90
1	L1	1988	G	N3-C4-C5	-5.69	125.75	128.60
46	S2	329	G	N3-C4-N9	5.69	129.42	126.00
1	L1	263	G	C5-C6-O6	5.69	132.02	128.60
46	S2	834	C	N3-C2-O2	-5.69	117.92	121.90
60	ST	64	LEU	CA-CB-CG	5.69	128.39	115.30
1	L1	693	C	C2-N1-C1'	5.69	125.06	118.80
1	L1	2102	G	N3-C4-N9	5.69	129.41	126.00
1	L1	962	C	N1-C2-O2	5.68	122.31	118.90
1	L1	2096	G	N3-C4-N9	5.67	129.40	126.00
16	LN	124	ASP	CB-CG-OD1	5.67	123.40	118.30
1	L1	2333	G	N9-C4-C5	5.66	107.66	105.40
1	L1	41	C	C6-N1-C2	-5.65	118.04	120.30
1	L1	112	C	C2-N1-C1'	5.64	125.01	118.80
46	S2	659	G	C8-N9-C1'	-5.64	119.67	127.00
1	L1	1994	C	C6-N1-C2	-5.63	118.05	120.30
46	S2	688	U	P-O3'-C3'	5.63	126.45	119.70
59	SS	21	ASP	CB-CG-OD1	5.62	123.36	118.30
1	L1	180	C	N3-C2-O2	-5.61	117.97	121.90
1	L1	2096	G	N3-C4-C5	-5.61	125.80	128.60
1	L1	3598	C	C6-N1-C2	-5.60	118.06	120.30
1	L1	739	G	N3-C4-N9	5.60	129.36	126.00
1	L1	131	C	C6-N1-C2	-5.60	118.06	120.30
46	S2	193	C	C6-N1-C2	-5.59	118.06	120.30
45	Lr	125	MET	CB-CG-SD	5.59	129.17	112.40
71	SM	42	LEU	CA-CB-CG	5.59	128.16	115.30
46	S2	322	C	C6-N1-C2	-5.58	118.07	120.30
1	L1	3598	C	C5-C6-N1	5.58	123.79	121.00
1	L1	489	C	C2-N1-C1'	5.57	124.93	118.80
46	S2	1520	G	N3-C4-C5	-5.57	125.81	128.60
1	L1	977	C	C2-N1-C1'	5.57	124.92	118.80
46	S2	206	G	N1-C2-N2	-5.57	111.19	116.20
1	L1	2333	G	N1-C6-O6	-5.57	116.56	119.90
46	S2	1772	C	C5-C6-N1	5.56	123.78	121.00
1	L1	234	G	C4-N9-C1'	5.56	133.73	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1002	U	N1-C2-O2	5.55	126.69	122.80
1	L1	1853	G	N3-C4-N9	5.54	129.32	126.00
1	L1	1079	C	C6-N1-C2	-5.54	118.08	120.30
1	L1	4266	G	C2-N3-C4	5.53	114.67	111.90
68	SC	104	ASP	CB-CG-OD1	5.53	123.27	118.30
49	SD	193	ASP	CB-CG-OD1	5.53	123.27	118.30
1	L1	3882	C	C6-N1-C2	-5.52	118.09	120.30
1	L1	3778	U	N3-C2-O2	-5.50	118.35	122.20
1	L1	2491	C	N1-C2-O2	5.48	122.19	118.90
1	L1	68	U	N3-C2-O2	-5.48	118.36	122.20
1	L1	2099	G	N1-C2-N2	-5.47	111.27	116.20
1	L1	1170	G	N1-C6-O6	-5.47	116.62	119.90
46	S2	118	C	N1-C2-O2	5.46	122.18	118.90
46	S2	1649	U	N1-C2-O2	5.46	126.62	122.80
1	L1	758	G	N1-C2-N2	-5.46	111.29	116.20
1	L1	1472	C	C2-N1-C1'	5.46	124.80	118.80
1	L1	2491	C	N3-C2-O2	-5.46	118.08	121.90
1	L1	74	G	C8-N9-C1'	-5.45	119.92	127.00
46	S2	178	C	N1-C2-O2	5.44	122.17	118.90
46	S2	1434	C	P-O3'-C3'	5.44	126.23	119.70
1	L1	3636	C	N3-C2-O2	-5.44	118.09	121.90
46	S2	112	U	P-O3'-C3'	5.44	126.23	119.70
46	S2	1696	C	C2-N1-C1'	5.43	124.77	118.80
1	L1	3924	C	C5-C6-N1	5.42	123.71	121.00
1	L1	1995	G	N9-C4-C5	-5.42	103.23	105.40
1	L1	129	C	N1-C2-O2	5.42	122.15	118.90
1	L1	2820	C	N3-C2-O2	-5.41	118.11	121.90
46	S2	1261	C	C6-N1-C2	-5.41	118.14	120.30
1	L1	1973	G	N1-C6-O6	-5.41	116.66	119.90
1	L1	4594	U	C2-N1-C1'	5.41	124.19	117.70
46	S2	4	C	C6-N1-C2	-5.40	118.14	120.30
46	S2	570	C	N3-C2-O2	-5.40	118.12	121.90
46	S2	563	G	P-O3'-C3'	5.40	126.18	119.70
69	SG	41	LEU	CA-CB-CG	5.40	127.72	115.30
1	L1	2304	U	N3-C2-O2	-5.38	118.43	122.20
1	L1	282	C	N3-C2-O2	-5.38	118.13	121.90
59	SS	16	LEU	CB-CG-CD1	5.38	120.14	111.00
1	L1	757	G	N3-C2-N2	5.37	123.66	119.90
1	L1	3657	U	N3-C2-O2	-5.37	118.44	122.20
1	L1	205	C	N3-C2-O2	-5.37	118.14	121.90
1	L1	1988	G	C6-C5-N7	-5.37	127.18	130.40
46	S2	1304	U	C2-N1-C1'	5.37	124.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	537	C	N1-C2-O2	5.36	122.11	118.90
46	S2	632	C	C2-N1-C1'	5.36	124.69	118.80
1	L1	96	U	N3-C2-O2	-5.34	118.46	122.20
1	L1	757	G	C5-C6-O6	5.34	131.80	128.60
1	L1	4241	C	C2-N1-C1'	5.34	124.67	118.80
1	L1	654	C	N1-C2-O2	5.33	122.10	118.90
1	L1	1995	G	C4-N9-C1'	5.33	133.43	126.50
1	L1	41	C	C5-C6-N1	5.33	123.66	121.00
1	L1	2627	C	C6-N1-C1'	-5.32	114.41	120.80
46	S2	168	C	N3-C2-O2	-5.32	118.18	121.90
46	S2	205	G	N3-C4-C5	-5.32	125.94	128.60
1	L1	4281	A	O4'-C1'-N9	5.32	112.45	108.20
1	L1	2528	G	N3-C4-N9	5.31	129.19	126.00
46	S2	666	U	C2-N1-C1'	5.31	124.07	117.70
1	L1	2099	G	N1-C6-O6	-5.30	116.72	119.90
1	L1	1243	C	N1-C2-O2	5.29	122.07	118.90
23	LU	24	ASP	CB-CG-OD2	5.29	123.06	118.30
1	L1	74	G	C4-N9-C1'	5.29	133.37	126.50
1	L1	255	C	N3-C2-O2	-5.28	118.20	121.90
1	L1	1973	G	N3-C2-N2	5.28	123.60	119.90
1	L1	1081	C	N1-C2-O2	5.28	122.07	118.90
1	L1	130	C	N1-C2-N3	5.28	122.90	119.20
1	L1	1995	G	C4-C5-N7	5.28	112.91	110.80
46	S2	579	C	N1-C2-O2	5.26	122.06	118.90
1	L1	1632	A	C2-N3-C4	5.26	113.23	110.60
1	L1	1893	C	C6-N1-C2	-5.26	118.20	120.30
46	S2	205	G	C4-N9-C1'	5.26	133.34	126.50
1	L1	4399	U	N3-C2-O2	-5.25	118.52	122.20
1	L1	923	C	C2-N1-C1'	5.25	124.58	118.80
1	L1	4681	A	C5-C6-N1	5.25	120.32	117.70
1	L1	2514	G	C4-C5-N7	5.23	112.89	110.80
1	L1	2744	A	N1-C6-N6	-5.23	115.46	118.60
1	L1	4862	G	N9-C4-C5	-5.23	103.31	105.40
1	L1	1868	A	N1-C6-N6	5.22	121.73	118.60
1	L1	3594	C	C5-C6-N1	5.22	123.61	121.00
1	L1	1607	C	N3-C2-O2	-5.21	118.25	121.90
59	SS	1	MET	CA-CB-CG	5.20	122.15	113.30
1	L1	2532	C	C2-N1-C1'	5.20	124.52	118.80
1	L1	2528	G	C8-N9-C1'	-5.20	120.25	127.00
46	S2	965	U	N3-C2-O2	-5.19	118.56	122.20
46	S2	1002	U	N3-C2-O2	-5.19	118.56	122.20
1	L1	4708	A	N7-C8-N9	5.19	116.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3636	C	C6-N1-C2	-5.19	118.23	120.30
1	L1	4266	G	N3-C4-N9	5.19	129.11	126.00
1	L1	406	C	P-O3'-C3'	5.18	125.92	119.70
1	L1	3772	U	N1-C2-O2	5.18	126.43	122.80
1	L1	263	G	N1-C6-O6	-5.18	116.79	119.90
1	L1	453	G	C8-N9-C1'	-5.18	120.27	127.00
1	L1	456	C	C6-N1-C2	-5.18	118.23	120.30
1	L1	4862	G	C6-C5-N7	-5.18	127.29	130.40
1	L1	4305	G	O4'-C1'-N9	5.17	112.34	108.20
46	S2	549	C	N1-C2-O2	5.17	122.00	118.90
1	L1	1458	C	N3-C2-O2	-5.17	118.28	121.90
2	L2	28	C	C6-N1-C2	-5.17	118.23	120.30
1	L1	1633	G	P-O3'-C3'	5.16	125.89	119.70
46	S2	1453	C	C6-N1-C2	-5.16	118.23	120.30
1	L1	4468	U	C5-C4-O4	5.16	129.00	125.90
1	L1	139	G	C8-N9-C4	-5.15	104.34	106.40
1	L1	2102	G	C4-N9-C1'	5.15	133.19	126.50
1	L1	3771	C	C2-N1-C1'	5.15	124.46	118.80
1	L1	2096	G	C8-N9-C1'	-5.14	120.32	127.00
1	L1	4945	G	N3-C4-N9	5.14	129.08	126.00
46	S2	329	G	N3-C4-C5	-5.13	126.04	128.60
46	S2	550	C	C5-C4-N4	5.13	123.79	120.20
49	SD	218	LEU	CA-CB-CG	5.12	127.09	115.30
1	L1	4133	C	C2-N1-C1'	5.12	124.44	118.80
16	LN	136	ASP	CB-CG-OD1	5.12	122.91	118.30
1	L1	1220	G	N1-C2-N2	-5.12	111.59	116.20
1	L1	2819	U	N3-C2-O2	-5.12	118.62	122.20
1	L1	1597	G	O4'-C1'-N9	5.12	112.29	108.20
46	S2	193	C	N1-C2-N3	5.12	122.78	119.20
1	L1	1995	G	C8-N9-C1'	-5.11	120.35	127.00
46	S2	1277	C	C5-C6-N1	5.11	123.55	121.00
6	LC	49	ARG	C-N-CA	5.10	134.46	121.70
46	S2	204	G	N1-C6-O6	-5.10	116.84	119.90
52	SH	132	ASP	CB-CG-OD1	5.10	122.89	118.30
1	L1	4404	U	C2-N1-C1'	5.10	123.82	117.70
1	L1	4360	U	N3-C2-O2	-5.10	118.63	122.20
1	L1	3930	U	N3-C2-O2	-5.10	118.63	122.20
1	L1	1726	U	N3-C2-O2	-5.09	118.63	122.20
1	L1	468	U	O4'-C1'-N1	5.09	112.27	108.20
2	L2	39	C	N1-C2-O2	5.08	121.95	118.90
1	L1	2487	G	N1-C6-O6	-5.08	116.85	119.90
46	S2	206	G	C8-N9-C4	-5.08	104.37	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3685	C	C5-C6-N1	5.08	123.54	121.00
6	LC	260	LEU	CB-CG-CD1	-5.08	102.37	111.00
1	L1	294	G	C4-N9-C1'	5.07	133.09	126.50
1	L1	1735	U	N1-C2-O2	5.07	126.35	122.80
1	L1	4303	C	C6-N1-C2	-5.07	118.27	120.30
1	L1	1973	G	C5-C6-O6	5.07	131.64	128.60
1	L1	1993	C	N3-C2-O2	-5.06	118.36	121.90
1	L1	1929	A	C4-N9-C1'	5.06	135.41	126.30
46	S2	1277	C	N1-C2-O2	5.05	121.93	118.90
46	S2	1520	G	C2-N3-C4	5.05	114.42	111.90
1	L1	138	G	C8-N9-C4	-5.04	104.38	106.40
1	L1	962	C	N3-C2-O2	-5.04	118.37	121.90
1	L1	643	C	N1-C2-O2	5.03	121.92	118.90
1	L1	2018	C	N1-C2-O2	5.03	121.92	118.90
1	L1	138	G	N1-C2-N2	-5.02	111.68	116.20
1	L1	3641	U	C2-N3-C4	-5.01	123.99	127.00
1	L1	1241	C	C5-C6-N1	5.01	123.51	121.00
1	L1	1989	G	C5-C6-O6	5.01	131.61	128.60
20	LR	177	LEU	CA-CB-CG	5.01	126.82	115.30
71	SM	12	MET	CA-CB-CG	5.00	121.81	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
61	SU	93	SER	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%)	233 (95%)	13 (5%)	0	100	100
5	LB	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
6	LC	363/427 (85%)	355 (98%)	8 (2%)	0	100	100
7	LD	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
8	LE	214/288 (74%)	208 (97%)	6 (3%)	0	100	100
9	LF	223/248 (90%)	215 (96%)	8 (4%)	0	100	100
10	LG	223/266 (84%)	220 (99%)	3 (1%)	0	100	100
11	LH	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
12	LI	198/214 (92%)	192 (97%)	6 (3%)	0	100	100
13	LJ	167/178 (94%)	163 (98%)	4 (2%)	0	100	100
14	LL	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
15	LM	137/215 (64%)	133 (97%)	4 (3%)	0	100	100
16	LN	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
17	LO	199/203 (98%)	199 (100%)	0	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	LQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
20	LR	185/196 (94%)	184 (100%)	1 (0%)	0	100	100
21	LS	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
22	LT	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
23	LU	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
24	LV	129/140 (92%)	122 (95%)	7 (5%)	0	100	100
25	LW	122/157 (78%)	117 (96%)	5 (4%)	0	100	100
26	LX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
27	LY	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
28	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
29	La	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
30	Lb	105/159 (66%)	99 (94%)	6 (6%)	0	100	100
31	Lc	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
32	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
33	Le	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
34	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
35	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
38	Lj	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
39	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
40	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
41	Lm	50/128 (39%)	50 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	100/106 (94%)	96 (96%)	4 (4%)	0	100	100
44	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	Lr	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
47	SA	220/295 (75%)	216 (98%)	4 (2%)	0	100	100
48	SB	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
49	SD	225/243 (93%)	218 (97%)	7 (3%)	0	100	100
50	SE	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
51	SF	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
52	SH	182/194 (94%)	162 (89%)	16 (9%)	4 (2%)	6	10
53	SI	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
54	SK	96/165 (58%)	92 (96%)	4 (4%)	0	100	100
55	SL	140/158 (89%)	132 (94%)	8 (6%)	0	100	100
56	SP	125/145 (86%)	124 (99%)	1 (1%)	0	100	100
57	SQ	142/146 (97%)	130 (92%)	11 (8%)	1 (1%)	22	39
58	SR	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
59	SS	143/152 (94%)	137 (96%)	6 (4%)	0	100	100
60	ST	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
61	SU	102/119 (86%)	96 (94%)	5 (5%)	1 (1%)	15	28
62	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
63	SX	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
64	Sa	100/115 (87%)	97 (97%)	2 (2%)	1 (1%)	15	28
65	Sc	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
66	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
67	Sg	311/317 (98%)	294 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	SC	220/293 (75%)	216 (98%)	4 (2%)	0	100	100
69	SG	235/249 (94%)	228 (97%)	7 (3%)	0	100	100
70	SJ	183/194 (94%)	176 (96%)	7 (4%)	0	100	100
71	SM	120/132 (91%)	111 (92%)	9 (8%)	0	100	100
72	SN	148/151 (98%)	148 (100%)	0	0	100	100
73	SO	133/151 (88%)	124 (93%)	8 (6%)	1 (1%)	19	35
74	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
75	SY	123/133 (92%)	121 (98%)	2 (2%)	0	100	100
76	SZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
77	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
78	Se	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
79	Sf	59/156 (38%)	55 (93%)	4 (7%)	0	100	100
All	All	11249/12687 (89%)	10882 (97%)	359 (3%)	8 (0%)	54	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	SH	34	SER
57	SQ	44	PRO
52	SH	11	PRO
52	SH	40	LEU
61	SU	94	PRO
64	Sa	46	GLU
52	SH	8	ILE
73	SO	89	GLY

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%)	185 (97%)	5 (3%)	46	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	LB	348/349 (100%)	325 (93%)	23 (7%)	16	32
6	LC	304/348 (87%)	294 (97%)	10 (3%)	38	64
7	LD	246/250 (98%)	239 (97%)	7 (3%)	43	70
8	LE	194/252 (77%)	190 (98%)	4 (2%)	53	78
9	LF	194/215 (90%)	190 (98%)	4 (2%)	53	78
10	LG	196/223 (88%)	190 (97%)	6 (3%)	40	67
11	LH	169/171 (99%)	161 (95%)	8 (5%)	26	49
12	LI	172/181 (95%)	168 (98%)	4 (2%)	50	76
13	LJ	142/149 (95%)	136 (96%)	6 (4%)	30	54
14	LL	176/177 (99%)	166 (94%)	10 (6%)	20	39
15	LM	118/161 (73%)	112 (95%)	6 (5%)	24	45
16	LN	171/172 (99%)	167 (98%)	4 (2%)	50	76
17	LO	173/174 (99%)	168 (97%)	5 (3%)	42	69
18	LP	134/163 (82%)	132 (98%)	2 (2%)	65	85
19	LQ	164/165 (99%)	161 (98%)	3 (2%)	59	81
20	LR	166/175 (95%)	159 (96%)	7 (4%)	30	54
21	LS	157/157 (100%)	152 (97%)	5 (3%)	39	65
22	LT	139/140 (99%)	132 (95%)	7 (5%)	24	46
23	LU	91/115 (79%)	85 (93%)	6 (7%)	16	32
24	LV	101/107 (94%)	98 (97%)	3 (3%)	41	68
25	LW	103/126 (82%)	98 (95%)	5 (5%)	25	47
26	LX	106/133 (80%)	103 (97%)	3 (3%)	43	70
27	LY	124/135 (92%)	119 (96%)	5 (4%)	31	56
28	LZ	117/117 (100%)	115 (98%)	2 (2%)	60	82
29	La	120/121 (99%)	114 (95%)	6 (5%)	24	46
30	Lb	88/126 (70%)	81 (92%)	7 (8%)	12	23
31	Lc	83/97 (86%)	81 (98%)	2 (2%)	49	74
32	Ld	98/110 (89%)	94 (96%)	4 (4%)	30	55
33	Le	114/121 (94%)	113 (99%)	1 (1%)	78	92
34	Lf	88/89 (99%)	82 (93%)	6 (7%)	16	30
35	Lg	98/100 (98%)	93 (95%)	5 (5%)	24	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Lh	109/110 (99%)	104 (95%)	5 (5%)	27	50
37	Li	86/89 (97%)	84 (98%)	2 (2%)	50	76
38	Lj	73/80 (91%)	70 (96%)	3 (4%)	30	55
39	Lk	64/65 (98%)	58 (91%)	6 (9%)	8	17
40	Ll	47/48 (98%)	44 (94%)	3 (6%)	17	33
41	Lm	48/116 (41%)	48 (100%)	0	100	100
42	Ln	23/24 (96%)	21 (91%)	2 (9%)	10	20
43	Lo	90/93 (97%)	86 (96%)	4 (4%)	28	52
44	Lp	74/75 (99%)	72 (97%)	2 (3%)	44	71
45	Lr	109/121 (90%)	103 (94%)	6 (6%)	21	41
47	SA	184/243 (76%)	177 (96%)	7 (4%)	33	58
48	SB	195/231 (84%)	183 (94%)	12 (6%)	18	35
49	SD	190/202 (94%)	180 (95%)	10 (5%)	22	43
50	SE	224/225 (100%)	213 (95%)	11 (5%)	25	47
51	SF	156/170 (92%)	147 (94%)	9 (6%)	20	38
52	SH	166/174 (95%)	146 (88%)	20 (12%)	5	9
53	SI	178/180 (99%)	171 (96%)	7 (4%)	32	57
54	SK	89/136 (65%)	80 (90%)	9 (10%)	7	14
55	SL	130/142 (92%)	122 (94%)	8 (6%)	18	35
56	SP	113/130 (87%)	105 (93%)	8 (7%)	14	28
57	SQ	119/121 (98%)	108 (91%)	11 (9%)	9	18
58	SR	122/122 (100%)	119 (98%)	3 (2%)	47	73
59	SS	126/132 (96%)	120 (95%)	6 (5%)	25	48
60	ST	113/115 (98%)	106 (94%)	7 (6%)	18	35
61	SU	94/107 (88%)	85 (90%)	9 (10%)	8	16
62	SV	67/67 (100%)	62 (92%)	5 (8%)	13	26
63	SX	113/115 (98%)	110 (97%)	3 (3%)	44	71
64	Sa	89/98 (91%)	88 (99%)	1 (1%)	73	89
65	Sc	57/62 (92%)	54 (95%)	3 (5%)	22	43
66	Sd	48/49 (98%)	47 (98%)	1 (2%)	53	78
67	Sg	272/275 (99%)	258 (95%)	14 (5%)	24	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	SC	188/225 (84%)	182 (97%)	6 (3%)	39	65
69	SG	207/218 (95%)	192 (93%)	15 (7%)	14	28
70	SJ	161/168 (96%)	154 (96%)	7 (4%)	29	53
71	SM	102/108 (94%)	91 (89%)	11 (11%)	6	12
72	SN	130/131 (99%)	124 (95%)	6 (5%)	27	50
73	SO	105/119 (88%)	101 (96%)	4 (4%)	33	58
74	SW	112/113 (99%)	105 (94%)	7 (6%)	18	34
75	SY	109/115 (95%)	102 (94%)	7 (6%)	17	33
76	SZ	66/103 (64%)	62 (94%)	4 (6%)	18	36
77	Sb	75/76 (99%)	70 (93%)	5 (7%)	16	31
78	Se	47/48 (98%)	44 (94%)	3 (6%)	17	33
79	Sf	54/140 (39%)	48 (89%)	6 (11%)	6	11
All	All	9808/10799 (91%)	9349 (95%)	459 (5%)	30	49

All (459) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	147	ARG
4	LA	149	LYS
4	LA	217	GLN
4	LA	221	LYS
4	LA	242	ARG
5	LB	53	MET
5	LB	58	ARG
5	LB	59	GLU
5	LB	60	VAL
5	LB	65	SER
5	LB	66	LYS
5	LB	69	LYS
5	LB	136	LYS
5	LB	137	TRP
5	LB	138	GLN
5	LB	141	ASP
5	LB	169	ARG
5	LB	208	ASN
5	LB	228	TYR
5	LB	287	ILE
5	LB	289	GLN

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Mol	Chain	Res	Type
5	LB	295	ASP
5	LB	300	LYS
5	LB	309	LEU
5	LB	310	SER
5	LB	343	ARG
5	LB	357	ARG
5	LB	358	ARG
6	LC	29	LYS
6	LC	48	ASN
6	LC	114	ARG
6	LC	122	TYR
6	LC	140	LYS
6	LC	155	GLU
6	LC	257	PHE
6	LC	312	ARG
6	LC	337	ARG
6	LC	348	LYS
7	LD	58	ARG
7	LD	128	ASP
7	LD	136	ASP
7	LD	194	VAL
7	LD	224	SER
7	LD	232	THR
7	LD	234	ASP
8	LE	50	LEU
8	LE	51	VAL
8	LE	56	ARG
8	LE	246	ARG
9	LF	68	GLU
9	LF	102	SER
9	LF	221	LYS
9	LF	223	LYS
10	LG	29	ASN
10	LG	44	ASP
10	LG	73	ARG
10	LG	175	ARG
10	LG	192	ARG
10	LG	257	LYS
11	LH	7	ASN
11	LH	15	ASN
11	LH	28	LYS
11	LH	50	LYS

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Mol	Chain	Res	Type
11	LH	52	LYS
11	LH	71	ARG
11	LH	137	SER
11	LH	177	ASP
12	LI	35	ASP
12	LI	66	GLU
12	LI	82	LYS
12	LI	123	GLN
13	LJ	28	GLU
13	LJ	58	ARG
13	LJ	72	CYS
13	LJ	114	ASP
13	LJ	128	LEU
13	LJ	129	ASP
14	LL	49	ARG
14	LL	52	SER
14	LL	67	HIS
14	LL	92	ARG
14	LL	103	ARG
14	LL	109	SER
14	LL	122	SER
14	LL	138	ASP
14	LL	161	TYR
14	LL	200	LYS
15	LM	39	ASP
15	LM	45	VAL
15	LM	54	CYS
15	LM	63	LYS
15	LM	116	LYS
15	LM	121	ARG
16	LN	10	LEU
16	LN	18	VAL
16	LN	126	THR
16	LN	166	SER
17	LO	5	GLN
17	LO	78	ARG
17	LO	171	LYS
17	LO	173	GLN
17	LO	187	LYS
18	LP	3	ARG
18	LP	57	CYS
19	LQ	16	LYS

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Mol	Chain	Res	Type
19	LQ	49	LYS
19	LQ	71	LYS
20	LR	16	ARG
20	LR	31	GLU
20	LR	43	LYS
20	LR	71	ARG
20	LR	112	SER
20	LR	151	ARG
20	LR	160	GLU
21	LS	42	SER
21	LS	49	SER
21	LS	99	ASP
21	LS	118	ARG
21	LS	135	SER
22	LT	83	LYS
22	LT	99	SER
22	LT	107	LYS
22	LT	116	LYS
22	LT	120	LYS
22	LT	129	LYS
22	LT	137	GLU
23	LU	31	ASP
23	LU	71	THR
23	LU	95	ASN
23	LU	99	TRP
23	LU	106	SER
23	LU	108	GLU
24	LV	48	ARG
24	LV	87	SER
24	LV	115	SER
25	LW	1	MET
25	LW	2	LYS
25	LW	101	ARG
25	LW	102	LYS
25	LW	116	LYS
26	LX	85	SER
26	LX	88	LYS
26	LX	152	LYS
27	LY	36	LYS
27	LY	41	LYS
27	LY	74	TYR
27	LY	91	ASN

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Mol	Chain	Res	Type
27	LY	105	VAL
28	LZ	73	LYS
28	LZ	112	ARG
29	La	6	ARG
29	La	82	VAL
29	La	92	LYS
29	La	106	SER
29	La	122	VAL
29	La	140	VAL
30	Lb	14	ARG
30	Lb	51	LYS
30	Lb	55	LYS
30	Lb	58	GLN
30	Lb	63	LYS
30	Lb	76	VAL
30	Lb	114	LYS
31	Lc	44	LYS
31	Lc	102	SER
32	Ld	40	LYS
32	Ld	50	ARG
32	Ld	55	LYS
32	Ld	98	SER
33	Le	126	ASN
34	Lf	24	HIS
34	Lf	25	THR
34	Lf	54	LYS
34	Lf	89	ARG
34	Lf	104	MET
34	Lf	105	LEU
35	Lg	63	VAL
35	Lg	65	MET
35	Lg	73	HIS
35	Lg	89	ASP
35	Lg	101	LYS
36	Lh	13	LYS
36	Lh	19	LYS
36	Lh	87	LYS
36	Lh	88	THR
36	Lh	94	ARG
37	Li	11	LEU
37	Li	12	ASN
38	Lj	24	SER

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Mol	Chain	Res	Type
38	Lj	32	SER
38	Lj	83	THR
39	Lk	9	LYS
39	Lk	18	LYS
39	Lk	19	ASP
39	Lk	22	SER
39	Lk	36	VAL
39	Lk	46	VAL
40	Ll	8	ARG
40	Ll	21	ARG
40	Ll	29	MET
42	Ln	16	LYS
42	Ln	24	SER
43	Lo	33	LEU
43	Lo	78	ARG
43	Lo	80	LYS
43	Lo	99	ARG
44	Lp	36	LYS
44	Lp	48	LYS
45	Lr	58	LYS
45	Lr	67	ARG
45	Lr	101	LYS
45	Lr	119	ARG
45	Lr	122	LYS
45	Lr	125	MET
47	SA	79	SER
47	SA	81	ASN
47	SA	102	ARG
47	SA	124	VAL
47	SA	191	ARG
47	SA	192	GLU
47	SA	200	ASP
48	SB	27	LYS
48	SB	38	MET
48	SB	52	THR
48	SB	60	ASP
48	SB	70	SER
48	SB	88	THR
48	SB	89	GLU
48	SB	92	GLN
48	SB	174	ARG
48	SB	203	SER

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Mol	Chain	Res	Type
48	SB	224	GLU
48	SB	232	HIS
49	SD	35	SER
49	SD	40	ARG
49	SD	76	ARG
49	SD	143	ARG
49	SD	156	LEU
49	SD	167	TYR
49	SD	178	ARG
49	SD	206	ASP
49	SD	215	ASP
49	SD	218	LEU
50	SE	62	LYS
50	SE	88	ASP
50	SE	93	ASP
50	SE	126	VAL
50	SE	143	ASP
50	SE	208	VAL
50	SE	211	LYS
50	SE	230	LYS
50	SE	232	ASN
50	SE	233	LYS
50	SE	255	ARG
51	SF	31	ASN
51	SF	36	GLN
51	SF	37	ASP
51	SF	59	LYS
51	SF	76	MET
51	SF	83	ASN
51	SF	135	ARG
51	SF	136	ARG
51	SF	140	ASP
52	SH	7	LYS
52	SH	8	ILE
52	SH	14	GLU
52	SH	17	ASP
52	SH	18	GLU
52	SH	20	GLU
52	SH	24	SER
52	SH	27	LEU
52	SH	28	LEU
52	SH	30	LEU

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Mol	Chain	Res	Type
52	SH	31	GLU
52	SH	32	MET
52	SH	39	GLN
52	SH	40	LEU
52	SH	45	ILE
52	SH	58	LYS
52	SH	107	LYS
52	SH	122	LEU
52	SH	137	SER
52	SH	184	ASP
53	SI	5	ARG
53	SI	69	SER
53	SI	73	THR
53	SI	106	SER
53	SI	115	SER
53	SI	133	GLU
53	SI	154	LYS
54	SK	1	MET
54	SK	6	LYS
54	SK	14	LEU
54	SK	18	GLU
54	SK	37	ASP
54	SK	38	LYS
54	SK	55	ARG
54	SK	81	ASP
54	SK	94	LEU
55	SL	12	LYS
55	SL	35	ARG
55	SL	69	ARG
55	SL	97	ARG
55	SL	109	MET
55	SL	114	SER
55	SL	141	ASN
55	SL	152	LYS
56	SP	12	PHE
56	SP	14	LYS
56	SP	37	TYR
56	SP	61	ARG
56	SP	76	VAL
56	SP	83	MET
56	SP	96	VAL
56	SP	130	ARG

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Mol	Chain	Res	Type
57	SQ	4	LYS
57	SQ	43	GLU
57	SQ	44	PRO
57	SQ	45	ARG
57	SQ	60	LYS
57	SQ	89	SER
57	SQ	105	LYS
57	SQ	107	GLU
57	SQ	118	THR
57	SQ	127	CYS
57	SQ	145	TYR
58	SR	77	GLU
58	SR	83	ASN
58	SR	111	PHE
59	SS	1	MET
59	SS	2	SER
59	SS	52	LEU
59	SS	77	TYR
59	SS	83	PHE
59	SS	104	ASP
60	ST	22	LEU
60	ST	50	GLU
60	ST	88	MET
60	ST	112	MET
60	ST	129	ARG
60	ST	132	ASP
60	ST	133	ARG
61	SU	19	ARG
61	SU	23	THR
61	SU	36	CYS
61	SU	41	ARG
61	SU	49	LYS
61	SU	78	ASP
61	SU	82	MET
61	SU	90	ASP
61	SU	111	GLU
62	SV	10	ASP
62	SV	34	MET
62	SV	38	GLU
62	SV	52	THR
62	SV	83	PHE
63	SX	88	ASP

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Mol	Chain	Res	Type
63	SX	105	PHE
63	SX	127	ASN
64	Sa	30	VAL
65	Sc	26	GLN
65	Sc	36	ASP
65	Sc	51	ARG
66	Sd	6	LEU
67	Sg	30	MET
67	Sg	49	GLU
67	Sg	57	ARG
67	Sg	64	HIS
67	Sg	113	PHE
67	Sg	118	ARG
67	Sg	135	LEU
67	Sg	223	GLU
67	Sg	228	TYR
67	Sg	235	ILE
67	Sg	246	TYR
67	Sg	249	CYS
67	Sg	297	THR
67	Sg	302	TYR
68	SC	61	MET
68	SC	73	MET
68	SC	104	ASP
68	SC	132	ASP
68	SC	236	PHE
68	SC	248	TYR
69	SG	19	ASP
69	SG	27	PHE
69	SG	39	ASP
69	SG	46	LYS
69	SG	65	GLN
69	SG	98	ARG
69	SG	107	SER
69	SG	116	LYS
69	SG	119	LYS
69	SG	159	ARG
69	SG	167	LYS
69	SG	168	LYS
69	SG	183	ARG
69	SG	216	ARG
69	SG	218	LYS

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Mol	Chain	Res	Type
70	SJ	92	MET
70	SJ	93	LYS
70	SJ	95	ASP
70	SJ	136	ARG
70	SJ	140	GLN
70	SJ	152	ASP
70	SJ	155	LYS
71	SM	12	MET
71	SM	31	LEU
71	SM	60	MET
71	SM	61	TYR
71	SM	63	LYS
71	SM	66	GLU
71	SM	76	LEU
71	SM	93	LYS
71	SM	109	VAL
71	SM	127	TYR
71	SM	132	LYS
72	SN	42	LYS
72	SN	69	ASN
72	SN	117	LEU
72	SN	132	LYS
72	SN	142	GLU
72	SN	150	VAL
73	SO	75	MET
73	SO	83	GLN
73	SO	149	ARG
73	SO	151	LEU
74	SW	20	ARG
74	SW	30	CYS
74	SW	43	LYS
74	SW	80	ASP
74	SW	84	LYS
74	SW	104	LEU
74	SW	112	ASP
75	SY	16	ARG
75	SY	24	VAL
75	SY	61	ARG
75	SY	74	MET
75	SY	83	LYS
75	SY	85	ASN
75	SY	93	ARG

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Mol	Chain	Res	Type
76	SZ	41	ARG
76	SZ	52	LYS
76	SZ	64	ASN
76	SZ	101	SER
77	Sb	42	LYS
77	Sb	44	THR
77	Sb	56	CYS
77	Sb	77	CYS
77	Sb	80	ARG
78	Se	23	GLU
78	Se	24	LYS
78	Se	41	ARG
79	Sf	102	VAL
79	Sf	111	ASN
79	Sf	120	GLU
79	Sf	132	MET
79	Sf	138	ARG
79	Sf	150	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
5	LB	258	HIS
10	LG	38	ASN
17	LO	63	ASN
52	SH	12	ASN
57	SQ	77	HIS
57	SQ	114	GLN
59	SS	76	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	3701/5070 (72%)	720 (19%)	11 (0%)
2	L2	119/120 (99%)	11 (9%)	0
3	L3	155/156 (99%)	31 (20%)	0
46	S2	1708/1869 (91%)	328 (19%)	9 (0%)
All	All	5683/7215 (78%)	1090 (19%)	20 (0%)

All (1090) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	15	A
1	L1	39	A
1	L1	42	A
1	L1	48	G
1	L1	56	A
1	L1	58	G
1	L1	59	A
1	L1	64	A
1	L1	65	A
1	L1	69	A
1	L1	73	A
1	L1	85	G
1	L1	91	G
1	L1	98	A
1	L1	108	A
1	L1	109	G
1	L1	110	C
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	157	U
1	L1	159	C
1	L1	169	G
1	L1	170	C
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	200	U
1	L1	210	C
1	L1	216	C
1	L1	218	A
1	L1	219	G
1	L1	220	C
1	L1	233	U
1	L1	234	G
1	L1	254	G

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Mol	Chain	Res	Type
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	340	C
1	L1	350	C
1	L1	373	G
1	L1	387	G
1	L1	388	A
1	L1	398	A2M
1	L1	407	A
1	L1	410	A
1	L1	412	G
1	L1	413	G
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

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Mol	Chain	Res	Type
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	512	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
1	L1	659	G
1	L1	665	C
1	L1	667	A
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	758	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

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Mol	Chain	Res	Type
1	L1	926	G
1	L1	932	A
1	L1	933	G
1	L1	934	C
1	L1	935	A
1	L1	941	C
1	L1	944	A
1	L1	945	U
1	L1	959	G
1	L1	960	A
1	L1	962	C
1	L1	965	G
1	L1	966	A
1	L1	967	C
1	L1	968	C
1	L1	970	G
1	L1	971	U
1	L1	982	U
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

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Mol	Chain	Res	Type
1	L1	1184	A
1	L1	1193	C
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	1220	G
1	L1	1221	G
1	L1	1222	A
1	L1	1241	C
1	L1	1246	G
1	L1	1253	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	1272	C
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	1313	C
1	L1	1326	A2M
1	L1	1337	A
1	L1	1340	OMC
1	L1	1344	C
1	L1	1354	A
1	L1	1358	G

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Mol	Chain	Res	Type
1	L1	1359	G
1	L1	1365	C
1	L1	1367	C
1	L1	1371	A
1	L1	1387	A
1	L1	1394	G
1	L1	1397	A
1	L1	1398	A
1	L1	1404	G
1	L1	1407	C
1	L1	1409	C
1	L1	1410	U
1	L1	1414	C
1	L1	1417	C
1	L1	1420	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	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	1624	G
1	L1	1625	OMG
1	L1	1631	A
1	L1	1633	G
1	L1	1634	A
1	L1	1638	A
1	L1	1640	C
1	L1	1642	A
1	L1	1654	G

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Mol	Chain	Res	Type
1	L1	1661	C
1	L1	1670	G
1	L1	1676	C
1	L1	1677	PSU
1	L1	1678	C
1	L1	1681	G
1	L1	1699	A
1	L1	1700	G
1	L1	1701	A
1	L1	1702	C
1	L1	1704	C
1	L1	1705	G
1	L1	1707	C
1	L1	1724	G
1	L1	1726	U
1	L1	1734	G
1	L1	1741	G
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	1764	G
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	1781	U
1	L1	1787	A
1	L1	1804	A
1	L1	1810	G
1	L1	1820	C
1	L1	1821	G
1	L1	1822	U
1	L1	1836	G

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Mol	Chain	Res	Type
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
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	1940	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	2011	C
1	L1	2017	A
1	L1	2018	C
1	L1	2026	A
1	L1	2044	U
1	L1	2046	G
1	L1	2048	U

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Mol	Chain	Res	Type
1	L1	2055	G
1	L1	2056	G
1	L1	2069	A
1	L1	2084	C
1	L1	2085	G
1	L1	2092	G
1	L1	2093	A
1	L1	2095	A
1	L1	2097	U
1	L1	2098	G
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	2261	G
1	L1	2289	C
1	L1	2300	A
1	L1	2301	G
1	L1	2313	A
1	L1	2333	G
1	L1	2348	G
1	L1	2351	OMC
1	L1	2360	A
1	L1	2395	A
1	L1	2397	G
1	L1	2417	A
1	L1	2421	G
1	L1	2422	OMC
1	L1	2424	OMG
1	L1	2425	U
1	L1	2447	U
1	L1	2450	G
1	L1	2453	A
1	L1	2464	C
1	L1	2465	C
1	L1	2471	G
1	L1	2474	G
1	L1	2475	G

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Mol	Chain	Res	Type
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	2494	U
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	2544	G
1	L1	2546	G
1	L1	2547	G
1	L1	2554	U
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
1	L1	2695	A
1	L1	2696	A
1	L1	2703	G
1	L1	2710	C
1	L1	2711	G

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Mol	Chain	Res	Type
1	L1	2712	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	2803	U
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	2902	G
1	L1	2903	G
1	L1	2906	G
1	L1	2907	G
1	L1	2908	U
1	L1	2909	C
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
1	L1	3596	A
1	L1	3597	G
1	L1	3601	C
1	L1	3604	A
1	L1	3606	U

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Mol	Chain	Res	Type
1	L1	3615	G
1	L1	3618	C
1	L1	3626	G
1	L1	3635	A
1	L1	3644	U
1	L1	3646	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	3736	A
1	L1	3748	A
1	L1	3750	G
1	L1	3753	G
1	L1	3754	G
1	L1	3760	A
1	L1	3771	C
1	L1	3775	A
1	L1	3776	G
1	L1	3777	G
1	L1	3783	A
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	3812	C
1	L1	3814	U
1	L1	3817	A
1	L1	3819	G
1	L1	3838	U
1	L1	3839	G
1	L1	3840	U
1	L1	3841	OMC
1	L1	3867	A2M
1	L1	3877	A
1	L1	3878	C

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Mol	Chain	Res	Type
1	L1	3879	G
1	L1	3897	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
1	L1	4042	G
1	L1	4043	G
1	L1	4044	U
1	L1	4046	A
1	L1	4048	A

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Mol	Chain	Res	Type
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	4061	G
1	L1	4062	A
1	L1	4064	C
1	L1	4076	G
1	L1	4086	G
1	L1	4094	G
1	L1	4095	G
1	L1	4096	C
1	L1	4097	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	4110	C
1	L1	4111	U
1	L1	4112	C
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
1	L1	4143	G
1	L1	4157	A
1	L1	4162	C
1	L1	4163	U
1	L1	4168	G
1	L1	4170	A

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Mol	Chain	Res	Type
1	L1	4183	G
1	L1	4184	G
1	L1	4191	G
1	L1	4203	A
1	L1	4222	G
1	L1	4225	G
1	L1	4229	U
1	L1	4233	A
1	L1	4251	A
1	L1	4254	G
1	L1	4257	A
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	4305	G
1	L1	4306	OMU
1	L1	4314	C
1	L1	4329	G
1	L1	4330	G
1	L1	4332	C
1	L1	4349	C
1	L1	4364	G
1	L1	4373	G
1	L1	4376	A
1	L1	4377	G
1	L1	4378	A
1	L1	4380	A
1	L1	4387	C
1	L1	4391	G
1	L1	4394	A
1	L1	4420	U
1	L1	4422	A
1	L1	4437	U
1	L1	4448	G
1	L1	4449	A
1	L1	4452	U
1	L1	4464	A
1	L1	4475	G
1	L1	4500	PSU

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Mol	Chain	Res	Type
1	L1	4512	U
1	L1	4513	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	4573	G
1	L1	4575	G
1	L1	4590	A
1	L1	4636	PSU
1	L1	4637	OMG
1	L1	4656	A
1	L1	4657	U
1	L1	4670	C
1	L1	4679	G
1	L1	4695	C
1	L1	4700	A
1	L1	4708	A
1	L1	4709	U
1	L1	4719	G
1	L1	4732	G
1	L1	4734	A
1	L1	4740	G
1	L1	4741	C
1	L1	4742	G
1	L1	4745	G
1	L1	4747	C
1	L1	4750	G
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	4775	C
1	L1	4776	G
1	L1	4859	C
1	L1	4862	G

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Mol	Chain	Res	Type
1	L1	4870	G
1	L1	4871	C
1	L1	4875	G
1	L1	4882	U
1	L1	4883	C
1	L1	4887	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	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	4985	U
1	L1	4988	U
1	L1	4989	U
1	L1	4991	U
1	L1	5007	A
1	L1	5009	G
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

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Mol	Chain	Res	Type
1	L1	5047	C
1	L1	5050	C
1	L1	5058	A
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	100	A
2	L2	110	G
2	L2	111	C
3	L3	2	G
3	L3	23	C
3	L3	34	U
3	L3	35	C
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	82	A
3	L3	83	C
3	L3	84	A
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	110	U
3	L3	111	U
3	L3	114	G
3	L3	123	U
3	L3	124	U

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Mol	Chain	Res	Type
3	L3	125	C
3	L3	126	C
3	L3	127	U
3	L3	128	C
3	L3	150	C
46	S2	17	C
46	S2	23	G
46	S2	33	G
46	S2	41	G
46	S2	46	A
46	S2	56	G
46	S2	58	C
46	S2	59	U
46	S2	64	A
46	S2	65	C
46	S2	67	C
46	S2	68	A
46	S2	71	G
46	S2	72	C
46	S2	73	C
46	S2	74	G
46	S2	76	U
46	S2	99	A2M
46	S2	103	A
46	S2	113	G
46	S2	114	G
46	S2	115	U
46	S2	126	G
46	S2	130	G
46	S2	139	C
46	S2	143	U
46	S2	149	A
46	S2	155	G
46	S2	159	A2M
46	S2	160	U
46	S2	162	C
46	S2	175	A
46	S2	184	G
46	S2	194	C
46	S2	196	C
46	S2	197	U
46	S2	198	U

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Mol	Chain	Res	Type
46	S2	200	G
46	S2	203	G
46	S2	204	G
46	S2	311	C
46	S2	318	A
46	S2	319	C
46	S2	323	C
46	S2	324	C
46	S2	325	C
46	S2	326	C
46	S2	328	U
46	S2	329	G
46	S2	332	G
46	S2	351	G
46	S2	360	A
46	S2	362	C
46	S2	364	A
46	S2	369	C
46	S2	370	G
46	S2	385	G
46	S2	386	C
46	S2	408	A
46	S2	409	C
46	S2	421	G
46	S2	438	G
46	S2	448	A
46	S2	449	A
46	S2	450	C
46	S2	452	G
46	S2	464	A
46	S2	471	G
46	S2	472	C
46	S2	473	A
46	S2	474	G
46	S2	476	A
46	S2	482	G
46	S2	487	U
46	S2	488	U
46	S2	492	C
46	S2	493	A
46	S2	500	A
46	S2	516	A

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Mol	Chain	Res	Type
46	S2	525	A
46	S2	530	U
46	S2	531	A
46	S2	532	C
46	S2	536	A
46	S2	537	C
46	S2	540	U
46	S2	544	G
46	S2	546	G
46	S2	547	G
46	S2	551	U
46	S2	554	A
46	S2	555	A
46	S2	556	U
46	S2	557	U
46	S2	558	G
46	S2	559	G
46	S2	560	A
46	S2	563	G
46	S2	564	A
46	S2	576	A2M
46	S2	583	A
46	S2	587	A
46	S2	589	G
46	S2	590	A2M
46	S2	591	U
46	S2	594	A
46	S2	597	G
46	S2	598	G
46	S2	604	A
46	S2	607	U
46	S2	614	C
46	S2	628	A
46	S2	629	A
46	S2	631	U
46	S2	643	A
46	S2	655	A
46	S2	660	C
46	S2	664	A
46	S2	668	A2M
46	S2	669	A
46	S2	671	A

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Mol	Chain	Res	Type
46	S2	672	A
46	S2	673	G
46	S2	688	U
46	S2	689	U
46	S2	690	G
46	S2	692	G
46	S2	696	G
46	S2	698	G
46	S2	732	U
46	S2	733	C
46	S2	736	C
46	S2	738	C
46	S2	739	C
46	S2	748	C
46	S2	751	G
46	S2	752	G
46	S2	753	C
46	S2	789	G
46	S2	791	C
46	S2	794	A
46	S2	797	C
46	S2	798	G
46	S2	799	U
46	S2	811	A
46	S2	821	G
46	S2	822	PSU
46	S2	823	PSU
46	S2	830	A
46	S2	834	C
46	S2	835	C
46	S2	836	G
46	S2	837	A
46	S2	838	G
46	S2	839	C
46	S2	840	C
46	S2	841	G
46	S2	842	C
46	S2	847	A
46	S2	867	OMG
46	S2	869	A
46	S2	870	A
46	S2	872	A

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Mol	Chain	Res	Type
46	S2	874	G
46	S2	877	C
46	S2	884	C
46	S2	888	U
46	S2	889	U
46	S2	891	G
46	S2	892	U
46	S2	896	U
46	S2	898	U
46	S2	899	U
46	S2	900	C
46	S2	901	G
46	S2	903	A
46	S2	909	G
46	S2	913	A
46	S2	917	U
46	S2	920	A
46	S2	930	C
46	S2	933	G
46	S2	934	G
46	S2	943	U
46	S2	955	A
46	S2	963	A
46	S2	990	A
46	S2	992	A
46	S2	999	G
46	S2	1001	A
46	S2	1017	U
46	S2	1023	A
46	S2	1027	A
46	S2	1061	U
46	S2	1062	A
46	S2	1067	C
46	S2	1083	A
46	S2	1085	C
46	S2	1109	C
46	S2	1114	U
46	S2	1116	C
46	S2	1118	C
46	S2	1133	A
46	S2	1138	C
46	S2	1153	C

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Mol	Chain	Res	Type
46	S2	1154	U
46	S2	1195	A
46	S2	1203	G
46	S2	1207	G
46	S2	1208	A
46	S2	1215	C
46	S2	1216	C
46	S2	1217	A
46	S2	1224	G
46	S2	1242	U
46	S2	1243	PSU
46	S2	1251	A
46	S2	1253	A
46	S2	1256	G
46	S2	1257	G
46	S2	1259	A
46	S2	1264	C
46	S2	1274	G
46	S2	1275	G
46	S2	1277	C
46	S2	1283	C
46	S2	1284	A
46	S2	1285	G
46	S2	1286	G
46	S2	1290	G
46	S2	1300	U
46	S2	1301	A
46	S2	1302	G
46	S2	1303	C
46	S2	1308	U
46	S2	1309	C
46	S2	1327	G
46	S2	1342	U
46	S2	1343	U
46	S2	1348	G
46	S2	1371	U
46	S2	1372	U
46	S2	1373	C
46	S2	1378	A
46	S2	1391	OMC
46	S2	1397	U
46	S2	1401	A

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Mol	Chain	Res	Type
46	S2	1402	A
46	S2	1404	U
46	S2	1419	C
46	S2	1421	A
46	S2	1423	C
46	S2	1435	C
46	S2	1436	C
46	S2	1438	A
46	S2	1442	OMU
46	S2	1454	A
46	S2	1462	U
46	S2	1463	U
46	S2	1480	A
46	S2	1487	A
46	S2	1489	A
46	S2	1490	OMG
46	S2	1494	U
46	S2	1495	G
46	S2	1497	G
46	S2	1498	A
46	S2	1506	A
46	S2	1507	G
46	S2	1508	A
46	S2	1510	G
46	S2	1520	G
46	S2	1521	C
46	S2	1522	A
46	S2	1533	A
46	S2	1548	G
46	S2	1552	G
46	S2	1553	C
46	S2	1556	A
46	S2	1560	U
46	S2	1579	A
46	S2	1580	A
46	S2	1585	U
46	S2	1586	U
46	S2	1587	G
46	S2	1588	A
46	S2	1601	A
46	S2	1621	U
46	S2	1623	A

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Mol	Chain	Res	Type
46	S2	1634	A
46	S2	1648	G
46	S2	1654	G
46	S2	1664	A
46	S2	1665	G
46	S2	1671	G
46	S2	1680	G
46	S2	1686	G
46	S2	1699	A
46	S2	1721	U
46	S2	1722	G
46	S2	1744	G
46	S2	1752	C
46	S2	1753	C
46	S2	1754	G
46	S2	1758	G
46	S2	1760	G
46	S2	1761	U
46	S2	1773	C
46	S2	1774	C
46	S2	1775	U
46	S2	1777	G
46	S2	1783	C
46	S2	1784	G
46	S2	1786	U
46	S2	1819	A
46	S2	1824	A
46	S2	1825	A
46	S2	1829	G
46	S2	1831	A
46	S2	1835	A
46	S2	1838	U
46	S2	1849	G
46	S2	1852	C
46	S2	1861	G
46	S2	1862	G
46	S2	1863	A
46	S2	1864	U
46	S2	1865	C

All (20) RNA pucker outliers are listed below:

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	1633	G
1	L1	2760	G
1	L1	3614	G
1	L1	3673	C
1	L1	4678	G
1	L1	4699	U
46	S2	112	U
46	S2	563	G
46	S2	628	A
46	S2	688	U
46	S2	867	OMG
46	S2	954	U
46	S2	1434	C
46	S2	1497	G
46	S2	1520	G

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

143 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$
46	5MU	S2	814	46	19,22,23	7.24	8 (42%)	28,32,35	3.31	12 (42%)
1	A2M	L1	1524	1	18,25,26	4.12	8 (44%)	18,36,39	3.48	3 (16%)
1	OMC	L1	2824	1	19,22,23	2.97	8 (42%)	26,31,34	0.97	2 (7%)
46	OMG	S2	867	46	18,26,27	2.58	8 (44%)	19,38,41	1.52	4 (21%)
46	OMC	S2	1272	46	19,22,23	3.06	8 (42%)	26,31,34	0.82	0
46	OMU	S2	172	46	19,22,23	2.89	6 (31%)	26,31,34	1.76	5 (19%)
46	A2M	S2	468	46	18,25,26	4.24	8 (44%)	18,36,39	3.41	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	OMU	S2	1442	46,80	19,22,23	2.91	8 (42%)	26,31,34	1.67	5 (19%)
46	MA6	S2	1850	46	19,26,27	1.15	2 (10%)	18,38,41	4.51	3 (16%)
1	A2M	L1	3830	1	18,25,26	4.20	7 (38%)	18,36,39	3.43	3 (16%)
3	OMG	L3	75	3	18,26,27	2.54	8 (44%)	19,38,41	1.53	4 (21%)
46	OMU	S2	116	46	19,22,23	2.86	6 (31%)	26,31,34	1.69	5 (19%)
1	OMC	L1	2351	1,80	19,22,23	2.95	8 (42%)	26,31,34	1.16	3 (11%)
1	A2M	L1	3825	1	18,25,26	4.24	7 (38%)	18,36,39	3.33	3 (16%)
1	OMG	L1	4494	1	18,26,27	2.52	8 (44%)	19,38,41	1.51	4 (21%)
1	PSU	L1	1683	1,81	18,21,22	1.11	1 (5%)	22,30,33	1.91	5 (22%)
1	OMG	L1	2876	1	18,26,27	2.53	8 (44%)	19,38,41	1.53	4 (21%)
1	OMG	L1	3792	1	18,26,27	2.48	8 (44%)	19,38,41	1.44	4 (21%)
46	OMG	S2	1490	46,80	18,26,27	2.49	8 (44%)	19,38,41	1.41	4 (21%)
1	PSU	L1	4636	1	18,21,22	1.10	1 (5%)	22,30,33	1.96	5 (22%)
1	PSU	L1	4403	1	18,21,22	1.05	1 (5%)	22,30,33	1.65	4 (18%)
1	PSU	L1	4450	1,80	18,21,22	1.03	1 (5%)	22,30,33	1.78	5 (22%)
43	MLZ	Lo	53	43	8,9,10	0.71	0	4,9,11	0.64	0
1	A2M	L1	2787	1	18,25,26	4.20	8 (44%)	18,36,39	3.40	4 (22%)
46	OMG	S2	644	46	18,26,27	2.50	8 (44%)	19,38,41	1.44	4 (21%)
1	OMU	L1	4306	1	19,22,23	2.82	6 (31%)	26,31,34	1.71	5 (19%)
1	PSU	L1	4293	1	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
46	A2M	S2	166	46	18,25,26	4.28	7 (38%)	18,36,39	3.49	3 (16%)
46	A2M	S2	159	46	18,25,26	4.25	7 (38%)	18,36,39	3.42	3 (16%)
1	A2M	L1	4523	1,80	18,25,26	4.22	7 (38%)	18,36,39	3.49	3 (16%)
1	OMG	L1	3627	1	18,26,27	2.50	8 (44%)	19,38,41	1.53	3 (15%)
46	5MC	S2	1374	46	18,22,23	3.56	7 (38%)	26,32,35	1.05	2 (7%)
1	UR3	L1	4530	1	19,22,23	2.71	7 (36%)	26,32,35	1.33	3 (11%)
1	PSU	L1	4442	1	18,21,22	1.03	1 (5%)	22,30,33	1.77	4 (18%)
46	6MZ	S2	1832	46,80	18,25,26	2.09	3 (16%)	16,36,39	2.41	4 (25%)
46	OMU	S2	1288	46	19,22,23	2.98	8 (42%)	26,31,34	1.69	5 (19%)
46	A2M	S2	99	46,80	18,25,26	4.24	6 (33%)	18,36,39	3.34	3 (16%)
1	A2M	L1	400	1	18,25,26	4.22	8 (44%)	18,36,39	3.32	3 (16%)
1	OMG	L1	1316	1,80	18,26,27	2.56	8 (44%)	19,38,41	1.61	3 (15%)
1	OMC	L1	4456	1	19,22,23	2.87	8 (42%)	26,31,34	0.82	1 (3%)
46	OMG	S2	601	46	18,26,27	2.52	8 (44%)	19,38,41	1.41	3 (15%)
1	PSU	L1	3764	1	18,21,22	1.05	1 (5%)	22,30,33	1.63	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	S2	119	46	18,21,22	1.00	1 (5%)	22,30,33	1.65	4 (18%)
46	4AC	S2	1842	46	21,24,25	3.32	10 (47%)	29,34,37	1.06	3 (10%)
46	A2M	S2	484	46	18,25,26	4.20	7 (38%)	18,36,39	3.51	3 (16%)
1	OMU	L1	2837	1	19,22,23	2.84	6 (31%)	26,31,34	1.74	6 (23%)
1	OMC	L1	1881	1,80	19,22,23	2.93	8 (42%)	26,31,34	0.92	0
1	1MA	L1	1322	1,80	16,25,26	3.51	4 (25%)	18,37,40	2.09	4 (22%)
1	OMU	L1	3925	1	19,22,23	2.92	7 (36%)	26,31,34	1.77	4 (15%)
1	PSU	L1	3715	1	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
1	A2M	L1	1326	1	18,25,26	4.16	7 (38%)	18,36,39	3.46	3 (16%)
46	A2M	S2	668	46,80	18,25,26	4.14	7 (38%)	18,36,39	3.62	3 (16%)
46	OMC	S2	174	46,80	19,22,23	2.99	8 (42%)	26,31,34	0.75	0
1	OMG	L1	2424	1	18,26,27	2.54	8 (44%)	19,38,41	1.49	4 (21%)
46	4AC	S2	1337	46	21,24,25	3.45	10 (47%)	29,34,37	1.06	2 (6%)
1	OMC	L1	3841	1	19,22,23	2.99	8 (42%)	26,31,34	0.95	1 (3%)
46	M7A	S2	1806	46	20,25,26	1.88	5 (25%)	28,37,40	3.87	8 (28%)
1	2MG	L1	1517	1	18,26,27	2.18	7 (38%)	16,38,41	1.55	4 (25%)
1	OMG	L1	4618	1	18,26,27	2.54	8 (44%)	19,38,41	1.53	5 (26%)
1	OMG	L1	4196	1	18,26,27	2.52	8 (44%)	19,38,41	1.51	4 (21%)
46	OMC	S2	1703	46	19,22,23	2.97	8 (42%)	26,31,34	0.72	0
46	PSU	S2	612	46	18,21,22	1.06	1 (5%)	22,30,33	1.78	5 (22%)
46	OMG	S2	683	46	18,26,27	2.53	8 (44%)	19,38,41	1.55	4 (21%)
46	PSU	S2	1243	46,80	18,21,22	1.07	1 (5%)	22,30,33	1.67	4 (18%)
1	OMC	L1	2861	1	19,22,23	2.96	8 (42%)	26,31,34	0.75	0
1	A2M	L1	3723	1	18,25,26	4.26	6 (33%)	18,36,39	3.37	3 (16%)
1	OMG	L1	3744	1	18,26,27	2.56	8 (44%)	19,38,41	1.49	4 (21%)
1	OMG	L1	4637	1	18,26,27	2.47	8 (44%)	19,38,41	1.42	3 (15%)
1	2MG	L1	729	1	18,26,27	2.14	8 (44%)	16,38,41	1.37	3 (18%)
46	UY1	S2	1326	46,80	19,22,23	4.34	12 (63%)	22,31,34	1.85	3 (13%)
1	JMH	L1	1456	1	18,22,23	2.64	5 (27%)	21,32,35	0.89	1 (4%)
46	OMG	S2	1328	46	18,26,27	2.58	8 (44%)	19,38,41	1.50	4 (21%)
1	A2M	L1	1871	1,80	18,25,26	4.22	6 (33%)	18,36,39	3.43	3 (16%)
1	OMC	L1	4536	1	19,22,23	2.84	8 (42%)	26,31,34	0.79	0
46	A2M	S2	1678	46	18,25,26	4.27	7 (38%)	18,36,39	3.45	3 (16%)
1	OMC	L1	3887	1	19,22,23	2.93	8 (42%)	26,31,34	0.81	0
1	A2M	L1	3867	1	18,25,26	4.16	8 (44%)	18,36,39	3.39	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	6MZ	L1	4220	1	18,25,26	1.95	3 (16%)	16,36,39	2.26	4 (25%)
1	A2M	L1	4571	1	18,25,26	4.28	7 (38%)	18,36,39	3.52	3 (16%)
46	JMH	S2	1219	46,80	18,22,23	2.78	5 (27%)	21,32,35	1.60	4 (19%)
1	PSU	L1	4531	1	18,21,22	1.12	1 (5%)	22,30,33	1.79	5 (22%)
1	PSU	L1	1582	1	18,21,22	1.07	1 (5%)	22,30,33	1.59	4 (18%)
46	OMU	S2	121	46	19,22,23	2.86	6 (31%)	26,31,34	1.75	5 (19%)
46	PSU	S2	1081	46	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
1	PSU	L1	4628	1	18,21,22	0.99	1 (5%)	22,30,33	1.78	5 (22%)
46	A2M	S2	27	46,80	18,25,26	4.22	7 (38%)	18,36,39	3.41	3 (16%)
46	OMU	S2	354	46	19,22,23	2.82	6 (31%)	26,31,34	1.73	5 (19%)
46	OMG	S2	509	46	18,26,27	2.46	8 (44%)	19,38,41	1.44	4 (21%)
1	A2M	L1	1534	1,80	18,25,26	4.30	8 (44%)	18,36,39	3.61	3 (16%)
46	A2M	S2	1031	46	18,25,26	4.18	7 (38%)	18,36,39	3.45	3 (16%)
1	PSU	L1	2508	1	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
46	OMC	S2	462	46	19,22,23	2.99	8 (42%)	26,31,34	0.76	0
1	OMC	L1	2422	1,80	19,22,23	2.89	8 (42%)	26,31,34	0.77	1 (3%)
46	PSU	S2	823	46	18,21,22	1.76	6 (33%)	22,30,33	2.06	4 (18%)
1	OMG	L1	4228	1	18,26,27	2.54	8 (44%)	19,38,41	1.54	4 (21%)
1	A2M	L1	2401	1	18,25,26	4.19	8 (44%)	18,36,39	3.51	3 (16%)
1	B8H	L1	3762	1	19,22,23	6.72	6 (31%)	22,32,35	2.35	5 (22%)
1	OMC	L1	1340	1	19,22,23	2.83	8 (42%)	26,31,34	0.82	0
46	OMC	S2	517	46	19,22,23	2.97	8 (42%)	26,31,34	0.80	1 (3%)
1	OMG	L1	4499	1	18,26,27	2.55	8 (44%)	19,38,41	1.48	4 (21%)
1	OMG	L1	4623	1	18,26,27	2.49	8 (44%)	19,38,41	1.46	3 (15%)
1	OMG	L1	2364	1	18,26,27	2.50	8 (44%)	19,38,41	1.57	4 (21%)
46	UR3	S2	1830	46	19,22,23	2.78	7 (36%)	26,32,35	1.54	4 (15%)
1	OMG	L1	4392	1	18,26,27	2.50	8 (44%)	19,38,41	1.45	4 (21%)
46	MA6	S2	1851	46	19,26,27	0.98	1 (5%)	18,38,41	4.80	3 (16%)
1	5MC	L1	4335	1	18,22,23	3.50	7 (38%)	26,32,35	1.06	2 (7%)
1	OMC	L1	3869	1	19,22,23	2.96	8 (42%)	26,31,34	0.94	1 (3%)
1	UY1	L1	3818	1,81,80	19,22,23	4.44	12 (63%)	22,31,34	1.92	4 (18%)
1	A2M	L1	2815	1	18,25,26	4.25	6 (33%)	18,36,39	3.39	3 (16%)
46	OMG	S2	436	46	18,26,27	2.53	8 (44%)	19,38,41	1.52	4 (21%)
46	A2M	S2	1383	46	18,25,26	4.27	6 (33%)	18,36,39	3.51	3 (16%)
1	A2M	L1	3718	1	18,25,26	4.22	6 (33%)	18,36,39	3.35	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	L1	3782	1,80	18,22,23	3.37	7 (38%)	26,32,35	1.10	2 (7%)
46	OMU	S2	428	46	19,22,23	2.88	6 (31%)	26,31,34	1.68	4 (15%)
46	OMC	S2	1710	46	19,22,23	2.99	8 (42%)	26,31,34	0.88	1 (3%)
1	PSU	L1	4500	1	18,21,22	0.95	1 (5%)	22,30,33	1.76	5 (22%)
1	OMU	L1	4620	1	19,22,23	2.83	7 (36%)	26,31,34	1.70	4 (15%)
1	OMG	L1	3944	1	18,26,27	2.56	8 (44%)	19,38,41	1.52	4 (21%)
46	A2M	S2	590	46	18,25,26	4.24	6 (33%)	18,36,39	3.43	3 (16%)
1	OMC	L1	3701	1,80	19,22,23	2.87	8 (42%)	26,31,34	0.86	0
46	OMC	S2	1391	46	19,22,23	2.98	8 (42%)	26,31,34	0.90	1 (3%)
1	OMU	L1	4498	1	19,22,23	2.86	6 (31%)	26,31,34	1.77	4 (15%)
1	PSU	L1	3729	1	18,21,22	1.03	1 (5%)	22,30,33	1.70	4 (18%)
1	5MC	L1	4447	1,80	18,22,23	3.51	7 (38%)	26,32,35	1.26	2 (7%)
1	OMC	L1	2365	1,80	19,22,23	2.85	8 (42%)	26,31,34	0.70	0
46	B8N	S2	1248	46	24,29,30	3.10	6 (25%)	29,42,45	1.72	6 (20%)
1	PSU	L1	1677	1,81	18,21,22	1.12	2 (11%)	22,30,33	1.69	4 (18%)
1	OMC	L1	3808	1	19,22,23	2.94	8 (42%)	26,31,34	0.98	1 (3%)
1	2MG	L1	978	1	18,26,27	2.26	8 (44%)	16,38,41	1.55	4 (25%)
3	OMU	L3	14	1,3	19,22,23	2.85	7 (36%)	26,31,34	1.79	4 (15%)
1	OMU	L1	4227	1	19,22,23	2.89	8 (42%)	26,31,34	1.74	4 (15%)
1	OMG	L1	3899	1	18,26,27	2.52	8 (44%)	19,38,41	1.57	5 (26%)
46	A2M	S2	512	46	18,25,26	4.22	6 (33%)	18,36,39	3.47	3 (16%)
1	A2M	L1	3785	1	18,25,26	3.94	8 (44%)	18,36,39	3.52	3 (16%)
1	OMG	L1	1522	1	18,26,27	2.54	8 (44%)	19,38,41	1.63	4 (21%)
1	OMG	L1	1625	1	18,26,27	2.52	8 (44%)	19,38,41	1.49	4 (21%)
1	OMG	L1	4370	1	18,26,27	2.53	8 (44%)	19,38,41	1.47	3 (15%)
46	PSU	S2	822	46	18,21,22	1.06	1 (5%)	22,30,33	1.82	5 (22%)
1	A2M	L1	398	1	18,25,26	4.23	7 (38%)	18,36,39	3.31	3 (16%)
1	B8T	L1	4671	1	19,22,23	3.19	8 (42%)	26,31,34	0.91	1 (3%)
1	OMC	L1	2804	1	19,22,23	2.92	8 (42%)	26,31,34	0.81	0
46	A2M	S2	576	46	18,25,26	4.22	6 (33%)	18,36,39	3.40	3 (16%)
1	A2M	L1	2363	1,80	18,25,26	4.21	8 (44%)	18,36,39	3.22	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
46	5MU	S2	814	46	-	0/7/25/26	0/2/2/2
1	A2M	L1	1524	1	-	0/5/27/28	0/3/3/3
1	OMC	L1	2824	1	-	1/9/27/28	0/2/2/2
46	OMG	S2	867	46	-	3/5/27/28	0/3/3/3
46	OMC	S2	1272	46	-	0/9/27/28	0/2/2/2
46	OMU	S2	172	46	-	0/9/27/28	0/2/2/2
46	A2M	S2	468	46	-	0/5/27/28	0/3/3/3
46	OMU	S2	1442	46,80	-	3/9/27/28	0/2/2/2
46	MA6	S2	1850	46	-	0/7/29/30	0/3/3/3
1	A2M	L1	3830	1	-	0/5/27/28	0/3/3/3
3	OMG	L3	75	3	-	1/5/27/28	0/3/3/3
46	OMU	S2	116	46	-	1/9/27/28	0/2/2/2
1	OMC	L1	2351	1,80	-	2/9/27/28	0/2/2/2
1	A2M	L1	3825	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	4494	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	1683	1,81	-	0/7/25/26	0/2/2/2
1	OMG	L1	2876	1	-	1/5/27/28	0/3/3/3
1	OMG	L1	3792	1	-	3/5/27/28	0/3/3/3
46	OMG	S2	1490	46,80	-	1/5/27/28	0/3/3/3
1	PSU	L1	4636	1	-	3/7/25/26	0/2/2/2
1	PSU	L1	4403	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	4450	1,80	-	2/7/25/26	0/2/2/2
43	MLZ	Lo	53	43	-	3/7/8/10	-
1	A2M	L1	2787	1	-	2/5/27/28	0/3/3/3
46	OMG	S2	644	46	-	1/5/27/28	0/3/3/3
1	OMU	L1	4306	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	4293	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	166	46	-	0/5/27/28	0/3/3/3
46	A2M	S2	159	46	-	2/5/27/28	0/3/3/3
1	A2M	L1	4523	1,80	-	0/5/27/28	0/3/3/3
1	OMG	L1	3627	1	-	0/5/27/28	0/3/3/3
46	5MC	S2	1374	46	-	0/7/25/26	0/2/2/2
1	UR3	L1	4530	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	4442	1	-	0/7/25/26	0/2/2/2
46	6MZ	S2	1832	46,80	-	0/5/27/28	0/3/3/3
46	OMU	S2	1288	46	-	1/9/27/28	0/2/2/2
46	A2M	S2	99	46,80	-	2/5/27/28	0/3/3/3
1	A2M	L1	400	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	1316	1,80	-	0/5/27/28	0/3/3/3
1	OMC	L1	4456	1	-	0/9/27/28	0/2/2/2
46	OMG	S2	601	46	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L1	3764	1	-	2/7/25/26	0/2/2/2
46	PSU	S2	119	46	-	0/7/25/26	0/2/2/2
46	4AC	S2	1842	46	-	0/11/29/30	0/2/2/2
46	A2M	S2	484	46	-	0/5/27/28	0/3/3/3
1	OMU	L1	2837	1	-	0/9/27/28	0/2/2/2
1	OMC	L1	1881	1,80	-	0/9/27/28	0/2/2/2
1	1MA	L1	1322	1,80	-	0/3/25/26	0/3/3/3
1	OMU	L1	3925	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	3715	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	1326	1	-	1/5/27/28	0/3/3/3
46	A2M	S2	668	46,80	-	2/5/27/28	0/3/3/3
46	OMC	S2	174	46,80	-	0/9/27/28	0/2/2/2
1	OMG	L1	2424	1	-	2/5/27/28	0/3/3/3
46	4AC	S2	1337	46	-	0/11/29/30	0/2/2/2
1	OMC	L1	3841	1	-	2/9/27/28	0/2/2/2
46	M7A	S2	1806	46	-	0/7/37/38	0/3/3/3
1	2MG	L1	1517	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	4618	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	4196	1	-	1/5/27/28	0/3/3/3
46	OMC	S2	1703	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	612	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	683	46	-	1/5/27/28	0/3/3/3
46	PSU	S2	1243	46,80	-	2/7/25/26	0/2/2/2
1	OMC	L1	2861	1	-	0/9/27/28	0/2/2/2
1	A2M	L1	3723	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	3744	1	-	1/5/27/28	0/3/3/3
1	OMG	L1	4637	1	-	1/5/27/28	0/3/3/3
1	2MG	L1	729	1	-	1/5/27/28	0/3/3/3
46	UY1	S2	1326	46,80	-	2/9/27/28	0/2/2/2
1	JMH	L1	1456	1	-	0/7/25/26	0/2/2/2
46	OMG	S2	1328	46	-	1/5/27/28	0/3/3/3
1	A2M	L1	1871	1,80	-	0/5/27/28	0/3/3/3
1	OMC	L1	4536	1	-	0/9/27/28	0/2/2/2
46	A2M	S2	1678	46	-	1/5/27/28	0/3/3/3
1	OMC	L1	3887	1	-	1/9/27/28	0/2/2/2
1	A2M	L1	3867	1	-	2/5/27/28	0/3/3/3
1	6MZ	L1	4220	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	4571	1	-	0/5/27/28	0/3/3/3
46	JMH	S2	1219	46,80	-	1/7/25/26	0/2/2/2
1	PSU	L1	4531	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	1582	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	OMU	S2	121	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	1081	46	-	1/7/25/26	0/2/2/2
1	PSU	L1	4628	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	27	46,80	-	0/5/27/28	0/3/3/3
46	OMU	S2	354	46	-	0/9/27/28	0/2/2/2
46	OMG	S2	509	46	-	0/5/27/28	0/3/3/3
1	A2M	L1	1534	1,80	-	3/5/27/28	0/3/3/3
46	A2M	S2	1031	46	-	0/5/27/28	0/3/3/3
1	PSU	L1	2508	1	-	0/7/25/26	0/2/2/2
46	OMC	S2	462	46	-	0/9/27/28	0/2/2/2
1	OMC	L1	2422	1,80	-	1/9/27/28	0/2/2/2
46	PSU	S2	823	46	-	2/7/25/26	0/2/2/2
1	OMG	L1	4228	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	2401	1	-	1/5/27/28	0/3/3/3
1	B8H	L1	3762	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	1340	1	-	2/9/27/28	0/2/2/2
46	OMC	S2	517	46	-	0/9/27/28	0/2/2/2
1	OMG	L1	4499	1	-	2/5/27/28	0/3/3/3
1	OMG	L1	4623	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	2364	1	-	2/5/27/28	0/3/3/3
46	UR3	S2	1830	46	-	2/7/25/26	0/2/2/2
1	OMG	L1	4392	1	-	0/5/27/28	0/3/3/3
46	MA6	S2	1851	46	-	2/7/29/30	0/3/3/3
1	5MC	L1	4335	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	3869	1	-	1/9/27/28	0/2/2/2
1	UY1	L1	3818	1,81,80	-	6/9/27/28	0/2/2/2
1	A2M	L1	2815	1	-	0/5/27/28	0/3/3/3
46	OMG	S2	436	46	-	0/5/27/28	0/3/3/3
46	A2M	S2	1383	46	-	0/5/27/28	0/3/3/3
1	A2M	L1	3718	1	-	0/5/27/28	0/3/3/3
1	5MC	L1	3782	1,80	-	0/7/25/26	0/2/2/2
46	OMU	S2	428	46	-	5/9/27/28	0/2/2/2
46	OMC	S2	1710	46	-	0/9/27/28	0/2/2/2
1	PSU	L1	4500	1	-	3/7/25/26	0/2/2/2
1	OMU	L1	4620	1	-	0/9/27/28	0/2/2/2
1	OMG	L1	3944	1	-	2/5/27/28	0/3/3/3
46	A2M	S2	590	46	-	3/5/27/28	0/3/3/3
1	OMC	L1	3701	1,80	-	4/9/27/28	0/2/2/2
46	OMC	S2	1391	46	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	L1	4498	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	3729	1	-	2/7/25/26	0/2/2/2
1	5MC	L1	4447	1,80	-	4/7/25/26	0/2/2/2
1	OMC	L1	2365	1,80	-	0/9/27/28	0/2/2/2
46	B8N	S2	1248	46	-	2/16/34/35	0/2/2/2
1	PSU	L1	1677	1,81	-	3/7/25/26	0/2/2/2
1	OMC	L1	3808	1	-	2/9/27/28	0/2/2/2
1	2MG	L1	978	1	-	0/5/27/28	0/3/3/3
3	OMU	L3	14	1,3	-	1/9/27/28	0/2/2/2
1	OMU	L1	4227	1	-	0/9/27/28	0/2/2/2
1	OMG	L1	3899	1	-	0/5/27/28	0/3/3/3
46	A2M	S2	512	46	-	2/5/27/28	0/3/3/3
1	A2M	L1	3785	1	-	2/5/27/28	0/3/3/3
1	OMG	L1	1522	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	1625	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	4370	1	-	0/5/27/28	0/3/3/3
46	PSU	S2	822	46	-	1/7/25/26	0/2/2/2
1	A2M	L1	398	1	-	2/5/27/28	0/3/3/3
1	B8T	L1	4671	1	-	0/7/27/28	0/2/2/2
1	OMC	L1	2804	1	-	0/9/27/28	0/2/2/2
46	A2M	S2	576	46	-	2/5/27/28	0/3/3/3
1	A2M	L1	2363	1,80	-	2/5/27/28	0/3/3/3

All (910) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	814	5MU	C4-C5	20.67	1.79	1.44
46	S2	814	5MU	C6-N1	16.38	1.66	1.38
1	L1	3762	B8H	C6-C5	-15.56	1.13	1.34
46	S2	166	A2M	O4'-C1'	15.50	1.62	1.41
46	S2	1383	A2M	O4'-C1'	15.48	1.62	1.41
1	L1	1534	A2M	O4'-C1'	15.40	1.62	1.41
1	L1	4571	A2M	O4'-C1'	15.37	1.62	1.41
1	L1	3723	A2M	O4'-C1'	15.33	1.62	1.41
1	L1	1871	A2M	O4'-C1'	15.24	1.62	1.41
1	L1	398	A2M	O4'-C1'	15.23	1.62	1.41
1	L1	2815	A2M	O4'-C1'	15.23	1.62	1.41
46	S2	99	A2M	O4'-C1'	15.23	1.62	1.41
46	S2	468	A2M	O4'-C1'	15.23	1.62	1.41
46	S2	1678	A2M	O4'-C1'	15.23	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4523	A2M	O4'-C1'	15.21	1.62	1.41
46	S2	159	A2M	O4'-C1'	15.20	1.62	1.41
46	S2	576	A2M	O4'-C1'	15.18	1.62	1.41
1	L1	3718	A2M	O4'-C1'	15.18	1.62	1.41
46	S2	590	A2M	O4'-C1'	15.16	1.62	1.41
1	L1	3825	A2M	O4'-C1'	15.15	1.62	1.41
46	S2	512	A2M	O4'-C1'	15.14	1.62	1.41
1	L1	400	A2M	O4'-C1'	15.13	1.62	1.41
46	S2	27	A2M	O4'-C1'	15.11	1.62	1.41
1	L1	2401	A2M	O4'-C1'	15.07	1.62	1.41
1	L1	3830	A2M	O4'-C1'	15.06	1.62	1.41
46	S2	484	A2M	O4'-C1'	15.04	1.62	1.41
1	L1	2363	A2M	O4'-C1'	15.03	1.62	1.41
46	S2	1031	A2M	O4'-C1'	15.03	1.62	1.41
1	L1	2787	A2M	O4'-C1'	15.01	1.62	1.41
1	L1	1326	A2M	O4'-C1'	14.89	1.61	1.41
1	L1	3762	B8H	C4-N3	-14.87	1.11	1.38
1	L1	3867	A2M	O4'-C1'	14.70	1.61	1.41
46	S2	668	A2M	O4'-C1'	14.51	1.61	1.41
1	L1	1524	A2M	O4'-C1'	14.42	1.61	1.41
1	L1	3762	B8H	C4-C5	14.06	1.84	1.44
1	L1	3785	A2M	O4'-C1'	13.93	1.60	1.41
1	L1	3762	B8H	C6-N1	12.59	1.67	1.36
1	L1	1322	1MA	C2-N3	12.39	1.44	1.29
1	L1	3818	UY1	O4'-C1'	-11.54	1.28	1.43
46	S2	1326	UY1	O4'-C1'	-11.21	1.28	1.43
46	S2	814	5MU	C4-N3	-11.12	1.18	1.38
46	S2	814	5MU	C6-C5	-10.71	1.17	1.34
1	L1	4447	5MC	C6-C5	9.30	1.49	1.34
46	S2	1374	5MC	C6-C5	9.07	1.49	1.34
1	L1	4335	5MC	C6-C5	8.88	1.49	1.34
1	L1	3782	5MC	C6-C5	8.80	1.49	1.34
46	S2	1219	JMH	C2-N1	8.01	1.50	1.38
46	S2	1832	6MZ	C6-N6	7.89	1.47	1.35
46	S2	1248	B8N	C6-N1	7.80	1.55	1.36
46	S2	1288	OMU	C2-N1	7.44	1.50	1.38
46	S2	1830	UR3	C2-N1	7.43	1.49	1.38
46	S2	1248	B8N	C4-N3	-7.38	1.26	1.40
1	L1	3925	OMU	C2-N1	7.25	1.50	1.38
1	L1	4671	B8T	C4-N3	7.18	1.45	1.32
1	L1	4220	6MZ	C6-N6	7.16	1.46	1.35
1	L1	3818	UY1	C3'-C4'	-7.13	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4498	OMU	C2-N1	7.13	1.49	1.38
3	L3	14	OMU	C2-N1	7.11	1.49	1.38
1	L1	4227	OMU	C2-N1	7.03	1.49	1.38
46	S2	1326	UY1	C3'-C4'	-7.03	1.35	1.53
46	S2	1442	OMU	C2-N1	6.97	1.49	1.38
46	S2	172	OMU	C2-N1	6.95	1.49	1.38
1	L1	1456	JMH	C2-N1	6.95	1.48	1.38
46	S2	1337	4AC	C4-N3	6.92	1.44	1.32
1	L1	2837	OMU	C2-N1	6.91	1.49	1.38
1	L1	4530	UR3	C2-N1	6.88	1.48	1.38
46	S2	116	OMU	C2-N1	6.86	1.49	1.38
1	L1	1524	A2M	O4'-C4'	-6.86	1.29	1.45
46	S2	428	OMU	C2-N1	6.83	1.49	1.38
46	S2	121	OMU	C2-N1	6.82	1.49	1.38
46	S2	668	A2M	O4'-C4'	-6.82	1.29	1.45
46	S2	1248	B8N	C6-C5	6.68	1.44	1.34
46	S2	354	OMU	C2-N1	6.67	1.49	1.38
1	L1	4306	OMU	C2-N1	6.66	1.49	1.38
46	S2	1288	OMU	C2-N3	6.65	1.49	1.38
1	L1	4620	OMU	C2-N1	6.64	1.49	1.38
46	S2	1842	4AC	C4-N3	6.64	1.44	1.32
1	L1	1534	A2M	O4'-C4'	-6.60	1.30	1.45
46	S2	1442	OMU	C2-N3	6.58	1.49	1.38
1	L1	3867	A2M	O4'-C4'	-6.58	1.30	1.45
46	S2	172	OMU	C2-N3	6.57	1.49	1.38
46	S2	590	A2M	O4'-C4'	-6.57	1.30	1.45
46	S2	1678	A2M	O4'-C4'	-6.51	1.30	1.45
46	S2	116	OMU	C2-N3	6.50	1.49	1.38
46	S2	428	OMU	C2-N3	6.49	1.49	1.38
46	S2	1272	OMC	C2-N3	6.48	1.49	1.36
46	S2	1248	B8N	C2-N1	6.48	1.58	1.39
46	S2	121	OMU	C2-N3	6.46	1.49	1.38
46	S2	1374	5MC	C4-N3	6.45	1.45	1.34
1	L1	400	A2M	O4'-C4'	-6.38	1.30	1.45
46	S2	468	A2M	O4'-C4'	-6.38	1.30	1.45
1	L1	4571	A2M	O4'-C4'	-6.38	1.30	1.45
46	S2	159	A2M	O4'-C4'	-6.38	1.30	1.45
1	L1	4523	A2M	O4'-C4'	-6.36	1.30	1.45
46	S2	1710	OMC	C2-N3	6.35	1.49	1.36
46	S2	27	A2M	O4'-C4'	-6.34	1.30	1.45
1	L1	2815	A2M	O4'-C4'	-6.33	1.30	1.45
1	L1	4498	OMU	C2-N3	6.32	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1337	4AC	C6-C5	6.32	1.49	1.35
1	L1	2363	A2M	O4'-C4'	-6.31	1.30	1.45
1	L1	398	A2M	O4'-C4'	-6.31	1.30	1.45
1	L1	3723	A2M	O4'-C4'	-6.31	1.30	1.45
46	S2	462	OMC	C2-N3	6.30	1.49	1.36
46	S2	1326	UY1	O4'-C4'	6.29	1.59	1.45
46	S2	512	A2M	O4'-C4'	-6.27	1.31	1.45
46	S2	1391	OMC	C2-N3	6.26	1.49	1.36
1	L1	2861	OMC	C2-N3	6.26	1.49	1.36
46	S2	576	A2M	O4'-C4'	-6.26	1.31	1.45
46	S2	517	OMC	C2-N3	6.25	1.49	1.36
46	S2	174	OMC	C2-N3	6.25	1.49	1.36
1	L1	4335	5MC	C4-N3	6.25	1.44	1.34
1	L1	4227	OMU	C2-N3	6.25	1.49	1.38
46	S2	484	A2M	O4'-C4'	-6.25	1.31	1.45
46	S2	99	A2M	O4'-C4'	-6.23	1.31	1.45
1	L1	3925	OMU	C2-N3	6.23	1.49	1.38
1	L1	4306	OMU	C2-N3	6.23	1.49	1.38
46	S2	1703	OMC	C2-N3	6.23	1.49	1.36
1	L1	3825	A2M	O4'-C4'	-6.22	1.31	1.45
1	L1	4620	OMU	C2-N3	6.21	1.49	1.38
46	S2	166	A2M	O4'-C4'	-6.21	1.31	1.45
46	S2	354	OMU	C2-N3	6.19	1.49	1.38
1	L1	3830	A2M	O4'-C4'	-6.18	1.31	1.45
46	S2	1031	A2M	O4'-C4'	-6.18	1.31	1.45
1	L1	2837	OMU	C2-N3	6.16	1.48	1.38
46	S2	1383	A2M	O4'-C4'	-6.16	1.31	1.45
1	L1	1326	A2M	O4'-C4'	-6.15	1.31	1.45
1	L1	4335	5MC	C2-N3	6.13	1.48	1.36
1	L1	3818	UY1	O4'-C4'	6.12	1.58	1.45
1	L1	2401	A2M	O4'-C4'	-6.11	1.31	1.45
1	L1	3718	A2M	O4'-C4'	-6.11	1.31	1.45
1	L1	2824	OMC	C2-N3	6.11	1.48	1.36
1	L1	3701	OMC	C6-C5	6.11	1.49	1.35
1	L1	2787	A2M	O4'-C4'	-6.10	1.31	1.45
3	L3	14	OMU	C2-N3	6.09	1.48	1.38
1	L1	2351	OMC	C6-C5	6.08	1.49	1.35
1	L1	3841	OMC	C2-N3	6.08	1.48	1.36
46	S2	1337	4AC	C2-N3	6.07	1.48	1.36
1	L1	2804	OMC	C2-N3	6.06	1.48	1.36
46	S2	1830	UR3	C6-C5	6.04	1.49	1.35
46	S2	1842	4AC	C6-C5	6.04	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1881	OMC	C2-N3	6.03	1.48	1.36
46	S2	1374	5MC	C2-N3	6.03	1.48	1.36
1	L1	3869	OMC	C6-C5	6.03	1.49	1.35
1	L1	2422	OMC	C6-C5	6.01	1.49	1.35
46	S2	462	OMC	C6-C5	6.01	1.49	1.35
46	S2	1272	OMC	C6-C5	5.98	1.49	1.35
1	L1	3808	OMC	C6-C5	5.97	1.48	1.35
46	S2	174	OMC	C6-C5	5.97	1.48	1.35
1	L1	3808	OMC	C2-N3	5.96	1.48	1.36
1	L1	1340	OMC	C2-N3	5.95	1.48	1.36
1	L1	1871	A2M	O4'-C4'	-5.95	1.31	1.45
46	S2	517	OMC	C6-C5	5.95	1.48	1.35
1	L1	4447	5MC	C4-N3	5.95	1.44	1.34
46	S2	1710	OMC	C6-C5	5.94	1.48	1.35
46	S2	1391	OMC	C6-C5	5.91	1.48	1.35
1	L1	2861	OMC	C6-C5	5.91	1.48	1.35
1	L1	4671	B8T	C6-C5	5.91	1.48	1.35
1	L1	2351	OMC	C2-N3	5.90	1.48	1.36
1	L1	3887	OMC	C6-C5	5.90	1.48	1.35
1	L1	3869	OMC	C2-N3	5.90	1.48	1.36
1	L1	3785	A2M	O4'-C4'	-5.90	1.31	1.45
1	L1	4530	UR3	C6-C5	5.90	1.48	1.35
1	L1	3841	OMC	C6-C5	5.89	1.48	1.35
1	L1	3887	OMC	C2-N3	5.88	1.48	1.36
46	S2	1703	OMC	C6-C5	5.88	1.48	1.35
1	L1	1456	JMH	C6-C5	5.87	1.48	1.35
1	L1	4456	OMC	C6-C5	5.87	1.48	1.35
1	L1	3782	5MC	C4-N3	5.86	1.44	1.34
1	L1	2804	OMC	C6-C5	5.85	1.48	1.35
1	L1	2365	OMC	C6-C5	5.84	1.48	1.35
1	L1	4536	OMC	C6-C5	5.83	1.48	1.35
46	S2	1288	OMU	C6-C5	5.81	1.48	1.35
1	L1	2422	OMC	C2-N3	5.81	1.48	1.36
1	L1	4447	5MC	C2-N3	5.79	1.48	1.36
46	S2	172	OMU	C6-C5	5.79	1.48	1.35
46	S2	1442	OMU	C6-C5	5.79	1.48	1.35
1	L1	4536	OMC	C2-N3	5.79	1.48	1.36
1	L1	3701	OMC	C2-N3	5.77	1.48	1.36
1	L1	1881	OMC	C6-C5	5.77	1.48	1.35
1	L1	3925	OMU	C6-C5	5.77	1.48	1.35
46	S2	428	OMU	C6-C5	5.76	1.48	1.35
1	L1	1340	OMC	C6-C5	5.75	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3782	5MC	C2-N3	5.74	1.48	1.36
46	S2	1842	4AC	C2-N3	5.74	1.48	1.36
1	L1	2837	OMU	C6-C5	5.74	1.48	1.35
46	S2	354	OMU	C6-C5	5.74	1.48	1.35
1	L1	4456	OMC	C2-N3	5.74	1.48	1.36
46	S2	1219	JMH	C6-C5	5.74	1.48	1.35
1	L1	2824	OMC	C6-C5	5.73	1.48	1.35
46	S2	1337	4AC	C7-N4	5.71	1.47	1.37
1	L1	4227	OMU	C6-C5	5.71	1.48	1.35
1	L1	4620	OMU	C6-C5	5.70	1.48	1.35
46	S2	121	OMU	C6-C5	5.69	1.48	1.35
1	L1	2365	OMC	C2-N3	5.67	1.47	1.36
1	L1	4306	OMU	C6-C5	5.66	1.48	1.35
3	L3	14	OMU	C6-C5	5.65	1.48	1.35
46	S2	116	OMU	C6-C5	5.60	1.48	1.35
1	L1	4671	B8T	C2-N3	5.59	1.47	1.36
46	S2	1337	4AC	C4-N4	5.58	1.47	1.39
1	L1	4499	OMG	C2-N3	5.51	1.46	1.33
1	L1	4498	OMU	C6-C5	5.51	1.47	1.35
46	S2	1328	OMG	C2-N3	5.49	1.46	1.33
1	L1	2876	OMG	C2-N3	5.47	1.46	1.33
1	L1	1625	OMG	C2-N3	5.45	1.46	1.33
1	L1	4637	OMG	C2-N3	5.45	1.46	1.33
1	L1	3818	UY1	O2-C2	-5.44	1.12	1.23
1	L1	4494	OMG	C2-N3	5.44	1.46	1.33
1	L1	3818	UY1	O4-C4	-5.42	1.13	1.23
46	S2	867	OMG	C2-N3	5.42	1.46	1.33
1	L1	3744	OMG	C2-N3	5.40	1.46	1.33
1	L1	3944	OMG	C2-N3	5.38	1.46	1.33
46	S2	601	OMG	C2-N3	5.37	1.46	1.33
1	L1	4228	OMG	C2-N3	5.37	1.46	1.33
46	S2	1842	4AC	C7-N4	5.35	1.47	1.37
1	L1	1522	OMG	C2-N3	5.34	1.46	1.33
1	L1	4370	OMG	C2-N3	5.34	1.46	1.33
46	S2	1326	UY1	O4-C4	-5.34	1.13	1.23
1	L1	3792	OMG	C2-N3	5.33	1.46	1.33
1	L1	4196	OMG	C2-N3	5.32	1.46	1.33
46	S2	644	OMG	C2-N3	5.31	1.46	1.33
46	S2	1490	OMG	C2-N3	5.31	1.46	1.33
1	L1	2364	OMG	C2-N3	5.30	1.46	1.33
46	S2	436	OMG	C2-N3	5.30	1.46	1.33
1	L1	4392	OMG	C2-N3	5.30	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	509	OMG	C2-N3	5.29	1.46	1.33
46	S2	683	OMG	C2-N3	5.28	1.46	1.33
1	L1	4618	OMG	C2-N3	5.28	1.46	1.33
3	L3	75	OMG	C2-N3	5.26	1.46	1.33
1	L1	1316	OMG	C2-N3	5.26	1.46	1.33
1	L1	2424	OMG	C2-N3	5.26	1.46	1.33
46	S2	1272	OMC	C4-N3	5.22	1.45	1.34
1	L1	3899	OMG	C2-N3	5.22	1.45	1.33
1	L1	3627	OMG	C2-N3	5.19	1.45	1.33
46	S2	814	5MU	C2-N3	5.17	1.47	1.38
1	L1	978	2MG	C2-N2	5.17	1.44	1.33
1	L1	3744	OMG	C4-N3	5.14	1.49	1.37
46	S2	1842	4AC	C4-N4	5.14	1.47	1.39
1	L1	4623	OMG	C2-N3	5.14	1.45	1.33
46	S2	1703	OMC	C4-N3	5.12	1.44	1.34
1	L1	4530	UR3	C2-N3	5.12	1.48	1.39
46	S2	174	OMC	C4-N3	5.06	1.44	1.34
46	S2	462	OMC	C4-N3	5.03	1.44	1.34
46	S2	436	OMG	C4-N3	5.03	1.49	1.37
1	L1	4618	OMG	C4-N3	5.01	1.49	1.37
1	L1	2876	OMG	C4-N3	4.99	1.49	1.37
1	L1	4370	OMG	C4-N3	4.99	1.49	1.37
1	L1	3944	OMG	C4-N3	4.98	1.49	1.37
1	L1	3792	OMG	C4-N3	4.98	1.49	1.37
46	S2	1490	OMG	C4-N3	4.97	1.49	1.37
46	S2	867	OMG	C4-N3	4.97	1.49	1.37
1	L1	2824	OMC	C4-N3	4.97	1.44	1.34
46	S2	683	OMG	C4-N3	4.97	1.49	1.37
46	S2	1328	OMG	C4-N3	4.97	1.49	1.37
1	L1	1522	OMG	C4-N3	4.96	1.49	1.37
1	L1	729	2MG	C2-N2	4.95	1.44	1.33
46	S2	1272	OMC	C4-N4	4.95	1.45	1.33
46	S2	1710	OMC	C4-N3	4.94	1.44	1.34
1	L1	4228	OMG	C4-N3	4.94	1.49	1.37
3	L3	75	OMG	C4-N3	4.94	1.49	1.37
46	S2	517	OMC	C4-N3	4.94	1.44	1.34
46	S2	1326	UY1	O2-C2	-4.93	1.13	1.23
46	S2	601	OMG	C4-N3	4.93	1.49	1.37
1	L1	1517	2MG	C2-N2	4.93	1.44	1.33
1	L1	1625	OMG	C4-N3	4.92	1.49	1.37
1	L1	1340	OMC	C4-N3	4.91	1.44	1.34
1	L1	4494	OMG	C4-N3	4.91	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1391	OMC	C4-N3	4.90	1.44	1.34
1	L1	1316	OMG	C4-N3	4.90	1.49	1.37
46	S2	462	OMC	C4-N4	4.88	1.45	1.33
46	S2	1391	OMC	C4-N4	4.88	1.45	1.33
46	S2	174	OMC	C4-N4	4.87	1.45	1.33
1	L1	2861	OMC	C4-N3	4.87	1.44	1.34
1	L1	3841	OMC	C4-N3	4.86	1.44	1.34
1	L1	3762	B8H	C2-N3	4.85	1.46	1.38
46	S2	1219	JMH	C2-N3	4.85	1.48	1.39
46	S2	1326	UY1	C1'-C5	4.84	1.61	1.50
1	L1	3899	OMG	C4-N3	4.83	1.49	1.37
1	L1	2351	OMC	C4-N4	4.83	1.45	1.33
1	L1	2424	OMG	C4-N3	4.83	1.49	1.37
46	S2	1710	OMC	C4-N4	4.83	1.45	1.33
1	L1	4499	OMG	C4-N3	4.82	1.49	1.37
1	L1	1881	OMC	C4-N3	4.81	1.44	1.34
1	L1	3869	OMC	C4-N3	4.81	1.44	1.34
46	S2	867	OMG	C2-N2	4.81	1.45	1.34
1	L1	2364	OMG	C4-N3	4.80	1.49	1.37
46	S2	1830	UR3	C2-N3	4.80	1.48	1.39
46	S2	644	OMG	C4-N3	4.79	1.49	1.37
1	L1	2424	OMG	C2-N2	4.79	1.45	1.34
1	L1	3841	OMC	C2-N1	4.78	1.50	1.40
1	L1	4392	OMG	C4-N3	4.78	1.49	1.37
1	L1	3887	OMC	C4-N3	4.78	1.44	1.34
1	L1	3627	OMG	C4-N3	4.77	1.48	1.37
1	L1	4196	OMG	C4-N3	4.76	1.48	1.37
46	S2	1703	OMC	C4-N4	4.76	1.45	1.33
1	L1	2861	OMC	C4-N4	4.76	1.45	1.33
46	S2	1328	OMG	C2-N2	4.75	1.45	1.34
1	L1	3808	OMC	C4-N4	4.74	1.45	1.33
1	L1	2365	OMC	C4-N3	4.74	1.44	1.34
46	S2	517	OMC	C4-N4	4.73	1.45	1.33
1	L1	4499	OMG	C2-N2	4.73	1.45	1.34
1	L1	2804	OMC	C4-N3	4.73	1.44	1.34
1	L1	3944	OMG	C2-N2	4.72	1.45	1.34
1	L1	4637	OMG	C4-N3	4.72	1.48	1.37
46	S2	1272	OMC	C2-N1	4.71	1.50	1.40
1	L1	3887	OMC	C4-N4	4.70	1.45	1.33
46	S2	509	OMG	C4-N3	4.69	1.48	1.37
1	L1	3869	OMC	C4-N4	4.68	1.44	1.33
1	L1	4671	B8T	C4-N4	4.68	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4623	OMG	C4-N3	4.68	1.48	1.37
46	S2	1391	OMC	C2-N1	4.67	1.50	1.40
46	S2	1710	OMC	C2-N1	4.67	1.50	1.40
1	L1	2824	OMC	C4-N4	4.67	1.44	1.33
46	S2	601	OMG	C2-N2	4.67	1.45	1.34
1	L1	2422	OMC	C4-N4	4.66	1.44	1.33
1	L1	3899	OMG	C2-N2	4.65	1.45	1.34
46	S2	1806	M7A	C6-N6	4.64	1.45	1.34
1	L1	1625	OMG	C2-N2	4.63	1.45	1.34
1	L1	2804	OMC	C4-N4	4.63	1.44	1.33
1	L1	2824	OMC	C2-N1	4.62	1.50	1.40
1	L1	4447	5MC	C6-N1	4.62	1.45	1.38
46	S2	1374	5MC	C6-N1	4.61	1.45	1.38
1	L1	3818	UY1	C1'-C5	4.60	1.60	1.50
1	L1	2351	OMC	C2-N1	4.60	1.50	1.40
1	L1	3808	OMC	C4-N3	4.60	1.43	1.34
46	S2	683	OMG	C2-N2	4.59	1.45	1.34
46	S2	644	OMG	C2-N2	4.58	1.45	1.34
46	S2	436	OMG	C2-N2	4.58	1.45	1.34
46	S2	1490	OMG	C2-N2	4.58	1.45	1.34
1	L1	3841	OMC	C4-N4	4.58	1.44	1.33
1	L1	1316	OMG	C2-N2	4.58	1.45	1.34
1	L1	4618	OMG	C2-N2	4.57	1.45	1.34
1	L1	4494	OMG	C2-N2	4.57	1.45	1.34
1	L1	3869	OMC	C2-N1	4.57	1.49	1.40
1	L1	3701	OMC	C4-N4	4.56	1.44	1.33
1	L1	4456	OMC	C4-N4	4.56	1.44	1.33
1	L1	2351	OMC	C4-N3	4.56	1.43	1.34
1	L1	2365	OMC	C4-N4	4.54	1.44	1.33
1	L1	4196	OMG	C2-N2	4.54	1.45	1.34
1	L1	4228	OMG	C2-N2	4.53	1.45	1.34
1	L1	3808	OMC	C2-N1	4.52	1.49	1.40
3	L3	75	OMG	C2-N2	4.52	1.44	1.34
1	L1	3744	OMG	C2-N2	4.52	1.44	1.34
1	L1	3701	OMC	C4-N3	4.51	1.43	1.34
1	L1	1340	OMC	C4-N4	4.51	1.44	1.33
1	L1	2861	OMC	C2-N1	4.51	1.49	1.40
1	L1	2364	OMG	C2-N2	4.50	1.44	1.34
1	L1	4536	OMC	C4-N4	4.50	1.44	1.33
1	L1	4370	OMG	C2-N2	4.50	1.44	1.34
1	L1	1881	OMC	C4-N4	4.49	1.44	1.33
1	L1	3627	OMG	C2-N2	4.48	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4623	OMG	C2-N2	4.48	1.44	1.34
1	L1	3792	OMG	C2-N2	4.47	1.44	1.34
1	L1	4456	OMC	C4-N3	4.47	1.43	1.34
46	S2	517	OMC	C2-N1	4.47	1.49	1.40
1	L1	1456	JMH	C2-N3	4.46	1.47	1.39
46	S2	509	OMG	C2-N2	4.46	1.44	1.34
1	L1	2876	OMG	C2-N2	4.45	1.44	1.34
46	S2	462	OMC	C2-N1	4.45	1.49	1.40
1	L1	2422	OMC	C4-N3	4.45	1.43	1.34
46	S2	174	OMC	C2-N1	4.45	1.49	1.40
1	L1	4637	OMG	C2-N2	4.44	1.44	1.34
1	L1	4392	OMG	C2-N2	4.44	1.44	1.34
1	L1	4536	OMC	C4-N3	4.44	1.43	1.34
1	L1	1881	OMC	C2-N1	4.39	1.49	1.40
1	L1	2804	OMC	C2-N1	4.37	1.49	1.40
1	L1	1522	OMG	C2-N2	4.35	1.44	1.34
1	L1	4456	OMC	C2-N1	4.31	1.49	1.40
46	S2	1374	5MC	C4-N4	4.30	1.45	1.34
1	L1	4335	5MC	C6-N1	4.29	1.45	1.38
1	L1	4335	5MC	C4-N4	4.27	1.45	1.34
46	S2	1703	OMC	C2-N1	4.26	1.49	1.40
1	L1	4536	OMC	C2-N1	4.25	1.49	1.40
1	L1	2422	OMC	C2-N1	4.25	1.49	1.40
1	L1	4335	5MC	C2-N1	4.24	1.49	1.40
1	L1	3887	OMC	C2-N1	4.24	1.49	1.40
46	S2	1374	5MC	C2-N1	4.23	1.49	1.40
46	S2	1337	4AC	C5-C4	4.21	1.49	1.40
1	L1	2365	OMC	C2-N1	4.20	1.49	1.40
46	S2	1326	UY1	C6-C5	4.19	1.40	1.35
1	L1	4671	B8T	C2-N1	4.19	1.49	1.40
1	L1	4447	5MC	C4-N4	4.19	1.45	1.34
1	L1	1322	1MA	C2-N1	4.17	1.43	1.35
46	S2	1842	4AC	C5-C4	4.16	1.49	1.40
1	L1	3782	5MC	C6-N1	4.06	1.45	1.38
1	L1	3818	UY1	C6-C5	4.03	1.40	1.35
1	L1	3701	OMC	C2-N1	4.02	1.48	1.40
1	L1	3782	5MC	C4-N4	4.01	1.44	1.34
46	S2	814	5MU	C2-N1	3.99	1.44	1.38
1	L1	1340	OMC	C2-N1	3.99	1.48	1.40
1	L1	3782	5MC	C2-N1	3.96	1.48	1.40
1	L1	3818	UY1	C2-N3	-3.95	1.30	1.37
46	S2	1337	4AC	C2-N1	3.94	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1842	4AC	C2-N1	3.87	1.48	1.40
1	L1	1322	1MA	C4-N3	3.81	1.49	1.37
1	L1	729	2MG	C4-N3	3.79	1.46	1.37
1	L1	978	2MG	C6-N1	3.75	1.43	1.37
1	L1	3887	OMC	C6-N1	3.70	1.46	1.38
46	S2	1326	UY1	C2-N3	-3.64	1.31	1.37
1	L1	3944	OMG	C6-N1	3.63	1.43	1.37
1	L1	4531	PSU	C6-C5	3.63	1.39	1.35
1	L1	1517	2MG	C6-N1	3.61	1.43	1.37
1	L1	978	2MG	C4-N3	3.60	1.46	1.37
1	L1	4447	5MC	C2-N1	3.60	1.47	1.40
46	S2	867	OMG	C6-N1	3.59	1.43	1.37
46	S2	1806	M7A	C2-N1	3.59	1.40	1.33
3	L3	75	OMG	C6-N1	3.57	1.43	1.37
1	L1	2424	OMG	C6-N1	3.57	1.43	1.37
46	S2	1328	OMG	C6-N1	3.56	1.43	1.37
1	L1	4671	B8T	C5-C4	3.55	1.48	1.40
46	S2	1243	PSU	C6-C5	3.54	1.39	1.35
46	S2	1806	M7A	C71-N7	-3.53	1.40	1.46
1	L1	2351	OMC	C6-N1	3.52	1.46	1.38
46	S2	1288	OMU	C4-N3	3.52	1.44	1.38
1	L1	1683	PSU	C6-C5	3.50	1.39	1.35
1	L1	1517	2MG	C4-N3	3.48	1.45	1.37
46	S2	1442	OMU	C4-N3	3.47	1.44	1.38
46	S2	683	OMG	C6-N1	3.46	1.43	1.37
46	S2	1081	PSU	C6-C5	3.46	1.39	1.35
1	L1	978	2MG	C2-N1	3.45	1.42	1.36
1	L1	4636	PSU	C6-C5	3.44	1.39	1.35
1	L1	3764	PSU	C6-C5	3.44	1.39	1.35
1	L1	4618	OMG	C6-N1	3.43	1.43	1.37
46	S2	116	OMU	C4-N3	3.42	1.44	1.38
1	L1	1582	PSU	C6-C5	3.42	1.39	1.35
1	L1	3869	OMC	C6-N1	3.42	1.46	1.38
1	L1	4671	B8T	C6-N1	3.39	1.46	1.38
1	L1	4392	OMG	C6-N1	3.39	1.42	1.37
1	L1	1881	OMC	O2-C2	-3.38	1.17	1.23
1	L1	4499	OMG	C6-N1	3.37	1.42	1.37
46	S2	822	PSU	C6-C5	3.37	1.39	1.35
1	L1	3899	OMG	C6-N1	3.37	1.42	1.37
1	L1	4403	PSU	C6-C5	3.36	1.39	1.35
1	L1	3744	OMG	C6-N1	3.36	1.42	1.37
1	L1	4228	OMG	C6-N1	3.36	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	172	OMU	C4-N3	3.35	1.44	1.38
1	L1	1316	OMG	C5-C6	3.35	1.54	1.47
46	S2	428	OMU	C4-N3	3.35	1.44	1.38
46	S2	436	OMG	C6-N1	3.35	1.42	1.37
46	S2	119	PSU	C6-C5	3.34	1.39	1.35
1	L1	4370	OMG	C6-N1	3.34	1.42	1.37
1	L1	4536	OMC	C6-N1	3.33	1.46	1.38
1	L1	1522	OMG	C6-N1	3.33	1.42	1.37
1	L1	1456	JMH	C6-N1	3.33	1.46	1.38
1	L1	4442	PSU	C6-C5	3.32	1.39	1.35
1	L1	2508	PSU	C6-C5	3.31	1.39	1.35
46	S2	823	PSU	C4-N3	-3.31	1.32	1.38
46	S2	1490	OMG	C6-N1	3.31	1.42	1.37
1	L1	2365	OMC	C6-N1	3.30	1.46	1.38
1	L1	3841	OMC	O2-C2	-3.30	1.17	1.23
1	L1	4456	OMC	O2-C2	-3.30	1.17	1.23
46	S2	1842	4AC	O2-C2	-3.30	1.17	1.23
1	L1	729	2MG	C6-N1	3.29	1.42	1.37
46	S2	644	OMG	C6-N1	3.28	1.42	1.37
1	L1	2422	OMC	C6-N1	3.27	1.45	1.38
1	L1	1517	2MG	C2-N1	3.26	1.41	1.36
1	L1	3808	OMC	C6-N1	3.26	1.45	1.38
46	S2	159	A2M	O3'-C3'	-3.26	1.35	1.43
1	L1	2804	OMC	C6-N1	3.25	1.45	1.38
46	S2	601	OMG	C6-N1	3.25	1.42	1.37
1	L1	4447	5MC	O2-C2	-3.25	1.17	1.23
1	L1	3701	OMC	C6-N1	3.24	1.45	1.38
46	S2	612	PSU	C6-C5	3.24	1.39	1.35
1	L1	3627	OMG	C6-N1	3.24	1.42	1.37
46	S2	174	OMC	C6-N1	3.24	1.45	1.38
1	L1	3729	PSU	C6-C5	3.24	1.39	1.35
1	L1	4293	PSU	C6-C5	3.24	1.39	1.35
1	L1	3715	PSU	C6-C5	3.23	1.39	1.35
1	L1	4227	OMU	C4-N3	3.23	1.44	1.38
46	S2	1337	4AC	C6-N1	3.22	1.45	1.38
1	L1	3925	OMU	O2-C2	-3.22	1.17	1.23
46	S2	462	OMC	C6-N1	3.21	1.45	1.38
1	L1	729	2MG	C2-N1	3.21	1.41	1.36
46	S2	1272	OMC	C6-N1	3.21	1.45	1.38
46	S2	517	OMC	C6-N1	3.21	1.45	1.38
1	L1	1677	PSU	C6-C5	3.20	1.39	1.35
1	L1	2876	OMG	C6-N1	3.20	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4671	B8T	O2-C2	-3.20	1.17	1.23
1	L1	4456	OMC	C6-N1	3.19	1.45	1.38
46	S2	121	OMU	C4-N3	3.19	1.44	1.38
1	L1	4392	OMG	C5-C6	3.19	1.53	1.47
1	L1	1316	OMG	C6-N1	3.18	1.42	1.37
1	L1	3841	OMC	C6-N1	3.18	1.45	1.38
46	S2	1391	OMC	C6-N1	3.18	1.45	1.38
46	S2	1248	B8N	O4-C4	-3.18	1.16	1.23
1	L1	3818	UY1	C2-N1	-3.18	1.32	1.36
46	S2	1703	OMC	C6-N1	3.17	1.45	1.38
1	L1	2861	OMC	C6-N1	3.17	1.45	1.38
46	S2	509	OMG	C6-N1	3.17	1.42	1.37
1	L1	4196	OMG	C6-N1	3.16	1.42	1.37
1	L1	3867	A2M	O3'-C3'	-3.16	1.35	1.43
1	L1	3701	OMC	O2-C2	-3.16	1.17	1.23
1	L1	4450	PSU	C6-C5	3.15	1.39	1.35
46	S2	354	OMU	C4-N3	3.15	1.44	1.38
46	S2	1326	UY1	C2-N1	-3.15	1.32	1.36
1	L1	1881	OMC	C6-N1	3.14	1.45	1.38
1	L1	4623	OMG	C6-N1	3.13	1.42	1.37
1	L1	2824	OMC	C6-N1	3.13	1.45	1.38
1	L1	2422	OMC	O2-C2	-3.13	1.17	1.23
46	S2	1710	OMC	C6-N1	3.13	1.45	1.38
1	L1	4494	OMG	C6-N1	3.13	1.42	1.37
1	L1	4571	A2M	C6-N6	3.12	1.45	1.34
46	S2	1678	A2M	C6-N6	3.12	1.45	1.34
46	S2	1703	OMC	O2-C2	-3.12	1.17	1.23
46	S2	1219	JMH	C6-N1	3.12	1.45	1.38
1	L1	3825	A2M	O3'-C3'	-3.12	1.35	1.43
46	S2	512	A2M	O3'-C3'	-3.12	1.35	1.43
1	L1	4536	OMC	O2-C2	-3.12	1.17	1.23
1	L1	3830	A2M	O3'-C3'	-3.11	1.35	1.43
46	S2	590	A2M	C6-N6	3.11	1.45	1.34
1	L1	2815	A2M	O3'-C3'	-3.11	1.35	1.43
46	S2	1842	4AC	C6-N1	3.11	1.45	1.38
1	L1	2364	OMG	C6-N1	3.11	1.42	1.37
46	S2	823	PSU	C2'-C1'	-3.11	1.49	1.53
3	L3	14	OMU	O4-C4	-3.11	1.18	1.24
46	S2	166	A2M	C6-N6	3.10	1.45	1.34
1	L1	2824	OMC	O2-C2	-3.10	1.18	1.23
1	L1	3825	A2M	C5-C4	-3.10	1.32	1.40
46	S2	99	A2M	O3'-C3'	-3.10	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1031	A2M	C6-N6	3.10	1.45	1.34
1	L1	3723	A2M	C6-N6	3.09	1.45	1.34
46	S2	159	A2M	C6-N6	3.09	1.45	1.34
1	L1	2815	A2M	C6-N6	3.09	1.45	1.34
1	L1	4623	OMG	C5-C6	3.09	1.53	1.47
46	S2	1678	A2M	O3'-C3'	-3.09	1.35	1.43
46	S2	484	A2M	C6-N6	3.08	1.45	1.34
46	S2	576	A2M	C6-N6	3.08	1.45	1.34
1	L1	3627	OMG	C5-C6	3.08	1.53	1.47
46	S2	1383	A2M	C6-N6	3.08	1.45	1.34
1	L1	2804	OMC	O2-C2	-3.08	1.18	1.23
46	S2	1806	M7A	C4-N9	3.08	1.43	1.38
1	L1	4306	OMU	C4-N3	3.07	1.44	1.38
3	L3	75	OMG	C5-C6	3.07	1.53	1.47
46	S2	468	A2M	O3'-C3'	-3.06	1.35	1.43
1	L1	4620	OMU	O2-C2	-3.06	1.17	1.23
46	S2	166	A2M	O3'-C3'	-3.06	1.35	1.43
1	L1	400	A2M	O3'-C3'	-3.05	1.35	1.43
1	L1	4571	A2M	O3'-C3'	-3.05	1.35	1.43
1	L1	3718	A2M	C6-N6	3.05	1.45	1.34
1	L1	4498	OMU	C4-N3	3.05	1.44	1.38
46	S2	468	A2M	C6-N6	3.05	1.45	1.34
1	L1	4620	OMU	O4-C4	-3.05	1.18	1.24
1	L1	4628	PSU	C6-C5	3.05	1.38	1.35
1	L1	4196	OMG	C5-C6	3.05	1.53	1.47
46	S2	668	A2M	O3'-C3'	-3.04	1.35	1.43
46	S2	512	A2M	C6-N6	3.04	1.45	1.34
1	L1	4306	OMU	O4-C4	-3.04	1.18	1.24
1	L1	3867	A2M	C6-N6	3.04	1.45	1.34
1	L1	3925	OMU	C4-N3	3.04	1.44	1.38
46	S2	590	A2M	O3'-C3'	-3.03	1.35	1.43
46	S2	27	A2M	O3'-C3'	-3.03	1.35	1.43
1	L1	2787	A2M	O3'-C3'	-3.03	1.35	1.43
46	S2	1328	OMG	C5-C6	3.03	1.53	1.47
1	L1	2837	OMU	C4-N3	3.03	1.44	1.38
1	L1	3744	OMG	C5-C6	3.03	1.53	1.47
46	S2	1830	UR3	C6-N1	3.02	1.45	1.38
1	L1	3830	A2M	C6-N6	3.02	1.45	1.34
46	S2	576	A2M	O3'-C3'	-3.02	1.35	1.43
1	L1	2365	OMC	O2-C2	-3.02	1.18	1.23
1	L1	3785	A2M	C5-C4	-3.01	1.33	1.40
1	L1	1326	A2M	O3'-C3'	-3.01	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	400	A2M	C6-N6	3.01	1.45	1.34
1	L1	4618	OMG	C5-C6	3.01	1.53	1.47
46	S2	27	A2M	C6-N6	3.01	1.45	1.34
1	L1	2401	A2M	O3'-C3'	-3.01	1.35	1.43
1	L1	1524	A2M	C6-N6	3.00	1.45	1.34
46	S2	1678	A2M	O2'-C2'	2.99	1.50	1.42
1	L1	4494	OMG	C5-C6	2.99	1.53	1.47
1	L1	2401	A2M	C6-N6	2.99	1.44	1.34
1	L1	4637	OMG	C6-N1	2.99	1.42	1.37
1	L1	3782	5MC	O2-C2	-2.99	1.18	1.23
46	S2	484	A2M	O2'-C2'	2.99	1.50	1.42
1	L1	4530	UR3	C6-N1	2.99	1.45	1.38
1	L1	4370	OMG	C5-C6	2.98	1.53	1.47
1	L1	398	A2M	C6-N6	2.98	1.44	1.34
1	L1	3723	A2M	O3'-C3'	-2.98	1.36	1.43
1	L1	3887	OMC	O2-C2	-2.98	1.18	1.23
1	L1	2815	A2M	O2'-C2'	2.98	1.50	1.42
3	L3	14	OMU	O2-C2	-2.98	1.17	1.23
1	L1	1871	A2M	O3'-C3'	-2.98	1.36	1.43
1	L1	1326	A2M	C6-N6	2.98	1.44	1.34
46	S2	867	OMG	C5-C6	2.97	1.53	1.47
46	S2	668	A2M	C5-C4	-2.97	1.33	1.40
1	L1	1625	OMG	C6-N1	2.97	1.42	1.37
46	S2	601	OMG	C5-C6	2.97	1.53	1.47
1	L1	3869	OMC	O2-C2	-2.97	1.18	1.23
46	S2	668	A2M	C6-N6	2.96	1.44	1.34
1	L1	1871	A2M	C6-N6	2.96	1.44	1.34
1	L1	2787	A2M	C6-N6	2.96	1.44	1.34
46	S2	644	OMG	C5-C6	2.95	1.53	1.47
1	L1	3944	OMG	C5-C6	2.95	1.53	1.47
1	L1	3825	A2M	C6-N6	2.95	1.44	1.34
46	S2	99	A2M	C6-N6	2.95	1.44	1.34
46	S2	121	OMU	O2-C2	-2.94	1.17	1.23
1	L1	4637	OMG	C5-C6	2.94	1.53	1.47
1	L1	3718	A2M	O2'-C2'	2.94	1.50	1.42
46	S2	1031	A2M	O2'-C2'	2.94	1.50	1.42
1	L1	2363	A2M	C6-N6	2.93	1.44	1.34
1	L1	1534	A2M	C6-N6	2.93	1.44	1.34
1	L1	1522	OMG	C5-C6	2.93	1.53	1.47
1	L1	4227	OMU	O2-C2	-2.93	1.17	1.23
1	L1	398	A2M	O3'-C3'	-2.93	1.36	1.43
1	L1	3808	OMC	O2-C2	-2.92	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1383	A2M	O3'-C3'	-2.92	1.36	1.43
46	S2	668	A2M	O2'-C2'	2.92	1.50	1.42
1	L1	4523	A2M	C6-N6	2.91	1.44	1.34
1	L1	1534	A2M	O3'-C3'	-2.91	1.36	1.43
1	L1	4620	OMU	C4-N3	2.91	1.43	1.38
1	L1	1340	OMC	O2-C2	-2.91	1.18	1.23
1	L1	2861	OMC	O2-C2	-2.91	1.18	1.23
46	S2	1850	MA6	C5-C4	-2.90	1.33	1.40
1	L1	3899	OMG	C5-C4	-2.90	1.35	1.43
1	L1	2837	OMU	O2-C2	-2.90	1.17	1.23
1	L1	1625	OMG	C5-C6	2.89	1.53	1.47
1	L1	3792	OMG	C5-C6	2.89	1.53	1.47
1	L1	3867	A2M	O2'-C2'	2.89	1.50	1.42
1	L1	1316	OMG	O6-C6	-2.88	1.17	1.23
1	L1	1322	1MA	C5-C4	-2.88	1.35	1.43
1	L1	4571	A2M	O2'-C2'	2.88	1.50	1.42
1	L1	3792	OMG	C6-N1	2.88	1.42	1.37
1	L1	4499	OMG	C5-C6	2.88	1.53	1.47
1	L1	4498	OMU	O4-C4	-2.87	1.18	1.24
46	S2	354	OMU	O4-C4	-2.87	1.18	1.24
1	L1	2837	OMU	O4-C4	-2.87	1.18	1.24
1	L1	1524	A2M	O2'-C2'	2.87	1.50	1.42
46	S2	428	OMU	O4-C4	-2.87	1.18	1.24
1	L1	4227	OMU	O4-C4	-2.87	1.18	1.24
46	S2	517	OMC	O2-C2	-2.87	1.18	1.23
1	L1	2364	OMG	C5-C6	2.86	1.53	1.47
1	L1	3925	OMU	O4-C4	-2.86	1.18	1.24
46	S2	99	A2M	C5-C4	-2.86	1.33	1.40
1	L1	398	A2M	C5-C4	-2.86	1.33	1.40
1	L1	3825	A2M	O2'-C2'	2.85	1.49	1.42
46	S2	1383	A2M	O2'-C2'	2.85	1.49	1.42
46	S2	509	OMG	C5-C6	2.85	1.53	1.47
46	S2	1337	4AC	O2-C2	-2.84	1.18	1.23
1	L1	4228	OMG	C5-C6	2.84	1.53	1.47
1	L1	4498	OMU	O2-C2	-2.84	1.17	1.23
1	L1	2363	A2M	C5-C4	-2.83	1.33	1.40
1	L1	4306	OMU	O2-C2	-2.83	1.17	1.23
1	L1	3723	A2M	C5-C4	-2.83	1.33	1.40
46	S2	512	A2M	O2'-C2'	2.82	1.49	1.42
46	S2	468	A2M	C5-C4	-2.82	1.33	1.40
46	S2	1806	M7A	C5-N7	2.82	1.46	1.39
1	L1	3723	A2M	O2'-C2'	2.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1374	5MC	O2-C2	-2.81	1.18	1.23
46	S2	166	A2M	O2'-C2'	2.81	1.49	1.42
46	S2	1678	A2M	C5-C4	-2.81	1.33	1.40
1	L1	2351	OMC	O2-C2	-2.81	1.18	1.23
1	L1	2363	A2M	O2'-C2'	2.80	1.49	1.42
46	S2	27	A2M	C5-C4	-2.80	1.33	1.40
46	S2	159	A2M	O2'-C2'	2.79	1.49	1.42
1	L1	4523	A2M	O3'-C3'	-2.79	1.36	1.43
1	L1	4571	A2M	C5-C4	-2.79	1.33	1.40
46	S2	174	OMC	O2-C2	-2.79	1.18	1.23
46	S2	1490	OMG	C5-C6	2.79	1.53	1.47
46	S2	576	A2M	O2'-C2'	2.79	1.49	1.42
46	S2	590	A2M	O2'-C2'	2.79	1.49	1.42
46	S2	462	OMC	O2-C2	-2.78	1.18	1.23
1	L1	1871	A2M	C5-C4	-2.78	1.33	1.40
1	L1	2363	A2M	O3'-C3'	-2.78	1.36	1.43
1	L1	1534	A2M	O2'-C2'	2.78	1.49	1.42
46	S2	99	A2M	O2'-C2'	2.78	1.49	1.42
46	S2	354	OMU	O2-C2	-2.78	1.18	1.23
1	L1	2364	OMG	C5-C4	-2.78	1.36	1.43
1	L1	1326	A2M	C5-C4	-2.78	1.33	1.40
1	L1	2876	OMG	C5-C6	2.78	1.53	1.47
46	S2	1383	A2M	C5-C4	-2.77	1.33	1.40
1	L1	4623	OMG	C5-C4	-2.77	1.36	1.43
46	S2	436	OMG	C5-C6	2.77	1.53	1.47
1	L1	1340	OMC	C6-N1	2.77	1.44	1.38
1	L1	3830	A2M	O2'-C2'	2.77	1.49	1.42
1	L1	4618	OMG	C5-C4	-2.77	1.36	1.43
1	L1	1522	OMG	C5-C4	-2.77	1.36	1.43
1	L1	1326	A2M	O2'-C2'	2.77	1.49	1.42
1	L1	1534	A2M	C5-C4	-2.77	1.33	1.40
1	L1	2787	A2M	O2'-C2'	2.76	1.49	1.42
1	L1	3718	A2M	O3'-C3'	-2.76	1.36	1.43
46	S2	1031	A2M	O3'-C3'	-2.75	1.36	1.43
1	L1	2424	OMG	C5-C4	-2.75	1.36	1.43
1	L1	1517	2MG	O6-C6	-2.75	1.17	1.23
1	L1	1871	A2M	O2'-C2'	2.75	1.49	1.42
1	L1	2401	A2M	C5-C4	-2.75	1.33	1.40
1	L1	1522	OMG	O6-C6	-2.75	1.17	1.23
1	L1	4196	OMG	C5-C4	-2.75	1.36	1.43
1	L1	398	A2M	O2'-C2'	2.75	1.49	1.42
46	S2	1851	MA6	C5-C4	-2.74	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1391	OMC	O2-C2	-2.74	1.18	1.23
46	S2	1710	OMC	O2-C2	-2.74	1.18	1.23
1	L1	3830	A2M	C5-C4	-2.74	1.33	1.40
1	L1	400	A2M	C5-C4	-2.74	1.33	1.40
1	L1	3785	A2M	O2'-C2'	2.74	1.49	1.42
46	S2	121	OMU	O4-C4	-2.74	1.19	1.24
1	L1	1517	2MG	C5-C4	-2.74	1.36	1.43
1	L1	1524	A2M	O3'-C3'	-2.74	1.36	1.43
1	L1	2401	A2M	O2'-C2'	2.73	1.49	1.42
3	L3	75	OMG	C5-C4	-2.73	1.36	1.43
46	S2	576	A2M	C5-C4	-2.73	1.33	1.40
46	S2	814	5MU	O4-C4	-2.73	1.18	1.23
46	S2	484	A2M	O3'-C3'	-2.73	1.36	1.43
46	S2	468	A2M	O2'-C2'	2.73	1.49	1.42
1	L1	2815	A2M	C5-C4	-2.73	1.33	1.40
46	S2	116	OMU	O4-C4	-2.73	1.19	1.24
1	L1	4370	OMG	C5-C4	-2.73	1.36	1.43
1	L1	3718	A2M	C5-C4	-2.73	1.33	1.40
1	L1	3899	OMG	C5-C6	2.73	1.52	1.47
46	S2	116	OMU	O2-C2	-2.73	1.18	1.23
1	L1	2424	OMG	C5-C6	2.72	1.52	1.47
1	L1	4523	A2M	O2'-C2'	2.71	1.49	1.42
1	L1	4228	OMG	C5-C4	-2.71	1.36	1.43
46	S2	512	A2M	C5-C4	-2.71	1.33	1.40
46	S2	428	OMU	O2-C2	-2.71	1.18	1.23
46	S2	683	OMG	C5-C6	2.71	1.52	1.47
1	L1	4499	OMG	C5-C4	-2.71	1.36	1.43
1	L1	4196	OMG	C2-N1	2.70	1.44	1.37
46	S2	166	A2M	C5-C4	-2.70	1.33	1.40
1	L1	2876	OMG	C5-C4	-2.70	1.36	1.43
46	S2	484	A2M	C5-C4	-2.70	1.33	1.40
1	L1	3627	OMG	C5-C4	-2.69	1.36	1.43
1	L1	3867	A2M	C5-C4	-2.69	1.33	1.40
46	S2	159	A2M	C5-C4	-2.69	1.33	1.40
1	L1	400	A2M	O2'-C2'	2.69	1.49	1.42
46	S2	509	OMG	C5-C4	-2.68	1.36	1.43
46	S2	1031	A2M	C5-C4	-2.68	1.33	1.40
3	L3	14	OMU	C4-N3	2.68	1.43	1.38
46	S2	1272	OMC	O2-C2	-2.68	1.18	1.23
1	L1	4335	5MC	O2-C2	-2.68	1.18	1.23
46	S2	172	OMU	O2-C2	-2.68	1.18	1.23
1	L1	2364	OMG	O6-C6	-2.68	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4392	OMG	C5-C4	-2.68	1.36	1.43
46	S2	814	5MU	O2-C2	-2.67	1.18	1.23
46	S2	867	OMG	C2-N1	2.67	1.44	1.37
1	L1	1625	OMG	O6-C6	-2.67	1.17	1.23
1	L1	2787	A2M	C5-C4	-2.67	1.33	1.40
46	S2	1328	OMG	C2-N1	2.66	1.44	1.37
46	S2	27	A2M	O2'-C2'	2.66	1.49	1.42
1	L1	4220	6MZ	C5-C4	-2.66	1.33	1.40
1	L1	4523	A2M	C5-C4	-2.66	1.33	1.40
46	S2	1442	OMU	O4-C4	-2.66	1.19	1.24
1	L1	3792	OMG	C5-C4	-2.66	1.36	1.43
1	L1	4623	OMG	O6-C6	-2.65	1.17	1.23
46	S2	683	OMG	C5-C4	-2.65	1.36	1.43
1	L1	2424	OMG	C2-N1	2.64	1.44	1.37
1	L1	3744	OMG	C5-C4	-2.64	1.36	1.43
1	L1	1524	A2M	C5-C4	-2.64	1.33	1.40
46	S2	172	OMU	O4-C4	-2.64	1.19	1.24
46	S2	644	OMG	C5-C4	-2.64	1.36	1.43
1	L1	3627	OMG	O6-C6	-2.63	1.18	1.23
1	L1	2876	OMG	O6-C6	-2.61	1.18	1.23
1	L1	3869	OMC	C5-C4	2.61	1.48	1.42
1	L1	4228	OMG	O6-C6	-2.61	1.18	1.23
1	L1	3944	OMG	C2-N1	2.61	1.44	1.37
1	L1	1316	OMG	C2-N1	2.61	1.44	1.37
46	S2	683	OMG	O6-C6	-2.61	1.18	1.23
1	L1	1316	OMG	C5-C4	-2.61	1.36	1.43
3	L3	75	OMG	C2-N1	2.60	1.44	1.37
1	L1	3785	A2M	C6-N6	2.60	1.43	1.34
46	S2	1288	OMU	O4-C4	-2.60	1.19	1.24
1	L1	4456	OMC	C5-C4	2.60	1.48	1.42
46	S2	590	A2M	C5-C4	-2.60	1.34	1.40
1	L1	3899	OMG	O6-C6	-2.60	1.18	1.23
46	S2	1490	OMG	C5-C4	-2.59	1.36	1.43
1	L1	4500	PSU	C6-C5	2.59	1.38	1.35
46	S2	1328	OMG	C5-C4	-2.59	1.36	1.43
1	L1	978	2MG	CM2-N2	2.59	1.50	1.45
46	S2	436	OMG	C5-C4	-2.59	1.36	1.43
1	L1	978	2MG	C5-C4	-2.58	1.36	1.43
46	S2	867	OMG	C5-C4	-2.58	1.36	1.43
1	L1	3944	OMG	C5-C4	-2.58	1.36	1.43
46	S2	1288	OMU	O2-C2	-2.57	1.18	1.23
1	L1	4623	OMG	C2-N1	2.57	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4637	OMG	C5-C4	-2.57	1.36	1.43
46	S2	1442	OMU	O2-C2	-2.57	1.18	1.23
1	L1	4228	OMG	C2-N1	2.57	1.44	1.37
46	S2	823	PSU	C2-N1	-2.57	1.33	1.36
46	S2	823	PSU	C2-N3	-2.57	1.33	1.37
1	L1	4196	OMG	O6-C6	-2.57	1.18	1.23
1	L1	4494	OMG	C5-C4	-2.57	1.36	1.43
1	L1	4499	OMG	C2-N1	2.57	1.44	1.37
1	L1	2364	OMG	C2-N1	2.56	1.44	1.37
1	L1	3701	OMC	C5-C4	2.55	1.48	1.42
46	S2	1272	OMC	C5-C4	2.55	1.48	1.42
46	S2	436	OMG	C2-N1	2.55	1.44	1.37
46	S2	644	OMG	C2-N1	2.55	1.44	1.37
1	L1	2422	OMC	C5-C4	2.54	1.48	1.42
1	L1	1881	OMC	C5-C4	2.54	1.48	1.42
1	L1	3762	B8H	O2-C2	-2.54	1.18	1.23
1	L1	3818	UY1	C4-C5	-2.54	1.36	1.44
46	S2	601	OMG	C2-N1	2.54	1.43	1.37
46	S2	601	OMG	C5-C4	-2.53	1.36	1.43
1	L1	3744	OMG	C2-N1	2.52	1.43	1.37
46	S2	174	OMC	C5-C4	2.51	1.48	1.42
1	L1	3627	OMG	C2-N1	2.51	1.43	1.37
46	S2	1830	UR3	O2-C2	-2.51	1.18	1.22
1	L1	1625	OMG	C5-C4	-2.50	1.36	1.43
1	L1	4494	OMG	O6-C6	-2.49	1.18	1.23
1	L1	1522	OMG	C2-N1	2.49	1.43	1.37
46	S2	436	OMG	O6-C6	-2.49	1.18	1.23
1	L1	2804	OMC	C5-C4	2.49	1.48	1.42
46	S2	509	OMG	C2-N1	2.47	1.43	1.37
1	L1	3744	OMG	O6-C6	-2.47	1.18	1.23
1	L1	4618	OMG	C2-N1	2.46	1.43	1.37
1	L1	729	2MG	C5-C4	-2.46	1.36	1.43
1	L1	4370	OMG	O6-C6	-2.45	1.18	1.23
1	L1	2861	OMC	C5-C4	2.45	1.48	1.42
46	S2	683	OMG	C2-N1	2.44	1.43	1.37
1	L1	978	2MG	O6-C6	-2.43	1.18	1.23
1	L1	3792	OMG	O6-C6	-2.43	1.18	1.23
1	L1	4370	OMG	C2-N1	2.43	1.43	1.37
1	L1	4618	OMG	O6-C6	-2.43	1.18	1.23
1	L1	3887	OMC	C5-C4	2.43	1.48	1.42
3	L3	75	OMG	O6-C6	-2.42	1.18	1.23
1	L1	3899	OMG	C2-N1	2.42	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4392	OMG	C2-N1	2.42	1.43	1.37
1	L1	4494	OMG	C2-N1	2.40	1.43	1.37
1	L1	1456	JMH	C5-C4	2.40	1.48	1.42
46	S2	517	OMC	C5-C4	2.40	1.48	1.42
46	S2	462	OMC	C5-C4	2.39	1.48	1.42
46	S2	1830	UR3	O4-C4	-2.38	1.18	1.23
1	L1	4637	OMG	C2-N1	2.38	1.43	1.37
1	L1	4637	OMG	O6-C6	-2.38	1.18	1.23
46	S2	823	PSU	C6-C5	2.38	1.38	1.35
1	L1	4499	OMG	O6-C6	-2.36	1.18	1.23
1	L1	1625	OMG	C2-N1	2.36	1.43	1.37
1	L1	3792	OMG	C2-N1	2.36	1.43	1.37
1	L1	2351	OMC	C5-C4	2.36	1.48	1.42
1	L1	729	2MG	O6-C6	-2.36	1.18	1.23
46	S2	1391	OMC	C5-C4	2.35	1.48	1.42
46	S2	644	OMG	O6-C6	-2.35	1.18	1.23
1	L1	2365	OMC	C5-C4	2.35	1.48	1.42
46	S2	1703	OMC	C5-C4	2.35	1.48	1.42
46	S2	1710	OMC	C5-C4	2.35	1.48	1.42
46	S2	1832	6MZ	C5-C4	-2.35	1.34	1.40
1	L1	4392	OMG	O6-C6	-2.34	1.18	1.23
46	S2	1326	UY1	C4-C5	-2.34	1.37	1.44
46	S2	1490	OMG	C2-N1	2.34	1.43	1.37
46	S2	509	OMG	O6-C6	-2.34	1.18	1.23
46	S2	601	OMG	O6-C6	-2.33	1.18	1.23
1	L1	3785	A2M	O5'-C5'	-2.33	1.39	1.44
1	L1	3808	OMC	C5-C4	2.32	1.48	1.42
1	L1	3841	OMC	C5-C4	2.32	1.48	1.42
1	L1	2424	OMG	O6-C6	-2.32	1.18	1.23
46	S2	1490	OMG	O6-C6	-2.30	1.18	1.23
1	L1	4536	OMC	C5-C4	2.29	1.48	1.42
1	L1	4530	UR3	O4-C4	-2.28	1.18	1.23
1	L1	4530	UR3	O2-C2	-2.28	1.18	1.22
1	L1	3944	OMG	O6-C6	-2.27	1.18	1.23
1	L1	2876	OMG	C2-N1	2.27	1.43	1.37
46	S2	1842	4AC	O7-C7	-2.26	1.18	1.23
46	S2	867	OMG	O6-C6	-2.25	1.18	1.23
46	S2	1328	OMG	O6-C6	-2.23	1.18	1.23
1	L1	2401	A2M	O5'-C5'	-2.23	1.39	1.44
1	L1	4530	UR3	C4-N3	2.23	1.45	1.40
1	L1	1517	2MG	CM2-N2	2.22	1.49	1.45
1	L1	2824	OMC	C5-C4	2.21	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4227	OMU	C5-C4	2.20	1.48	1.43
46	S2	1850	MA6	C2-N3	2.19	1.35	1.32
1	L1	3785	A2M	O3'-C3'	-2.18	1.37	1.43
1	L1	2401	A2M	C2-N3	2.17	1.35	1.32
46	S2	1830	UR3	C5-C4	2.17	1.49	1.43
1	L1	3818	UY1	O3'-C3'	2.16	1.48	1.43
1	L1	2787	A2M	C2-N3	2.16	1.35	1.32
46	S2	1031	A2M	O5'-C5'	-2.16	1.39	1.44
1	L1	3818	UY1	O2'-C2'	-2.15	1.37	1.42
1	L1	2363	A2M	O5'-C5'	-2.15	1.39	1.44
1	L1	1524	A2M	C2-N3	2.14	1.35	1.32
1	L1	3867	A2M	O5'-C5'	-2.14	1.39	1.44
3	L3	14	OMU	C5-C4	2.14	1.48	1.43
46	S2	1288	OMU	C6-N1	2.13	1.43	1.38
46	S2	159	A2M	C2-N3	2.13	1.35	1.32
1	L1	4523	A2M	O5'-C5'	-2.13	1.39	1.44
46	S2	1337	4AC	O7-C7	-2.12	1.18	1.23
46	S2	484	A2M	C2-N3	2.12	1.35	1.32
1	L1	729	2MG	CM2-N2	2.11	1.49	1.45
46	S2	166	A2M	C2-N3	2.10	1.35	1.32
1	L1	978	2MG	C5-C6	2.10	1.51	1.47
1	L1	1524	A2M	O5'-C5'	-2.09	1.39	1.44
46	S2	1678	A2M	C2-N3	2.09	1.35	1.32
1	L1	1677	PSU	O4'-C1'	-2.09	1.40	1.43
1	L1	3830	A2M	O5'-C5'	-2.08	1.39	1.44
1	L1	1534	A2M	O5'-C5'	-2.07	1.39	1.44
1	L1	3825	A2M	O5'-C5'	-2.06	1.39	1.44
1	L1	3925	OMU	C6-N1	2.06	1.43	1.38
1	L1	1534	A2M	C2-N3	2.06	1.35	1.32
1	L1	1326	A2M	C2-N3	2.06	1.35	1.32
46	S2	1326	UY1	O3'-C3'	2.05	1.47	1.43
1	L1	729	2MG	C5-C6	2.05	1.51	1.47
46	S2	1326	UY1	O2'-C2'	-2.05	1.37	1.42
1	L1	400	A2M	O5'-C5'	-2.05	1.39	1.44
1	L1	1340	OMC	C5-C4	2.04	1.47	1.42
46	S2	823	PSU	C6-N1	-2.04	1.32	1.36
1	L1	2787	A2M	C5-N7	-2.04	1.32	1.39
1	L1	398	A2M	C2-N3	2.04	1.35	1.32
46	S2	468	A2M	O5'-C5'	-2.04	1.39	1.44
46	S2	668	A2M	O5'-C5'	-2.03	1.39	1.44
46	S2	1442	OMU	C6-N1	2.03	1.42	1.38
46	S2	1219	JMH	C5-C4	2.03	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1288	OMU	C5-C4	2.03	1.48	1.43
1	L1	400	A2M	C2-N3	2.03	1.35	1.32
46	S2	468	A2M	C2-N3	2.03	1.35	1.32
1	L1	2363	A2M	C2-N3	2.03	1.35	1.32
1	L1	4220	6MZ	C2-N3	2.02	1.35	1.32
1	L1	4571	A2M	C2-N3	2.02	1.35	1.32
1	L1	3785	A2M	C2-N3	2.02	1.35	1.32
1	L1	4620	OMU	C5-C4	2.01	1.48	1.43
46	S2	1442	OMU	C5-C4	2.01	1.48	1.43
46	S2	1248	B8N	C32-C33	2.01	1.57	1.53
46	S2	1832	6MZ	C2-N3	2.01	1.35	1.32
1	L1	4227	OMU	C6-N1	2.01	1.42	1.38
1	L1	3867	A2M	C2-N3	2.01	1.35	1.32
46	S2	27	A2M	O5'-C5'	-2.00	1.39	1.44

All (469) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1851	MA6	N1-C6-N6	-17.56	98.57	117.06
46	S2	1850	MA6	N1-C6-N6	-15.65	100.58	117.06
46	S2	1806	M7A	C5-C6-N6	13.64	147.03	123.74
46	S2	1806	M7A	N6-C6-N1	-11.50	93.16	118.35
1	L1	1534	A2M	C5-C6-N6	11.37	137.63	120.35
46	S2	668	A2M	C5-C6-N6	11.18	137.34	120.35
1	L1	4571	A2M	C5-C6-N6	11.12	137.25	120.35
46	S2	484	A2M	C5-C6-N6	11.10	137.22	120.35
46	S2	1383	A2M	C5-C6-N6	11.08	137.18	120.35
1	L1	2401	A2M	C5-C6-N6	11.01	137.09	120.35
46	S2	166	A2M	C5-C6-N6	11.00	137.07	120.35
1	L1	1524	A2M	C5-C6-N6	10.99	137.05	120.35
1	L1	1326	A2M	C5-C6-N6	10.99	137.05	120.35
1	L1	4523	A2M	C5-C6-N6	10.97	137.02	120.35
46	S2	512	A2M	C5-C6-N6	10.97	137.02	120.35
1	L1	3718	A2M	C5-C6-N6	10.90	136.91	120.35
1	L1	3830	A2M	C5-C6-N6	10.85	136.84	120.35
46	S2	1031	A2M	C5-C6-N6	10.84	136.82	120.35
46	S2	576	A2M	C5-C6-N6	10.81	136.78	120.35
46	S2	1678	A2M	C5-C6-N6	10.81	136.78	120.35
46	S2	159	A2M	C5-C6-N6	10.76	136.70	120.35
46	S2	468	A2M	C5-C6-N6	10.75	136.69	120.35
1	L1	1871	A2M	C5-C6-N6	10.75	136.68	120.35
46	S2	27	A2M	C5-C6-N6	10.70	136.62	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	2815	A2M	C5-C6-N6	10.67	136.57	120.35
1	L1	3723	A2M	C5-C6-N6	10.65	136.53	120.35
46	S2	590	A2M	C5-C6-N6	10.64	136.52	120.35
1	L1	3785	A2M	C5-C6-N6	10.61	136.47	120.35
1	L1	2787	A2M	C5-C6-N6	10.58	136.42	120.35
1	L1	3867	A2M	C5-C6-N6	10.57	136.42	120.35
46	S2	99	A2M	C5-C6-N6	10.56	136.41	120.35
1	L1	400	A2M	C5-C6-N6	10.52	136.33	120.35
1	L1	3825	A2M	C5-C6-N6	10.47	136.26	120.35
1	L1	398	A2M	C5-C6-N6	10.40	136.15	120.35
1	L1	2363	A2M	C5-C6-N6	10.35	136.08	120.35
46	S2	814	5MU	C5-C4-N3	10.06	123.90	115.31
46	S2	1850	MA6	C1'-N9-C4	-9.32	110.26	126.64
46	S2	1851	MA6	C1'-N9-C4	-8.17	112.30	126.64
46	S2	814	5MU	C5-C6-N1	-8.00	115.11	123.34
1	L1	1534	A2M	N6-C6-N1	-7.82	102.35	118.57
1	L1	2401	A2M	N6-C6-N1	-7.70	102.59	118.57
1	L1	4571	A2M	N6-C6-N1	-7.69	102.61	118.57
1	L1	3785	A2M	N6-C6-N1	-7.68	102.64	118.57
46	S2	668	A2M	N6-C6-N1	-7.66	102.67	118.57
46	S2	484	A2M	N6-C6-N1	-7.65	102.69	118.57
46	S2	166	A2M	N6-C6-N1	-7.63	102.74	118.57
46	S2	1383	A2M	N6-C6-N1	-7.53	102.94	118.57
1	L1	1524	A2M	N6-C6-N1	-7.51	102.98	118.57
46	S2	590	A2M	N6-C6-N1	-7.46	103.08	118.57
46	S2	468	A2M	N6-C6-N1	-7.44	103.13	118.57
46	S2	27	A2M	N6-C6-N1	-7.43	103.15	118.57
46	S2	1678	A2M	N6-C6-N1	-7.42	103.17	118.57
1	L1	4523	A2M	N6-C6-N1	-7.41	103.19	118.57
1	L1	3830	A2M	N6-C6-N1	-7.41	103.20	118.57
46	S2	159	A2M	N6-C6-N1	-7.40	103.21	118.57
46	S2	576	A2M	N6-C6-N1	-7.40	103.21	118.57
46	S2	512	A2M	N6-C6-N1	-7.37	103.28	118.57
46	S2	99	A2M	N6-C6-N1	-7.32	103.38	118.57
1	L1	3723	A2M	N6-C6-N1	-7.31	103.39	118.57
1	L1	3718	A2M	N6-C6-N1	-7.25	103.53	118.57
1	L1	2815	A2M	N6-C6-N1	-7.23	103.57	118.57
1	L1	400	A2M	N6-C6-N1	-7.23	103.57	118.57
1	L1	3867	A2M	N6-C6-N1	-7.21	103.62	118.57
46	S2	1031	A2M	N6-C6-N1	-7.20	103.64	118.57
1	L1	398	A2M	N6-C6-N1	-7.19	103.66	118.57
1	L1	1326	A2M	N6-C6-N1	-7.17	103.68	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3825	A2M	N6-C6-N1	-7.14	103.76	118.57
1	L1	1871	A2M	N6-C6-N1	-7.08	103.88	118.57
1	L1	2787	A2M	N6-C6-N1	-7.07	103.90	118.57
1	L1	2363	A2M	N6-C6-N1	-6.84	104.38	118.57
1	L1	3762	B8H	C4-N3-C2	-6.75	118.61	127.35
46	S2	814	5MU	C4-N3-C2	-6.67	118.72	127.35
1	L1	1322	1MA	N1-C2-N3	-6.64	118.28	126.02
46	S2	823	PSU	N1-C2-N3	6.53	122.52	115.13
1	L1	1871	A2M	N3-C2-N1	-6.28	118.87	128.68
46	S2	668	A2M	N3-C2-N1	-6.19	119.01	128.68
46	S2	1031	A2M	N3-C2-N1	-6.17	119.03	128.68
46	S2	512	A2M	N3-C2-N1	-6.12	119.12	128.68
46	S2	1832	6MZ	N3-C2-N1	-6.08	119.17	128.68
1	L1	1326	A2M	N3-C2-N1	-6.01	119.29	128.68
46	S2	1832	6MZ	C2-N1-C6	5.99	121.72	116.59
1	L1	3762	B8H	N3-C2-N1	5.96	121.58	115.14
1	L1	4220	6MZ	N3-C2-N1	-5.93	119.41	128.68
46	S2	27	A2M	N3-C2-N1	-5.85	119.53	128.68
1	L1	2815	A2M	N3-C2-N1	-5.82	119.58	128.68
1	L1	3818	UY1	N1-C2-N3	5.81	121.72	115.13
1	L1	3825	A2M	N3-C2-N1	-5.80	119.61	128.68
1	L1	3867	A2M	N3-C2-N1	-5.79	119.64	128.68
46	S2	1678	A2M	N3-C2-N1	-5.75	119.69	128.68
1	L1	2401	A2M	N3-C2-N1	-5.75	119.69	128.68
46	S2	590	A2M	N3-C2-N1	-5.74	119.71	128.68
1	L1	3830	A2M	N3-C2-N1	-5.73	119.72	128.68
46	S2	166	A2M	N3-C2-N1	-5.73	119.72	128.68
1	L1	4571	A2M	N3-C2-N1	-5.73	119.73	128.68
46	S2	1383	A2M	N3-C2-N1	-5.72	119.74	128.68
46	S2	1851	MA6	N3-C2-N1	-5.70	119.77	128.68
1	L1	4523	A2M	N3-C2-N1	-5.67	119.81	128.68
46	S2	468	A2M	N3-C2-N1	-5.67	119.81	128.68
1	L1	398	A2M	N3-C2-N1	-5.65	119.85	128.68
1	L1	3723	A2M	N3-C2-N1	-5.64	119.86	128.68
46	S2	99	A2M	N3-C2-N1	-5.64	119.87	128.68
1	L1	1524	A2M	N3-C2-N1	-5.64	119.87	128.68
1	L1	1534	A2M	N3-C2-N1	-5.63	119.88	128.68
3	L3	14	OMU	C4-N3-C2	-5.62	119.17	126.58
1	L1	4498	OMU	C4-N3-C2	-5.61	119.17	126.58
46	S2	159	A2M	N3-C2-N1	-5.58	119.96	128.68
46	S2	484	A2M	N3-C2-N1	-5.53	120.03	128.68
46	S2	576	A2M	N3-C2-N1	-5.52	120.05	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1850	MA6	N3-C2-N1	-5.51	120.06	128.68
1	L1	3785	A2M	N3-C2-N1	-5.47	120.12	128.68
1	L1	400	A2M	N3-C2-N1	-5.45	120.17	128.68
1	L1	2787	A2M	N3-C2-N1	-5.44	120.17	128.68
1	L1	4227	OMU	C4-N3-C2	-5.43	119.42	126.58
46	S2	1326	UY1	N1-C2-N3	5.39	121.23	115.13
1	L1	2363	A2M	N3-C2-N1	-5.37	120.29	128.68
46	S2	1806	M7A	N3-C2-N1	-5.35	120.23	128.60
1	L1	3925	OMU	C4-N3-C2	-5.34	119.54	126.58
1	L1	1683	PSU	N1-C2-N3	5.32	121.16	115.13
46	S2	172	OMU	C4-N3-C2	-5.29	119.60	126.58
1	L1	4306	OMU	C4-N3-C2	-5.27	119.63	126.58
46	S2	354	OMU	C4-N3-C2	-5.25	119.65	126.58
1	L1	4636	PSU	C4-N3-C2	-5.20	118.85	126.34
46	S2	121	OMU	C4-N3-C2	-5.17	119.77	126.58
46	S2	428	OMU	C4-N3-C2	-5.13	119.81	126.58
1	L1	2837	OMU	C4-N3-C2	-5.12	119.82	126.58
1	L1	4220	6MZ	C2-N1-C6	5.12	120.98	116.59
46	S2	1442	OMU	C4-N3-C2	-5.12	119.83	126.58
1	L1	3718	A2M	N3-C2-N1	-5.11	120.69	128.68
1	L1	4620	OMU	C4-N3-C2	-5.00	119.98	126.58
46	S2	1806	M7A	N3-C4-N9	4.99	133.17	126.87
46	S2	1288	OMU	C4-N3-C2	-4.99	120.00	126.58
46	S2	116	OMU	C4-N3-C2	-4.97	120.02	126.58
46	S2	1248	B8N	C5-C4-N3	4.95	125.33	116.17
46	S2	1219	JMH	C1'-N1-C2	4.94	125.33	116.99
1	L1	4636	PSU	N1-C2-N3	4.92	120.71	115.13
1	L1	4628	PSU	N1-C2-N3	4.73	120.49	115.13
46	S2	822	PSU	N1-C2-N3	4.71	120.46	115.13
1	L1	2508	PSU	N1-C2-N3	4.67	120.42	115.13
1	L1	4450	PSU	C4-N3-C2	-4.63	119.66	126.34
46	S2	814	5MU	N3-C2-N1	4.62	121.02	114.89
1	L1	4450	PSU	N1-C2-N3	4.59	120.33	115.13
46	S2	1081	PSU	N1-C2-N3	4.59	120.33	115.13
1	L1	4531	PSU	N1-C2-N3	4.58	120.32	115.13
1	L1	3715	PSU	N1-C2-N3	4.57	120.31	115.13
46	S2	612	PSU	N1-C2-N3	4.56	120.29	115.13
1	L1	2508	PSU	C4-N3-C2	-4.54	119.79	126.34
1	L1	4442	PSU	N1-C2-N3	4.54	120.28	115.13
1	L1	1677	PSU	C4-N3-C2	-4.53	119.82	126.34
1	L1	4531	PSU	C4-N3-C2	-4.51	119.84	126.34
1	L1	1677	PSU	N1-C2-N3	4.49	120.22	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4442	PSU	C4-N3-C2	-4.48	119.89	126.34
1	L1	4293	PSU	N1-C2-N3	4.47	120.20	115.13
1	L1	1683	PSU	C4-N3-C2	-4.46	119.91	126.34
1	L1	4628	PSU	C4-N3-C2	-4.46	119.91	126.34
1	L1	4500	PSU	N1-C2-N3	4.45	120.17	115.13
46	S2	612	PSU	C4-N3-C2	-4.43	119.95	126.34
1	L1	4293	PSU	C4-N3-C2	-4.42	119.96	126.34
1	L1	3729	PSU	C4-N3-C2	-4.40	120.00	126.34
46	S2	119	PSU	N1-C2-N3	4.39	120.11	115.13
46	S2	822	PSU	C4-N3-C2	-4.38	120.03	126.34
46	S2	1830	UR3	C4-N3-C2	-4.37	120.45	124.56
1	L1	3715	PSU	C4-N3-C2	-4.37	120.05	126.34
1	L1	3729	PSU	N1-C2-N3	4.35	120.06	115.13
46	S2	1243	PSU	N1-C2-N3	4.35	120.06	115.13
3	L3	14	OMU	N3-C2-N1	4.30	120.59	114.89
1	L1	4403	PSU	C4-N3-C2	-4.29	120.16	126.34
1	L1	3764	PSU	N1-C2-N3	4.26	119.96	115.13
46	S2	1243	PSU	C4-N3-C2	-4.26	120.20	126.34
1	L1	4500	PSU	C4-N3-C2	-4.26	120.20	126.34
46	S2	119	PSU	C4-N3-C2	-4.23	120.24	126.34
1	L1	1582	PSU	N1-C2-N3	4.20	119.89	115.13
1	L1	3925	OMU	N3-C2-N1	4.20	120.47	114.89
46	S2	1081	PSU	C4-N3-C2	-4.19	120.30	126.34
1	L1	4227	OMU	N3-C2-N1	4.17	120.43	114.89
1	L1	4403	PSU	N1-C2-N3	4.16	119.84	115.13
1	L1	4620	OMU	N3-C2-N1	4.11	120.34	114.89
1	L1	3764	PSU	C4-N3-C2	-4.10	120.44	126.34
46	S2	1248	B8N	C4-N3-C2	-4.09	120.29	125.46
1	L1	4530	UR3	C4-N3-C2	-4.07	120.73	124.56
1	L1	1522	OMG	C5-C6-N1	4.04	121.09	113.95
46	S2	121	OMU	N3-C2-N1	4.01	120.21	114.89
46	S2	814	5MU	C5M-C5-C6	-4.01	117.50	122.85
1	L1	4306	OMU	N3-C2-N1	4.00	120.20	114.89
1	L1	1582	PSU	C4-N3-C2	-3.98	120.61	126.34
1	L1	3818	UY1	C4-N3-C2	-3.97	120.62	126.34
46	S2	1326	UY1	C4-N3-C2	-3.97	120.62	126.34
46	S2	814	5MU	O4-C4-C5	-3.95	120.33	124.90
46	S2	823	PSU	O2-C2-N1	-3.94	118.46	122.79
46	S2	172	OMU	N3-C2-N1	3.91	120.08	114.89
1	L1	4498	OMU	N3-C2-N1	3.86	120.02	114.89
1	L1	2837	OMU	N3-C2-N1	3.86	120.01	114.89
46	S2	354	OMU	N3-C2-N1	3.85	119.99	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4447	5MC	C5-C6-N1	-3.83	119.40	123.34
46	S2	1806	M7A	C4-N9-C1'	-3.82	117.53	126.60
46	S2	1219	JMH	C6-N1-C2	-3.72	118.46	121.79
46	S2	1830	UR3	C1'-N1-C2	3.70	123.23	116.99
46	S2	1442	OMU	N3-C2-N1	3.69	119.79	114.89
1	L1	2364	OMG	C5-C6-N1	3.67	120.43	113.95
1	L1	1316	OMG	C5-C6-N1	3.67	120.43	113.95
1	L1	3899	OMG	C5-C6-N1	3.66	120.41	113.95
46	S2	1288	OMU	N3-C2-N1	3.65	119.74	114.89
46	S2	823	PSU	C4-N3-C2	-3.65	121.08	126.34
46	S2	116	OMU	N3-C2-N1	3.65	119.73	114.89
1	L1	4498	OMU	C5-C4-N3	3.63	120.28	114.84
46	S2	683	OMG	C5-C6-N1	3.61	120.33	113.95
1	L1	4494	OMG	C5-C6-N1	3.58	120.28	113.95
3	L3	75	OMG	C5-C6-N1	3.58	120.27	113.95
1	L1	4228	OMG	C5-C6-N1	3.58	120.27	113.95
46	S2	436	OMG	C5-C6-N1	3.56	120.24	113.95
1	L1	4618	OMG	C5-C6-N1	3.55	120.22	113.95
46	S2	428	OMU	N3-C2-N1	3.55	119.60	114.89
1	L1	3744	OMG	C5-C6-N1	3.54	120.21	113.95
1	L1	2876	OMG	C5-C6-N1	3.52	120.17	113.95
1	L1	3944	OMG	C5-C6-N1	3.52	120.16	113.95
46	S2	1328	OMG	C5-C6-N1	3.50	120.14	113.95
1	L1	3627	OMG	C5-C6-N1	3.50	120.13	113.95
46	S2	867	OMG	C5-C6-N1	3.49	120.12	113.95
1	L1	4370	OMG	C5-C6-N1	3.46	120.06	113.95
1	L1	4499	OMG	C5-C6-N1	3.46	120.06	113.95
1	L1	978	2MG	C5-C6-N1	3.44	120.03	113.95
1	L1	4530	UR3	C6-N1-C2	-3.44	118.71	121.79
1	L1	1517	2MG	C5-C6-N1	3.43	120.01	113.95
1	L1	1625	OMG	C5-C6-N1	3.42	120.00	113.95
3	L3	14	OMU	C5-C4-N3	3.41	119.94	114.84
46	S2	814	5MU	C6-C5-C4	3.41	120.88	118.03
1	L1	3792	OMG	C5-C6-N1	3.40	119.95	113.95
46	S2	354	OMU	C5-C4-N3	3.39	119.92	114.84
1	L1	4227	OMU	C5-C4-N3	3.39	119.92	114.84
46	S2	1490	OMG	C5-C6-N1	3.39	119.94	113.95
1	L1	4196	OMG	C5-C6-N1	3.38	119.92	113.95
1	L1	1522	OMG	C2-N1-C6	-3.37	118.90	125.10
46	S2	1832	6MZ	C9-N6-C6	3.37	125.77	122.87
1	L1	2364	OMG	C2-N1-C6	-3.36	118.91	125.10
46	S2	509	OMG	C5-C6-N1	3.36	119.88	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4392	OMG	C5-C6-N1	3.35	119.87	113.95
1	L1	1322	1MA	C5-C6-N1	3.34	118.88	113.90
46	S2	116	OMU	C5-C4-N3	3.34	119.84	114.84
1	L1	3762	B8H	C5-C4-N3	3.34	124.13	116.58
1	L1	4306	OMU	C5-C4-N3	3.33	119.83	114.84
1	L1	2424	OMG	C5-C6-N1	3.33	119.83	113.95
46	S2	428	OMU	C5-C4-N3	3.33	119.81	114.84
46	S2	644	OMG	C5-C6-N1	3.30	119.79	113.95
1	L1	4196	OMG	C2-N1-C6	-3.29	119.04	125.10
46	S2	601	OMG	C5-C6-N1	3.29	119.76	113.95
1	L1	1625	OMG	C2-N1-C6	-3.27	119.07	125.10
46	S2	1442	OMU	C5-C4-N3	3.27	119.73	114.84
1	L1	4623	OMG	C5-C6-N1	3.27	119.72	113.95
1	L1	3762	B8H	O2-C2-N1	-3.26	119.20	122.87
1	L1	2837	OMU	C5-C4-N3	3.25	119.71	114.84
46	S2	1288	OMU	C5-C4-N3	3.25	119.71	114.84
46	S2	121	OMU	C5-C4-N3	3.25	119.70	114.84
1	L1	729	2MG	C5-C6-N1	3.24	119.68	113.95
46	S2	1374	5MC	C5-C6-N1	-3.24	120.00	123.34
1	L1	4220	6MZ	C9-N6-C6	-3.23	120.09	122.87
1	L1	1316	OMG	C2-N1-C6	-3.22	119.17	125.10
46	S2	172	OMU	C5-C4-N3	3.21	119.65	114.84
1	L1	2876	OMG	C2-N1-C6	-3.19	119.23	125.10
1	L1	3627	OMG	C2-N1-C6	-3.18	119.24	125.10
1	L1	3782	5MC	C5-C6-N1	-3.18	120.07	123.34
46	S2	1326	UY1	O2-C2-N1	-3.18	119.29	122.79
46	S2	1248	B8N	N3-C2-N1	3.17	121.24	116.76
1	L1	4637	OMG	C5-C6-N1	3.17	119.55	113.95
46	S2	1830	UR3	C6-N1-C2	-3.15	118.97	121.79
1	L1	3925	OMU	C5-C4-N3	3.14	119.53	114.84
46	S2	1806	M7A	C2-N3-C4	3.12	119.12	111.75
46	S2	436	OMG	C2-N1-C6	-3.11	119.36	125.10
1	L1	4620	OMU	C5-C4-N3	3.11	119.50	114.84
46	S2	509	OMG	C2-N1-C6	-3.11	119.38	125.10
1	L1	3944	OMG	C2-N1-C6	-3.10	119.39	125.10
1	L1	3818	UY1	O2-C2-N1	-3.10	119.38	122.79
1	L1	1683	PSU	C6-N1-C2	-3.10	119.52	122.68
1	L1	4494	OMG	C2-N1-C6	-3.10	119.40	125.10
1	L1	4442	PSU	O2-C2-N1	-3.09	119.39	122.79
1	L1	3744	OMG	C2-N1-C6	-3.09	119.41	125.10
46	S2	867	OMG	C2-N1-C6	-3.07	119.45	125.10
46	S2	1328	OMG	C2-N1-C6	-3.07	119.45	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	428	OMU	O4-C4-C5	-3.07	119.77	125.16
46	S2	683	OMG	C2-N1-C6	-3.06	119.47	125.10
1	L1	4447	5MC	C1'-N1-C6	3.05	126.20	121.12
1	L1	4637	OMG	C2-N1-C6	-3.04	119.50	125.10
46	S2	644	OMG	C2-N1-C6	-3.04	119.51	125.10
46	S2	1806	M7A	C71-N7-C5	-3.03	112.37	124.01
1	L1	2351	OMC	O2-C2-N3	-3.00	117.45	122.33
1	L1	1316	OMG	C8-N7-C5	2.99	108.69	102.99
46	S2	116	OMU	O4-C4-C5	-2.99	119.91	125.16
3	L3	75	OMG	C2-N1-C6	-2.99	119.60	125.10
1	L1	4228	OMG	C2-N1-C6	-2.98	119.60	125.10
1	L1	2424	OMG	C2-N1-C6	-2.98	119.61	125.10
1	L1	4335	5MC	C5-C6-N1	-2.97	120.28	123.34
1	L1	4392	OMG	C2-N1-C6	-2.95	119.66	125.10
1	L1	4500	PSU	C6-N1-C2	-2.95	119.66	122.68
46	S2	601	OMG	C2-N1-C6	-2.94	119.69	125.10
1	L1	1517	2MG	C8-N7-C5	2.92	108.55	102.99
1	L1	4499	OMG	C2-N1-C6	-2.92	119.73	125.10
1	L1	4623	OMG	C2-N1-C6	-2.91	119.73	125.10
46	S2	121	OMU	O4-C4-C5	-2.91	120.04	125.16
46	S2	1442	OMU	O4-C4-C5	-2.90	120.06	125.16
1	L1	978	2MG	CM2-N2-C2	-2.89	117.49	123.86
1	L1	3782	5MC	CM5-C5-C6	-2.88	119.00	122.85
46	S2	172	OMU	O4-C4-C5	-2.86	120.14	125.16
1	L1	3792	OMG	C2-N1-C6	-2.86	119.84	125.10
1	L1	4293	PSU	O2-C2-N1	-2.85	119.65	122.79
1	L1	3899	OMG	C2-N1-C6	-2.85	119.86	125.10
1	L1	4370	OMG	C2-N1-C6	-2.84	119.86	125.10
1	L1	4618	OMG	C2-N1-C6	-2.83	119.88	125.10
1	L1	4531	PSU	C6-C5-C4	2.83	120.18	118.20
1	L1	978	2MG	C8-N7-C5	2.83	108.38	102.99
46	S2	1288	OMU	O4-C4-C5	-2.81	120.22	125.16
1	L1	4498	OMU	O4-C4-C5	-2.80	120.23	125.16
1	L1	729	2MG	C8-N7-C5	2.79	108.31	102.99
1	L1	2876	OMG	C8-N7-C5	2.78	108.30	102.99
46	S2	1490	OMG	C2-N1-C6	-2.77	120.00	125.10
3	L3	75	OMG	C8-N7-C5	2.76	108.25	102.99
1	L1	4628	PSU	O2-C2-N1	-2.75	119.76	122.79
1	L1	3899	OMG	C8-N7-C5	2.74	108.21	102.99
1	L1	4196	OMG	C8-N7-C5	2.74	108.21	102.99
1	L1	2364	OMG	C8-N7-C5	2.72	108.18	102.99
1	L1	4370	OMG	C8-N7-C5	2.72	108.18	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1830	UR3	O2-C2-N3	-2.71	117.52	121.34
1	L1	3627	OMG	C8-N7-C5	2.71	108.15	102.99
46	S2	1337	4AC	C6-C5-C4	2.69	120.26	116.96
1	L1	1677	PSU	O2-C2-N1	-2.69	119.83	122.79
1	L1	4335	5MC	CM5-C5-C6	-2.67	119.28	122.85
1	L1	3744	OMG	C8-N7-C5	2.67	108.07	102.99
1	L1	4623	OMG	C8-N7-C5	2.66	108.06	102.99
1	L1	4637	OMG	C8-N7-C5	2.65	108.05	102.99
1	L1	3729	PSU	O2-C2-N1	-2.65	119.87	122.79
1	L1	4403	PSU	O2-C2-N1	-2.65	119.87	122.79
46	S2	354	OMU	O4-C4-C5	-2.65	120.50	125.16
46	S2	822	PSU	O2-C2-N1	-2.63	119.90	122.79
1	L1	3925	OMU	O4-C4-C5	-2.63	120.54	125.16
46	S2	644	OMG	C8-N7-C5	2.62	107.98	102.99
46	S2	1328	OMG	C8-N7-C5	2.62	107.98	102.99
1	L1	1517	2MG	CM2-N2-C2	-2.62	118.08	123.86
1	L1	3944	OMG	C8-N7-C5	2.61	107.97	102.99
1	L1	2508	PSU	O2-C2-N1	-2.61	119.92	122.79
1	L1	4671	B8T	C6-C5-C4	2.60	120.14	116.96
1	L1	4499	OMG	C8-N7-C5	2.59	107.93	102.99
46	S2	814	5MU	C5M-C5-C4	2.59	121.62	118.77
1	L1	4456	OMC	O2-C2-N3	-2.59	118.12	122.33
1	L1	2424	OMG	O6-C6-C5	-2.59	119.32	124.37
1	L1	4227	OMU	O4-C4-C5	-2.58	120.62	125.16
1	L1	4500	PSU	O2-C2-N1	-2.58	119.95	122.79
1	L1	4228	OMG	O6-C6-C5	-2.58	119.33	124.37
1	L1	3792	OMG	C8-N7-C5	2.58	107.91	102.99
1	L1	1456	JMH	C6-N1-C2	-2.58	119.48	121.79
46	S2	601	OMG	C8-N7-C5	2.58	107.90	102.99
1	L1	4392	OMG	C8-N7-C5	2.58	107.90	102.99
46	S2	1219	JMH	O2-C2-N3	-2.58	117.71	121.34
1	L1	4442	PSU	C6-N1-C2	-2.57	120.05	122.68
46	S2	612	PSU	O2-C2-N1	-2.57	119.96	122.79
46	S2	683	OMG	C8-N7-C5	2.57	107.89	102.99
46	S2	1288	OMU	C1'-N1-C2	2.57	122.22	117.57
1	L1	4228	OMG	C8-N7-C5	2.56	107.87	102.99
1	L1	4618	OMG	C8-N7-C5	2.56	107.86	102.99
1	L1	1322	1MA	CM1-N1-C2	-2.55	115.18	120.55
1	L1	4306	OMU	O2-C2-N1	-2.55	119.40	122.79
1	L1	4494	OMG	C8-N7-C5	2.54	107.83	102.99
1	L1	1522	OMG	C8-N7-C5	2.54	107.83	102.99
46	S2	867	OMG	C8-N7-C5	2.54	107.83	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3762	B8H	O4-C4-N3	-2.54	115.25	120.12
1	L1	3715	PSU	C6-N1-C2	-2.54	120.09	122.68
1	L1	4636	PSU	O2-C2-N1	-2.53	120.00	122.79
46	S2	436	OMG	C8-N7-C5	2.53	107.81	102.99
3	L3	14	OMU	O4-C4-C5	-2.52	120.72	125.16
1	L1	1582	PSU	C6-N1-C2	-2.52	120.11	122.68
46	S2	1081	PSU	C6-N1-C2	-2.51	120.11	122.68
46	S2	1832	6MZ	C4-C5-N7	-2.51	106.78	109.40
1	L1	3808	OMC	O2-C2-N3	-2.51	118.25	122.33
46	S2	822	PSU	C6-N1-C2	-2.50	120.12	122.68
46	S2	612	PSU	C6-N1-C2	-2.48	120.14	122.68
46	S2	814	5MU	O2-C2-N3	-2.48	116.88	121.50
1	L1	1625	OMG	O6-C6-C5	-2.48	119.53	124.37
46	S2	1243	PSU	O2-C2-N1	-2.47	120.07	122.79
1	L1	1522	OMG	O6-C6-C5	-2.47	119.55	124.37
46	S2	436	OMG	O6-C6-C5	-2.45	119.58	124.37
1	L1	1625	OMG	C8-N7-C5	2.45	107.66	102.99
1	L1	1322	1MA	C8-N7-C5	2.45	107.65	102.99
46	S2	1806	M7A	C5-C4-N3	-2.44	120.89	126.62
1	L1	3764	PSU	C6-N1-C2	-2.44	120.19	122.68
46	S2	1842	4AC	C5-C4-N3	-2.44	118.67	122.59
1	L1	4306	OMU	O4-C4-C5	-2.42	120.91	125.16
1	L1	1677	PSU	C6-N1-C2	-2.41	120.21	122.68
1	L1	2424	OMG	C8-N7-C5	2.41	107.58	102.99
46	S2	1248	B8N	C31-N3-C4	2.41	120.86	117.31
1	L1	3899	OMG	O6-C6-C5	-2.40	119.67	124.37
46	S2	119	PSU	C6-N1-C2	-2.40	120.23	122.68
46	S2	509	OMG	C8-N7-C5	2.40	107.56	102.99
46	S2	814	5MU	C1'-N1-C2	2.40	121.91	117.57
1	L1	4499	OMG	O6-C6-C5	-2.40	119.69	124.37
46	S2	822	PSU	O4'-C1'-C2'	2.40	108.52	105.14
1	L1	4628	PSU	C6-N1-C2	-2.39	120.24	122.68
46	S2	1842	4AC	C6-C5-C4	2.39	119.89	116.96
1	L1	3869	OMC	O2-C2-N3	-2.39	118.45	122.33
1	L1	2824	OMC	O2-C2-N3	-2.38	118.46	122.33
46	S2	867	OMG	O6-C6-C5	-2.38	119.73	124.37
1	L1	3715	PSU	O2-C2-N1	-2.37	120.19	122.79
1	L1	2837	OMU	O4-C4-C5	-2.35	121.02	125.16
46	S2	1337	4AC	C5-C4-N3	-2.35	118.81	122.59
1	L1	4293	PSU	C6-N1-C2	-2.34	120.29	122.68
46	S2	1243	PSU	C6-N1-C2	-2.33	120.30	122.68
1	L1	4196	OMG	O6-C6-C5	-2.33	119.83	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	683	OMG	O6-C6-C5	-2.33	119.83	124.37
1	L1	4530	UR3	C1'-N1-C2	2.32	120.91	116.99
1	L1	4450	PSU	O2-C2-N1	-2.32	120.24	122.79
46	S2	1710	OMC	O2-C2-N3	-2.32	118.56	122.33
46	S2	1490	OMG	C8-N7-C5	2.32	107.41	102.99
1	L1	978	2MG	O6-C6-C5	-2.32	119.85	124.37
1	L1	3729	PSU	C6-N1-C2	-2.32	120.31	122.68
1	L1	2876	OMG	O6-C6-C5	-2.32	119.85	124.37
1	L1	3744	OMG	O6-C6-C5	-2.32	119.85	124.37
1	L1	2364	OMG	O6-C6-C5	-2.31	119.86	124.37
1	L1	1517	2MG	O6-C6-C5	-2.31	119.87	124.37
1	L1	4620	OMU	O4-C4-C5	-2.30	121.11	125.16
1	L1	4450	PSU	C6-C5-C4	2.30	119.81	118.20
46	S2	1248	B8N	O4'-C1'-C2'	2.29	108.38	105.14
46	S2	814	5MU	O4-C4-N3	-2.29	115.73	120.12
46	S2	119	PSU	O2-C2-N1	-2.29	120.27	122.79
46	S2	1328	OMG	O6-C6-C5	-2.28	119.91	124.37
46	S2	1490	OMG	O6-C6-C5	-2.26	119.95	124.37
1	L1	2837	OMU	C2'-C1'-N1	-2.26	109.83	114.22
1	L1	3764	PSU	O2-C2-N1	-2.26	120.30	122.79
46	S2	354	OMU	O2-C2-N1	-2.26	119.78	122.79
1	L1	4618	OMG	O6-C6-C5	-2.25	119.99	124.37
46	S2	612	PSU	O4'-C1'-C2'	2.24	108.31	105.14
1	L1	2824	OMC	C1'-N1-C2	2.24	123.41	118.42
1	L1	3841	OMC	O2-C2-N3	-2.23	118.70	122.33
1	L1	3944	OMG	O6-C6-C5	-2.23	120.01	124.37
1	L1	4531	PSU	O2-C2-N1	-2.22	120.35	122.79
46	S2	1081	PSU	O4'-C1'-C2'	2.22	108.27	105.14
46	S2	509	OMG	O6-C6-C5	-2.22	120.05	124.37
46	S2	116	OMU	C1'-N1-C2	2.21	121.58	117.57
3	L3	75	OMG	O6-C6-C5	-2.21	120.06	124.37
1	L1	4494	OMG	O6-C6-C5	-2.21	120.06	124.37
1	L1	2351	OMC	O2-C2-N1	2.21	123.45	118.89
46	S2	1374	5MC	CM5-C5-C6	-2.20	119.91	122.85
46	S2	1842	4AC	O2-C2-N3	-2.19	118.77	122.33
1	L1	1582	PSU	O2-C2-N1	-2.19	120.38	122.79
1	L1	3899	OMG	N1-C2-N3	-2.18	119.25	123.32
46	S2	1391	OMC	O2-C2-N3	-2.17	118.80	122.33
1	L1	4500	PSU	O4'-C1'-C2'	2.16	108.19	105.14
46	S2	1248	B8N	O4-C4-N3	-2.16	116.31	119.98
1	L1	4450	PSU	C6-N1-C2	-2.16	120.47	122.68
1	L1	4636	PSU	O4'-C1'-C2'	2.15	108.18	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4636	PSU	C6-C5-C4	2.14	119.69	118.20
1	L1	2351	OMC	C1'-N1-C2	2.13	123.18	118.42
46	S2	823	PSU	C5-C6-N1	-2.13	118.91	122.11
46	S2	517	OMC	O2-C2-N3	-2.13	118.87	122.33
46	S2	1219	JMH	C1'-N1-C6	-2.13	116.20	120.84
1	L1	4531	PSU	C6-N1-C2	-2.12	120.52	122.68
1	L1	2422	OMC	O2-C2-N3	-2.12	118.88	122.33
46	S2	644	OMG	O6-C6-C5	-2.11	120.25	124.37
1	L1	2508	PSU	C6-N1-C2	-2.10	120.53	122.68
46	S2	121	OMU	O2-C2-N1	-2.10	120.00	122.79
46	S2	172	OMU	O2-C2-N1	-2.09	120.01	122.79
1	L1	3792	OMG	O6-C6-C5	-2.07	120.33	124.37
1	L1	1683	PSU	O2-C2-N1	-2.06	120.52	122.79
1	L1	2787	A2M	C5'-C4'-C3'	-2.05	107.49	115.18
1	L1	4392	OMG	O6-C6-C5	-2.05	120.37	124.37
46	S2	814	5MU	C1'-N1-C6	-2.04	117.73	121.12
1	L1	729	2MG	O6-C6-C5	-2.04	120.39	124.37
1	L1	4618	OMG	N1-C2-N3	-2.04	119.52	123.32
1	L1	4220	6MZ	C1'-N9-C4	-2.02	123.09	126.64
1	L1	3818	UY1	C5-C6-N1	-2.02	119.08	122.11
1	L1	1683	PSU	C6-C5-C4	2.02	119.61	118.20
1	L1	2837	OMU	O2-C2-N1	-2.01	120.11	122.79
46	S2	1442	OMU	O2-C2-N1	-2.01	120.12	122.79
1	L1	4628	PSU	O4'-C1'-C2'	2.01	107.97	105.14
1	L1	4403	PSU	O4'-C1'-C2'	2.00	107.97	105.14

There are no chirality outliers.

All (127) 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	1534	A2M	C3'-C2'-O2'-CM'
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	3744	OMG	C1'-C2'-O2'-CM2
1	L1	3792	OMG	C1'-C2'-O2'-CM2
1	L1	3808	OMC	C3'-C4'-C5'-O5'
1	L1	3818	UY1	C2'-C1'-C5-C4
1	L1	3818	UY1	O4'-C4'-C5'-O5'
1	L1	3841	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L1	3841	OMC	O4'-C4'-C5'-O5'
1	L1	3867	A2M	O4'-C4'-C5'-O5'
1	L1	3867	A2M	C3'-C4'-C5'-O5'
1	L1	3944	OMG	C3'-C4'-C5'-O5'
1	L1	4196	OMG	C1'-C2'-O2'-CM2
1	L1	4450	PSU	C2'-C1'-C5-C4
1	L1	4636	PSU	C3'-C4'-C5'-O5'
1	L1	4637	OMG	C1'-C2'-O2'-CM2
3	L3	14	OMU	C1'-C2'-O2'-CM2
3	L3	75	OMG	C1'-C2'-O2'-CM2
46	S2	116	OMU	C1'-C2'-O2'-CM2
46	S2	159	A2M	C3'-C4'-C5'-O5'
46	S2	576	A2M	O4'-C4'-C5'-O5'
46	S2	576	A2M	C3'-C4'-C5'-O5'
46	S2	601	OMG	C1'-C2'-O2'-CM2
46	S2	668	A2M	C3'-C4'-C5'-O5'
46	S2	867	OMG	C3'-C4'-C5'-O5'
46	S2	867	OMG	C1'-C2'-O2'-CM2
46	S2	1248	B8N	O4'-C4'-C5'-O5'
46	S2	1248	B8N	C3'-C4'-C5'-O5'
46	S2	1326	UY1	C2'-C1'-C5-C4
46	S2	1328	OMG	C1'-C2'-O2'-CM2
46	S2	1391	OMC	C3'-C4'-C5'-O5'
46	S2	1391	OMC	O4'-C4'-C5'-O5'
46	S2	1442	OMU	C1'-C2'-O2'-CM2
46	S2	1442	OMU	O4'-C4'-C5'-O5'
46	S2	1678	A2M	C1'-C2'-O2'-CM2
46	S2	1851	MA6	O4'-C4'-C5'-O5'
46	S2	1830	UR3	O4'-C1'-N1-C2
1	L1	3701	OMC	C2'-C1'-N1-C2
1	L1	398	A2M	O4'-C4'-C5'-O5'
1	L1	1677	PSU	C3'-C4'-C5'-O5'
1	L1	3785	A2M	O4'-C4'-C5'-O5'
1	L1	3785	A2M	C3'-C4'-C5'-O5'
1	L1	4500	PSU	C3'-C4'-C5'-O5'
1	L1	4500	PSU	O4'-C4'-C5'-O5'
46	S2	159	A2M	O4'-C4'-C5'-O5'
46	S2	590	A2M	O4'-C4'-C5'-O5'
46	S2	590	A2M	C3'-C4'-C5'-O5'
46	S2	668	A2M	O4'-C4'-C5'-O5'
46	S2	823	PSU	C3'-C4'-C5'-O5'
46	S2	1851	MA6	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L1	1677	PSU	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'
46	S2	99	A2M	O4'-C4'-C5'-O5'
46	S2	512	A2M	O4'-C4'-C5'-O5'
46	S2	867	OMG	O4'-C4'-C5'-O5'
46	S2	1442	OMU	C3'-C4'-C5'-O5'
46	S2	1830	UR3	O4'-C1'-N1-C6
46	S2	428	OMU	C2'-C1'-N1-C6
1	L1	398	A2M	C3'-C4'-C5'-O5'
1	L1	3764	PSU	C3'-C4'-C5'-O5'
46	S2	823	PSU	O4'-C4'-C5'-O5'
1	L1	4447	5MC	C2'-C1'-N1-C6
43	Lo	53	MLZ	CE-CD-CG-CB
1	L1	2364	OMG	O4'-C4'-C5'-O5'
1	L1	3764	PSU	O4'-C4'-C5'-O5'
46	S2	512	A2M	C3'-C4'-C5'-O5'
46	S2	428	OMU	C2'-C1'-N1-C2
1	L1	3729	PSU	O4'-C4'-C5'-O5'
46	S2	99	A2M	C3'-C4'-C5'-O5'
46	S2	1243	PSU	O4'-C4'-C5'-O5'
46	S2	428	OMU	O4'-C1'-N1-C6
1	L1	4499	OMG	O4'-C4'-C5'-O5'
1	L1	1326	A2M	C4'-C5'-O5'-P
1	L1	2787	A2M	C3'-C4'-C5'-O5'
1	L1	3701	OMC	O4'-C1'-N1-C2
1	L1	4447	5MC	C2'-C1'-N1-C2
1	L1	3869	OMC	C3'-C2'-O2'-CM2
1	L1	3701	OMC	O4'-C1'-N1-C6
1	L1	4447	5MC	O4'-C1'-N1-C6
1	L1	1534	A2M	C4'-C5'-O5'-P
46	S2	590	A2M	C4'-C5'-O5'-P
1	L1	1582	PSU	C3'-C4'-C5'-O5'
1	L1	2364	OMG	C3'-C4'-C5'-O5'
1	L1	3818	UY1	C4'-C5'-O5'-P
1	L1	4447	5MC	O4'-C1'-N1-C2
46	S2	428	OMU	O4'-C1'-N1-C2
1	L1	2363	A2M	C3'-C2'-O2'-CM2
46	S2	644	OMG	C4'-C5'-O5'-P
46	S2	1490	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	L1	2824	OMC	C3'-C4'-C5'-O5'
1	L1	4499	OMG	C3'-C4'-C5'-O5'
1	L1	1677	PSU	O4'-C1'-C5-C4
1	L1	3818	UY1	O4'-C1'-C5-C4
1	L1	4450	PSU	O4'-C1'-C5-C4
46	S2	1326	UY1	O4'-C1'-C5-C4
1	L1	3792	OMG	O4'-C4'-C5'-O5'
43	Lo	53	MLZ	CD-CE-NZ-CM
1	L1	4500	PSU	C4'-C5'-O5'-P
1	L1	729	2MG	O4'-C4'-C5'-O5'
1	L1	2422	OMC	O4'-C4'-C5'-O5'
1	L1	2876	OMG	C3'-C4'-C5'-O5'
43	Lo	53	MLZ	CA-CB-CG-CD
46	S2	683	OMG	O4'-C4'-C5'-O5'
46	S2	822	PSU	C3'-C4'-C5'-O5'
46	S2	1243	PSU	C3'-C4'-C5'-O5'
1	L1	2363	A2M	C1'-C2'-O2'-CM'
1	L1	2351	OMC	C2'-C1'-N1-C2
46	S2	1219	JMH	C2'-C1'-N1-C2
46	S2	1288	OMU	C2'-C1'-N1-C2
1	L1	2787	A2M	O4'-C4'-C5'-O5'
1	L1	3729	PSU	C3'-C4'-C5'-O5'
46	S2	428	OMU	O4'-C4'-C5'-O5'
1	L1	3818	UY1	O4'-C1'-C5-C6
1	L1	4636	PSU	O4'-C1'-C5-C6
1	L1	1534	A2M	O4'-C4'-C5'-O5'
46	S2	1081	PSU	C4'-C5'-O5'-P
1	L1	2401	A2M	C3'-C2'-O2'-CM'
1	L1	2351	OMC	O4'-C4'-C5'-O5'
1	L1	3887	OMC	C4'-C5'-O5'-P
1	L1	3792	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides 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.

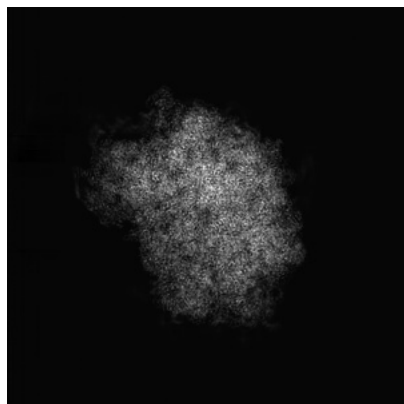
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33330. These allow visual inspection of the internal detail of the map and identification of artifacts.

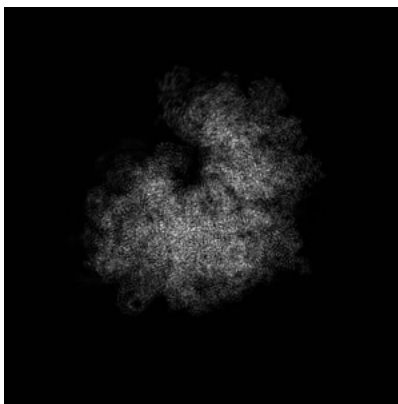
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

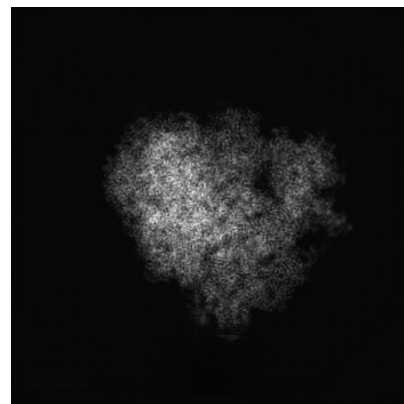
6.1.1 Primary map



X

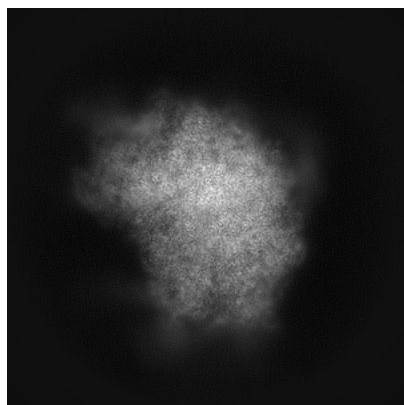


Y

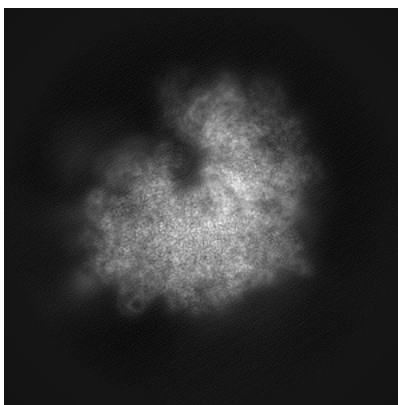


Z

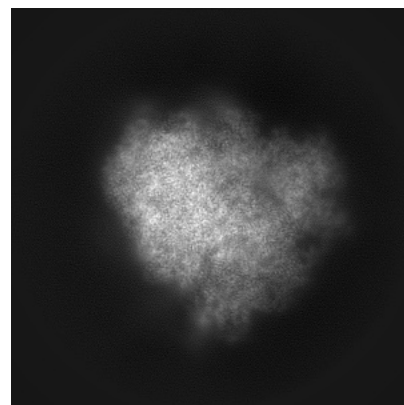
6.1.2 Raw map



X



Y

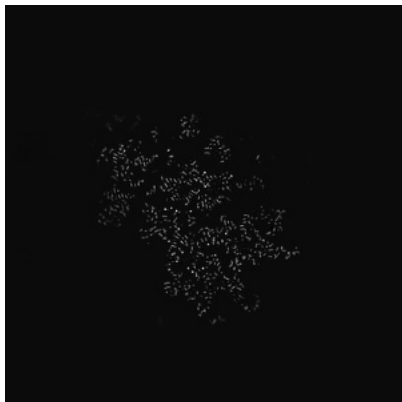


Z

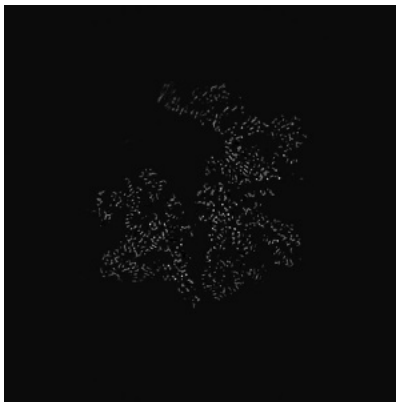
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210

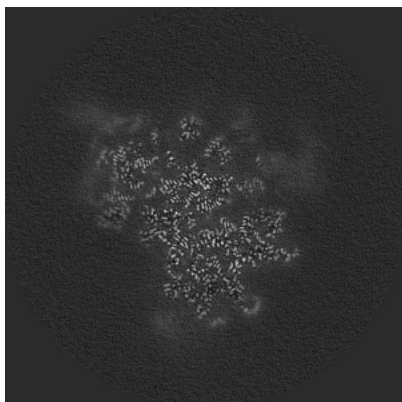


Y Index: 210

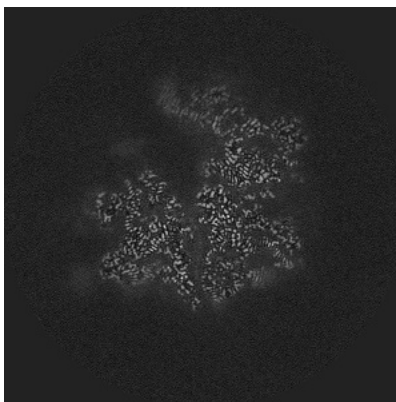


Z Index: 210

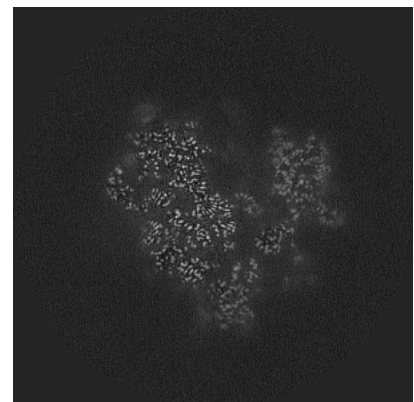
6.2.2 Raw map



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: 170

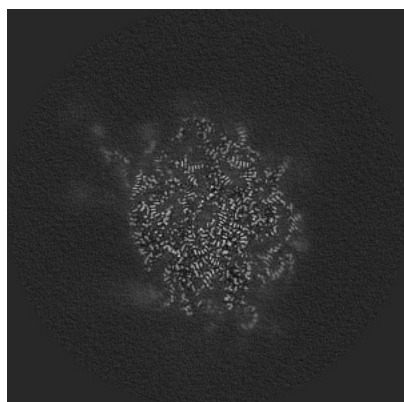


Y Index: 203

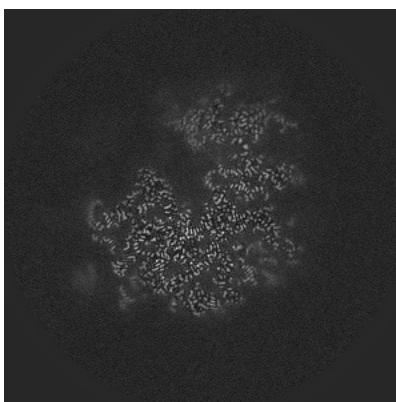


Z Index: 232

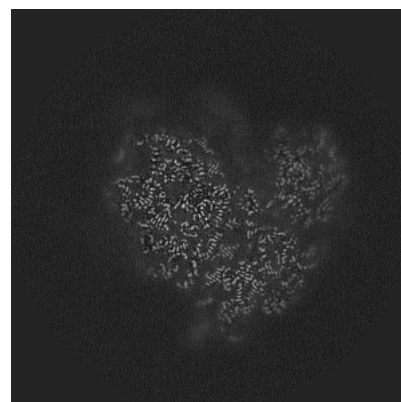
6.3.2 Raw map



X Index: 187



Y Index: 224

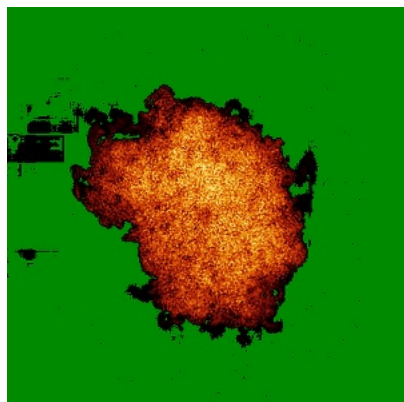


Z Index: 230

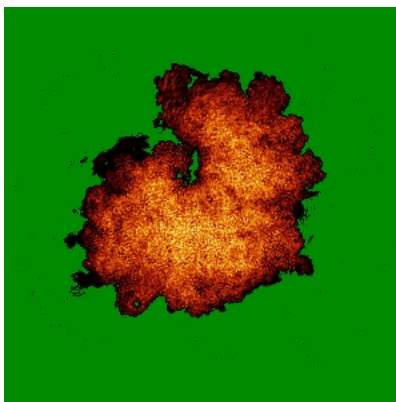
The images above show the largest variance slices of the map in three orthogonal directions.

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

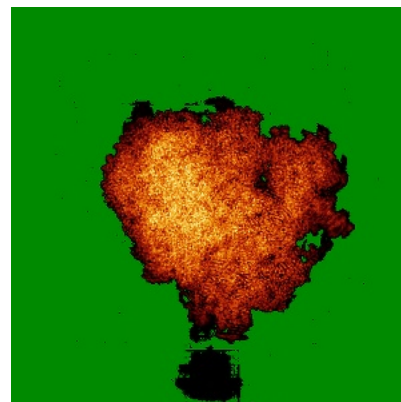
6.4.1 Primary map



X

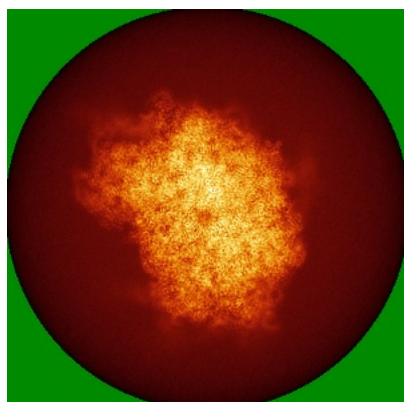


Y

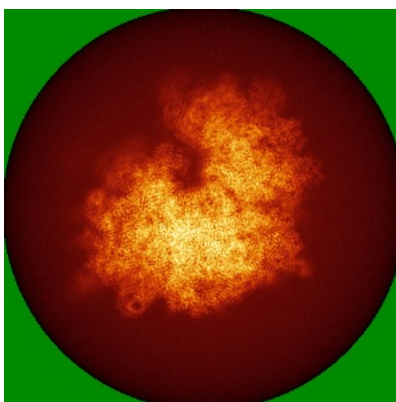


Z

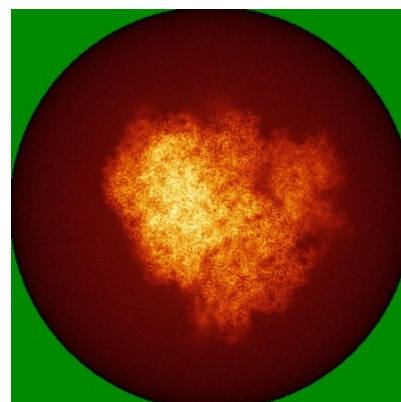
6.4.2 Raw map



X



Y



Z

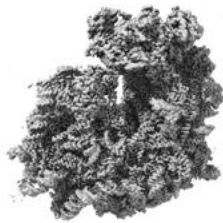
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



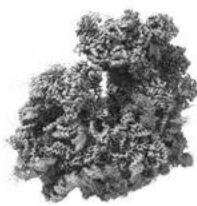
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

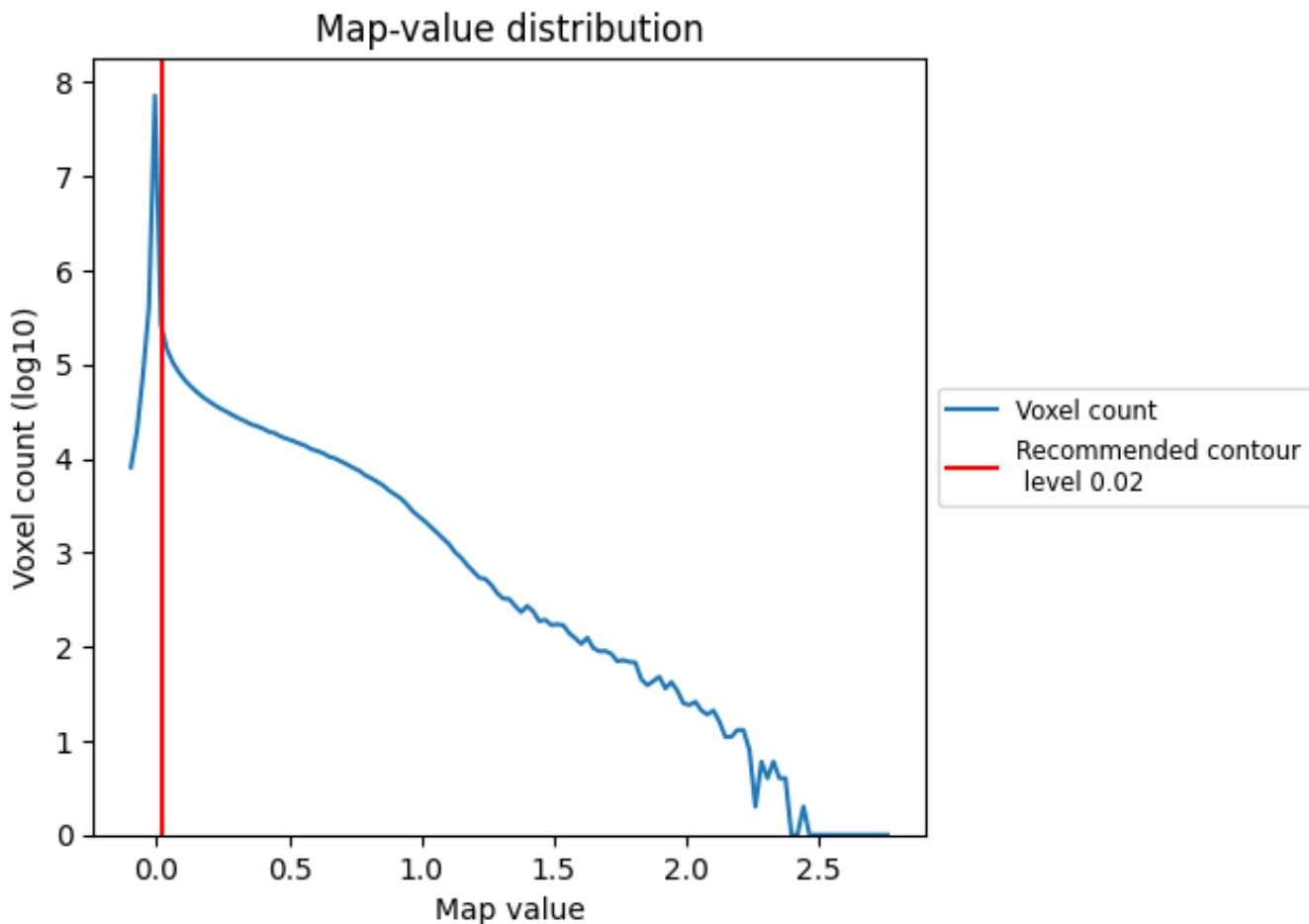
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

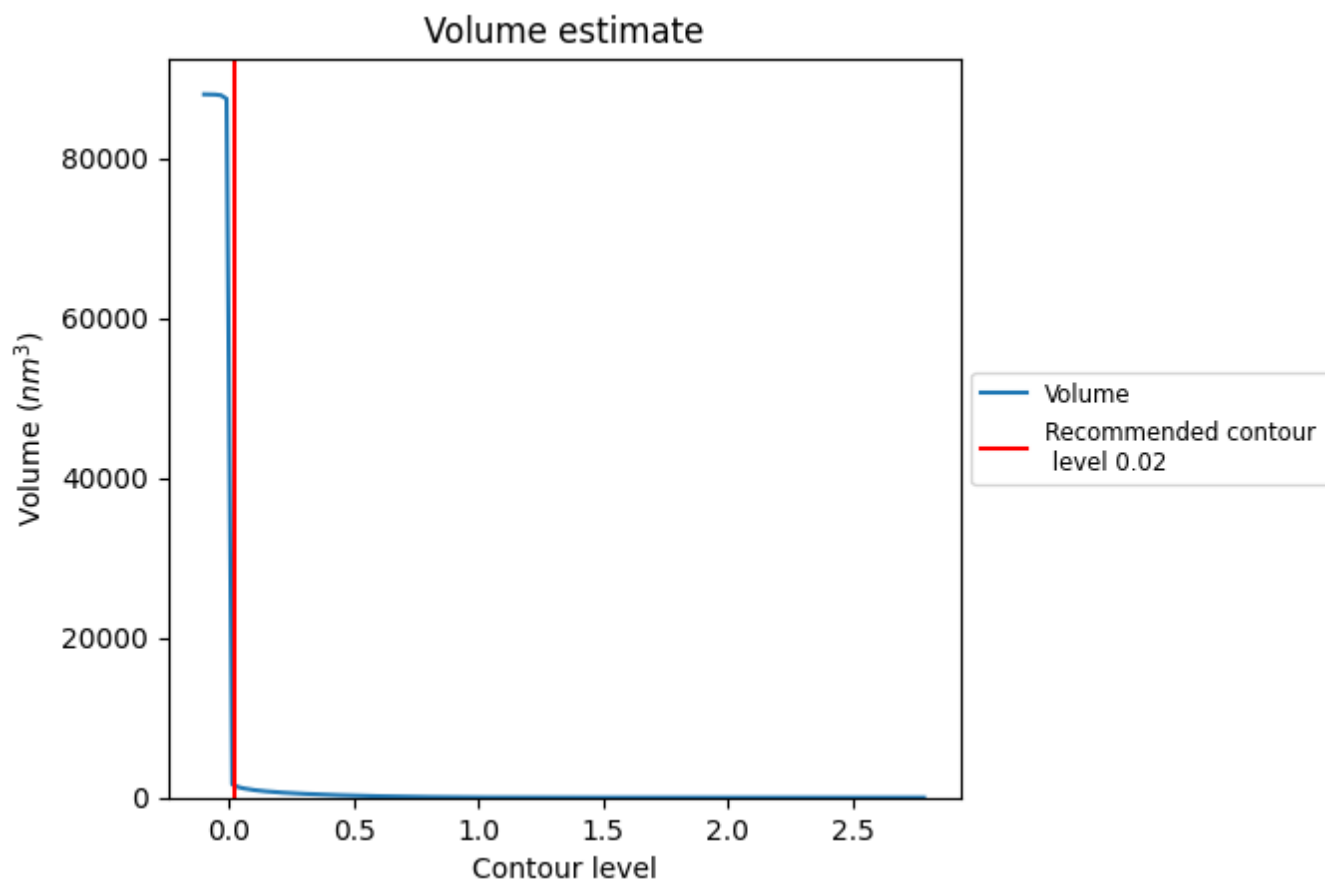
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

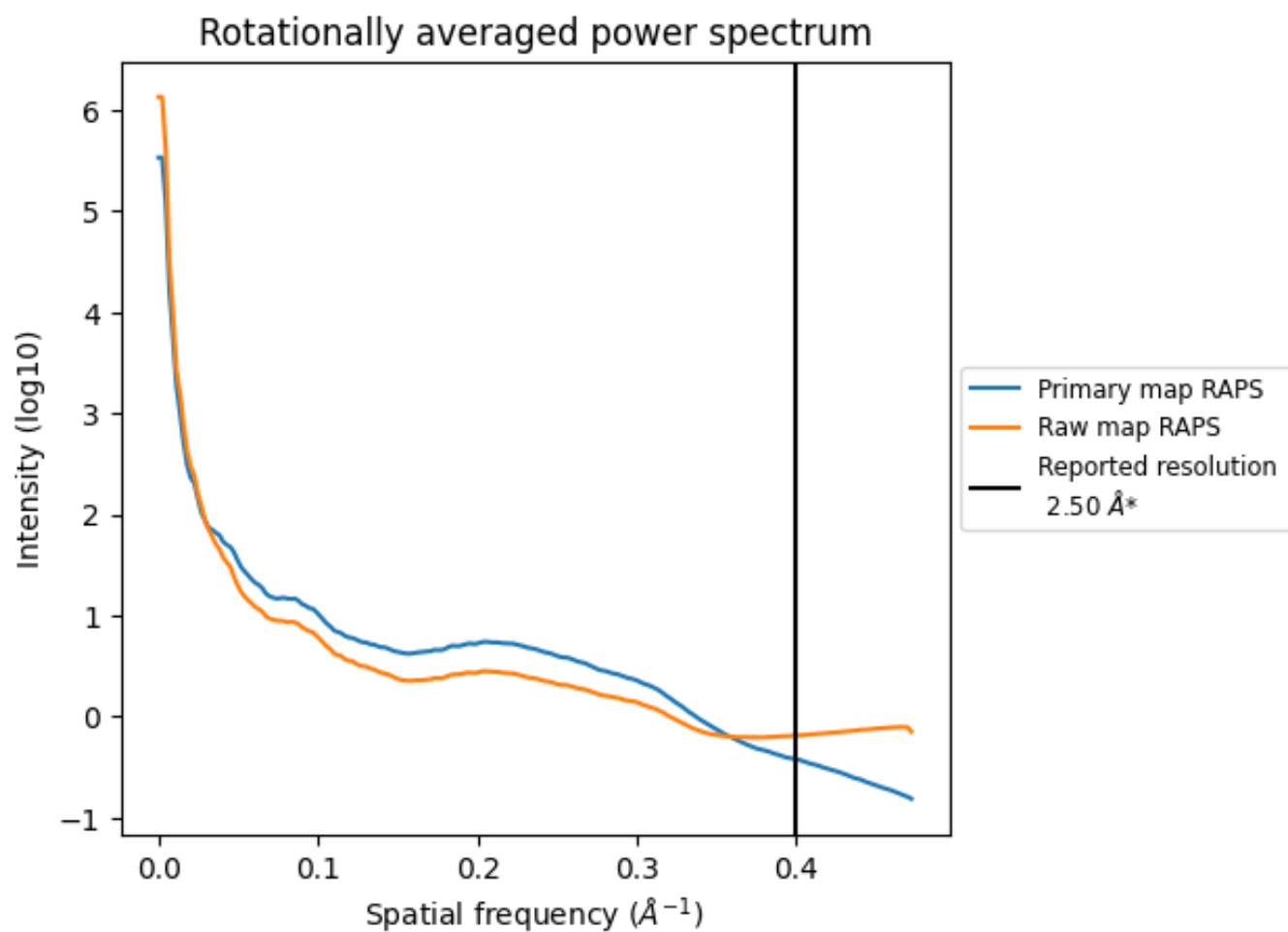
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1583 nm^3 ; this corresponds to an approximate mass of 1430 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

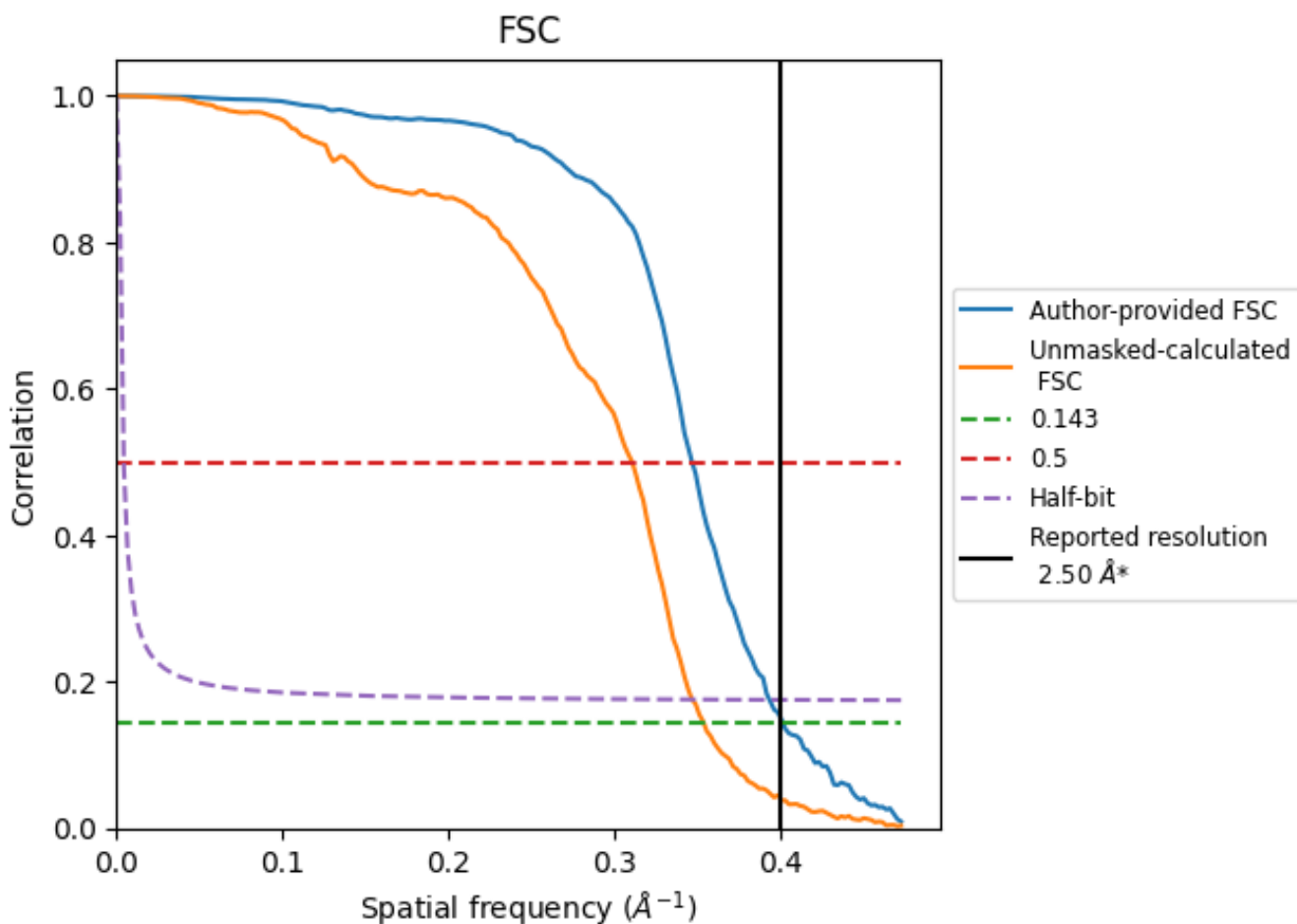


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

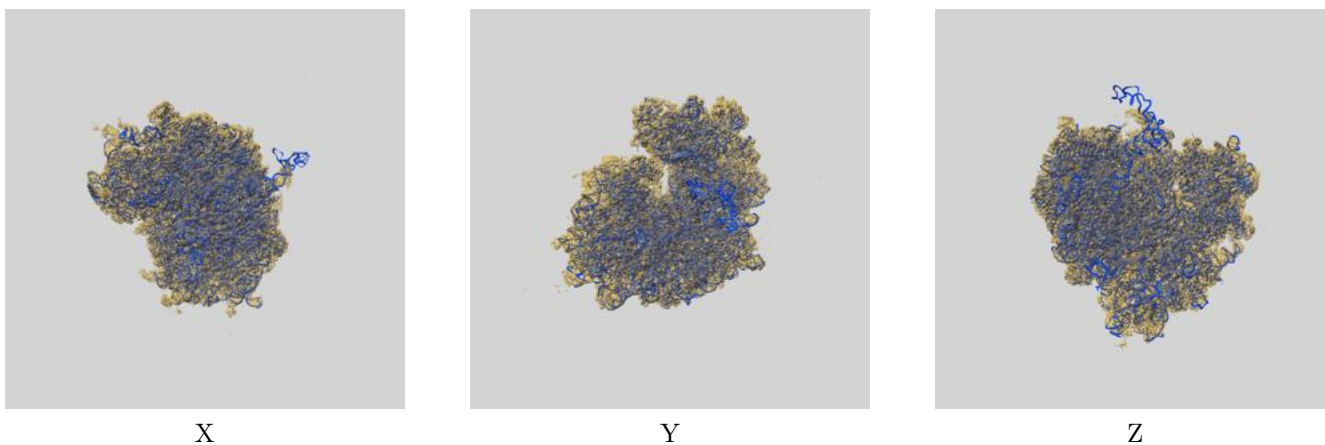
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.89	2.55
Unmasked-calculated*	2.83	3.22	2.89

*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 2.83 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

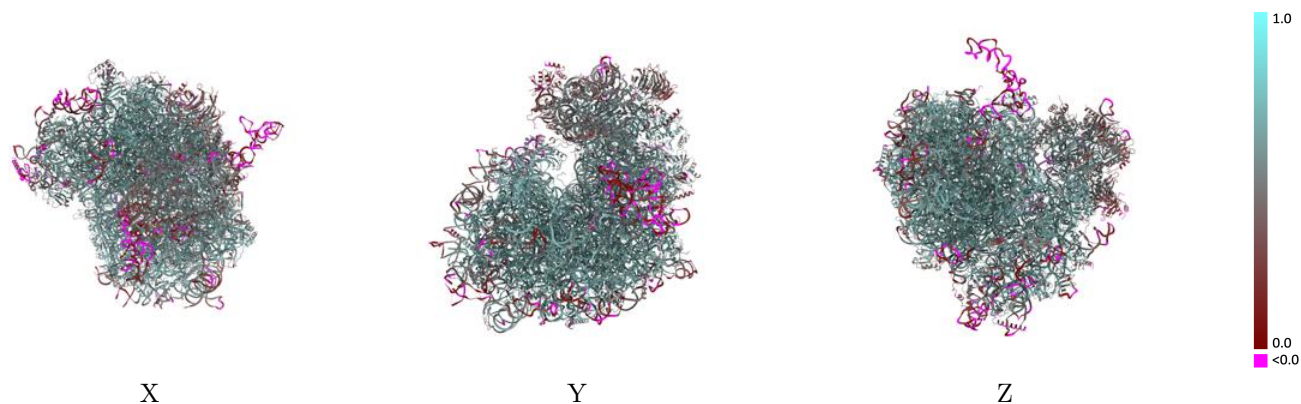
This section contains information regarding the fit between EMDB map EMD-33330 and PDB model 7XNY. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



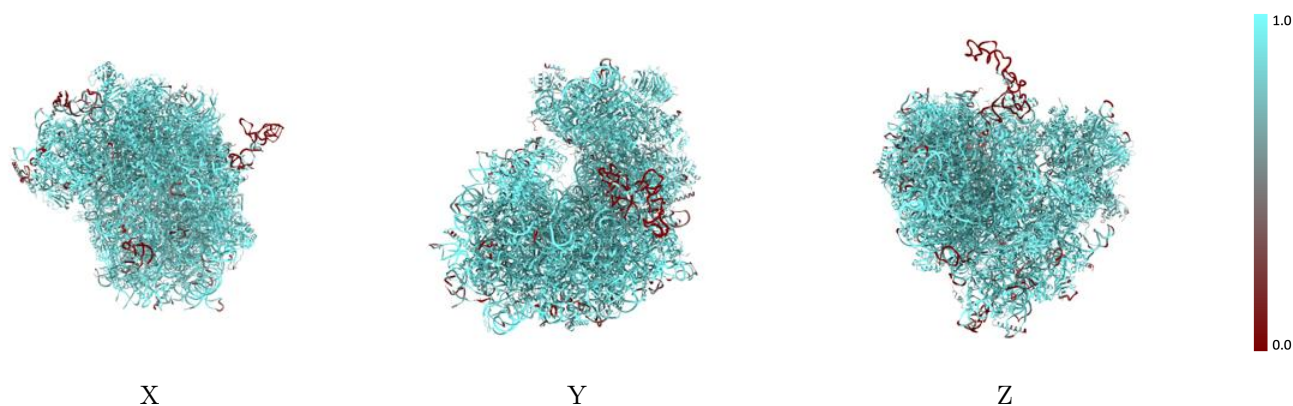
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



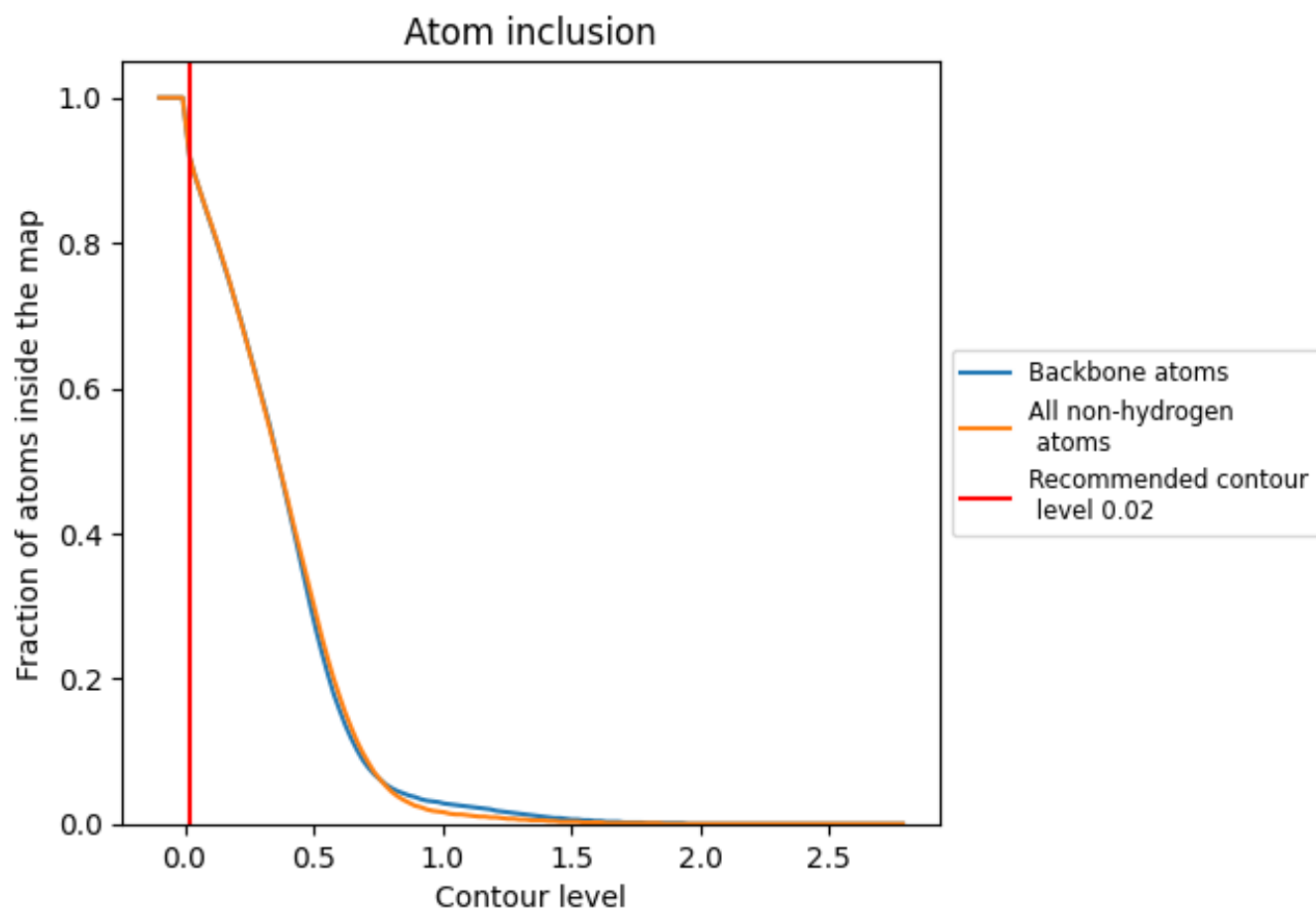
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.5600
L1	 0.9070	 0.5570
L2	 0.9920	 0.6420
L3	 0.9310	 0.5930
LA	 0.9800	 0.6660
LB	 0.9490	 0.6340
LC	 0.9560	 0.6380
LD	 0.9370	 0.5890
LE	 0.9480	 0.5930
LF	 0.9620	 0.6540
LG	 0.9210	 0.5740
LH	 0.9450	 0.6000
LI	 0.9560	 0.6220
LJ	 0.9160	 0.5370
LL	 0.9180	 0.5870
LM	 0.9490	 0.6120
LN	 0.9820	 0.6700
LO	 0.9520	 0.6360
LP	 0.9490	 0.6450
LQ	 0.9660	 0.6550
LR	 0.9090	 0.5840
LS	 0.9790	 0.6550
LT	 0.9380	 0.6080
LU	 0.8760	 0.4830
LV	 0.9560	 0.6440
LW	 0.7220	 0.3800
LX	 0.9370	 0.6200
LY	 0.9310	 0.6040
LZ	 0.9550	 0.6050
La	 0.9690	 0.6530
Lb	 0.8680	 0.5420
Lc	 0.9370	 0.6280
Ld	 0.9320	 0.6100
Le	 0.9670	 0.6480
Lf	 0.9750	 0.6590









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Chain	Atom inclusion	Q-score
Lg	0.9450	0.6200
Lh	0.9220	0.5900
Li	0.9390	0.5890
Lj	0.9720	0.6370
Lk	0.8890	0.5310
Ll	0.9360	0.6000
Lm	0.9420	0.6180
Ln	0.9380	0.6130
Lo	0.9390	0.6240
Lp	0.9350	0.6340
Lr	0.9670	0.6430
S2	0.9320	0.5450
SA	0.9460	0.5840
SB	0.9410	0.5860
SC	0.9530	0.6080
SD	0.8840	0.4580
SE	0.9500	0.5920
SF	0.9170	0.4870
SG	0.8720	0.4700
SH	0.8820	0.4870
SI	0.9210	0.5630
SJ	0.9190	0.5490
SK	0.8600	0.3830
SL	0.9390	0.6210
SM	0.6410	0.1100
SN	0.9620	0.6210
SO	0.9470	0.5980
SP	0.7840	0.3350
SQ	0.8900	0.4770
SR	0.8900	0.4920
SS	0.8610	0.3910
ST	0.8780	0.4270
SU	0.8750	0.4150
SV	0.9570	0.5940
SW	0.9680	0.6410
SX	0.9490	0.6160
SY	0.9190	0.5260
SZ	0.7940	0.3540
Sa	0.9300	0.5740
Sb	0.9170	0.5410
Sc	0.8520	0.4740
Sd	0.9190	0.5200

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Chain	Atom inclusion	Q-score
Se	 0.7720	 0.4650
Sf	 0.7400	 0.1880
Sg	 0.8670	 0.3790