Full wwPDB EM Validation Report (i)

Nov 4, 2023 – 05:33 PM EDT

PDB ID	:	8G61
EMDB ID	:	EMD-29760
Title	:	mRNA decoding in human is kinetically and structurally distinct from bacteria (AC state)
Authors	:	Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Altman, R.B.; Blanchard, S.C.
Deposited on	:	2023-02-14
Resolution	:	2.94 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 (i) 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 (1)) were used in the production of this report:

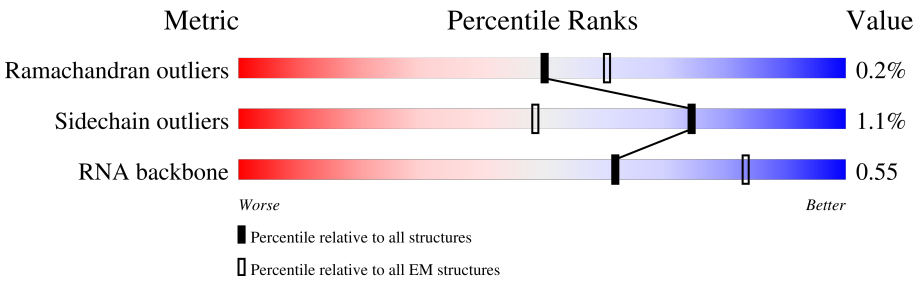
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.94 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	S2	1869	• 69% 20% • 10%
2	L8	156	• 79% 21%
3	L5	5069	• 57% 15% 28%
4	L7	120	• 93% 7%
5	SB	264	7% 81% 19%
6	SA	295	5% 75% • 25%
7	SD	243	9% 93% 7%
8	SJ	194	7% 95% 5%

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Mol	Chain	Length	Quality of chain
9	SE	263	98%
10	SC	293	74% 24%
11	SG	249	14% 94% 5%
12	SF	204	5% 93% 7%
13	SH	194	16% 96%
14	SW	130	98%
15	SI	208	6% 98%
16	SQ	146	95%
17	SU	119	10% 85% 15%
18	SK	165	53% 5% 42%
19	SO	151	7% 87% 11%
20	SX	143	97%
21	SM	132	82% 89% 8%
22	SS	152	5% 96%
23	Sd	56	96%
24	SN	151	99%
25	SL	158	91% 8%
26	SR	135	21% 99%
27	SP	145	10% 92% 7%
28	ST	145	98%
29	SV	83	5% 99%
30	SY	133	11% 95%
31	SZ	125	12% 69% 31%
32	Sa	115	6% 86% 14%
33	Sb	84	10% 99%

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Mol	Chain	Length	Quality of chain
34	Sc	69	14% 94% 6%
35	Se	133	5% 43% 57%
36	Sf	156	21% 39% 60%
37	Sg	317	27% 97%
38	Lz	217	55% 94%
39	LA	257	96%
40	LB	403	99%
41	LC	427	86% 14%
42	LJ	178	94% 5%
43	LH	192	99%
44	LE	288	76% 23%
45	LG	266	8% 89% 10%
46	LO	203	98%
47	LL	211	96%
48	LV	140	94% 5%
49	LM	215	63% 37%
50	La	148	98%
51	LN	204	99%
52	LI	214	95% 5%
53	LD	297	98%
54	LQ	188	99%
55	LR	196	6% 94% 5%
56	LS	176	100%
57	LT	160	98%
58	LP	184	83% 17%

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Mol	Chain	Length	Quality of chain
59	LU	128	77% 23%
60	LX	156	76% 24%
61	LY	145	91% 8%
62	LW	157	15% 71% 25%
63	LZ	136	98%
64	Lr	137	90% 9%
65	Lh	123	99%
66	Lb	159	8% 67% 31%
67	LF	248	90% 9%
68	Lc	115	85% 15%
69	Ld	125	86% 14%
70	Le	135	92% 5%
71	Lf	110	99%
72	Lg	117	6% 97%
73	Li	105	95%
74	Lj	97	87% 11%
75	Lk	70	99%
76	Ll	51	96%
77	Lm	128	41% 59%
78	Ln	25	96%
79	Lo	106	97%
80	Lp	92	99%
81	5A	154	23% 92% 5%
82	mR	60	17% 83%
83	At	76	11% 75% 21%

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Mol	Chain	Length	Quality of chain
84	Pt	77	8% 69% 26% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SAC	SA	2	-	X	-	-

2 Entry composition (i)

There are 92 unique types of molecules in this entry. The entry contains 219329 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	S2	1682	35978	16086	6447	11762	1683	1	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L8	156	3320	1482	585	1097	156	0	0

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L5	3657	78479	34987	14355	25480	3657	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L7	120	2562	1141	456	845	120	0	0

- Molecule 5 is a protein called 40S ribosomal protein S3a.

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

- Molecule 6 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SA	222	1750	1111	306	325	8	0	0

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SD	226	1756	1119	315	314	8	0	0

- Molecule 8 is a protein called 40S ribosomal protein S9.

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

- Molecule 9 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 10 is a protein called 40S ribosomal protein S2.

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

- Molecule 11 is a protein called 40S ribosomal protein S6.

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

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SF	189	1494	934	284	269	7	0	0

- Molecule 13 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SH	189	1517	966	279	271	1	0	0

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S8.

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

- Molecule 16 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	SQ	141	1123	715	212	193	3	0	0

- Molecule 17 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SU	101	803	504	153	142	4	0	0

- Molecule 18 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	SK	96	810	530	143	131	6	0	0

- Molecule 19 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	SO	135	1009	618	198	187	6	0	0

- Molecule 20 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	SX	140	1088	687	215	183	3	0	0

- Molecule 21 is a protein called 40S ribosomal protein S12.

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

- Molecule 22 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	SS	148	1214	761	245	207	1	0	0

- Molecule 23 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Sd	54	454	284	93	72	5	0	0

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	SN	150	1214	778	231	204	1	1	0

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	SL	145	1189	757	225	201	6	0	0

- Molecule 26 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	SR	134	1083	680	201	198	4	0	0

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	SP	135	1110	707	209	187	7	0	0

- Molecule 28 is a protein called 40S ribosomal protein S19.

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

- Molecule 29 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	SV	83	639	395	117	122	5	0	0

- Molecule 30 is a protein called 40S ribosomal protein S24.

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

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	SZ	86	688	442	129	116	1	0	0

- Molecule 32 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Sa	99	792	492	165	130	5	0	0

- Molecule 33 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Sb	83	650	408	121	114	7	0	0

- Molecule 34 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Sc	65	517	314	106	95	2	0	0

- Molecule 35 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Se	57	452	281	99	71	1	0	0

- Molecule 36 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Sf	63	515	324	98	86	7	0	0

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 38 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Lz	213	1714	1097	309	300	8	0	0

- Molecule 39 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LA	251	1930	1209	396	319	6	1	0

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	LB	402	3240	2061	608	557	14	0	0

- Molecule 41 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	LC	368	2927	1840	583	489	15	0	0

- Molecule 42 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	LJ	169	1358	859	253	240	6	0	0

- Molecule 43 is a protein called 60S ribosomal protein L9.

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

- Molecule 44 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	LE	223	1787	1150	339	294	4	0	0

- Molecule 45 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	LG	239	1913	1218	368	323	4	0	0

- Molecule 46 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	LO	200	1641	1058	320	258	5	0	0

- Molecule 47 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	LL	206	1664	1041	345	274	4	0	0

- Molecule 48 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	LV	133	988	623	186	174	5	0	0

- Molecule 49 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	LM	136	1120	719	215	179	7	0	0

- Molecule 50 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	La	147	1163	736	237	187	3	0	0

- Molecule 51 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	LN	203	1700	1072	359	265	4	0	0

- Molecule 52 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	LI	203	1646	1045	317	271	13	0	0

- Molecule 53 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	LD	294	2391	1513	436	428	14	0	0

- Molecule 54 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	LQ	187	1512	944	314	249	5	0	0

- Molecule 55 is a protein called 60S ribosomal protein L19.

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

- Molecule 56 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	LS	176	1460	930	284	235	11	0	0

- Molecule 57 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	LT	159	1297	823	252	216	6	0	0

- Molecule 58 is a protein called 60S ribosomal protein L17.

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

- Molecule 59 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	LU	99	808	518	141	147	2	0	0

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

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

- Molecule 61 is a protein called 60S ribosomal protein L26.

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

- Molecule 62 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	LW	118	950	595	192	159	4	0	0

- Molecule 63 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	LZ	135	1106	714	208	181	3	0	0

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	Lr	125	1005	624	207	169	5	0	0

- Molecule 65 is a protein called 60S ribosomal protein L35.

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

- Molecule 66 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	Lb	109	885	552	192	137	4	0	0

- Molecule 67 is a protein called 60S ribosomal protein L7.

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

- Molecule 68 is a protein called 60S ribosomal protein L30.

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

- Molecule 69 is a protein called 60S ribosomal protein L31.

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

- Molecule 70 is a protein called 60S ribosomal protein L32.

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

- Molecule 71 is a protein called 60S ribosomal protein L35a.

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

- Molecule 72 is a protein called 60S ribosomal protein L34.

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

- Molecule 73 is a protein called 60S ribosomal protein L36.

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

- Molecule 74 is a protein called 60S ribosomal protein L37.

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

- Molecule 75 is a protein called 60S ribosomal protein L38.

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

- Molecule 76 is a protein called 60S ribosomal protein L39.

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

- Molecule 77 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	Lm	52	431	269	90	66	6	0	0

- Molecule 78 is a protein called 60S ribosomal protein L41.

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

- Molecule 79 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Lo	104	852	534	174	138	6	0	0

- Molecule 80 is a protein called 60S ribosomal protein L37a.

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

- Molecule 81 is a protein called eIF5A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	5A	150	1144	716	194	225	9	0	0

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
82	mR	10	210	94	34	72	10	0	0

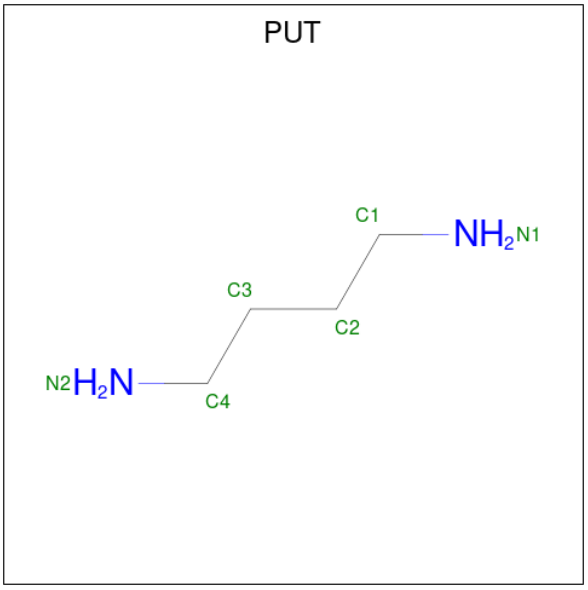
- Molecule 83 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
83	At	76	1624	724	290	533	76	1	0	0

- Molecule 84 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
84	Pt	77	1645	734	298	535	77	1	0	0

- Molecule 85 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
85	S2	1	6	4	2	0
85	L5	1	6	4	2	0
85	L5	1	6	4	2	0
85	L5	1	6	4	2	0

- Molecule 86 is POTASSIUM ION (three-letter code: K) (formula: K).

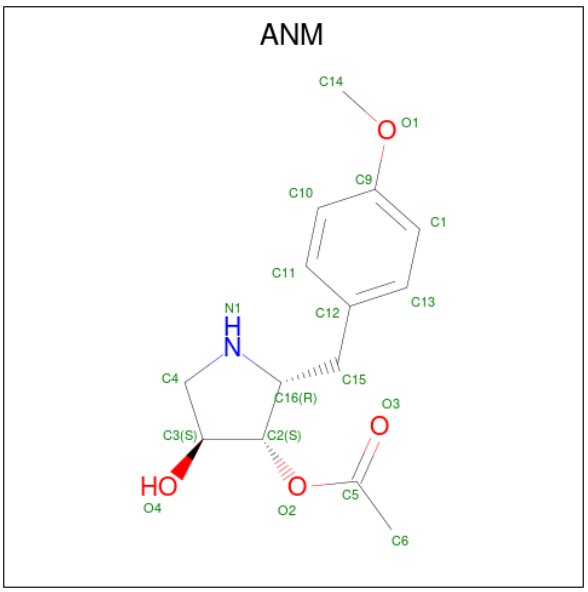
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
86	S2	1	1	1	0
86	L5	13	13	13	0
86	LA	1	1	1	0
86	Lf	1	1	1	0

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
87	S2	67	67	67	0
87	L8	6	6	6	0
87	L5	231	231	231	0
87	L7	4	4	4	0
87	SC	1	1	1	0
87	SS	1	1	1	0
87	SN	1	1	1	0
87	Sa	1	1	1	0
87	LA	1	1	1	0
87	LB	1	1	1	0
87	LV	1	1	1	0
87	LN	2	2	2	0
87	LP	1	1	1	0
87	Le	1	1	1	0
87	Lg	1	1	1	0
87	Ln	1	1	1	0
87	Lo	1	1	1	0
87	5A	1	1	1	0
87	At	1	1	1	0
87	Pt	2	2	2	0

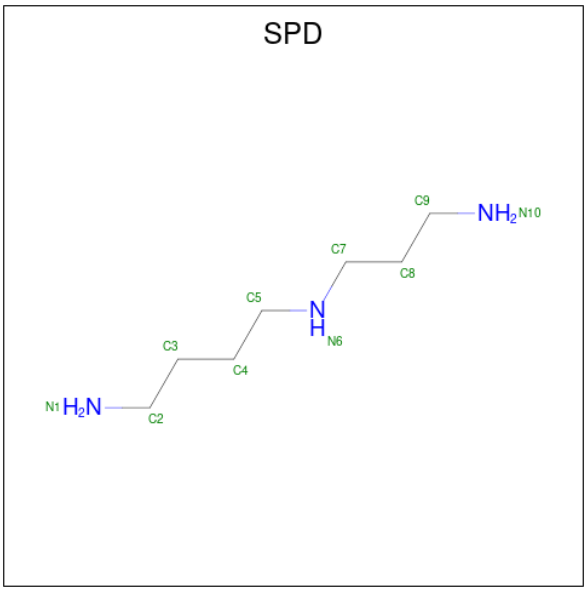
- Molecule 88 is ANISOMYCIN (three-letter code: ANM) (formula: $C_{14}H_{19}NO_4$) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
88	L5	1	19	14	1	4	0

- Molecule 89 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
89	L5	1	10	7	3	0
			Total	C	N	
89	L5	1	10	7	3	0

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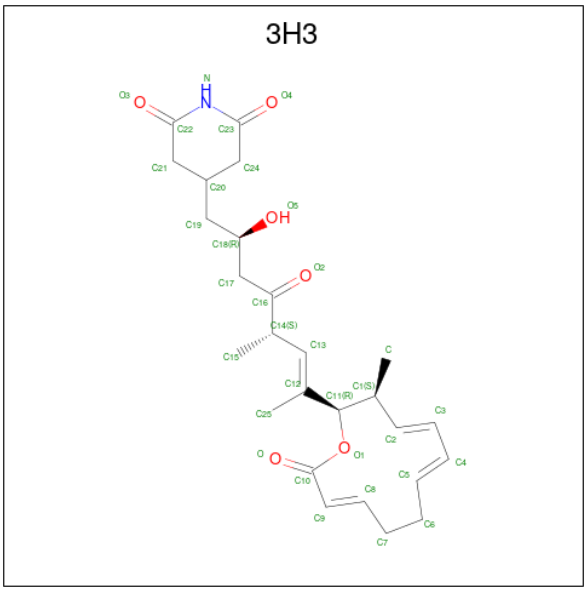
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
89	L5	1	10	7	3	0
			Total	C	N	
89	L5	1	10	7	3	0
			Total	C	N	
89	L5	1	10	7	3	0

- Molecule 90 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxoo xacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (three-letter code: 3H3) (formula: $C_{26}H_{35}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
90	L5	1	33	26	1	6	0

- Molecule 91 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
91	Sd	1	1	1	0
			Total	Zn	
91	Sa	1	1	1	0
			Total	Zn	
91	Sf	1	1	1	0
			Total	Zn	
91	Lg	1	1	1	0

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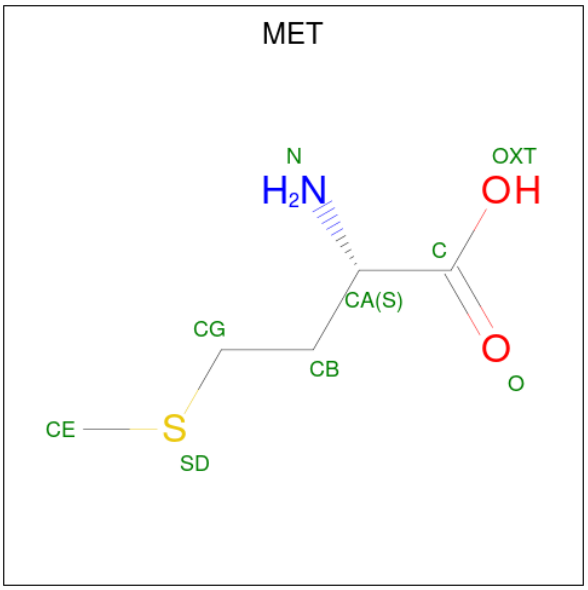
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
91	Lj	1	1	1	0
91	Lm	1	1	1	0
91	Lo	1	1	1	0
91	Lp	1	1	1	0

- Molecule 92 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



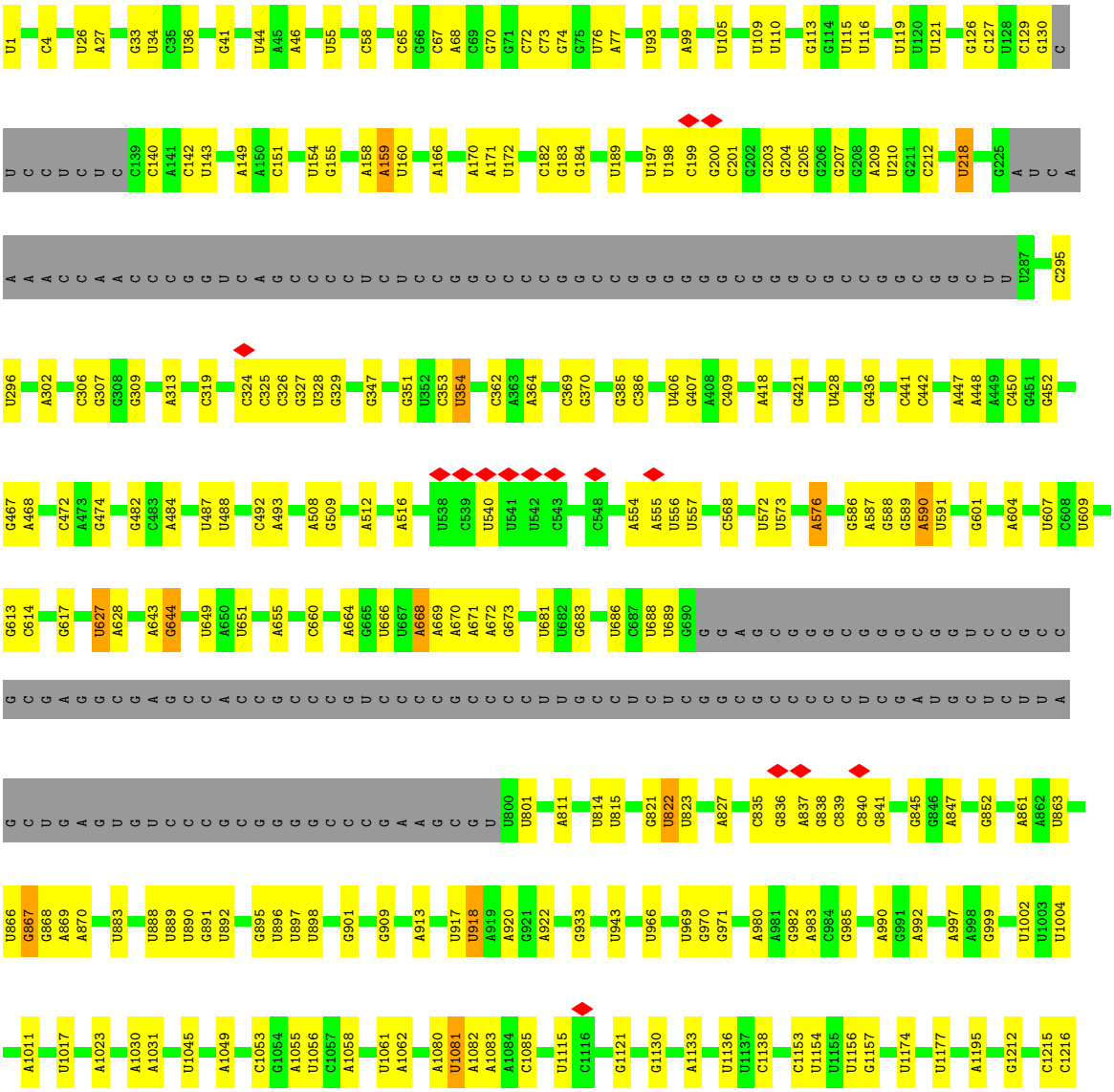
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
92	Pt	1	8	5	1	1	1	0

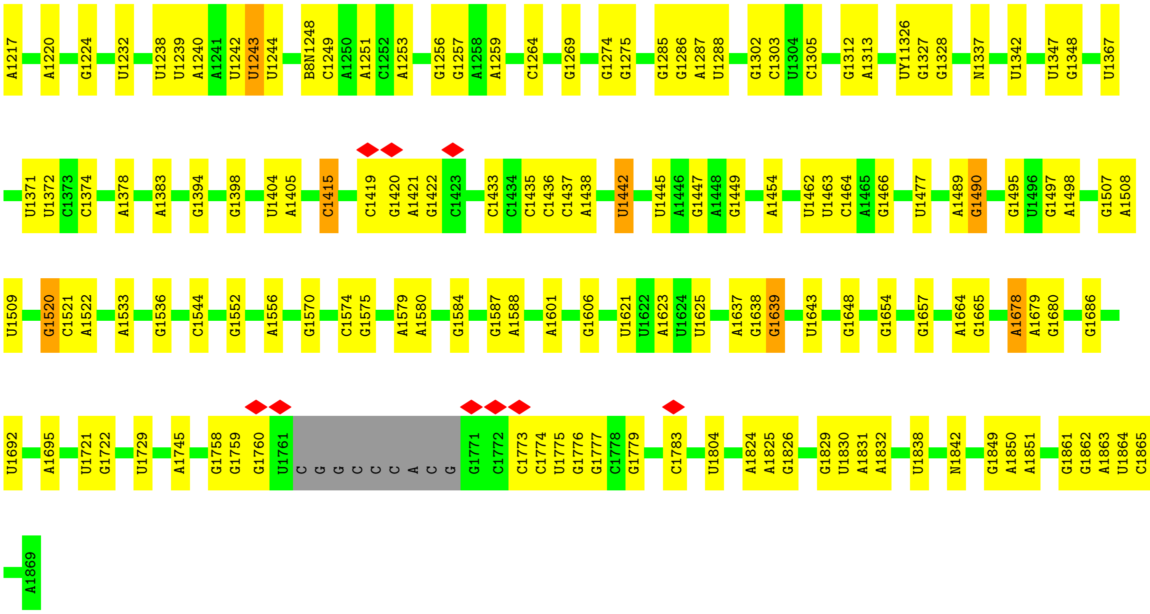
3 Residue-property plots (i)

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

- Molecule 1: 18S rRNA

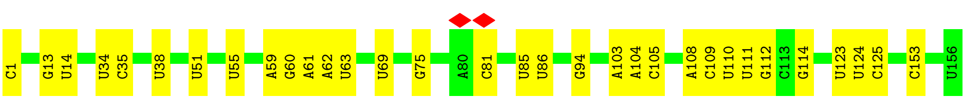
Chain S2:





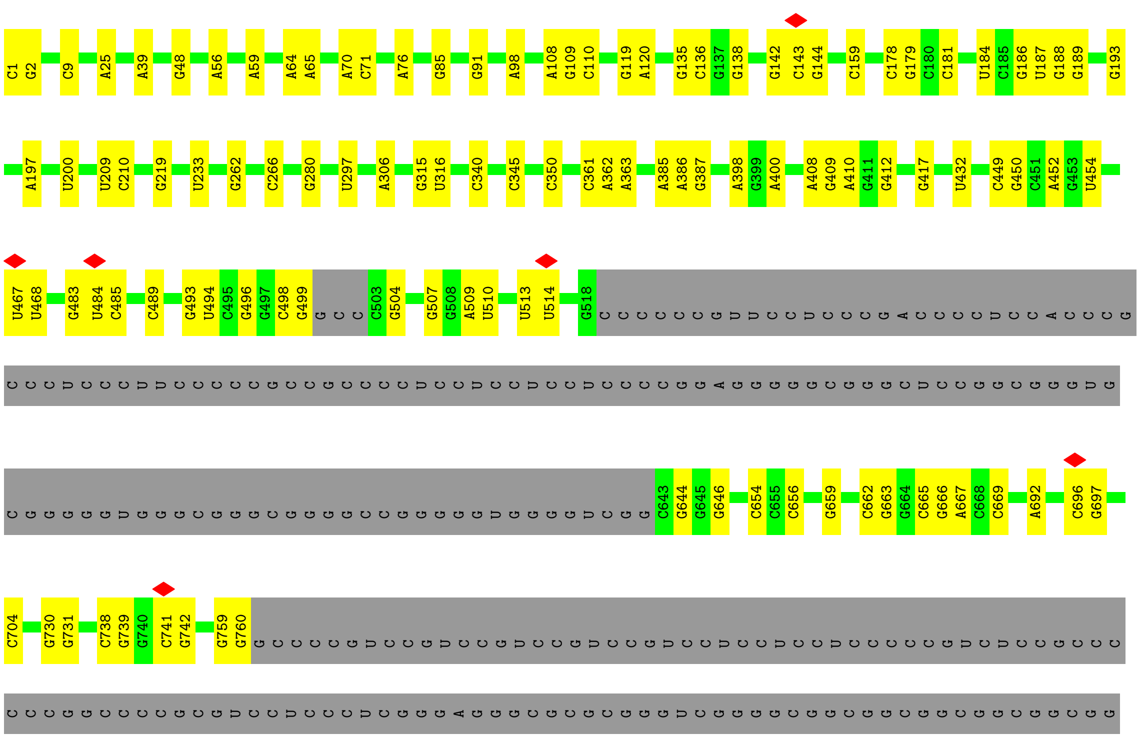
• Molecule 2: 5.8S rRNA

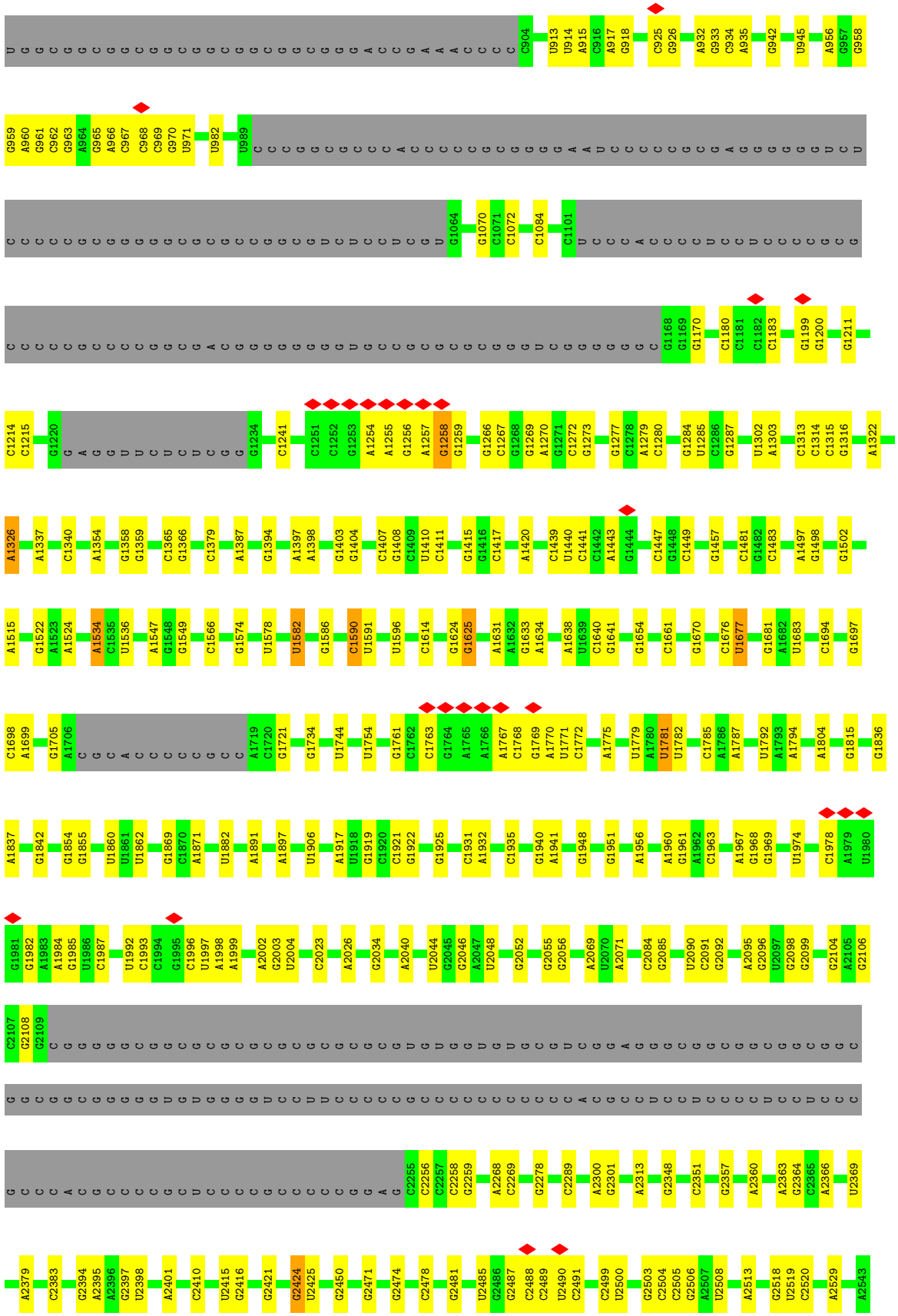
Chain L8:



• Molecule 3: 28S rRNA

Chain L5:

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G959 A960 G961 C962 G963 A964 G965 A966 C967 C968 C969 G970 U971 U982 U989 C C C G G C G G C C C A C C C C G C G G G G A A U C C C C C G C G G A G C G G C U C C U
C C C C C G C G G G G C G C G C C G G C G C G U C U C C U C C G U G1064 G1070 C1071 C1072 C1084 C1101 U C C C A C C C C U C C U
C C C C C G C C C C C G G C G A C G G G G G G G G U G G C C C G C G G G G G G G G G G C G1168 G1169 G1170 C1180 C1181 C1182 C1183 G1199 G1200 G1211
C1214 C1215 G1220 G A G U U C U C U C G G G1234 C1241 C1251 C1252 G1253 A1254 A1255 G1256 A1257 G1258 G1259 G1266 C1267 G1268 G1269 A1270 G1271 C1272 G1273 G1277 G1278 A1279 C1280 G1284 U1285 G1286 G1287 U1302 A1303 C1313 C1314 C1315 G1316 A1322
A1326 A1337 C1340 A1354 G1358 G1359 C1365 G1366 C1379 A1387 G1394 A1397 A1398 G1403 G1404 C1407 G1408 C1409 U1410 C1411 G1415 G1416 C1417 A1420 C1439 U1440 C1441 C1442 A1443 G1444 C1447 C1448 C1449 G1457 C1481 G1482 C1483 A1497 G1498 G1502
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C1698 A1699 G1705 A1706 C G C A C C C C G C C A1719 C1720 G1721 G1734 U1744 U1754 G1761 C1762 C1763 G1764 A1765 A1766 A1767 C1768 G1769 A1770 U1771 C1772 A1775 U1779 A1780 U1781 U1782 C1785 A1786 A1787 U1792 A1793 A1794 A1804 G1815 G1836
A1837 G1842 G1854 G1855 U1860 U1861 U1862 G1869 C1870 A1871 U1882 A1891 A1897 U1906 A1917 U1918 G1919 C1920 C1921 G1922 G1925 C1931 A1932 C1935 G1940 A1941 G1948 G1951 A1956 A1960 G1961 A1962 C1963 A1967 G1968 G1969 U1974 C1978 A1979 U1980
G1981 G1982 A1983 A1984 G1985 U1986 C1987 U1992 C1993 C1994 G1995 C1996 U1997 A1998 A1999 A2002 G2003 U2004 C2023 A2026 G2034 A2040 U2044 G2045 G2046 A2047 U2048 G2052 G2055 G2056 A2069 U2070 A2071 C2084 G2085 U2090 C2091 G2092 A2095 G2096 U2097 C2098 G2099 G2104 A2105 G2106
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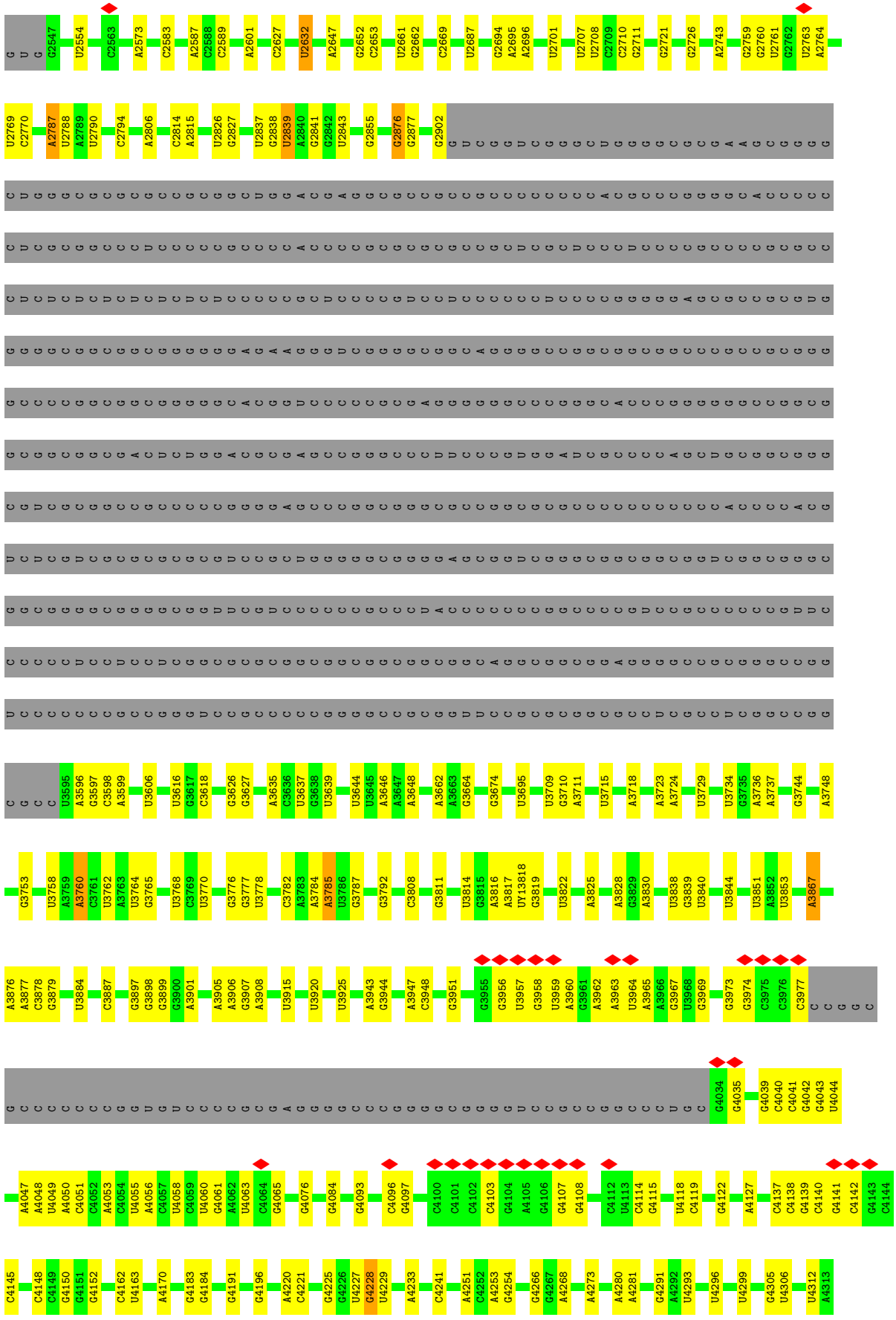
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C2653
U2661
G2662
C2669
U2687
G2694
A2695
A2696
U2701
U2707
U2708
C2709
C2710
G2711
G2721
G2726
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U2788
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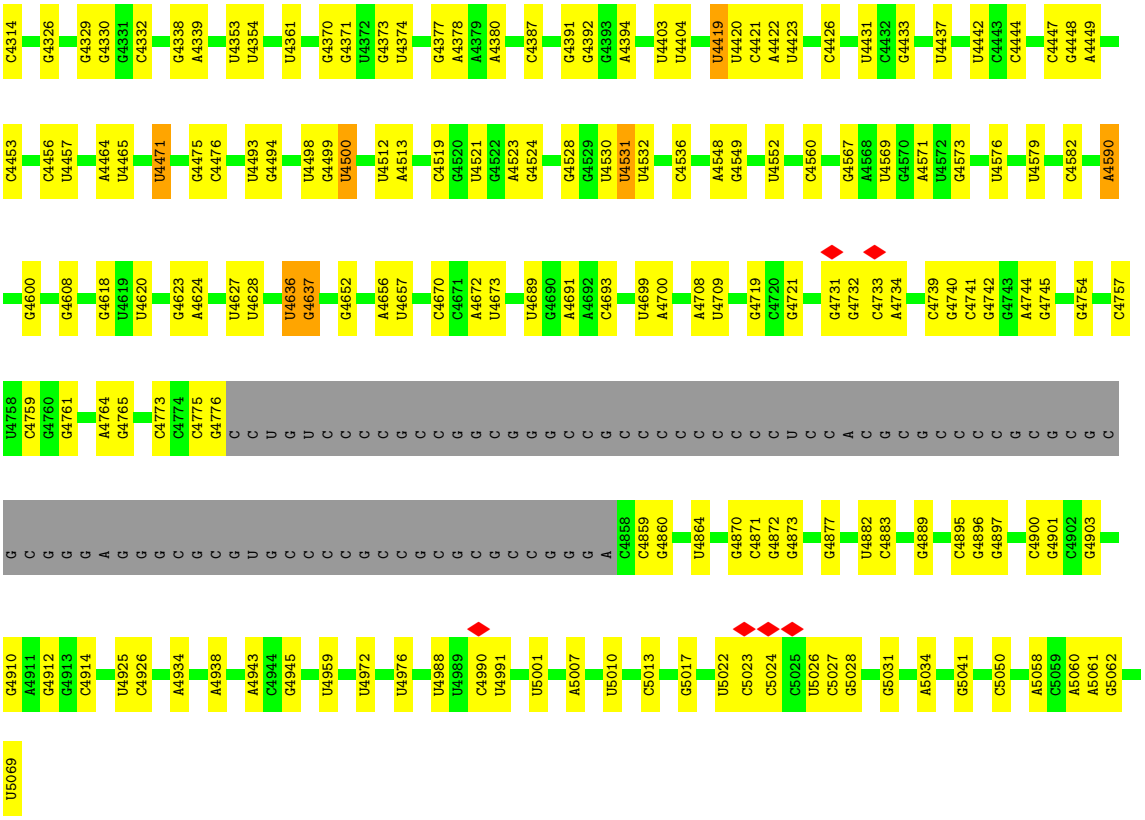
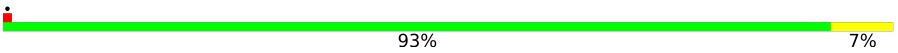
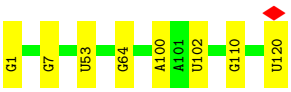


- Molecule 4: 5S rRNA

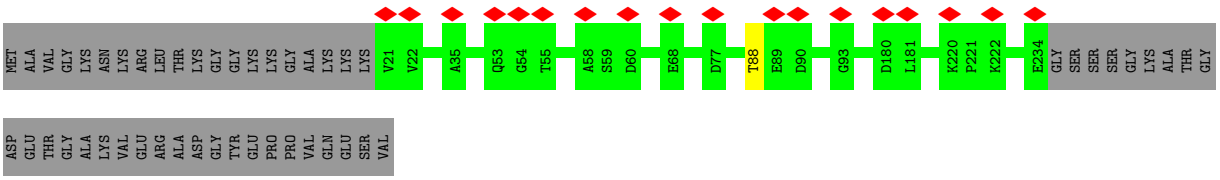
Chain L7:





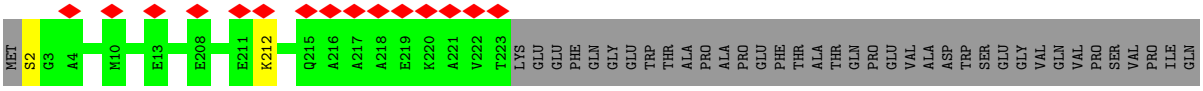
- Molecule 5: 40S ribosomal protein S3a

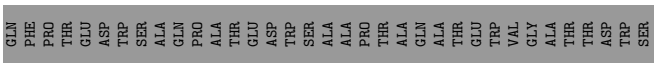
Chain SB:



- Molecule 6: 40S ribosomal protein SA

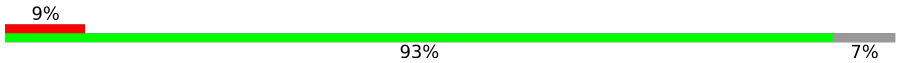
Chain SA:

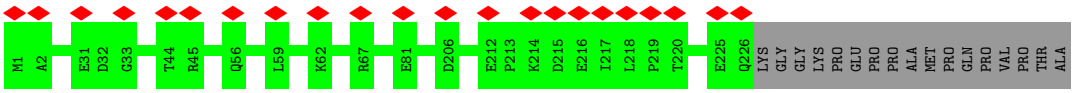




• Molecule 7: 40S ribosomal protein S3

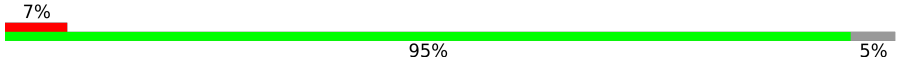
Chain SD:

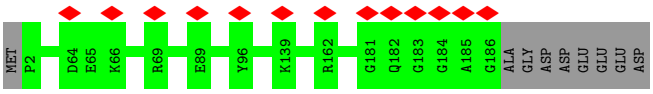




• Molecule 8: 40S ribosomal protein S9

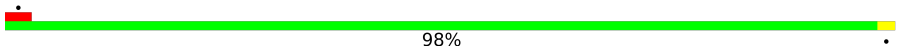
Chain SJ:

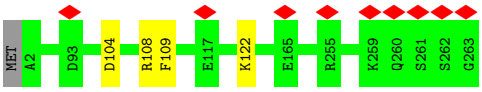




• Molecule 9: 40S ribosomal protein S4, X isoform

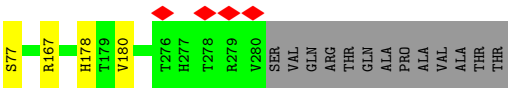
Chain SE:





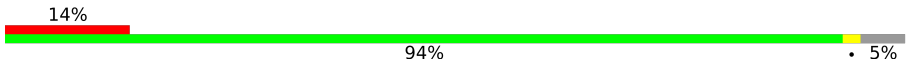
• Molecule 10: 40S ribosomal protein S2

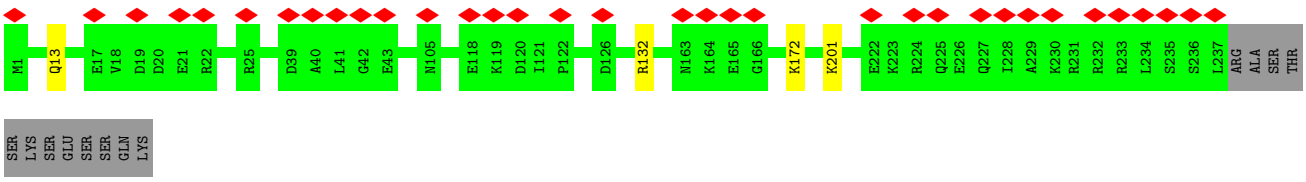
Chain SC:



• Molecule 11: 40S ribosomal protein S6

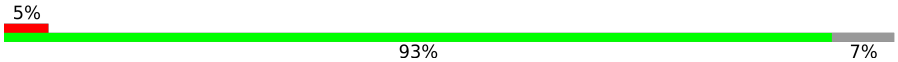
Chain SG:

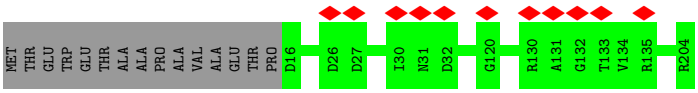




• Molecule 12: 40S ribosomal protein S5

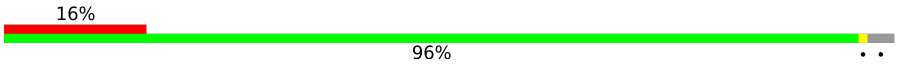
Chain SF:

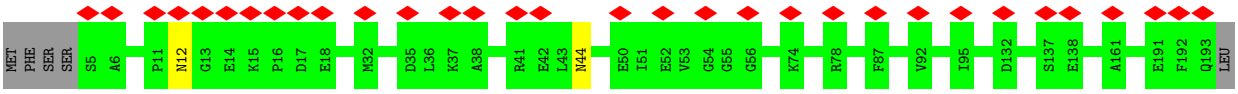




• Molecule 13: 40S ribosomal protein S7

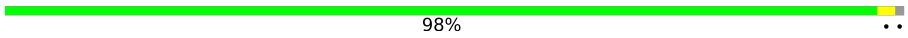
Chain SH:

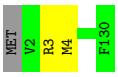




• Molecule 14: 40S ribosomal protein S15a

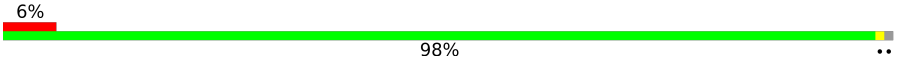
Chain SW:

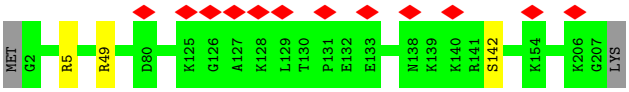




• Molecule 15: 40S ribosomal protein S8

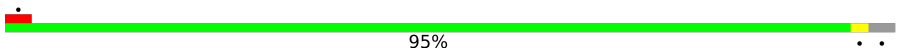
Chain SI:

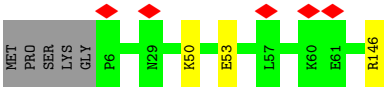




• Molecule 16: 40S ribosomal protein S16

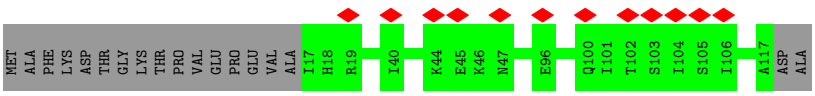
Chain SQ:





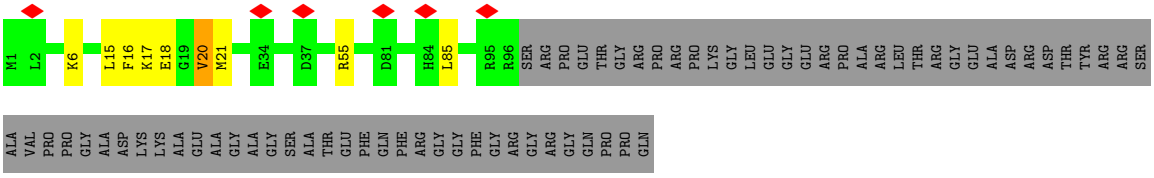
• Molecule 17: 40S ribosomal protein S20

Chain SU:



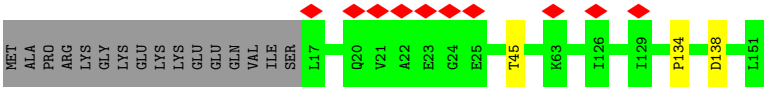
• Molecule 18: 40S ribosomal protein S10

Chain SK:



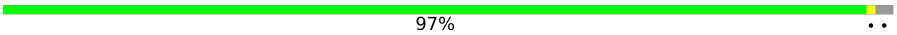
• Molecule 19: 40S ribosomal protein S14

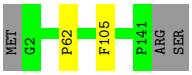
Chain SO:



• Molecule 20: uS12

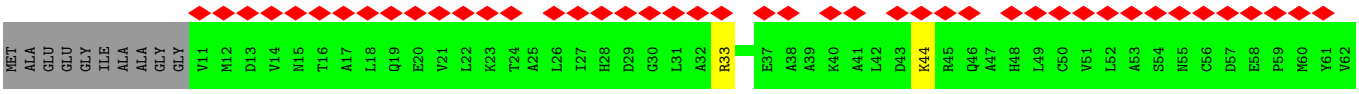
Chain SX:

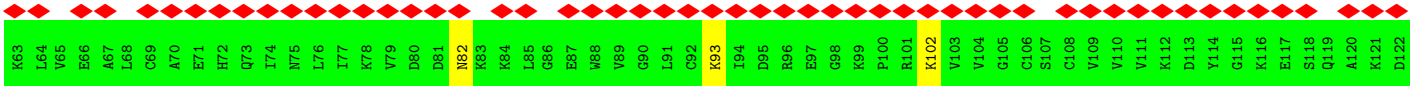


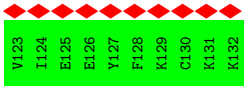


• Molecule 21: 40S ribosomal protein S12

Chain SM:

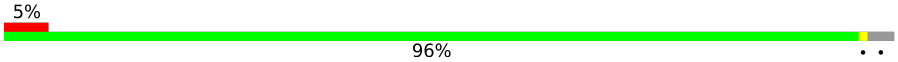


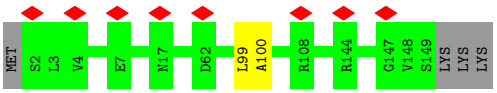




• Molecule 22: 40S ribosomal protein S18

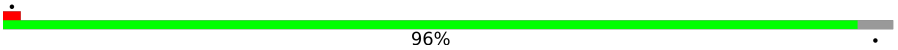
Chain SS:

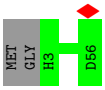




• Molecule 23: 40S ribosomal protein S29

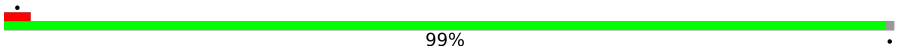
Chain Sd:

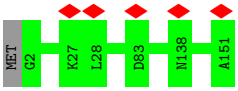




• Molecule 24: 40S ribosomal protein S13

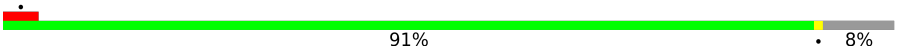
Chain SN:

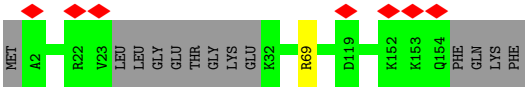




• Molecule 25: 40S ribosomal protein S11

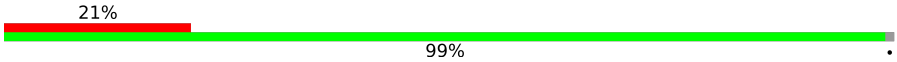
Chain SL:

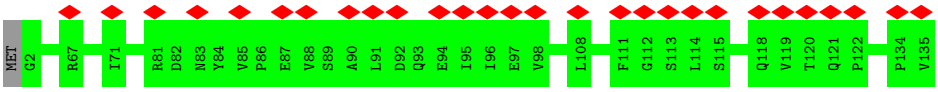




• Molecule 26: 40S ribosomal protein S17

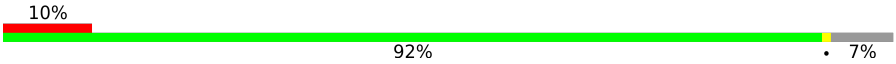
Chain SR:

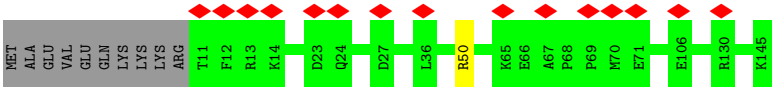




• Molecule 27: 40S ribosomal protein S15

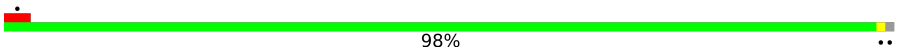
Chain SP:

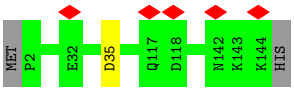




• Molecule 28: 40S ribosomal protein S19

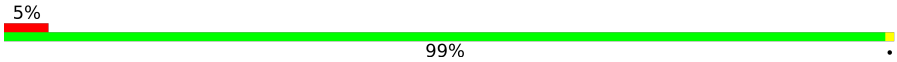
Chain ST:

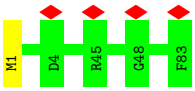




• Molecule 29: 40S ribosomal protein S21

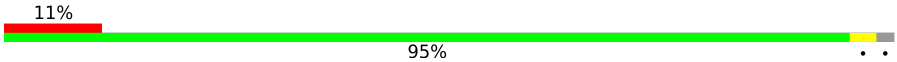
Chain SV:

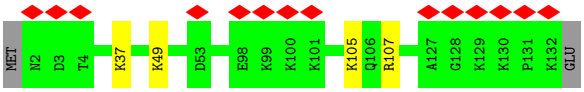




• Molecule 30: 40S ribosomal protein S24

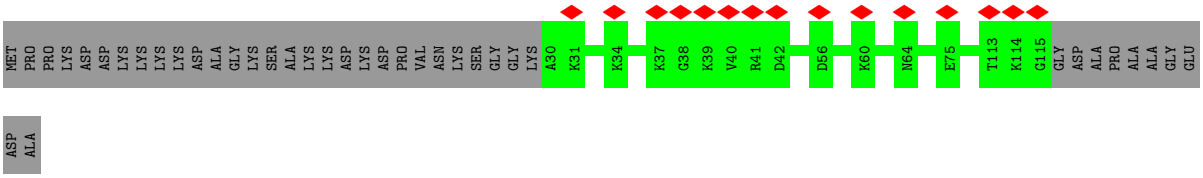
Chain SY:





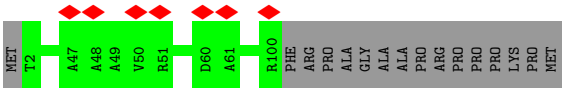
• Molecule 31: 40S ribosomal protein S25

Chain SZ:



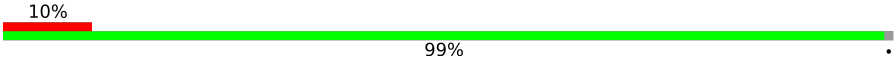
- Molecule 32: 40S ribosomal protein S26

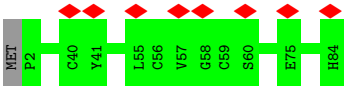
Chain Sa:



- Molecule 33: 40S ribosomal protein S27

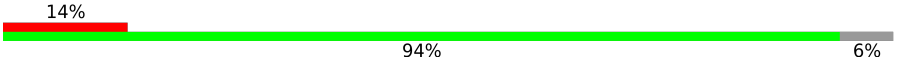
Chain Sb:

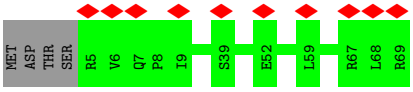




- Molecule 34: 40S ribosomal protein S28

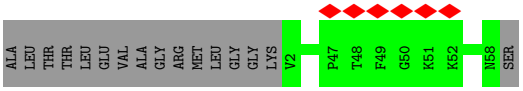
Chain Sc:





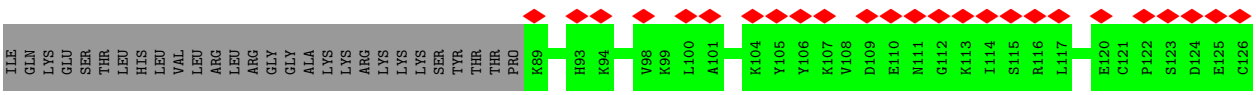
- Molecule 35: FAU ubiquitin-like and ribosomal protein S30

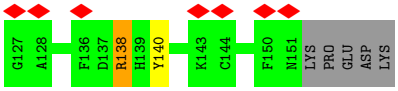
Chain Se:



- Molecule 36: Ubiquitin-40S ribosomal protein S27a

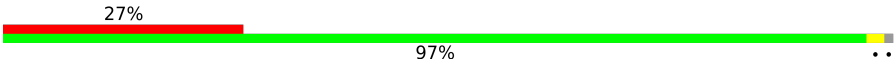
Chain Sf:

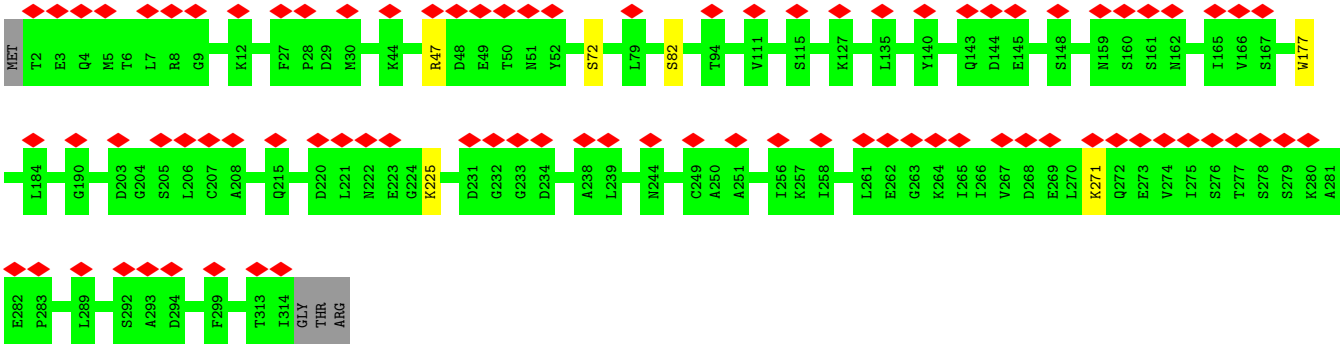




- Molecule 37: Receptor of activated protein C kinase 1

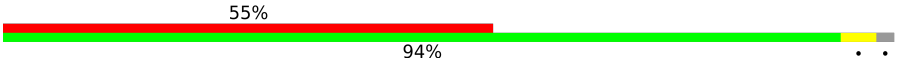
Chain Sg:

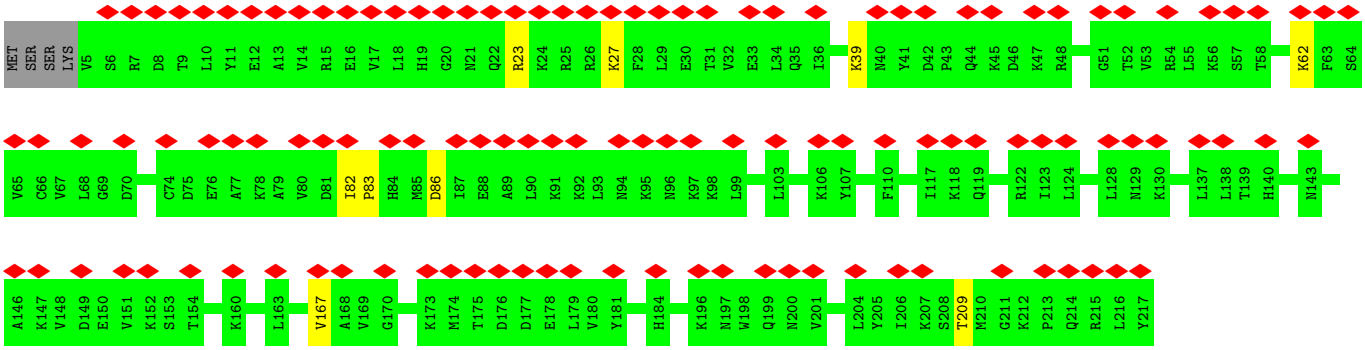




- Molecule 38: 60S ribosomal protein L10a

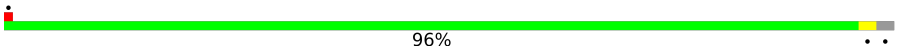
Chain Lz:

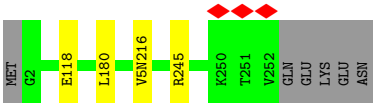




- Molecule 39: uL2

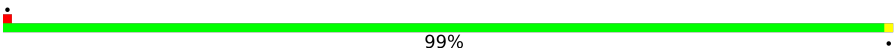
Chain LA:

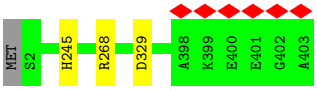




- Molecule 40: 60S ribosomal protein L3

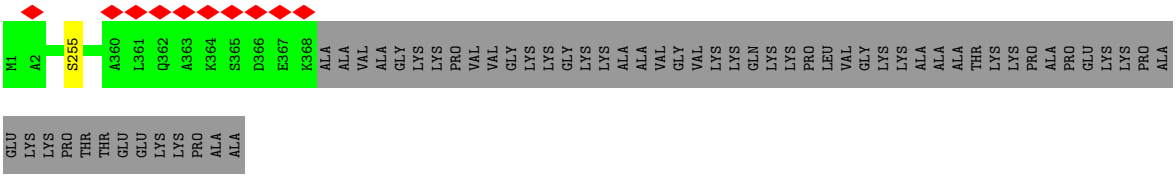
Chain LB:





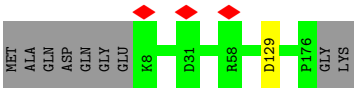
- Molecule 41: 60S ribosomal protein L4

Chain LC: 86% 14%



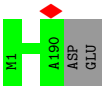
- Molecule 42: 60S ribosomal protein L11

Chain LJ: 94% 5%



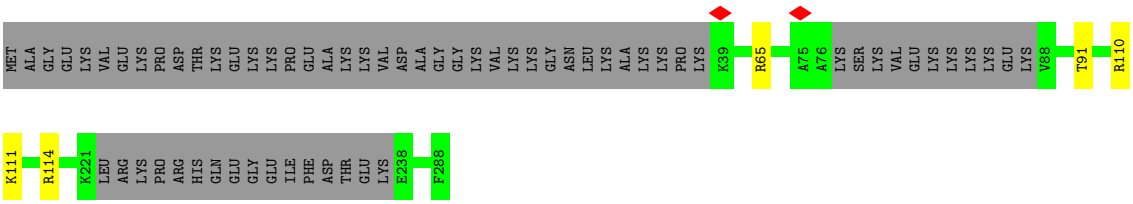
- Molecule 43: 60S ribosomal protein L9

Chain LH: 99%



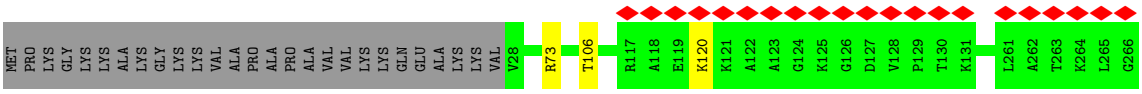
- Molecule 44: 60S ribosomal protein L6

Chain LE: 76% 23%



- Molecule 45: 60S ribosomal protein L7a

Chain LG: 8% 89% 10%

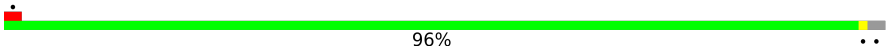


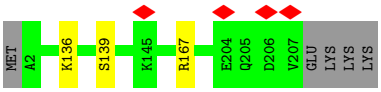
- Molecule 46: 60S ribosomal protein L13a

Chain LO: 98%

- Molecule 47: 60S ribosomal protein L13

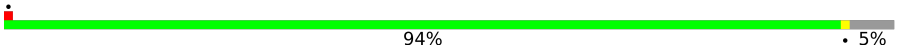
Chain LL:

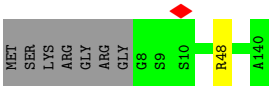




• Molecule 48: 60S ribosomal protein L23

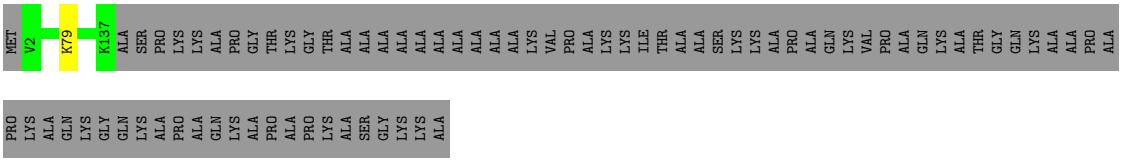
Chain LV:





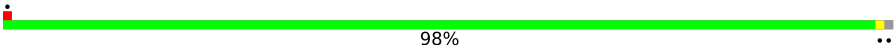
• Molecule 49: 60S ribosomal protein L14

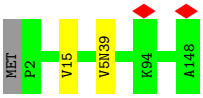
Chain LM:



• Molecule 50: 60S ribosomal protein L27a

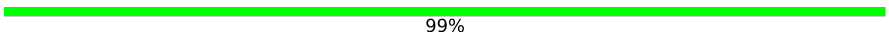
Chain La:





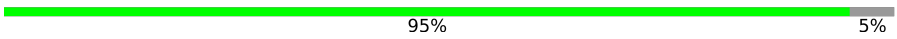
• Molecule 51: 60S ribosomal protein L15

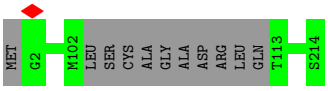
Chain LN:



• Molecule 52: 60S ribosomal protein L10

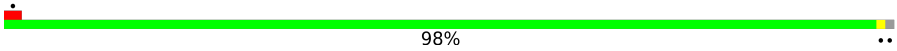
Chain LI:

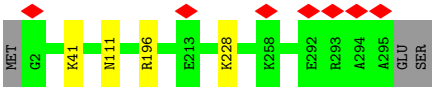




• Molecule 53: 60S ribosomal protein L5

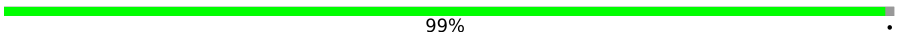
Chain LD:





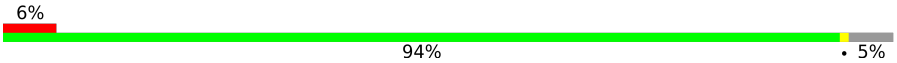
• Molecule 54: 60S ribosomal protein L18

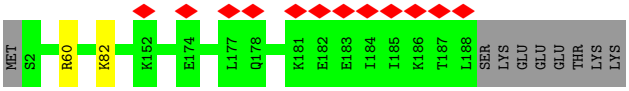
Chain LQ:



• Molecule 55: 60S ribosomal protein L19

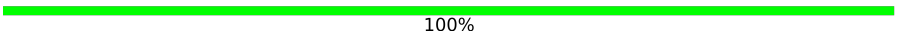
Chain LR:





• Molecule 56: 60S ribosomal protein L18a

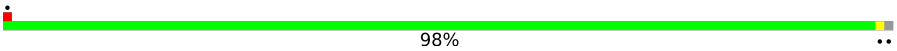
Chain LS:

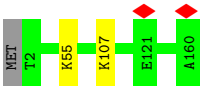


There are no outlier residues recorded for this chain.

• Molecule 57: 60S ribosomal protein L21

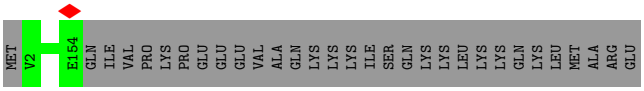
Chain LT:





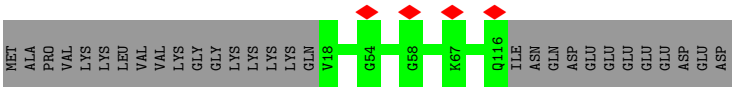
• Molecule 58: 60S ribosomal protein L17

Chain LP:



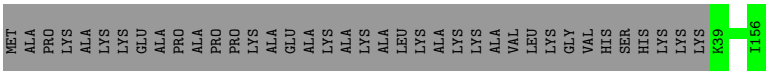
• Molecule 59: 60S ribosomal protein L22

Chain LU:



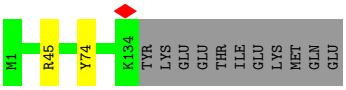
• Molecule 60: 60S ribosomal protein L23a

Chain LX:



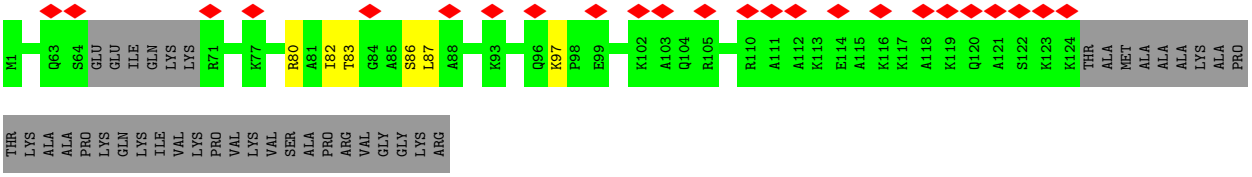
• Molecule 61: 60S ribosomal protein L26

Chain LY:



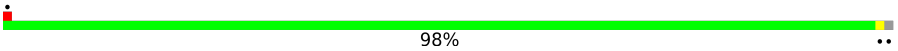
• Molecule 62: 60S ribosomal protein L24

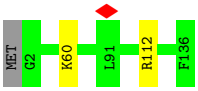
Chain LW:



• Molecule 63: 60S ribosomal protein L27

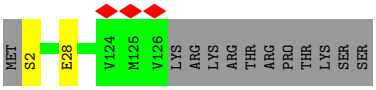
Chain LZ:





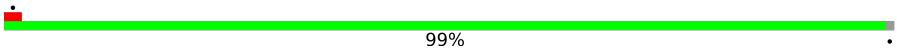
• Molecule 64: 60S ribosomal protein L28

Chain Lr:



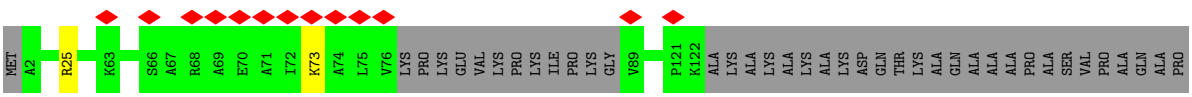
• Molecule 65: 60S ribosomal protein L35

Chain Lh:



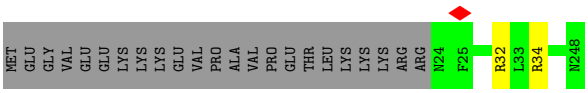
• Molecule 66: 60S ribosomal protein L29

Chain Lb:



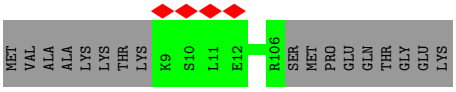
• Molecule 67: 60S ribosomal protein L7

Chain LF:



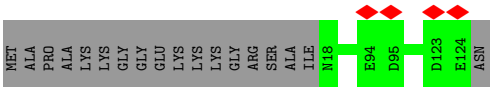
• Molecule 68: 60S ribosomal protein L30

Chain Lc:



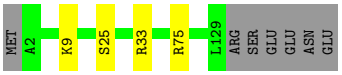
• Molecule 69: 60S ribosomal protein L31

Chain Ld:



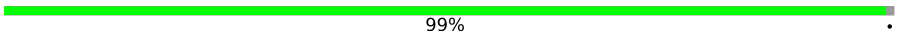
• Molecule 70: 60S ribosomal protein L32

Chain Le:



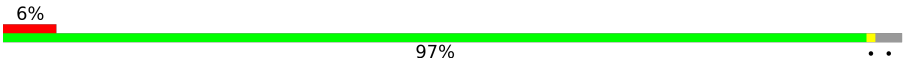
• Molecule 71: 60S ribosomal protein L35a

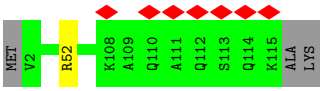
Chain Lf:



• Molecule 72: 60S ribosomal protein L34

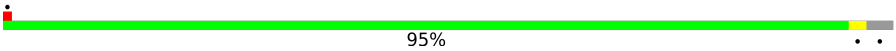
Chain Lg:

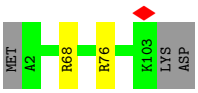




• Molecule 73: 60S ribosomal protein L36

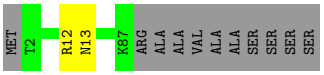
Chain Li:





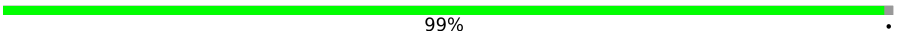
• Molecule 74: 60S ribosomal protein L37

Chain Lj:



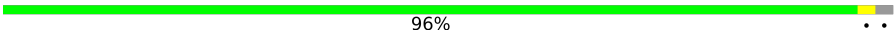
• Molecule 75: 60S ribosomal protein L38

Chain Lk:



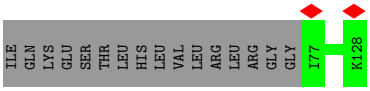
• Molecule 76: 60S ribosomal protein L39

Chain Ll:



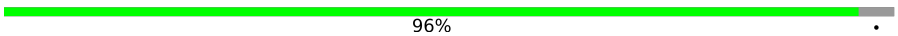
• Molecule 77: eL40

Chain Lm:



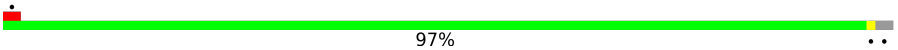
• Molecule 78: 60S ribosomal protein L41

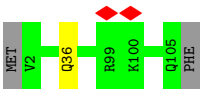
Chain Ln:



• Molecule 79: 60S ribosomal protein L36a

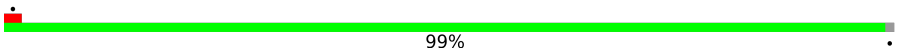
Chain Lo:

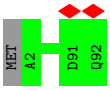




• Molecule 80: 60S ribosomal protein L37a

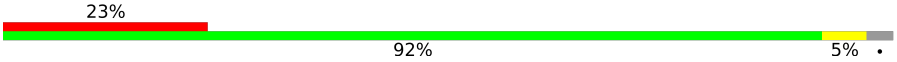
Chain Lp:

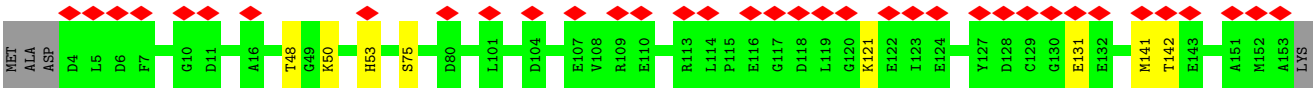




- Molecule 81: eIF5A1

Chain 5A:



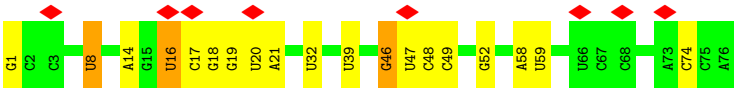


- Molecule 82: mRNA

Chain mR:

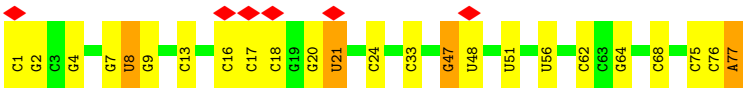
- Molecule 83: A-site tRNA

Chain At:



- Molecule 84: RNA (77-MER)

Chain Pt:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	79	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	528.64, 528.64, 528.64	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82600003, 0.82600003, 0.82600003	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: ZN, 4AC, PUT, 3H3, HY3, 7MG, V5N, OMG, 6MZ, ANM, SAC, UY1, MA6, OMC, MLZ, PSU, UR3, A2M, MG, 5CT, 1MA, K, HIC, M3L, G7M, OMU, AME, 4SU, H2U, B8N, 5MC, SPD

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	S2	0.33	1/38205 (0.0%)	0.76	3/59545 (0.0%)
2	L8	0.51	1/3613 (0.0%)	0.76	0/5627
3	L5	0.50	1/84727 (0.0%)	0.80	8/132180 (0.0%)
4	L7	0.48	1/2862 (0.0%)	0.77	0/4459
5	SB	0.27	0/1765	0.52	0/2362
6	SA	0.28	0/1778	0.53	0/2416
7	SD	0.28	0/1784	0.53	0/2403
8	SJ	0.28	0/1550	0.57	0/2069
9	SE	0.30	0/2118	0.54	0/2849
10	SC	0.29	0/1762	0.51	0/2381
11	SG	0.30	0/1946	0.59	0/2590
12	SF	0.27	0/1515	0.54	0/2037
13	SH	0.27	0/1540	0.53	0/2064
14	SW	0.30	0/1051	0.54	0/1406
15	SI	0.30	0/1715	0.56	0/2287
16	SQ	0.30	0/1141	0.57	0/1528
17	SU	0.25	0/813	0.57	0/1092
18	SK	0.39	0/834	0.57	0/1125
19	SO	0.33	0/1022	0.61	0/1372
20	SX	0.28	0/1096	0.53	0/1461
21	SM	0.26	0/950	0.52	0/1275
22	SS	0.28	0/1232	0.61	0/1651
23	Sd	0.30	0/465	0.55	0/618
24	SN	0.27	0/1242	0.52	0/1671
25	SL	0.29	0/1209	0.54	0/1616
26	SR	0.27	0/1098	0.57	0/1474
27	SP	0.28	0/1133	0.56	0/1515
28	ST	0.28	0/1131	0.51	0/1515
29	SV	0.27	0/635	0.53	0/850
30	SY	0.30	0/1083	0.60	0/1438
31	SZ	0.27	0/696	0.56	0/929

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Sa	0.27	0/805	0.57	0/1079
33	Sb	0.25	0/664	0.50	0/891
34	Sc	0.26	0/519	0.61	0/694
35	Se	0.30	0/458	0.57	0/604
36	Sf	0.32	0/525	0.55	0/695
37	Sg	0.28	0/2493	0.53	0/3394
38	Lz	0.29	0/1742	0.56	0/2338
39	LA	0.37	0/1958	0.62	0/2623
40	LB	0.33	0/3295	0.55	0/4406
41	LC	0.33	0/2981	0.56	0/4002
42	LJ	0.29	0/1381	0.56	0/1847
43	LH	0.29	0/1537	0.56	0/2066
44	LE	0.30	0/1821	0.52	0/2442
45	LG	0.28	0/1946	0.52	0/2620
46	LO	0.34	0/1673	0.55	0/2238
47	LL	0.32	0/1695	0.59	0/2270
48	LV	0.32	0/1002	0.56	0/1345
49	LM	0.30	0/1142	0.53	0/1527
50	La	0.33	0/1179	0.55	0/1573
51	LN	0.36	0/1745	0.61	0/2338
52	LI	0.32	0/1684	0.54	0/2247
53	LD	0.30	0/2437	0.52	0/3263
54	LQ	0.35	0/1536	0.61	0/2052
55	LR	0.29	0/1582	0.56	0/2091
56	LS	0.35	0/1500	0.57	0/2013
57	LT	0.33	0/1325	0.55	0/1770
58	LP	0.34	0/1268	0.54	0/1701
59	LU	0.29	0/822	0.55	0/1103
60	LX	0.31	0/984	0.54	0/1323
61	LY	0.33	0/1132	0.57	0/1504
62	LW	0.33	0/964	0.55	0/1278
63	LZ	0.33	0/1129	0.52	0/1507
64	Lr	0.33	0/1011	0.57	0/1356
65	Lh	0.28	0/1023	0.54	0/1351
66	Lb	0.29	0/887	0.54	0/1171
67	LF	0.33	0/1905	0.55	0/2539
68	Lc	0.30	0/774	0.51	0/1038
69	Ld	0.31	0/903	0.56	0/1216
70	Le	0.35	0/1071	0.56	0/1429
71	Lf	0.35	0/895	0.60	0/1198
72	Lg	0.32	0/916	0.59	0/1220
73	Li	0.29	0/843	0.58	0/1115
74	Lj	0.38	0/720	0.62	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	Lk	0.28	0/575	0.52	0/761
76	Ll	0.32	0/454	0.60	0/599
77	Lm	0.35	0/425	0.59	0/564
78	Ln	0.32	0/231	0.71	0/294
79	Lo	0.35	0/854	0.55	0/1125
80	Lp	0.33	0/718	0.53	0/953
81	5A	0.31	0/1144	0.56	0/1539
82	mR	0.33	0/233	0.78	0/360
83	At	0.34	1/1677 (0.1%)	0.76	0/2612
84	Pt	0.61	6/1721 (0.3%)	1.01	8/2679 (0.3%)
All	All	0.40	11/229615 (0.0%)	0.71	19/336720 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Pt	77	A	C5-C4	13.22	1.48	1.38
84	Pt	1	C	OP3-P	-10.71	1.48	1.61
1	S2	1	U	OP3-P	-10.70	1.48	1.61
2	L8	1	C	OP3-P	-10.67	1.48	1.61
4	L7	1	G	OP3-P	-10.61	1.48	1.61
83	At	1	G	OP3-P	-10.60	1.48	1.61
3	L5	1	C	OP3-P	-10.18	1.49	1.61
84	Pt	77	A	C5-C6	9.14	1.49	1.41
84	Pt	77	A	N7-C5	-7.42	1.34	1.39
84	Pt	77	A	C8-N7	6.69	1.36	1.31
84	Pt	77	A	N9-C4	-5.46	1.34	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	Pt	77	A	C2-N3-C4	21.89	121.55	110.60
84	Pt	77	A	N3-C4-C5	-12.48	118.06	126.80
84	Pt	77	A	N1-C2-N3	-11.22	123.69	129.30
84	Pt	77	A	N3-C4-N9	9.94	135.35	127.40
84	Pt	77	A	C4-C5-N7	-8.36	106.52	110.70
84	Pt	77	A	C5-N7-C8	6.99	107.40	103.90
3	L5	4404	U	C2-N1-C1'	5.72	124.57	117.70
84	Pt	77	A	C6-C5-N7	5.55	136.18	132.30
3	L5	2410	C	C2-N1-C1'	5.54	124.89	118.80
1	S2	1520	G	C4-N9-C1'	5.39	133.51	126.50
3	L5	1259	G	N1-C2-N2	-5.33	111.41	116.20
3	L5	4945	G	C5-C6-O6	-5.31	125.42	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	Pt	77	A	C6-N1-C2	5.31	121.78	118.60
1	S2	666	U	C2-N1-C1'	5.30	124.06	117.70
1	S2	1415	C	N1-C2-O2	5.27	122.06	118.90
3	L5	417	G	O4'-C1'-N9	5.26	112.41	108.20
3	L5	1258	G	N3-C4-N9	5.25	129.15	126.00
3	L5	4419	U	N1-C2-O2	5.20	126.44	122.80
3	L5	1590	C	P-O3'-C3'	5.18	125.92	119.70

There are no chirality outliers.

There are no planarity outliers.

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	
5	SB	212/264 (80%)	204 (96%)	8 (4%)	0	100	100
6	SA	220/295 (75%)	213 (97%)	7 (3%)	0	100	100
7	SD	224/243 (92%)	221 (99%)	3 (1%)	0	100	100
8	SJ	183/194 (94%)	174 (95%)	9 (5%)	0	100	100
9	SE	260/263 (99%)	251 (96%)	8 (3%)	1 (0%)	34	64
10	SC	220/293 (75%)	215 (98%)	4 (2%)	1 (0%)	29	60
11	SG	235/249 (94%)	221 (94%)	13 (6%)	1 (0%)	34	64
12	SF	187/204 (92%)	169 (90%)	18 (10%)	0	100	100
13	SH	187/194 (96%)	178 (95%)	8 (4%)	1 (0%)	29	60
14	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	SI	204/208 (98%)	194 (95%)	9 (4%)	1 (0%)	29	60
16	SQ	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
17	SU	99/119 (83%)	97 (98%)	2 (2%)	0	100	100
18	SK	94/165 (57%)	82 (87%)	8 (8%)	4 (4%)	2	9
19	SO	133/151 (88%)	122 (92%)	9 (7%)	2 (2%)	10	32
20	SX	137/143 (96%)	131 (96%)	6 (4%)	0	100	100
21	SM	120/132 (91%)	113 (94%)	5 (4%)	2 (2%)	9	29
22	SS	146/152 (96%)	136 (93%)	9 (6%)	1 (1%)	22	52
23	Sd	52/56 (93%)	49 (94%)	3 (6%)	0	100	100
24	SN	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
25	SL	141/158 (89%)	134 (95%)	7 (5%)	0	100	100
26	SR	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
27	SP	133/145 (92%)	125 (94%)	8 (6%)	0	100	100
28	ST	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
29	SV	81/83 (98%)	81 (100%)	0	0	100	100
30	SY	129/133 (97%)	123 (95%)	6 (5%)	0	100	100
31	SZ	84/125 (67%)	79 (94%)	5 (6%)	0	100	100
32	Sa	97/115 (84%)	93 (96%)	4 (4%)	0	100	100
33	Sb	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
34	Sc	63/69 (91%)	60 (95%)	3 (5%)	0	100	100
35	Se	55/133 (41%)	51 (93%)	4 (7%)	0	100	100
36	Sf	61/156 (39%)	53 (87%)	7 (12%)	1 (2%)	9	30
37	Sg	311/317 (98%)	285 (92%)	25 (8%)	1 (0%)	41	69
38	Lz	211/217 (97%)	170 (81%)	36 (17%)	5 (2%)	6	21
39	LA	249/257 (97%)	240 (96%)	8 (3%)	1 (0%)	34	64
40	LB	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
41	LC	366/427 (86%)	358 (98%)	8 (2%)	0	100	100
42	LJ	167/178 (94%)	163 (98%)	4 (2%)	0	100	100
43	LH	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
44	LE	217/288 (75%)	207 (95%)	10 (5%)	0	100	100
45	LG	237/266 (89%)	223 (94%)	13 (6%)	1 (0%)	34	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	LO	198/203 (98%)	192 (97%)	6 (3%)	0	100	100
47	LL	204/211 (97%)	192 (94%)	12 (6%)	0	100	100
48	LV	131/140 (94%)	125 (95%)	6 (5%)	0	100	100
49	LM	134/215 (62%)	131 (98%)	3 (2%)	0	100	100
50	La	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	22	52
51	LN	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
52	LI	199/214 (93%)	192 (96%)	7 (4%)	0	100	100
53	LD	292/297 (98%)	285 (98%)	7 (2%)	0	100	100
54	LQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
55	LR	185/196 (94%)	184 (100%)	1 (0%)	0	100	100
56	LS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
57	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
58	LP	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
59	LU	97/128 (76%)	91 (94%)	6 (6%)	0	100	100
60	LX	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
61	LY	132/145 (91%)	127 (96%)	5 (4%)	0	100	100
62	LW	114/157 (73%)	107 (94%)	6 (5%)	1 (1%)	17	46
63	LZ	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
64	Lr	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
65	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
66	Lb	104/159 (65%)	100 (96%)	4 (4%)	0	100	100
67	LF	223/248 (90%)	212 (95%)	11 (5%)	0	100	100
68	Lc	96/115 (84%)	92 (96%)	4 (4%)	0	100	100
69	Ld	105/125 (84%)	101 (96%)	4 (4%)	0	100	100
70	Le	126/135 (93%)	121 (96%)	5 (4%)	0	100	100
71	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
72	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
73	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
74	Lj	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
75	Lk	67/70 (96%)	67 (100%)	0	0	100	100
76	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	Lm	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
78	Ln	22/25 (88%)	21 (96%)	1 (4%)	0	100	100
79	Lo	101/106 (95%)	96 (95%)	5 (5%)	0	100	100
80	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
81	5A	147/154 (96%)	130 (88%)	14 (10%)	3 (2%)	7	25
All	All	11641/13133 (89%)	11127 (96%)	486 (4%)	28 (0%)	50	76

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	SM	82	ASN
38	Lz	82	ILE
38	Lz	86	ASP
81	5A	75	SER
81	5A	131	GLU
11	SG	132	ARG
18	SK	20	VAL
38	Lz	167	VAL
62	LW	97	LYS
15	SI	142	SER
18	SK	17	LYS
10	SC	77	SER
36	Sf	138	ARG
37	Sg	177	TRP
38	Lz	83	PRO
38	Lz	209	THR
81	5A	48	THR
13	SH	12	ASN
18	SK	15	LEU
19	SO	138	ASP
21	SM	102	LYS
22	SS	100	ALA
39	LA	180	LEU
45	LG	106	THR
9	SE	109	PHE
18	SK	6	LYS
50	La	15	VAL
19	SO	134	PRO

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	
5	SB	195/231 (84%)	194 (100%)	1 (0%)	88	96
6	SA	183/242 (76%)	182 (100%)	1 (0%)	88	96
7	SD	189/202 (94%)	189 (100%)	0	100	100
8	SJ	161/168 (96%)	161 (100%)	0	100	100
9	SE	224/225 (100%)	221 (99%)	3 (1%)	69	88
10	SC	188/225 (84%)	185 (98%)	3 (2%)	62	84
11	SG	207/218 (95%)	204 (99%)	3 (1%)	67	86
12	SF	159/170 (94%)	159 (100%)	0	100	100
13	SH	168/174 (97%)	167 (99%)	1 (1%)	86	95
14	SW	112/113 (99%)	110 (98%)	2 (2%)	59	82
15	SI	178/180 (99%)	176 (99%)	2 (1%)	73	90
16	SQ	117/121 (97%)	114 (97%)	3 (3%)	46	75
17	SU	93/107 (87%)	93 (100%)	0	100	100
18	SK	87/136 (64%)	81 (93%)	6 (7%)	15	40
19	SO	105/119 (88%)	104 (99%)	1 (1%)	76	91
20	SX	111/114 (97%)	110 (99%)	1 (1%)	78	92
21	SM	102/108 (94%)	99 (97%)	3 (3%)	42	73
22	SS	128/132 (97%)	127 (99%)	1 (1%)	81	93
23	Sd	48/49 (98%)	48 (100%)	0	100	100
24	SN	131/131 (100%)	131 (100%)	0	100	100
25	SL	131/142 (92%)	130 (99%)	1 (1%)	81	93
26	SR	121/122 (99%)	121 (100%)	0	100	100
27	SP	121/130 (93%)	120 (99%)	1 (1%)	81	93
28	ST	113/115 (98%)	112 (99%)	1 (1%)	78	92
29	SV	66/66 (100%)	66 (100%)	0	100	100
30	SY	113/115 (98%)	109 (96%)	4 (4%)	36	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	SZ	75/103 (73%)	75 (100%)	0	100	100
32	Sa	86/98 (88%)	86 (100%)	0	100	100
33	Sb	75/76 (99%)	75 (100%)	0	100	100
34	Sc	58/62 (94%)	58 (100%)	0	100	100
35	Se	46/104 (44%)	46 (100%)	0	100	100
36	Sf	56/140 (40%)	54 (96%)	2 (4%)	35	66
37	Sg	272/275 (99%)	267 (98%)	5 (2%)	59	82
38	Lz	192/196 (98%)	188 (98%)	4 (2%)	53	79
39	LA	193/198 (98%)	190 (98%)	3 (2%)	62	84
40	LB	347/348 (100%)	345 (99%)	2 (1%)	86	95
41	LC	306/348 (88%)	305 (100%)	1 (0%)	92	97
42	LJ	143/149 (96%)	142 (99%)	1 (1%)	84	94
43	LH	169/171 (99%)	169 (100%)	0	100	100
44	LE	196/252 (78%)	191 (97%)	5 (3%)	46	75
45	LG	202/223 (91%)	200 (99%)	2 (1%)	76	91
46	LO	172/174 (99%)	170 (99%)	2 (1%)	71	89
47	LL	172/177 (97%)	169 (98%)	3 (2%)	60	83
48	LV	102/107 (95%)	101 (99%)	1 (1%)	76	91
49	LM	116/161 (72%)	115 (99%)	1 (1%)	78	92
50	La	119/120 (99%)	119 (100%)	0	100	100
51	LN	171/172 (99%)	170 (99%)	1 (1%)	86	95
52	LI	173/181 (96%)	173 (100%)	0	100	100
53	LD	247/250 (99%)	243 (98%)	4 (2%)	62	84
54	LQ	164/165 (99%)	164 (100%)	0	100	100
55	LR	166/175 (95%)	164 (99%)	2 (1%)	71	89
56	LS	157/157 (100%)	157 (100%)	0	100	100
57	LT	139/140 (99%)	137 (99%)	2 (1%)	67	86
58	LP	134/163 (82%)	134 (100%)	0	100	100
59	LU	89/115 (77%)	89 (100%)	0	100	100
60	LX	106/133 (80%)	106 (100%)	0	100	100
61	LY	124/135 (92%)	122 (98%)	2 (2%)	62	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	LW	95/126 (75%)	90 (95%)	5 (5%)	22	52
63	LZ	117/118 (99%)	115 (98%)	2 (2%)	60	83
64	Lr	108/120 (90%)	107 (99%)	1 (1%)	78	92
65	Lh	109/110 (99%)	109 (100%)	0	100	100
66	Lb	89/125 (71%)	87 (98%)	2 (2%)	52	78
67	LF	194/215 (90%)	192 (99%)	2 (1%)	76	91
68	Lc	83/97 (86%)	83 (100%)	0	100	100
69	Ld	98/110 (89%)	98 (100%)	0	100	100
70	Le	114/121 (94%)	110 (96%)	4 (4%)	36	67
71	Lf	88/89 (99%)	88 (100%)	0	100	100
72	Lg	98/100 (98%)	97 (99%)	1 (1%)	76	91
73	Li	86/89 (97%)	84 (98%)	2 (2%)	50	78
74	Lj	73/80 (91%)	71 (97%)	2 (3%)	44	74
75	Lk	64/65 (98%)	64 (100%)	0	100	100
76	Ll	47/48 (98%)	46 (98%)	1 (2%)	53	79
77	Lm	47/115 (41%)	47 (100%)	0	100	100
78	Ln	23/24 (96%)	23 (100%)	0	100	100
79	Lo	91/93 (98%)	90 (99%)	1 (1%)	73	90
80	Lp	74/75 (99%)	74 (100%)	0	100	100
81	5A	122/127 (96%)	118 (97%)	4 (3%)	38	69
All	All	10138/11170 (91%)	10030 (99%)	108 (1%)	74	90

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	SB	88	THR
6	SA	212	LYS
9	SE	104	ASP
9	SE	108	ARG
9	SE	122	LYS
10	SC	167	ARG
10	SC	178	HIS
10	SC	180	VAL
11	SG	13	GLN
11	SG	172	LYS

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Mol	Chain	Res	Type
11	SG	201	LYS
13	SH	44	ASN
14	SW	3	ARG
14	SW	4	MET
15	SI	5	ARG
15	SI	49	ARG
16	SQ	50	LYS
16	SQ	53	GLU
16	SQ	146	ARG
18	SK	16	PHE
18	SK	18	GLU
18	SK	20	VAL
18	SK	21	MET
18	SK	55	ARG
18	SK	85	LEU
19	SO	45	THR
20	SX	105	PHE
21	SM	33	ARG
21	SM	44	LYS
21	SM	93	LYS
22	SS	99	LEU
25	SL	69	ARG
27	SP	50	ARG
28	ST	35	ASP
30	SY	37	LYS
30	SY	49	LYS
30	SY	105	LYS
30	SY	107	ARG
36	Sf	138	ARG
36	Sf	140	TYR
37	Sg	47	ARG
37	Sg	72	SER
37	Sg	82	SER
37	Sg	225	LYS
37	Sg	271	LYS
38	Lz	23	ARG
38	Lz	27	LYS
38	Lz	39	LYS
38	Lz	62	LYS
39	LA	118	GLU
39	LA	245[A]	ARG
39	LA	245[B]	ARG

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Mol	Chain	Res	Type
40	LB	268	ARG
40	LB	329	ASP
41	LC	255	SER
42	LJ	129	ASP
44	LE	65	ARG
44	LE	91	THR
44	LE	110	ARG
44	LE	111	LYS
44	LE	114	ARG
45	LG	73	ARG
45	LG	120	LYS
46	LO	49	ARG
46	LO	61	ARG
47	LL	136	LYS
47	LL	139	SER
47	LL	167	ARG
48	LV	48	ARG
49	LM	79	LYS
51	LN	38	ARG
53	LD	41	LYS
53	LD	111	ASN
53	LD	196	ARG
53	LD	228	LYS
55	LR	60	ARG
55	LR	82	LYS
57	LT	55	LYS
57	LT	107	LYS
61	LY	45	ARG
61	LY	74	TYR
62	LW	80	ARG
62	LW	82	ILE
62	LW	83	THR
62	LW	86	SER
62	LW	87	LEU
63	LZ	60	LYS
63	LZ	112	ARG
64	Lr	28	GLU
66	Lb	25	ARG
66	Lb	73	LYS
67	LF	32	ARG
67	LF	34	ARG
70	Le	9	LYS

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Mol	Chain	Res	Type
70	Le	25	SER
70	Le	33	ARG
70	Le	75	ARG
72	Lg	52	ARG
73	Li	68	ARG
73	Li	76	ARG
74	Lj	12	ARG
74	Lj	13	ASN
76	Ll	36	ARG
79	Lo	36	GLN
81	5A	53	HIS
81	5A	121	LYS
81	5A	141	MET
81	5A	142	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
5	SB	232	HIS
6	SA	113	GLN
9	SE	36	HIS
10	SC	178	HIS
11	SG	163	ASN
13	SH	39	GLN
13	SH	68	GLN
13	SH	91	HIS
14	SW	90	GLN
16	SQ	86	GLN
18	SK	66	HIS
20	SX	73	GLN
30	SY	15	ASN
30	SY	22	GLN
33	Sb	26	GLN
37	Sg	178	ASN
37	Sg	191	HIS
38	Lz	35	GLN
38	Lz	84	HIS
38	Lz	129	ASN
38	Lz	141	ASN
38	Lz	182	ASN
41	LC	212	ASN
41	LC	299	GLN

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Mol	Chain	Res	Type
42	LJ	110	GLN
43	LH	63	ASN
53	LD	111	ASN
58	LP	93	HIS
58	LP	137	ASN
63	LZ	28	ASN
66	Lb	50	ASN
67	LF	131	ASN
68	Lc	15	ASN
70	Le	23	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1669/1869 (89%)	324 (19%)	11 (0%)
2	L8	155/156 (99%)	27 (17%)	0
3	L5	3642/5069 (71%)	676 (18%)	21 (0%)
4	L7	119/120 (99%)	7 (5%)	0
82	mR	9/60 (15%)	0	0
83	At	75/76 (98%)	15 (20%)	0
84	Pt	76/77 (98%)	21 (27%)	0
All	All	5745/7427 (77%)	1070 (18%)	32 (0%)

All (1070) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	4	C
1	S2	26	U
1	S2	33	G
1	S2	41	G
1	S2	44	U
1	S2	46	A
1	S2	55	U
1	S2	58	C
1	S2	65	C
1	S2	67	C
1	S2	68	A
1	S2	70	G
1	S2	72	C
1	S2	73	C
1	S2	74	G

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Mol	Chain	Res	Type
1	S2	76	U
1	S2	77	A
1	S2	110	U
1	S2	113	G
1	S2	115	U
1	S2	126	G
1	S2	127	C
1	S2	129	C
1	S2	130	G
1	S2	140	C
1	S2	142	C
1	S2	143	U
1	S2	149	A
1	S2	151	C
1	S2	154	U
1	S2	155	G
1	S2	158	A
1	S2	159	A2M
1	S2	160	U
1	S2	170	A
1	S2	171	A
1	S2	182	C
1	S2	183	G
1	S2	184	G
1	S2	189	U
1	S2	197	U
1	S2	198	U
1	S2	199	C
1	S2	200	G
1	S2	201	C
1	S2	203	G
1	S2	204	G
1	S2	205	G
1	S2	207	G
1	S2	209	A
1	S2	210	U
1	S2	212	C
1	S2	218	PSU
1	S2	295	C
1	S2	302	A
1	S2	306	C
1	S2	307	G

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Mol	Chain	Res	Type
1	S2	309	G
1	S2	313	A
1	S2	319	C
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	327	G
1	S2	328	U
1	S2	329	G
1	S2	347	G
1	S2	351	G
1	S2	353	C
1	S2	354	OMU
1	S2	362	C
1	S2	364	A
1	S2	369	C
1	S2	370	G
1	S2	385	G
1	S2	386	C
1	S2	407	G
1	S2	409	C
1	S2	418	A
1	S2	421	G
1	S2	441	C
1	S2	442	C
1	S2	447	A
1	S2	448	A
1	S2	450	C
1	S2	452	G
1	S2	467	G
1	S2	472	C
1	S2	474	G
1	S2	482	G
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	493	A
1	S2	508	A
1	S2	516	A
1	S2	540	U
1	S2	555	A
1	S2	556	U

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Mol	Chain	Res	Type
1	S2	557	U
1	S2	568	C
1	S2	576	A2M
1	S2	586	G
1	S2	587	A
1	S2	588	G
1	S2	589	G
1	S2	590	A2M
1	S2	591	U
1	S2	604	A
1	S2	607	U
1	S2	613	G
1	S2	614	C
1	S2	617	G
1	S2	627	OMU
1	S2	628	A
1	S2	643	A
1	S2	644	OMG
1	S2	655	A
1	S2	660	C
1	S2	664	A
1	S2	668	A2M
1	S2	669	A
1	S2	670	A
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	688	U
1	S2	689	U
1	S2	811	A
1	S2	821	G
1	S2	822	PSU
1	S2	823	U
1	S2	827	A
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	840	C
1	S2	841	G
1	S2	845	G

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Mol	Chain	Res	Type
1	S2	847	A
1	S2	852	G
1	S2	861	A
1	S2	867	OMG
1	S2	868	G
1	S2	869	A
1	S2	870	A
1	S2	883	U
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	892	U
1	S2	895	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	901	G
1	S2	909	G
1	S2	913	A
1	S2	917	U
1	S2	920	A
1	S2	922	A
1	S2	933	G
1	S2	943	U
1	S2	969	U
1	S2	970	G
1	S2	971	G
1	S2	980	A
1	S2	982	G
1	S2	983	A
1	S2	985	G
1	S2	990	A
1	S2	992	A
1	S2	997	A
1	S2	999	G
1	S2	1002	U
1	S2	1011	A
1	S2	1017	U
1	S2	1023	A
1	S2	1030	A
1	S2	1045	U

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Mol	Chain	Res	Type
1	S2	1049	A
1	S2	1053	C
1	S2	1055	A
1	S2	1058	A
1	S2	1061	U
1	S2	1062	A
1	S2	1080	A
1	S2	1082	A
1	S2	1083	A
1	S2	1085	C
1	S2	1115	U
1	S2	1121	G
1	S2	1130	G
1	S2	1133	A
1	S2	1138	C
1	S2	1153	C
1	S2	1154	U
1	S2	1156	U
1	S2	1157	G
1	S2	1195	A
1	S2	1212	G
1	S2	1215	C
1	S2	1216	C
1	S2	1217	A
1	S2	1220	A
1	S2	1224	G
1	S2	1240	A
1	S2	1242	U
1	S2	1243	PSU
1	S2	1249	C
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1259	A
1	S2	1264	C
1	S2	1269	G
1	S2	1274	G
1	S2	1275	G
1	S2	1285	G
1	S2	1286	G
1	S2	1287	A

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Mol	Chain	Res	Type
1	S2	1302	G
1	S2	1303	C
1	S2	1305	C
1	S2	1312	G
1	S2	1313	A
1	S2	1327	G
1	S2	1342	U
1	S2	1348	G
1	S2	1371	U
1	S2	1372	U
1	S2	1374	C
1	S2	1378	A
1	S2	1394	G
1	S2	1398	G
1	S2	1404	U
1	S2	1405	A
1	S2	1415	C
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1433	C
1	S2	1435	C
1	S2	1437	C
1	S2	1438	A
1	S2	1442	OMU
1	S2	1449	G
1	S2	1454	A
1	S2	1462	U
1	S2	1463	U
1	S2	1464	C
1	S2	1466	G
1	S2	1477	U
1	S2	1489	A
1	S2	1490	OMG
1	S2	1495	G
1	S2	1497	G
1	S2	1498	A
1	S2	1507	G
1	S2	1508	A
1	S2	1509	U
1	S2	1520	G
1	S2	1521	C

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Mol	Chain	Res	Type
1	S2	1522	A
1	S2	1533	A
1	S2	1536	G
1	S2	1544	C
1	S2	1552	G
1	S2	1556	A
1	S2	1570	G
1	S2	1574	C
1	S2	1575	G
1	S2	1579	A
1	S2	1580	A
1	S2	1584	G
1	S2	1587	G
1	S2	1588	A
1	S2	1601	A
1	S2	1606	G
1	S2	1621	U
1	S2	1623	A
1	S2	1637	A
1	S2	1638	G
1	S2	1639	G7M
1	S2	1648	G
1	S2	1654	G
1	S2	1657	G
1	S2	1664	A
1	S2	1665	G
1	S2	1678	A2M
1	S2	1679	A
1	S2	1680	G
1	S2	1686	G
1	S2	1695	A
1	S2	1721	U
1	S2	1722	G
1	S2	1729	U
1	S2	1745	A
1	S2	1758	G
1	S2	1759	G
1	S2	1760	G
1	S2	1773	C
1	S2	1774	C
1	S2	1775	U
1	S2	1776	G

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Mol	Chain	Res	Type
1	S2	1777	G
1	S2	1779	G
1	S2	1783	C
1	S2	1824	A
1	S2	1826	G
1	S2	1829	G
1	S2	1830	U
1	S2	1831	A
1	S2	1838	U
1	S2	1849	G
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1864	U
1	S2	1865	C
2	L8	13	G
2	L8	34	U
2	L8	35	C
2	L8	38	U
2	L8	51	U
2	L8	59	A
2	L8	60	G
2	L8	61	A
2	L8	62	A
2	L8	63	U
2	L8	81	C
2	L8	85	U
2	L8	86	U
2	L8	94	G
2	L8	103	A
2	L8	104	A
2	L8	105	C
2	L8	108	A
2	L8	109	C
2	L8	110	U
2	L8	111	U
2	L8	112	G
2	L8	114	G
2	L8	123	U
2	L8	124	U
2	L8	125	C
2	L8	153	C

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Mol	Chain	Res	Type
3	L5	2	G
3	L5	9	C
3	L5	25	A
3	L5	39	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	70	A
3	L5	71	C
3	L5	76	A
3	L5	85	G
3	L5	91	G
3	L5	98	A
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	120	A
3	L5	135	G
3	L5	136	C
3	L5	138	G
3	L5	142	G
3	L5	143	C
3	L5	144	G
3	L5	159	C
3	L5	178	C
3	L5	179	G
3	L5	181	C
3	L5	184	U
3	L5	186	G
3	L5	187	U
3	L5	188	G
3	L5	189	G
3	L5	193	G
3	L5	197	A
3	L5	200	U
3	L5	209	U
3	L5	210	C
3	L5	219	G
3	L5	233	U

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Mol	Chain	Res	Type
3	L5	262	G
3	L5	266	C
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	340	C
3	L5	345	C
3	L5	350	C
3	L5	361	C
3	L5	362	A
3	L5	363	A
3	L5	386	A
3	L5	387	G
3	L5	409	G
3	L5	410	A
3	L5	412	G
3	L5	432	U
3	L5	449	C
3	L5	450	G
3	L5	452	A
3	L5	454	U
3	L5	467	U
3	L5	468	U
3	L5	483	G
3	L5	484	U
3	L5	485	C
3	L5	489	C
3	L5	493	G
3	L5	494	U
3	L5	496	G
3	L5	498	C
3	L5	499	G
3	L5	504	G
3	L5	507	G
3	L5	509	A
3	L5	510	U
3	L5	513	U
3	L5	514	U
3	L5	644	G
3	L5	646	G

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Mol	Chain	Res	Type
3	L5	654	C
3	L5	656	C
3	L5	659	G
3	L5	662	C
3	L5	663	G
3	L5	665	C
3	L5	666	G
3	L5	667	A
3	L5	669	C
3	L5	692	A
3	L5	696	C
3	L5	697	G
3	L5	704	C
3	L5	730	G
3	L5	731	G
3	L5	738	C
3	L5	739	G
3	L5	741	C
3	L5	742	G
3	L5	759	G
3	L5	760	G
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	917	A
3	L5	918	G
3	L5	925	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	942	G
3	L5	945	U
3	L5	956	A
3	L5	958	G
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	963	G
3	L5	965	G
3	L5	966	A

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Mol	Chain	Res	Type
3	L5	967	C
3	L5	968	C
3	L5	969	C
3	L5	970	G
3	L5	971	U
3	L5	982	U
3	L5	1070	G
3	L5	1072	C
3	L5	1084	C
3	L5	1170	G
3	L5	1180	C
3	L5	1183	C
3	L5	1199	G
3	L5	1200	G
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1241	C
3	L5	1254	A
3	L5	1255	A
3	L5	1256	G
3	L5	1257	A
3	L5	1258	G
3	L5	1266	G
3	L5	1267	C
3	L5	1269	G
3	L5	1270	A
3	L5	1272	C
3	L5	1273	G
3	L5	1277	G
3	L5	1279	A
3	L5	1280	C
3	L5	1284	G
3	L5	1285	U
3	L5	1287	G
3	L5	1302	U
3	L5	1303	A
3	L5	1313	C
3	L5	1314	C
3	L5	1315	C
3	L5	1326	A2M
3	L5	1337	A

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Mol	Chain	Res	Type
3	L5	1354	A
3	L5	1358	G
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G
3	L5	1379	C
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1398	A
3	L5	1403	G
3	L5	1404	G
3	L5	1408	G
3	L5	1410	U
3	L5	1411	C
3	L5	1415	G
3	L5	1417	C
3	L5	1420	A
3	L5	1439	C
3	L5	1440	U
3	L5	1441	C
3	L5	1443	A
3	L5	1447	C
3	L5	1449	C
3	L5	1457	G
3	L5	1481	C
3	L5	1483	C
3	L5	1497	A
3	L5	1498	G
3	L5	1502	G
3	L5	1515	A
3	L5	1534	A2M
3	L5	1547	A
3	L5	1549	G
3	L5	1566	C
3	L5	1574	G
3	L5	1578	U
3	L5	1582	PSU
3	L5	1586	G
3	L5	1591	U
3	L5	1596	U
3	L5	1614	C

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Mol	Chain	Res	Type
3	L5	1624	G
3	L5	1625	OMG
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1638	A
3	L5	1640	C
3	L5	1641	G
3	L5	1654	G
3	L5	1661	C
3	L5	1670	G
3	L5	1676	C
3	L5	1677	PSU
3	L5	1681	G
3	L5	1694	C
3	L5	1697	G
3	L5	1698	C
3	L5	1699	A
3	L5	1705	G
3	L5	1721	G
3	L5	1734	G
3	L5	1754	U
3	L5	1761	G
3	L5	1763	C
3	L5	1767	A
3	L5	1768	C
3	L5	1769	G
3	L5	1770	A
3	L5	1771	U
3	L5	1772	C
3	L5	1775	A
3	L5	1781	PSU
3	L5	1785	C
3	L5	1787	A
3	L5	1794	A
3	L5	1804	A
3	L5	1815	G
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1854	G
3	L5	1855	G

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Mol	Chain	Res	Type
3	L5	1869	G
3	L5	1882	U
3	L5	1891	A
3	L5	1897	A
3	L5	1906	U
3	L5	1917	A
3	L5	1919	G
3	L5	1921	C
3	L5	1922	G
3	L5	1925	G
3	L5	1931	C
3	L5	1932	A
3	L5	1935	C
3	L5	1940	G
3	L5	1941	A
3	L5	1948	G
3	L5	1951	G
3	L5	1956	A
3	L5	1960	A
3	L5	1961	G
3	L5	1963	C
3	L5	1967	A
3	L5	1968	G
3	L5	1969	G
3	L5	1974	U
3	L5	1978	C
3	L5	1982	G
3	L5	1984	A
3	L5	1985	G
3	L5	1987	C
3	L5	1992	U
3	L5	1993	C
3	L5	1996	C
3	L5	1997	U
3	L5	1998	A
3	L5	1999	A
3	L5	2002	A
3	L5	2003	G
3	L5	2004	U
3	L5	2023	C
3	L5	2026	A
3	L5	2034	G

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Mol	Chain	Res	Type
3	L5	2040	A
3	L5	2044	U
3	L5	2046	G
3	L5	2048	U
3	L5	2052	G
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A
3	L5	2071	A
3	L5	2084	C
3	L5	2085	G
3	L5	2090	U
3	L5	2091	C
3	L5	2092	G
3	L5	2095	A
3	L5	2096	G
3	L5	2098	G
3	L5	2099	G
3	L5	2104	G
3	L5	2106	G
3	L5	2108	G
3	L5	2256	C
3	L5	2258	C
3	L5	2259	G
3	L5	2268	A
3	L5	2269	C
3	L5	2278	G
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2313	A
3	L5	2348	G
3	L5	2351	OMC
3	L5	2357	G
3	L5	2360	A
3	L5	2366	A
3	L5	2369	U
3	L5	2379	A
3	L5	2383	C
3	L5	2394	G
3	L5	2395	A
3	L5	2397	G

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Mol	Chain	Res	Type
3	L5	2398	U
3	L5	2416	G
3	L5	2421	G
3	L5	2424	OMG
3	L5	2425	U
3	L5	2450	G
3	L5	2471	G
3	L5	2474	G
3	L5	2478	C
3	L5	2481	G
3	L5	2485	U
3	L5	2487	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2491	C
3	L5	2499	C
3	L5	2500	U
3	L5	2503	G
3	L5	2504	C
3	L5	2505	C
3	L5	2506	G
3	L5	2513	A
3	L5	2518	G
3	L5	2519	U
3	L5	2520	C
3	L5	2529	A
3	L5	2554	U
3	L5	2573	A
3	L5	2583	C
3	L5	2587	A
3	L5	2589	C
3	L5	2601	A
3	L5	2627	C
3	L5	2632	PSU
3	L5	2647	A
3	L5	2653	C
3	L5	2661	U
3	L5	2662	G
3	L5	2669	C
3	L5	2687	U
3	L5	2694	G

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Mol	Chain	Res	Type
3	L5	2695	A
3	L5	2696	A
3	L5	2701	U
3	L5	2707	U
3	L5	2708	U
3	L5	2710	C
3	L5	2711	G
3	L5	2721	G
3	L5	2726	G
3	L5	2743	A
3	L5	2759	G
3	L5	2760	G
3	L5	2761	U
3	L5	2763	U
3	L5	2764	A
3	L5	2769	U
3	L5	2770	C
3	L5	2787	A2M
3	L5	2788	U
3	L5	2790	U
3	L5	2794	C
3	L5	2806	A
3	L5	2814	C
3	L5	2826	U
3	L5	2827	G
3	L5	2838	G
3	L5	2839	PSU
3	L5	2841	G
3	L5	2855	G
3	L5	2877	G
3	L5	2902	G
3	L5	3596	A
3	L5	3597	G
3	L5	3598	C
3	L5	3599	A
3	L5	3606	U
3	L5	3616	U
3	L5	3618	C
3	L5	3626	G
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A

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Mol	Chain	Res	Type
3	L5	3648	A
3	L5	3662	A
3	L5	3664	G
3	L5	3674	G
3	L5	3709	U
3	L5	3710	G
3	L5	3711	A
3	L5	3736	A
3	L5	3737	A
3	L5	3748	A
3	L5	3753	G
3	L5	3760	A2M
3	L5	3765	G
3	L5	3776	G
3	L5	3777	G
3	L5	3778	U
3	L5	3784	A
3	L5	3785	A2M
3	L5	3787	G
3	L5	3811	G
3	L5	3814	U
3	L5	3816	A
3	L5	3817	A
3	L5	3819	G
3	L5	3822	U
3	L5	3828	A
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3867	A2M
3	L5	3876	A
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3887	OMC
3	L5	3897	G
3	L5	3898	G
3	L5	3901	A
3	L5	3905	A
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A

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Mol	Chain	Res	Type
3	L5	3915	U
3	L5	3943	A
3	L5	3947	A
3	L5	3948	C
3	L5	3951	G
3	L5	3956	G
3	L5	3957	U
3	L5	3958	G
3	L5	3959	U
3	L5	3960	A
3	L5	3962	A
3	L5	3963	A
3	L5	3964	U
3	L5	3965	A
3	L5	3967	G
3	L5	3969	G
3	L5	3973	G
3	L5	3974	G
3	L5	3977	C
3	L5	4035	G
3	L5	4039	G
3	L5	4040	C
3	L5	4041	C
3	L5	4042	G
3	L5	4043	G
3	L5	4044	U
3	L5	4047	A
3	L5	4048	A
3	L5	4049	U
3	L5	4050	A
3	L5	4051	C
3	L5	4053	A
3	L5	4055	U
3	L5	4056	A
3	L5	4058	U
3	L5	4060	U
3	L5	4061	G
3	L5	4063	U
3	L5	4065	G
3	L5	4076	G
3	L5	4084	G
3	L5	4093	G

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Mol	Chain	Res	Type
3	L5	4096	C
3	L5	4097	G
3	L5	4103	C
3	L5	4107	G
3	L5	4108	G
3	L5	4114	C
3	L5	4115	G
3	L5	4118	U
3	L5	4119	C
3	L5	4122	G
3	L5	4127	A
3	L5	4137	C
3	L5	4138	C
3	L5	4139	G
3	L5	4140	C
3	L5	4142	C
3	L5	4145	C
3	L5	4148	C
3	L5	4150	G
3	L5	4152	G
3	L5	4162	C
3	L5	4163	U
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4221	C
3	L5	4225	G
3	L5	4228	OMG
3	L5	4229	U
3	L5	4233	A
3	L5	4241	C
3	L5	4251	A
3	L5	4253	A
3	L5	4254	G
3	L5	4266	G
3	L5	4268	A
3	L5	4273	A
3	L5	4280	A
3	L5	4281	A
3	L5	4291	G
3	L5	4305	G

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Mol	Chain	Res	Type
3	L5	4314	C
3	L5	4326	G
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4338	G
3	L5	4339	A
3	L5	4354	U
3	L5	4371	G
3	L5	4373	G
3	L5	4374	U
3	L5	4377	G
3	L5	4378	A
3	L5	4380	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4419	U
3	L5	4421	C
3	L5	4422	A
3	L5	4426	C
3	L5	4433	G
3	L5	4437	U
3	L5	4444	C
3	L5	4448	G
3	L5	4449	A
3	L5	4453	C
3	L5	4464	A
3	L5	4465	U
3	L5	4471	PSU
3	L5	4475	G
3	L5	4476	C
3	L5	4500	PSU
3	L5	4512	U
3	L5	4513	A
3	L5	4519	C
3	L5	4524	G
3	L5	4528	G
3	L5	4531	PSU
3	L5	4548	A
3	L5	4549	G
3	L5	4560	C

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Mol	Chain	Res	Type
3	L5	4567	G
3	L5	4573	G
3	L5	4582	C
3	L5	4590	A2M
3	L5	4600	G
3	L5	4608	G
3	L5	4624	A
3	L5	4627	U
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
3	L5	4656	A
3	L5	4657	U
3	L5	4670	C
3	L5	4672	A
3	L5	4691	A
3	L5	4693	C
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4719	G
3	L5	4721	G
3	L5	4731	G
3	L5	4732	G
3	L5	4733	C
3	L5	4734	A
3	L5	4739	C
3	L5	4740	G
3	L5	4741	C
3	L5	4742	G
3	L5	4744	A
3	L5	4745	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4764	A
3	L5	4765	G
3	L5	4773	C
3	L5	4775	C
3	L5	4776	G
3	L5	4859	C

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Mol	Chain	Res	Type
3	L5	4860	G
3	L5	4864	U
3	L5	4870	G
3	L5	4871	C
3	L5	4873	G
3	L5	4877	G
3	L5	4882	U
3	L5	4883	C
3	L5	4889	G
3	L5	4895	C
3	L5	4896	G
3	L5	4897	G
3	L5	4900	C
3	L5	4901	G
3	L5	4903	G
3	L5	4910	G
3	L5	4912	G
3	L5	4914	C
3	L5	4925	U
3	L5	4926	C
3	L5	4934	A
3	L5	4938	A
3	L5	4943	A
3	L5	4959	U
3	L5	4976	U
3	L5	4988	U
3	L5	4990	C
3	L5	4991	U
3	L5	5007	A
3	L5	5013	C
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5026	U
3	L5	5027	C
3	L5	5028	G
3	L5	5031	G
3	L5	5034	A
3	L5	5041	G
3	L5	5050	C
3	L5	5058	A

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Mol	Chain	Res	Type
3	L5	5060	A
3	L5	5061	A
3	L5	5062	G
3	L5	5069	U
4	L7	7	G
4	L7	53	U
4	L7	64	G
4	L7	100	A
4	L7	102	U
4	L7	110	G
4	L7	120	U
83	At	8	4SU
83	At	14	A
83	At	16	H2U
83	At	17	C
83	At	18	G
83	At	19	G
83	At	21	A
83	At	46	7MG
83	At	47	U
83	At	48	C
83	At	49	C
83	At	52	G
83	At	58	A
83	At	59	U
83	At	74	C
84	Pt	2	G
84	Pt	4	G
84	Pt	7	G
84	Pt	8	4SU
84	Pt	9	G
84	Pt	13	C
84	Pt	16	C
84	Pt	17	C
84	Pt	18	C
84	Pt	20	G
84	Pt	21	H2U
84	Pt	24	C
84	Pt	47	G7M
84	Pt	48	U
84	Pt	51	U
84	Pt	62	C

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Mol	Chain	Res	Type
84	Pt	64	G
84	Pt	68	C
84	Pt	75	C
84	Pt	76	C
84	Pt	77	A

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	203	G
1	S2	329	G
1	S2	554	A
1	S2	867	OMG
1	S2	869	A
1	S2	918	PSU
1	S2	1081	PSU
1	S2	1419	C
1	S2	1436	C
1	S2	1776	G
1	S2	1825	A
3	L5	385	A
3	L5	408	A
3	L5	409	G
3	L5	934	C
3	L5	1407	C
3	L5	1590	C
3	L5	1633	G
3	L5	2652	G
3	L5	2876	OMG
3	L5	3876	A
3	L5	4048	A
3	L5	4076	G
3	L5	4141	G
3	L5	4378	A
3	L5	4475	G
3	L5	4699	U
3	L5	4733	C
3	L5	4872	G
3	L5	4925	U
3	L5	5027	C
3	L5	5060	A

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

240 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	$\#\|Z\| > 2$
3	OMG	L5	3627	3	18,26,27	0.95	1 (5%)	19,38,41	1.19	2 (10%)
1	A2M	S2	668	87,1	18,25,26	0.94	1 (5%)	18,36,39	1.25	2 (11%)
3	PSU	L5	1744	3,86	18,21,22	1.39	3 (16%)	22,30,33	1.93	4 (18%)
3	PSU	L5	3758	3	18,21,22	1.56	4 (22%)	22,30,33	2.00	5 (22%)
3	PSU	L5	3764	3	18,21,22	1.49	4 (22%)	22,30,33	2.17	5 (22%)
3	A2M	L5	4523	87,3	18,25,26	0.90	1 (5%)	18,36,39	1.27	2 (11%)
3	PSU	L5	1792	3	18,21,22	1.41	3 (16%)	22,30,33	1.89	3 (13%)
3	OMC	L5	1881	87,3	19,22,23	0.80	0	26,31,34	0.76	0
3	OMC	L5	3808	3	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
3	PSU	L5	4361	3	18,21,22	1.41	3 (16%)	22,30,33	1.92	3 (13%)
3	PSU	L5	4689	3	18,21,22	1.42	4 (22%)	22,30,33	1.93	3 (13%)
83	PSU	At	39	83	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
3	A2M	L5	3718	3	18,25,26	1.02	2 (11%)	18,36,39	1.11	2 (11%)
3	PSU	L5	4531	3	18,21,22	1.44	2 (11%)	22,30,33	2.10	4 (18%)
1	PSU	S2	1177	1	18,21,22	1.40	3 (16%)	22,30,33	1.92	3 (13%)
29	AME	SV	1	29	9,10,11	3.35	2 (22%)	9,11,13	4.51	5 (55%)
3	OMG	L5	3899	3	18,26,27	0.95	1 (5%)	19,38,41	1.14	2 (10%)
1	PSU	S2	296	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
3	PSU	L5	2508	3	18,21,22	1.42	3 (16%)	22,30,33	1.96	4 (18%)
3	OMC	L5	3701	3,86	19,22,23	0.79	0	26,31,34	0.73	0
3	PSU	L5	2839	3	18,21,22	1.31	2 (11%)	22,30,33	1.96	3 (13%)
1	4AC	S2	1337	1	21,24,25	1.22	2 (9%)	29,34,37	1.11	3 (10%)
1	OMU	S2	1442	87,1	19,22,23	1.20	2 (10%)	26,31,34	1.71	4 (15%)
1	PSU	S2	93	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
84	G7M	Pt	47	84	20,26,27	2.41	3 (15%)	17,39,42	0.63	0
3	PSU	L5	4420	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	PSU	S2	866	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
3	A2M	L5	3825	3	18,25,26	0.95	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	S2	814	1	18,21,22	1.37	3 (16%)	22,30,33	1.89	4 (18%)
3	A2M	L5	2787	3	18,25,26	1.01	2 (11%)	18,36,39	1.41	3 (16%)
3	PSU	L5	4423	87,3	18,21,22	1.38	3 (16%)	22,30,33	1.93	4 (18%)
3	OMG	L5	4494	3	18,26,27	0.95	1 (5%)	19,38,41	1.06	2 (10%)
1	OMG	S2	436	1	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
3	OMG	L5	2424	3	18,26,27	0.98	1 (5%)	19,38,41	0.99	2 (10%)
3	OMC	L5	4456	3	19,22,23	0.82	0	26,31,34	0.82	1 (3%)
3	PSU	L5	5010	3	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
3	PSU	L5	3770	3	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	S2	863	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
3	PSU	L5	4576	3	18,21,22	1.40	3 (16%)	22,30,33	1.86	3 (13%)
6	SAC	SA	2	6	7,8,9	3.74	2 (28%)	8,9,11	4.49	5 (62%)
40	HIC	LB	245	40	8,11,12	1.58	2 (25%)	6,14,16	1.30	0
1	PSU	S2	681	1	18,21,22	1.42	3 (16%)	22,30,33	1.96	4 (18%)
3	A2M	L5	1524	3	18,25,26	0.96	1 (5%)	18,36,39	1.25	3 (16%)
3	PSU	L5	1582	3	18,21,22	1.46	3 (16%)	22,30,33	2.05	5 (22%)
1	OMU	S2	627	1	19,22,23	1.20	2 (10%)	26,31,34	1.69	5 (19%)
1	PSU	S2	1238	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	S2	1445	1	18,21,22	1.32	2 (11%)	22,30,33	1.89	4 (18%)
3	PSU	L5	4296	3	18,21,22	1.39	3 (16%)	22,30,33	1.95	4 (18%)
3	PSU	L5	3762	3	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	S2	576	1	18,25,26	0.96	1 (5%)	18,36,39	1.23	2 (11%)
1	A2M	S2	99	87,1	18,25,26	1.03	1 (5%)	18,36,39	1.26	2 (11%)
1	PSU	S2	109	1	18,21,22	1.55	5 (27%)	22,30,33	2.10	4 (18%)
3	6MZ	L5	4220	3	18,25,26	0.83	1 (5%)	16,36,39	2.20	4 (25%)
1	OMC	S2	462	1	19,22,23	0.81	0	26,31,34	0.82	0
1	PSU	S2	1347	1	18,21,22	1.34	3 (16%)	22,30,33	1.86	4 (18%)
3	PSU	L5	4569	3	18,21,22	1.43	3 (16%)	22,30,33	1.95	3 (13%)
3	OMU	L5	4306	3	19,22,23	1.27	3 (15%)	26,31,34	1.71	5 (19%)
3	PSU	L5	3853	87,3	18,21,22	1.42	4 (22%)	22,30,33	1.95	4 (18%)
3	OMG	L5	3944	3	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
1	PSU	S2	822	1	18,21,22	1.33	2 (11%)	22,30,33	2.07	5 (22%)
3	OMG	L5	4618	3	18,26,27	1.03	1 (5%)	19,38,41	1.16	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OMG	L5	1625	87,3	18,26,27	1.00	1 (5%)	19,38,41	1.08	2 (10%)
3	PSU	L5	5001	3	18,21,22	1.40	3 (16%)	22,30,33	1.95	4 (18%)
1	A2M	S2	484	1	18,25,26	0.97	1 (5%)	18,36,39	1.24	2 (11%)
1	PSU	S2	1081	1	18,21,22	1.48	4 (22%)	22,30,33	2.06	5 (22%)
83	7MG	At	46	83	22,26,27	1.35	3 (13%)	29,39,42	2.67	9 (31%)
3	PSU	L5	1860	3	18,21,22	1.43	4 (22%)	22,30,33	1.94	3 (13%)
39	V5N	LA	216	39	4,11,12	0.74	0	5,14,16	1.81	3 (60%)
3	OMG	L5	4623	3	18,26,27	0.95	1 (5%)	19,38,41	1.12	2 (10%)
1	PSU	S2	1643	87,1	18,21,22	1.34	2 (11%)	22,30,33	1.87	4 (18%)
3	OMG	L5	4228	3	18,26,27	0.86	1 (5%)	19,38,41	1.10	2 (10%)
3	A2M	L5	4590	3	18,25,26	0.98	1 (5%)	18,36,39	1.23	2 (11%)
3	OMG	L5	4370	3	18,26,27	0.97	1 (5%)	19,38,41	1.05	2 (10%)
3	A2M	L5	2401	3	18,25,26	0.97	1 (5%)	18,36,39	1.40	3 (16%)
3	PSU	L5	3695	3	18,21,22	1.40	3 (16%)	22,30,33	1.93	4 (18%)
3	OMC	L5	3869	3	19,22,23	0.83	0	26,31,34	0.82	0
3	A2M	L5	4571	3	18,25,26	1.00	1 (5%)	18,36,39	1.20	2 (11%)
3	OMG	L5	2364	3	18,26,27	0.88	1 (5%)	19,38,41	1.16	2 (10%)
3	OMC	L5	3841	3	19,22,23	0.82	0	26,31,34	0.82	0
3	PSU	L5	4521	87,3	18,21,22	1.44	3 (16%)	22,30,33	1.93	5 (22%)
3	A2M	L5	1534	87,3	18,25,26	0.99	1 (5%)	18,36,39	1.48	3 (16%)
1	A2M	S2	1383	1	18,25,26	1.02	1 (5%)	18,36,39	1.24	2 (11%)
1	A2M	S2	1678	1	18,25,26	0.96	1 (5%)	18,36,39	1.41	2 (11%)
3	UY1	L5	3818	87,3	19,22,23	1.41	4 (21%)	22,31,34	1.96	4 (18%)
1	OMG	S2	1328	1	18,26,27	0.95	1 (5%)	19,38,41	1.05	2 (10%)
1	A2M	S2	1031	1	18,25,26	0.98	1 (5%)	18,36,39	1.20	2 (11%)
1	PSU	S2	34	1	18,21,22	1.34	2 (11%)	22,30,33	1.94	3 (13%)
1	PSU	S2	105	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
64	SAC	Lr	2	64	7,8,9	3.74	2 (28%)	8,9,11	4.55	4 (50%)
1	A2M	S2	590	1	18,25,26	1.04	1 (5%)	18,36,39	1.20	2 (11%)
3	PSU	L5	4500	83,3	18,21,22	1.37	2 (11%)	22,30,33	1.94	3 (13%)
3	OMG	L5	1316	3	18,26,27	1.02	1 (5%)	19,38,41	1.01	2 (10%)
1	A2M	S2	27	1	18,25,26	0.99	1 (5%)	18,36,39	1.22	2 (11%)
3	A2M	L5	2363	87,3	18,25,26	0.96	1 (5%)	18,36,39	1.15	2 (11%)
1	PSU	S2	1244	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
3	A2M	L5	3760	87,3	18,25,26	1.01	1 (5%)	18,36,39	1.45	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMU	S2	121	1	19,22,23	1.23	3 (15%)	26,31,34	1.66	4 (15%)
84	PSU	Pt	56	84	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	S2	649	1	18,21,22	1.38	2 (11%)	22,30,33	1.92	3 (13%)
2	PSU	L8	69	2	18,21,22	1.41	3 (16%)	22,30,33	1.95	4 (18%)
3	5MC	L5	4447	3,86	18,22,23	1.01	2 (11%)	26,32,35	1.33	4 (15%)
3	PSU	L5	4471	3	18,21,22	1.37	3 (16%)	22,30,33	1.85	4 (18%)
1	PSU	S2	406	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
3	PSU	L5	3637	3	18,21,22	1.45	3 (16%)	22,30,33	1.92	5 (22%)
2	OMG	L8	75	2	18,26,27	0.90	1 (5%)	19,38,41	1.16	2 (10%)
83	H2U	At	20	83	18,21,22	0.96	2 (11%)	21,30,33	1.33	2 (9%)
1	PSU	S2	609	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
83	H2U	At	16	83	18,21,22	1.02	2 (11%)	21,30,33	1.56	3 (14%)
3	OMU	L5	2415	3	19,22,23	1.31	3 (15%)	26,31,34	1.81	5 (19%)
3	PSU	L5	4431	3	18,21,22	1.34	2 (11%)	22,30,33	1.94	3 (13%)
1	OMU	S2	172	1	19,22,23	1.34	4 (21%)	26,31,34	1.88	6 (23%)
1	PSU	S2	1056	1	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	S2	159	1	18,25,26	1.01	1 (5%)	18,36,39	1.30	2 (11%)
3	A2M	L5	3785	87,3	18,25,26	0.91	0	18,36,39	1.43	3 (16%)
3	A2M	L5	1326	3	18,25,26	0.95	1 (5%)	18,36,39	1.20	2 (11%)
3	PSU	L5	4493	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	3 (13%)
1	PSU	S2	651	1	18,21,22	1.38	2 (11%)	22,30,33	1.96	4 (18%)
1	UY1	S2	1326	87,1	19,22,23	1.31	2 (10%)	22,31,34	1.91	4 (18%)
1	MA6	S2	1851	1	19,26,27	0.92	1 (5%)	18,38,41	1.24	3 (16%)
1	OMC	S2	1391	1	19,22,23	0.82	0	26,31,34	0.83	0
1	OMC	S2	517	1	19,22,23	0.81	0	26,31,34	0.82	0
3	OMU	L5	4227	3	19,22,23	1.25	3 (15%)	26,31,34	1.72	5 (19%)
1	PSU	S2	1136	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
3	PSU	L5	4403	3	18,21,22	1.45	4 (22%)	22,30,33	1.98	4 (18%)
3	PSU	L5	4552	3	18,21,22	1.42	4 (22%)	22,30,33	2.00	3 (13%)
3	OMC	L5	3887	3	19,22,23	0.77	0	26,31,34	0.81	0
1	B8N	S2	1248	1	24,29,30	1.03	2 (8%)	29,42,45	1.62	6 (20%)
3	OMG	L5	2876	3	18,26,27	1.01	1 (5%)	19,38,41	1.21	2 (10%)
1	OMG	S2	867	1	18,26,27	1.00	1 (5%)	19,38,41	1.22	2 (10%)
1	PSU	S2	918	1	18,21,22	1.37	2 (11%)	22,30,33	2.18	4 (18%)
1	PSU	S2	686	1	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OMU	L5	4620	3	19,22,23	1.30	3 (15%)	26,31,34	1.79	4 (15%)
1	PSU	S2	1367	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
20	HY3	SX	62	20	6,8,9	1.54	1 (16%)	5,10,12	1.27	0
3	PSU	L5	4353	3	18,21,22	1.40	3 (16%)	22,30,33	1.92	3 (13%)
3	PSU	L5	1782	3	18,21,22	1.39	3 (16%)	22,30,33	1.92	3 (13%)
3	OMC	L5	2804	3	19,22,23	0.81	0	26,31,34	0.84	0
1	PSU	S2	1692	1	18,21,22	1.53	4 (22%)	22,30,33	2.06	4 (18%)
3	OMU	L5	3925	3	19,22,23	1.22	2 (10%)	26,31,34	1.83	5 (19%)
1	G7M	S2	1639	84,1	20,26,27	2.59	4 (20%)	17,39,42	1.36	2 (11%)
3	A2M	L5	3724	3	18,25,26	1.01	1 (5%)	18,36,39	1.17	2 (11%)
3	A2M	L5	3867	3	18,25,26	0.97	1 (5%)	18,36,39	1.15	2 (11%)
3	PSU	L5	4532	3	18,21,22	1.49	3 (16%)	22,30,33	1.91	4 (18%)
83	PSU	At	32	83	18,21,22	1.34	2 (11%)	22,30,33	1.83	3 (13%)
3	PSU	L5	4628	3	18,21,22	1.41	2 (11%)	22,30,33	1.92	3 (13%)
3	PSU	L5	2632	3	18,21,22	1.40	4 (22%)	22,30,33	1.80	3 (13%)
1	OMG	S2	644	1	18,26,27	0.95	1 (5%)	19,38,41	1.07	2 (10%)
1	PSU	S2	119	1	18,21,22	1.32	2 (11%)	22,30,33	1.76	4 (18%)
84	OMC	Pt	33	84	19,22,23	0.85	0	26,31,34	1.02	2 (7%)
1	PSU	S2	1239	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	S2	1625	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
3	PSU	L5	1683	3	18,21,22	1.49	4 (22%)	22,30,33	1.84	3 (13%)
1	OMG	S2	1447	1	18,26,27	0.93	1 (5%)	19,38,41	1.04	2 (10%)
1	OMG	S2	1490	87,1	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
3	PSU	L5	3734	3	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
3	OMC	L5	4536	3	19,22,23	0.86	0	26,31,34	0.79	1 (3%)
1	A2M	S2	512	1	18,25,26	1.01	1 (5%)	18,36,39	1.26	2 (11%)
1	A2M	S2	166	1	18,25,26	0.98	1 (5%)	18,36,39	1.27	2 (11%)
3	PSU	L5	4299	3	18,21,22	1.44	3 (16%)	22,30,33	1.92	4 (18%)
3	OMC	L5	1340	3	19,22,23	0.88	1 (5%)	26,31,34	0.81	0
3	PSU	L5	4972	3	18,21,22	1.35	3 (16%)	22,30,33	1.83	3 (13%)
1	PSU	S2	572	1	18,21,22	1.41	2 (11%)	22,30,33	2.01	5 (22%)
1	A2M	S2	468	1	18,25,26	1.00	1 (5%)	18,36,39	1.17	2 (11%)
3	OMG	L5	4392	3	18,26,27	0.90	1 (5%)	19,38,41	1.01	2 (10%)
3	PSU	L5	3715	3	18,21,22	1.37	3 (16%)	22,30,33	1.88	3 (13%)
3	OMC	L5	2824	3	19,22,23	0.78	0	26,31,34	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	PSU	L5	4579	3	18,21,22	1.38	3 (16%)	22,30,33	1.96	4 (18%)
3	A2M	L5	3723	3	18,25,26	1.04	1 (5%)	18,36,39	1.22	2 (11%)
3	PSU	L5	3884	3	18,21,22	1.44	4 (22%)	22,30,33	1.95	3 (13%)
3	PSU	L5	1677	3	18,21,22	1.53	4 (22%)	22,30,33	1.97	3 (13%)
3	PSU	L5	3729	3	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
3	1MA	L5	1322	87,3	16,25,26	1.38	2 (12%)	18,37,40	1.06	2 (11%)
3	PSU	L5	3844	3	18,21,22	1.45	3 (16%)	22,30,33	1.87	3 (13%)
3	A2M	L5	2815	87,3	18,25,26	0.99	1 (5%)	18,36,39	1.23	2 (11%)
1	OMG	S2	509	87,1	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
3	PSU	L5	4293	3	18,21,22	1.43	3 (16%)	22,30,33	1.84	3 (13%)
1	OMC	S2	1703	1	19,22,23	0.81	0	26,31,34	0.69	0
3	PSU	L5	2843	3	18,21,22	1.43	3 (16%)	22,30,33	1.98	4 (18%)
1	OMC	S2	174	1	19,22,23	0.81	0	26,31,34	0.78	0
77	M3L	Lm	98	77	10,11,12	0.46	0	9,14,16	0.10	0
1	OMU	S2	354	1	19,22,23	1.27	3 (15%)	26,31,34	1.80	5 (19%)
1	PSU	S2	218	1	18,21,22	1.33	2 (11%)	22,30,33	1.85	4 (18%)
84	H2U	Pt	21	84	18,21,22	0.96	2 (11%)	21,30,33	1.35	2 (9%)
3	UR3	L5	4530	3	19,22,23	0.94	0	26,32,35	1.44	2 (7%)
3	PSU	L5	4636	3	18,21,22	1.50	4 (22%)	22,30,33	2.21	6 (27%)
1	6MZ	S2	1832	87,1	18,25,26	0.83	1 (5%)	16,36,39	2.09	3 (18%)
3	OMU	L5	2837	3	19,22,23	1.27	2 (10%)	26,31,34	1.78	4 (15%)
3	OMU	L5	4498	3	19,22,23	1.21	3 (15%)	26,31,34	1.77	5 (19%)
3	5MC	L5	3782	87,3	18,22,23	0.94	2 (11%)	26,32,35	1.15	3 (11%)
3	PSU	L5	4442	3	18,21,22	1.50	4 (22%)	22,30,33	2.17	5 (22%)
1	PSU	S2	1243	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
3	OMG	L5	4499	83,3	18,26,27	0.90	1 (5%)	19,38,41	1.06	2 (10%)
1	OMU	S2	116	1	19,22,23	1.23	3 (15%)	26,31,34	1.68	6 (23%)
3	OMG	L5	3744	3	18,26,27	0.95	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	S2	36	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
3	OMG	L5	4196	84,3	18,26,27	1.04	1 (5%)	19,38,41	1.16	3 (15%)
3	PSU	L5	1536	3	18,21,22	1.48	3 (16%)	22,30,33	1.85	4 (18%)
1	OMU	S2	1288	1	19,22,23	1.19	2 (10%)	26,31,34	1.66	4 (15%)
3	OMC	L5	2861	3	19,22,23	0.79	0	26,31,34	0.70	0
3	A2M	L5	1871	3	18,25,26	0.97	1 (5%)	18,36,39	1.35	2 (11%)
1	OMG	S2	601	1	18,26,27	0.89	1 (5%)	19,38,41	1.08	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PSU	L5	3768	3	18,21,22	1.49	4 (22%)	22,30,33	2.07	5 (22%)
3	A2M	L5	3830	3	18,25,26	0.92	1 (5%)	18,36,39	1.21	2 (11%)
1	PSU	S2	1174	87,1	18,21,22	1.37	4 (22%)	22,30,33	1.87	3 (13%)
1	OMG	S2	683	1	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
3	OMG	L5	4637	3	18,26,27	1.06	1 (5%)	19,38,41	1.15	2 (10%)
3	PSU	L5	4457	3	18,21,22	1.42	3 (16%)	22,30,33	1.92	4 (18%)
3	PSU	L5	1779	3	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	S2	966	1	18,21,22	1.34	2 (11%)	22,30,33	1.95	4 (18%)
1	PSU	S2	801	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	3 (13%)
3	OMC	L5	2351	3	19,22,23	0.84	0	26,31,34	0.75	0
3	PSU	L5	1781	3	18,21,22	1.44	3 (16%)	22,30,33	1.87	3 (13%)
2	PSU	L8	55	2	18,21,22	1.40	3 (16%)	22,30,33	1.90	4 (18%)
3	PSU	L5	4312	3	18,21,22	1.39	4 (22%)	22,30,33	1.96	3 (13%)
1	4AC	S2	1842	1	21,24,25	1.03	1 (4%)	29,34,37	1.09	4 (13%)
1	OMU	S2	428	1	19,22,23	1.20	3 (15%)	26,31,34	1.75	5 (19%)
3	OMC	L5	2365	3	19,22,23	0.81	0	26,31,34	0.76	0
3	PSU	L5	3920	87,3	18,21,22	1.41	3 (16%)	22,30,33	2.00	4 (18%)
50	V5N	La	39	50	4,11,12	0.62	0	5,14,16	1.91	2 (40%)
79	MLZ	Lo	53	79	8,9,10	0.78	0	4,9,11	0.60	0
66	MLZ	Lb	5	66	8,9,10	0.79	0	4,9,11	0.69	0
3	OMC	L5	2422	87,3	19,22,23	0.83	0	26,31,34	0.84	0
1	PSU	S2	1232	1	18,21,22	1.35	2 (11%)	22,30,33	1.96	3 (13%)
3	OMG	L5	3792	3	18,26,27	0.91	1 (5%)	19,38,41	1.07	3 (15%)
3	PSU	L5	4673	3	18,21,22	1.57	4 (22%)	22,30,33	2.01	4 (18%)
83	4SU	At	8	83	18,21,22	1.78	4 (22%)	26,30,33	2.24	5 (19%)
1	PSU	S2	1004	1	18,21,22	1.46	3 (16%)	22,30,33	2.06	5 (22%)
1	PSU	S2	815	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	S2	573	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
3	A2M	L5	400	3	18,25,26	0.98	1 (5%)	18,36,39	1.21	2 (11%)
3	PSU	L5	3851	3	18,21,22	1.41	4 (22%)	22,30,33	1.90	4 (18%)
3	PSU	L5	3639	3	18,21,22	1.47	4 (22%)	22,30,33	1.93	4 (18%)
1	OMU	S2	1804	1	19,22,23	1.26	2 (10%)	26,31,34	1.68	4 (15%)
3	OMG	L5	1522	3	18,26,27	0.96	1 (5%)	19,38,41	1.18	3 (15%)
3	A2M	L5	398	3	18,25,26	0.96	1 (5%)	18,36,39	1.25	2 (11%)
84	4SU	Pt	8	84	18,21,22	1.73	4 (22%)	26,30,33	2.19	4 (15%)
2	OMU	L8	14	2,3	19,22,23	1.26	3 (15%)	26,31,34	1.71	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MA6	S2	1850	1	19,26,27	0.92	1 (5%)	18,38,41	1.24	2 (11%)
81	5CT	5A	50	81	13,14,15	0.75	1 (7%)	9,15,17	2.37	4 (44%)
3	PSU	L5	1862	3	18,21,22	1.43	3 (16%)	22,30,33	2.06	4 (18%)

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
3	OMG	L5	3627	3	-	0/5/27/28	0/3/3/3
1	A2M	S2	668	87,1	-	3/5/27/28	0/3/3/3
3	PSU	L5	1744	3,86	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3764	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	87,3	-	1/5/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	1881	87,3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
83	PSU	At	39	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4531	3	-	2/7/25/26	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
29	AME	SV	1	29	-	2/9/10/12	-
3	OMG	L5	3899	3	-	0/5/27/28	0/3/3/3
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3701	3,86	-	4/9/27/28	0/2/2/2
3	PSU	L5	2839	3	-	2/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	2/11/29/30	0/2/2/2
1	OMU	S2	1442	87,1	-	1/9/27/28	0/2/2/2
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
84	G7M	Pt	47	84	-	2/3/25/26	0/3/3/3
3	PSU	L5	4420	3	-	4/7/25/26	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/5/27/28	0/3/3/3
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4423	87,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	0/5/27/28	0/3/3/3
1	OMG	S2	436	1	-	0/5/27/28	0/3/3/3
3	OMG	L5	2424	3	-	3/5/27/28	0/3/3/3
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	863	1	-	2/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
6	SAC	SA	2	6	-	5/7/8/10	-
40	HIC	LB	245	40	-	3/5/6/8	0/1/1/1
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
1	OMU	S2	627	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	576	1	-	2/5/27/28	0/3/3/3
1	A2M	S2	99	87,1	-	0/5/27/28	0/3/3/3
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	0/5/27/28	0/3/3/3
1	OMC	S2	462	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3853	87,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3944	3	-	0/5/27/28	0/3/3/3
1	PSU	S2	822	1	-	1/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	1/5/27/28	0/3/3/3
3	OMG	L5	1625	87,3	-	1/5/27/28	0/3/3/3
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	0/5/27/28	0/3/3/3
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
83	7MG	At	46	83	-	3/7/37/38	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
39	V5N	LA	216	39	-	1/5/10/12	0/1/1/1
3	OMG	L5	4623	3	-	0/5/27/28	0/3/3/3
1	PSU	S2	1643	87,1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	4228	3	-	2/5/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/5/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	2401	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	1/5/27/28	0/3/3/3
3	OMG	L5	2364	3	-	3/5/27/28	0/3/3/3
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4521	87,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	87,3	-	2/5/27/28	0/3/3/3
1	A2M	S2	1383	1	-	1/5/27/28	0/3/3/3
1	A2M	S2	1678	1	-	3/5/27/28	0/3/3/3
3	UY1	L5	3818	87,3	-	4/9/27/28	0/2/2/2
1	OMG	S2	1328	1	-	0/5/27/28	0/3/3/3
1	A2M	S2	1031	1	-	0/5/27/28	0/3/3/3
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
64	SAC	Lr	2	64	-	1/7/8/10	-
1	A2M	S2	590	1	-	1/5/27/28	0/3/3/3
3	PSU	L5	4500	83,3	-	1/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	0/5/27/28	0/3/3/3
1	A2M	S2	27	1	-	1/5/27/28	0/3/3/3
3	A2M	L5	2363	87,3	-	0/5/27/28	0/3/3/3
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3760	87,3	-	0/5/27/28	0/3/3/3
1	OMU	S2	121	1	-	1/9/27/28	0/2/2/2
84	PSU	Pt	56	84	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
2	PSU	L8	69	2	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3,86	-	4/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	2/7/25/26	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
2	OMG	L8	75	2	-	0/5/27/28	0/3/3/3
83	H2U	At	20	83	-	0/7/38/39	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
83	H2U	At	16	83	-	1/7/38/39	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	159	1	-	3/5/27/28	0/3/3/3
3	A2M	L5	3785	87,3	-	3/5/27/28	0/3/3/3
3	A2M	L5	1326	3	-	3/5/27/28	0/3/3/3
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
1	UY1	S2	1326	87,1	-	1/9/27/28	0/2/2/2
1	MA6	S2	1851	1	-	2/7/29/30	0/3/3/3
1	OMC	S2	1391	1	-	1/9/27/28	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
3	OMU	L5	4227	3	-	1/9/27/28	0/2/2/2
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	2/9/27/28	0/2/2/2
1	B8N	S2	1248	1	-	3/16/34/35	0/2/2/2
3	OMG	L5	2876	3	-	0/5/27/28	0/3/3/3
1	OMG	S2	867	1	-	3/5/27/28	0/3/3/3
1	PSU	S2	918	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	1/9/27/28	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
20	HY3	SX	62	20	-	1/1/12/14	0/1/1/1
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
1	G7M	S2	1639	84,1	-	2/3/25/26	0/3/3/3
3	A2M	L5	3724	3	-	1/5/27/28	0/3/3/3
3	A2M	L5	3867	3	-	3/5/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
83	PSU	At	32	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	3/7/25/26	0/2/2/2
1	OMG	S2	644	1	-	4/5/27/28	0/3/3/3
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
84	OMC	Pt	33	84	-	3/9/27/28	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	1447	1	-	2/5/27/28	0/3/3/3
1	OMG	S2	1490	87,1	-	1/5/27/28	0/3/3/3
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
1	A2M	S2	512	1	-	1/5/27/28	0/3/3/3
1	A2M	S2	166	1	-	1/5/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	1/5/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3729	3	-	2/7/25/26	0/2/2/2
3	1MA	L5	1322	87,3	-	0/3/25/26	0/3/3/3
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	2815	87,3	-	1/5/27/28	0/3/3/3
1	OMG	S2	509	87,1	-	0/5/27/28	0/3/3/3
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
1	OMC	S2	1703	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
77	M3L	Lm	98	77	-	4/9/10/12	-
1	OMU	S2	354	1	-	2/9/27/28	0/2/2/2
1	PSU	S2	218	1	-	3/7/25/26	0/2/2/2
84	H2U	Pt	21	84	-	6/7/38/39	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4636	3	-	3/7/25/26	0/2/2/2
1	6MZ	S2	1832	87,1	-	2/5/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	5MC	L5	3782	87,3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
3	OMG	L5	4499	83,3	-	0/5/27/28	0/3/3/3
1	OMU	S2	116	1	-	1/9/27/28	0/2/2/2
3	OMG	L5	3744	3	-	1/5/27/28	0/3/3/3
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	84,3	-	1/5/27/28	0/3/3/3
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	1288	1	-	1/9/27/28	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	1871	3	-	0/5/27/28	0/3/3/3
1	OMG	S2	601	1	-	0/5/27/28	0/3/3/3
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	1/5/27/28	0/3/3/3
1	PSU	S2	1174	87,1	-	0/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	3/5/27/28	0/3/3/3
3	OMG	L5	4637	3	-	3/5/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
1	4AC	S2	1842	1	-	2/11/29/30	0/2/2/2
1	OMU	S2	428	1	-	6/9/27/28	0/2/2/2
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3920	87,3	-	0/7/25/26	0/2/2/2
50	V5N	La	39	50	-	0/5/10/12	0/1/1/1
79	MLZ	Lo	53	79	-	1/7/8/10	-
66	MLZ	Lb	5	66	-	3/7/8/10	-
3	OMC	L5	2422	87,3	-	3/9/27/28	0/2/2/2
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
83	4SU	At	8	83	-	0/7/25/26	0/2/2/2
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	573	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	1804	1	-	1/9/27/28	0/2/2/2
3	OMG	L5	1522	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	398	3	-	1/5/27/28	0/3/3/3
84	4SU	Pt	8	84	-	0/7/25/26	0/2/2/2
2	OMU	L8	14	2,3	-	1/9/27/28	0/2/2/2
1	MA6	S2	1850	1	-	0/7/29/30	0/3/3/3
81	5CT	5A	50	81	-	8/13/14/16	-
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2

All (462) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SV	1	AME	OT-CT1	9.02	1.43	1.23
6	SA	2	SAC	OAC-C1A	8.92	1.43	1.23
64	Lr	2	SAC	OAC-C1A	8.90	1.43	1.23
1	S2	1639	G7M	C8-N9	7.28	1.46	1.33
84	Pt	47	G7M	C8-N9	7.28	1.46	1.33
84	Pt	47	G7M	C8-N7	6.89	1.45	1.33
1	S2	1639	G7M	C8-N7	6.84	1.45	1.33
83	At	8	4SU	C4-S4	-4.71	1.59	1.68
84	Pt	8	4SU	C4-S4	-4.44	1.60	1.68
1	S2	1639	G7M	C5-C4	4.05	1.47	1.39
3	L5	1322	1MA	C2-N3	4.04	1.33	1.29
6	SA	2	SAC	C1A-N	3.86	1.47	1.34
29	SV	1	AME	CT1-N	3.84	1.47	1.34
64	Lr	2	SAC	C1A-N	3.83	1.47	1.34
3	L5	4532	PSU	C6-C5	3.72	1.39	1.35
20	SX	62	HY3	C3-CA	-3.51	1.51	1.55
3	L5	4531	PSU	C6-C5	3.50	1.39	1.35
1	S2	863	PSU	C6-C5	3.44	1.39	1.35
1	S2	1337	4AC	C4-N4	-3.38	1.34	1.39
40	LB	245	HIC	CD2-CG	3.35	1.41	1.36
3	L5	3637	PSU	C4-N3	-3.34	1.32	1.38
83	At	8	4SU	C4-N3	-3.31	1.34	1.37
3	L5	3758	PSU	C4-N3	-3.31	1.32	1.38
3	L5	4636	PSU	C4-N3	-3.30	1.32	1.38
1	S2	1081	PSU	C4-N3	-3.28	1.32	1.38
3	L5	1582	PSU	C4-N3	-3.27	1.32	1.38
3	L5	3764	PSU	C4-N3	-3.27	1.32	1.38
3	L5	4673	PSU	C4-N3	-3.27	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	866	PSU	C6-C5	3.26	1.39	1.35
3	L5	4442	PSU	C4-N3	-3.25	1.32	1.38
3	L5	1536	PSU	C4-N3	-3.24	1.32	1.38
84	Pt	8	4SU	C4-N3	-3.24	1.34	1.37
1	S2	686	PSU	C6-C5	3.23	1.39	1.35
3	L5	5010	PSU	C6-C5	3.23	1.39	1.35
3	L5	4521	PSU	C4-N3	-3.22	1.32	1.38
1	S2	609	PSU	C6-C5	3.22	1.39	1.35
1	S2	1692	PSU	C4-N3	-3.20	1.32	1.38
3	L5	3844	PSU	C6-C5	3.20	1.39	1.35
3	L5	3639	PSU	C4-N3	-3.20	1.32	1.38
84	Pt	56	PSU	C6-C5	3.19	1.39	1.35
1	S2	109	PSU	C4-N3	-3.18	1.32	1.38
3	L5	2843	PSU	C4-N3	-3.18	1.32	1.38
3	L5	1779	PSU	C6-C5	3.18	1.39	1.35
3	L5	1677	PSU	O4'-C1'	-3.17	1.39	1.43
3	L5	3818	UY1	C4-N3	-3.17	1.33	1.38
3	L5	4457	PSU	C4-N3	-3.15	1.33	1.38
3	L5	3768	PSU	C4-N3	-3.15	1.33	1.38
1	S2	801	PSU	C6-C5	3.13	1.39	1.35
3	L5	4576	PSU	C6-C5	3.12	1.39	1.35
1	S2	573	PSU	C6-C5	3.12	1.39	1.35
1	S2	1243	PSU	C6-C5	3.12	1.39	1.35
1	S2	1239	PSU	C6-C5	3.12	1.39	1.35
3	L5	3920	PSU	C6-C5	3.12	1.39	1.35
1	S2	1004	PSU	C4-N3	-3.11	1.33	1.38
3	L5	1683	PSU	C4-N3	-3.11	1.33	1.38
3	L5	4293	PSU	C6-C5	3.10	1.38	1.35
3	L5	3715	PSU	C6-C5	3.10	1.38	1.35
3	L5	4361	PSU	C6-C5	3.10	1.38	1.35
3	L5	1792	PSU	C4-N3	-3.09	1.33	1.38
3	L5	4628	PSU	C6-C5	3.09	1.38	1.35
3	L5	3920	PSU	C4-N3	-3.09	1.33	1.38
1	S2	822	PSU	C6-C5	3.08	1.38	1.35
83	At	46	7MG	C4-N9	-3.08	1.34	1.37
3	L5	1860	PSU	C4-N3	-3.07	1.33	1.38
3	L5	1316	OMG	C6-N1	-3.06	1.33	1.37
3	L5	3853	PSU	C4-N3	-3.06	1.33	1.38
1	S2	966	PSU	C6-C5	3.06	1.38	1.35
1	S2	1232	PSU	C6-C5	3.06	1.38	1.35
83	At	32	PSU	C6-C5	3.05	1.38	1.35
3	L5	3899	OMG	C6-N1	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4569	PSU	C6-C5	3.04	1.38	1.35
1	S2	815	PSU	C6-C5	3.04	1.38	1.35
1	S2	681	PSU	C4-N3	-3.03	1.33	1.38
3	L5	3884	PSU	C6-C5	3.03	1.38	1.35
1	S2	34	PSU	C6-C5	3.03	1.38	1.35
1	S2	649	PSU	C6-C5	3.03	1.38	1.35
3	L5	4423	PSU	C6-C5	3.03	1.38	1.35
1	S2	814	PSU	C6-C5	3.03	1.38	1.35
3	L5	4296	PSU	C4-N3	-3.02	1.33	1.38
1	S2	1238	PSU	C6-C5	3.02	1.38	1.35
1	S2	1177	PSU	C6-C5	3.01	1.38	1.35
3	L5	1792	PSU	C6-C5	3.01	1.38	1.35
3	L5	1744	PSU	C6-C5	3.01	1.38	1.35
3	L5	3762	PSU	C6-C5	3.01	1.38	1.35
2	L8	55	PSU	C6-C5	3.01	1.38	1.35
3	L5	1781	PSU	C6-C5	3.01	1.38	1.35
3	L5	4637	OMG	C6-N1	-3.00	1.33	1.37
3	L5	4403	PSU	C4-N3	-3.00	1.33	1.38
3	L5	3695	PSU	C4-N3	-3.00	1.33	1.38
3	L5	2508	PSU	C4-N3	-3.00	1.33	1.38
3	L5	3844	PSU	C4-N3	-2.99	1.33	1.38
3	L5	1782	PSU	C6-C5	2.99	1.38	1.35
3	L5	3884	PSU	C4-N3	-2.99	1.33	1.38
3	L5	4579	PSU	C6-C5	2.99	1.38	1.35
3	L5	4299	PSU	C4-N3	-2.99	1.33	1.38
1	S2	218	PSU	C6-C5	2.98	1.38	1.35
3	L5	3770	PSU	C6-C5	2.98	1.38	1.35
3	L5	1625	OMG	C6-N1	-2.98	1.33	1.37
1	S2	918	PSU	C6-C5	2.98	1.38	1.35
1	S2	1367	PSU	C6-C5	2.98	1.38	1.35
3	L5	4531	PSU	C4-N3	-2.98	1.33	1.38
2	L8	55	PSU	C4-N3	-2.97	1.33	1.38
1	S2	651	PSU	C6-C5	2.97	1.38	1.35
3	L5	3851	PSU	C4-N3	-2.97	1.33	1.38
3	L5	4532	PSU	C4-N3	-2.97	1.33	1.38
3	L5	1862	PSU	C4-N3	-2.97	1.33	1.38
1	S2	296	PSU	C6-C5	2.97	1.38	1.35
1	S2	1625	PSU	C6-C5	2.96	1.38	1.35
3	L5	3729	PSU	C6-C5	2.96	1.38	1.35
3	L5	4493	PSU	C4-N3	-2.96	1.33	1.38
3	L5	4579	PSU	C4-N3	-2.96	1.33	1.38
3	L5	4361	PSU	C4-N3	-2.96	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2424	OMG	C6-N1	-2.95	1.33	1.37
3	L5	2837	OMU	C4-N3	-2.95	1.33	1.38
1	S2	119	PSU	C6-C5	2.95	1.38	1.35
3	L5	4293	PSU	C4-N3	-2.95	1.33	1.38
1	S2	572	PSU	C4-N3	-2.94	1.33	1.38
3	L5	3639	PSU	C6-C5	2.94	1.38	1.35
3	L5	4569	PSU	C4-N3	-2.94	1.33	1.38
3	L5	1744	PSU	C4-N3	-2.94	1.33	1.38
3	L5	4689	PSU	C6-C5	2.94	1.38	1.35
3	L5	4623	OMG	C6-N1	-2.93	1.33	1.37
3	L5	1677	PSU	C4-N3	-2.93	1.33	1.38
3	L5	1683	PSU	C6-C5	2.93	1.38	1.35
3	L5	4370	OMG	C6-N1	-2.93	1.33	1.37
3	L5	2839	PSU	C4-N3	-2.92	1.33	1.38
3	L5	4552	PSU	C4-N3	-2.92	1.33	1.38
3	L5	4620	OMU	C4-N3	-2.92	1.33	1.38
1	S2	1244	PSU	C6-C5	2.92	1.38	1.35
1	S2	36	PSU	C6-C5	2.92	1.38	1.35
1	S2	1056	PSU	C6-C5	2.92	1.38	1.35
3	L5	1862	PSU	C6-C5	2.92	1.38	1.35
3	L5	4353	PSU	C6-C5	2.92	1.38	1.35
3	L5	3734	PSU	C6-C5	2.92	1.38	1.35
2	L8	69	PSU	C4-N3	-2.92	1.33	1.38
3	L5	4447	5MC	C6-C5	2.91	1.39	1.34
3	L5	4493	PSU	C6-C5	2.91	1.38	1.35
3	L5	4471	PSU	C4-N3	-2.90	1.33	1.38
3	L5	1322	1MA	C6-N6	2.90	1.34	1.27
3	L5	3768	PSU	C6-C5	2.90	1.38	1.35
1	S2	814	PSU	C4-N3	-2.90	1.33	1.38
3	L5	2632	PSU	C4-N3	-2.90	1.33	1.38
3	L5	4196	OMG	C6-N1	-2.90	1.33	1.37
3	L5	4628	PSU	C4-N3	-2.90	1.33	1.38
3	L5	4494	OMG	C6-N1	-2.90	1.33	1.37
1	S2	1326	UY1	C6-C5	2.90	1.38	1.35
3	L5	1782	PSU	C4-N3	-2.90	1.33	1.38
1	S2	406	PSU	C6-C5	2.90	1.38	1.35
3	L5	4521	PSU	C6-C5	2.90	1.38	1.35
3	L5	1522	OMG	C6-N1	-2.90	1.33	1.37
3	L5	4972	PSU	C6-C5	2.89	1.38	1.35
1	S2	1347	PSU	C6-C5	2.89	1.38	1.35
3	L5	1781	PSU	C4-N3	-2.89	1.33	1.38
3	L5	4299	PSU	C6-C5	2.88	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	At	39	PSU	C6-C5	2.88	1.38	1.35
3	L5	4353	PSU	C4-N3	-2.88	1.33	1.38
1	S2	93	PSU	C6-C5	2.88	1.38	1.35
3	L5	3695	PSU	C6-C5	2.88	1.38	1.35
1	S2	572	PSU	C6-C5	2.87	1.38	1.35
1	S2	1177	PSU	C4-N3	-2.87	1.33	1.38
1	S2	1248	B8N	C6-C5	2.87	1.39	1.34
3	L5	4689	PSU	C4-N3	-2.87	1.33	1.38
3	L5	5001	PSU	C6-C5	2.86	1.38	1.35
3	L5	1536	PSU	C6-C5	2.86	1.38	1.35
1	S2	1804	OMU	C4-N3	-2.85	1.33	1.38
3	L5	5001	PSU	C4-N3	-2.85	1.33	1.38
1	S2	918	PSU	C4-N3	-2.85	1.33	1.38
1	S2	1347	PSU	C4-N3	-2.84	1.33	1.38
1	S2	1174	PSU	C6-C5	2.84	1.38	1.35
1	S2	1326	UY1	C4-N3	-2.84	1.33	1.38
3	L5	4618	OMG	C6-N1	-2.84	1.33	1.37
3	L5	4312	PSU	C6-C5	2.84	1.38	1.35
83	At	46	7MG	C5-C4	2.83	1.47	1.38
3	L5	4576	PSU	C4-N3	-2.83	1.33	1.38
3	L5	4296	PSU	C6-C5	2.83	1.38	1.35
1	S2	1136	PSU	C6-C5	2.83	1.38	1.35
1	S2	651	PSU	C4-N3	-2.83	1.33	1.38
3	L5	4423	PSU	C4-N3	-2.83	1.33	1.38
2	L8	69	PSU	C6-C5	2.83	1.38	1.35
3	L5	4420	PSU	C6-C5	2.82	1.38	1.35
3	L5	4972	PSU	C4-N3	-2.82	1.33	1.38
3	L5	4431	PSU	C4-N3	-2.82	1.33	1.38
1	S2	649	PSU	C4-N3	-2.82	1.33	1.38
3	L5	3637	PSU	C6-C5	2.82	1.38	1.35
3	L5	2508	PSU	C6-C5	2.82	1.38	1.35
1	S2	1643	PSU	C6-C5	2.81	1.38	1.35
3	L5	1860	PSU	C6-C5	2.80	1.38	1.35
3	L5	4500	PSU	C6-C5	2.80	1.38	1.35
1	S2	815	PSU	C4-N3	-2.79	1.33	1.38
1	S2	172	OMU	C4-N3	-2.79	1.33	1.38
3	L5	4312	PSU	C4-N3	-2.79	1.33	1.38
3	L5	3744	OMG	C6-N1	-2.78	1.33	1.37
3	L5	4552	PSU	C6-C5	2.78	1.38	1.35
3	L5	3715	PSU	C4-N3	-2.78	1.33	1.38
3	L5	1779	PSU	C4-N3	-2.78	1.33	1.38
1	S2	105	PSU	C4-N3	-2.78	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1445	PSU	C6-C5	2.78	1.38	1.35
1	S2	573	PSU	C4-N3	-2.77	1.33	1.38
83	At	39	PSU	C4-N3	-2.77	1.33	1.38
3	L5	2415	OMU	C4-N3	-2.76	1.33	1.38
3	L5	2632	PSU	C6-C5	2.76	1.38	1.35
2	L8	14	OMU	C4-N3	-2.76	1.33	1.38
1	S2	1232	PSU	C4-N3	-2.75	1.33	1.38
1	S2	1239	PSU	C4-N3	-2.75	1.33	1.38
1	S2	966	PSU	C4-N3	-2.75	1.33	1.38
1	S2	406	PSU	C4-N3	-2.75	1.33	1.38
3	L5	3734	PSU	C4-N3	-2.75	1.33	1.38
3	L5	3925	OMU	C4-N3	-2.75	1.33	1.38
1	S2	296	PSU	C4-N3	-2.75	1.33	1.38
1	S2	34	PSU	C4-N3	-2.74	1.33	1.38
3	L5	2364	OMG	C6-N1	-2.74	1.33	1.37
3	L5	4392	OMG	C6-N1	-2.73	1.33	1.37
1	S2	686	PSU	C4-N3	-2.73	1.33	1.38
1	S2	1238	PSU	C4-N3	-2.73	1.33	1.38
3	L5	4306	OMU	C4-N3	-2.73	1.33	1.38
1	S2	1056	PSU	C4-N3	-2.73	1.33	1.38
1	S2	1244	PSU	C4-N3	-2.72	1.33	1.38
3	L5	5010	PSU	C4-N3	-2.72	1.33	1.38
1	S2	681	PSU	C6-C5	2.72	1.38	1.35
3	L5	4498	OMU	C4-N3	-2.71	1.33	1.38
3	L5	3627	OMG	C6-N1	-2.71	1.33	1.37
1	S2	1174	PSU	C4-N3	-2.71	1.33	1.38
3	L5	3851	PSU	C6-C5	2.70	1.38	1.35
3	L5	3792	OMG	C6-N1	-2.70	1.33	1.37
1	S2	1243	PSU	C4-N3	-2.70	1.33	1.38
1	S2	1136	PSU	C4-N3	-2.70	1.33	1.38
1	S2	822	PSU	C4-N3	-2.69	1.33	1.38
3	L5	4471	PSU	C6-C5	2.69	1.38	1.35
3	L5	4227	OMU	C4-N3	-2.69	1.33	1.38
3	L5	4457	PSU	C6-C5	2.69	1.38	1.35
3	L5	3770	PSU	C4-N3	-2.69	1.33	1.38
1	S2	116	OMU	C4-N3	-2.69	1.33	1.38
3	L5	3782	5MC	C6-C5	2.68	1.39	1.34
3	L5	4500	PSU	C4-N3	-2.68	1.33	1.38
1	S2	36	PSU	C4-N3	-2.68	1.33	1.38
1	S2	105	PSU	C6-C5	2.68	1.38	1.35
3	L5	2843	PSU	C6-C5	2.68	1.38	1.35
1	S2	121	OMU	C4-N3	-2.68	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	801	PSU	C4-N3	-2.68	1.33	1.38
3	L5	3729	PSU	C4-N3	-2.68	1.33	1.38
3	L5	1582	PSU	C6-C5	2.68	1.38	1.35
1	S2	863	PSU	C4-N3	-2.67	1.33	1.38
84	Pt	56	PSU	C4-N3	-2.67	1.33	1.38
1	S2	354	OMU	C4-N3	-2.67	1.33	1.38
3	L5	1677	PSU	C6-C5	2.67	1.38	1.35
2	L8	14	OMU	C2-N3	-2.67	1.33	1.38
3	L5	4403	PSU	C6-C5	2.66	1.38	1.35
1	S2	1367	PSU	C4-N3	-2.66	1.33	1.38
1	S2	93	PSU	C4-N3	-2.66	1.33	1.38
1	S2	1643	PSU	C4-N3	-2.65	1.33	1.38
1	S2	1625	PSU	C4-N3	-2.65	1.33	1.38
83	At	32	PSU	C4-N3	-2.65	1.33	1.38
1	S2	866	PSU	C4-N3	-2.64	1.33	1.38
1	S2	1842	4AC	C4-N4	-2.64	1.35	1.39
3	L5	3762	PSU	C4-N3	-2.64	1.33	1.38
84	Pt	8	4SU	C5-C4	-2.64	1.39	1.42
3	L5	3758	PSU	C6-C5	2.64	1.38	1.35
1	S2	109	PSU	C6-C5	2.62	1.38	1.35
83	At	8	4SU	C5-C4	-2.62	1.39	1.42
1	S2	436	OMG	C6-N1	-2.61	1.34	1.37
1	S2	218	PSU	C4-N3	-2.61	1.34	1.38
1	S2	609	PSU	C4-N3	-2.61	1.34	1.38
1	S2	1328	OMG	C6-N1	-2.61	1.34	1.37
1	S2	119	PSU	C4-N3	-2.60	1.34	1.38
3	L5	4499	OMG	C6-N1	-2.60	1.34	1.37
1	S2	1445	PSU	C4-N3	-2.59	1.34	1.38
1	S2	428	OMU	C4-N3	-2.59	1.33	1.38
3	L5	4431	PSU	C6-C5	2.58	1.38	1.35
3	L5	1683	PSU	C2-N3	-2.58	1.33	1.37
1	S2	644	OMG	C6-N1	-2.57	1.34	1.37
3	L5	4306	OMU	C2-N3	-2.57	1.33	1.38
3	L5	4620	OMU	C2-N3	-2.57	1.33	1.38
1	S2	1490	OMG	C6-N1	-2.57	1.34	1.37
1	S2	683	OMG	C6-N1	-2.56	1.34	1.37
3	L5	4636	PSU	C6-C5	2.56	1.38	1.35
1	S2	867	OMG	C6-N1	-2.55	1.34	1.37
3	L5	4299	PSU	C2-N3	-2.55	1.33	1.37
1	S2	509	OMG	C6-N1	-2.55	1.34	1.37
83	At	46	7MG	C6-N1	-2.55	1.34	1.38
1	S2	627	OMU	C4-N3	-2.54	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1692	PSU	C2'-C1'	-2.54	1.50	1.53
1	S2	1442	OMU	C4-N3	-2.53	1.34	1.38
1	S2	1004	PSU	C6-C5	2.53	1.38	1.35
1	S2	1447	OMG	C6-N1	-2.52	1.34	1.37
3	L5	4420	PSU	C4-N3	-2.52	1.34	1.38
84	Pt	21	H2U	C2-N3	-2.52	1.33	1.38
2	L8	75	OMG	C6-N1	-2.51	1.34	1.37
1	S2	109	PSU	C2'-C1'	-2.51	1.50	1.53
1	S2	1639	G7M	C6-N1	-2.50	1.34	1.37
1	S2	1804	OMU	C2-N3	-2.50	1.33	1.38
3	L5	2876	OMG	C6-N1	-2.50	1.34	1.37
3	L5	3758	PSU	C2'-C1'	-2.50	1.50	1.53
3	L5	4673	PSU	C2-N3	-2.50	1.33	1.37
3	L5	3764	PSU	C2-N3	-2.49	1.33	1.37
3	L5	4228	OMG	C6-N1	-2.49	1.34	1.37
83	At	16	H2U	C2-N3	-2.49	1.33	1.38
3	L5	3818	UY1	C6-C5	2.48	1.38	1.35
3	L5	2837	OMU	C2-N3	-2.48	1.33	1.38
1	S2	1851	MA6	C5-C4	2.48	1.47	1.40
1	S2	1248	B8N	O4'-C1'	-2.48	1.40	1.43
1	S2	1692	PSU	C6-C5	2.47	1.38	1.35
1	S2	172	OMU	C2-N3	-2.47	1.33	1.38
1	S2	159	A2M	C5-C4	2.46	1.47	1.40
1	S2	590	A2M	C5-C4	2.46	1.47	1.40
3	L5	3723	A2M	C5-C4	2.46	1.47	1.40
3	L5	1536	PSU	C2-N3	-2.46	1.33	1.37
3	L5	3925	OMU	C2-N3	-2.44	1.33	1.38
3	L5	4673	PSU	C2'-C1'	-2.44	1.50	1.53
3	L5	2843	PSU	C2-N3	-2.44	1.33	1.37
1	S2	1337	4AC	C7-N4	-2.44	1.32	1.37
1	S2	1850	MA6	C5-C4	2.43	1.47	1.40
1	S2	1288	OMU	C4-N3	-2.43	1.34	1.38
3	L5	4498	OMU	C2-N3	-2.42	1.33	1.38
83	At	20	H2U	C2-N3	-2.42	1.33	1.38
1	S2	512	A2M	C5-C4	2.41	1.47	1.40
1	S2	601	OMG	C6-N1	-2.41	1.34	1.37
3	L5	4457	PSU	C2-N3	-2.41	1.33	1.37
3	L5	3637	PSU	C2-N3	-2.41	1.33	1.37
1	S2	1081	PSU	C2-N3	-2.40	1.33	1.37
3	L5	4636	PSU	C2-N3	-2.40	1.33	1.37
1	S2	576	A2M	C5-C4	2.39	1.47	1.40
3	L5	4442	PSU	C2-N3	-2.39	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1832	6MZ	C5-C4	2.39	1.47	1.40
3	L5	2415	OMU	C5-C4	-2.39	1.38	1.43
1	S2	172	OMU	C5-C4	-2.38	1.38	1.43
3	L5	2415	OMU	C2-N3	-2.38	1.33	1.38
3	L5	4532	PSU	C2-N3	-2.38	1.33	1.37
1	S2	1383	A2M	C5-C4	2.38	1.47	1.40
3	L5	2839	PSU	C6-C5	2.38	1.38	1.35
3	L5	3944	OMG	C6-N1	-2.38	1.34	1.37
1	S2	468	A2M	C5-C4	2.37	1.47	1.40
1	S2	354	OMU	C2-N3	-2.37	1.33	1.38
3	L5	3782	5MC	C6-N1	-2.37	1.34	1.38
3	L5	4227	OMU	C2-N3	-2.37	1.33	1.38
3	L5	3724	A2M	C5-C4	2.37	1.47	1.40
3	L5	1582	PSU	C2-N3	-2.37	1.33	1.37
84	Pt	47	G7M	C6-N1	2.36	1.41	1.37
83	At	16	H2U	C4-N3	-2.36	1.33	1.37
3	L5	3867	A2M	C5-C4	2.35	1.47	1.40
3	L5	3818	UY1	C2-N3	-2.35	1.33	1.37
3	L5	4220	6MZ	C5-C4	2.34	1.47	1.40
3	L5	4571	A2M	C5-C4	2.34	1.47	1.40
3	L5	4447	5MC	C6-N1	-2.34	1.34	1.38
1	S2	484	A2M	C5-C4	2.34	1.47	1.40
3	L5	4590	A2M	C5-C4	2.34	1.47	1.40
3	L5	4521	PSU	C2-N3	-2.33	1.33	1.37
1	S2	1692	PSU	C2-N3	-2.33	1.33	1.37
3	L5	4403	PSU	C2-N3	-2.33	1.33	1.37
3	L5	4673	PSU	C6-C5	2.32	1.38	1.35
81	5A	50	5CT	CB-CA	-2.32	1.50	1.53
3	L5	3758	PSU	C2-N3	-2.32	1.33	1.37
3	L5	3639	PSU	C2-N3	-2.32	1.33	1.37
1	S2	27	A2M	C5-C4	2.31	1.47	1.40
3	L5	3853	PSU	C6-C5	2.31	1.38	1.35
3	L5	3768	PSU	C2-N3	-2.31	1.33	1.37
3	L5	400	A2M	C5-C4	2.31	1.47	1.40
3	L5	1524	A2M	C5-C4	2.30	1.47	1.40
1	S2	99	A2M	C5-C4	2.30	1.47	1.40
1	S2	428	OMU	C2-N3	-2.30	1.33	1.38
1	S2	681	PSU	C2-N3	-2.30	1.33	1.37
3	L5	3844	PSU	C2-N3	-2.30	1.33	1.37
3	L5	4296	PSU	C2-N3	-2.30	1.33	1.37
3	L5	3718	A2M	C5-C4	2.29	1.47	1.40
2	L8	14	OMU	C5-C4	-2.29	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2401	A2M	C5-C4	2.28	1.47	1.40
3	L5	4442	PSU	C6-C5	2.28	1.38	1.35
1	S2	1678	A2M	C5-C4	2.28	1.47	1.40
1	S2	121	OMU	C2-N3	-2.28	1.33	1.38
3	L5	2815	A2M	C5-C4	2.27	1.46	1.40
1	S2	1081	PSU	C6-C5	2.27	1.38	1.35
1	S2	1004	PSU	C2-N3	-2.27	1.33	1.37
3	L5	4227	OMU	C5-C4	-2.26	1.38	1.43
3	L5	3764	PSU	C2'-C1'	-2.26	1.50	1.53
3	L5	3695	PSU	C2-N3	-2.26	1.33	1.37
3	L5	1326	A2M	C5-C4	2.26	1.46	1.40
3	L5	3853	PSU	C2-N1	-2.25	1.33	1.36
3	L5	4620	OMU	C5-C4	-2.25	1.38	1.43
1	S2	354	OMU	C5-C4	-2.24	1.38	1.43
3	L5	3760	A2M	C5-C4	2.24	1.46	1.40
1	S2	668	A2M	C5-C4	2.24	1.46	1.40
1	S2	1031	A2M	C5-C4	2.24	1.46	1.40
3	L5	3830	A2M	C5-C4	2.24	1.46	1.40
3	L5	1340	OMC	C6-N1	-2.23	1.32	1.38
3	L5	4552	PSU	C2-N1	-2.23	1.33	1.36
1	S2	1442	OMU	C2-N3	-2.23	1.34	1.38
3	L5	4353	PSU	C2-N3	-2.23	1.33	1.37
3	L5	1860	PSU	C2-N3	-2.22	1.33	1.37
3	L5	4403	PSU	C2-N1	-2.22	1.33	1.36
1	S2	116	OMU	C2-N3	-2.22	1.34	1.38
1	S2	166	A2M	C5-C4	2.22	1.46	1.40
3	L5	2363	A2M	C5-C4	2.22	1.46	1.40
3	L5	3884	PSU	C2-N3	-2.22	1.33	1.37
3	L5	4306	OMU	C5-C4	-2.21	1.38	1.43
3	L5	3851	PSU	C2-N3	-2.21	1.33	1.37
83	At	8	4SU	C2-N3	-2.20	1.34	1.38
3	L5	1871	A2M	C5-C4	2.20	1.46	1.40
3	L5	4493	PSU	C2-N3	-2.20	1.33	1.37
1	S2	627	OMU	C2-N3	-2.19	1.34	1.38
3	L5	4293	PSU	C2-N3	-2.19	1.33	1.37
3	L5	1683	PSU	C2-N1	-2.18	1.33	1.36
3	L5	1792	PSU	C2-N3	-2.18	1.33	1.37
3	L5	398	A2M	C5-C4	2.18	1.46	1.40
3	L5	1534	A2M	C5-C4	2.17	1.46	1.40
84	Pt	21	H2U	C4-N3	-2.17	1.33	1.37
3	L5	3853	PSU	C2-N3	-2.17	1.33	1.37
40	LB	245	HIC	CZ-NE2	-2.17	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3825	A2M	C5-C4	2.16	1.46	1.40
3	L5	2508	PSU	C2-N3	-2.16	1.33	1.37
3	L5	4471	PSU	C2-N3	-2.15	1.33	1.37
3	L5	2787	A2M	C5-C4	2.15	1.46	1.40
3	L5	3884	PSU	C2-N1	-2.14	1.33	1.36
2	L8	55	PSU	C2-N3	-2.13	1.33	1.37
3	L5	3764	PSU	C6-C5	2.13	1.37	1.35
1	S2	109	PSU	C2-N3	-2.13	1.33	1.37
1	S2	1288	OMU	C2-N3	-2.12	1.34	1.38
84	Pt	8	4SU	C2-N3	-2.12	1.34	1.38
3	L5	4442	PSU	C2-N1	-2.12	1.33	1.36
3	L5	1781	PSU	C2-N3	-2.12	1.33	1.37
2	L8	69	PSU	O4'-C1'	-2.12	1.40	1.43
3	L5	2632	PSU	C2-N3	-2.12	1.33	1.37
3	L5	4636	PSU	C2'-C1'	-2.11	1.51	1.53
1	S2	1174	PSU	C2-N1	-2.11	1.33	1.36
3	L5	1744	PSU	C2-N3	-2.11	1.33	1.37
1	S2	1081	PSU	C2'-C1'	-2.11	1.51	1.53
1	S2	116	OMU	C5-C4	-2.11	1.39	1.43
3	L5	4361	PSU	C2-N3	-2.11	1.33	1.37
3	L5	4689	PSU	C2-N1	-2.11	1.33	1.36
83	At	20	H2U	C4-N3	-2.11	1.34	1.37
1	S2	121	OMU	C5-C4	-2.11	1.39	1.43
1	S2	172	OMU	C6-N1	-2.10	1.32	1.38
1	S2	428	OMU	C5-C4	-2.10	1.39	1.43
3	L5	4569	PSU	C2-N3	-2.10	1.33	1.37
3	L5	4420	PSU	O4'-C1'	-2.09	1.40	1.43
3	L5	1862	PSU	C2-N1	-2.09	1.33	1.36
3	L5	4498	OMU	C5-C4	-2.08	1.39	1.43
3	L5	4523	A2M	C5-C4	2.07	1.46	1.40
3	L5	4689	PSU	C2-N3	-2.07	1.34	1.37
3	L5	1860	PSU	C2-N1	-2.07	1.33	1.36
1	S2	1174	PSU	C2-N3	-2.06	1.34	1.37
3	L5	4312	PSU	C2-N1	-2.06	1.33	1.36
3	L5	4312	PSU	C2-N3	-2.05	1.34	1.37
1	S2	1177	PSU	C2-N3	-2.05	1.34	1.37
3	L5	5001	PSU	C2-N3	-2.05	1.34	1.37
3	L5	4552	PSU	C2-N3	-2.05	1.34	1.37
3	L5	4579	PSU	C2-N3	-2.05	1.34	1.37
1	S2	1347	PSU	C2-N3	-2.04	1.34	1.37
3	L5	1677	PSU	C2-N3	-2.04	1.34	1.37
1	S2	109	PSU	C2-N1	-2.04	1.34	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4972	PSU	C2-N3	-2.03	1.34	1.37
3	L5	1782	PSU	C2-N3	-2.03	1.34	1.37
3	L5	3639	PSU	C2-N1	-2.03	1.34	1.36
3	L5	3818	UY1	C2-N1	-2.03	1.34	1.36
3	L5	2787	A2M	O4'-C1'	2.03	1.43	1.41
3	L5	4423	PSU	C2-N3	-2.02	1.34	1.37
3	L5	3715	PSU	C2-N3	-2.02	1.34	1.37
3	L5	3920	PSU	C2-N3	-2.02	1.34	1.37
3	L5	3851	PSU	C2-N1	-2.01	1.34	1.36
3	L5	3768	PSU	C2'-C1'	-2.01	1.51	1.53
3	L5	2632	PSU	C2-N1	-2.01	1.34	1.36
3	L5	3718	A2M	O4'-C1'	2.00	1.43	1.41
1	S2	814	PSU	C2-N3	-2.00	1.34	1.37
3	L5	4576	PSU	C2-N3	-2.00	1.34	1.37

All (698) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	At	46	7MG	N9-C4-N3	9.01	138.95	125.47
29	SV	1	AME	CA-N-CT1	-7.69	108.96	123.15
64	Lr	2	SAC	CA-N-C1A	-7.33	109.64	123.15
6	SA	2	SAC	OAC-C1A-C2A	-7.10	108.86	122.06
29	SV	1	AME	OT-CT1-N	-7.05	108.98	121.95
1	S2	1832	6MZ	C2-N1-C6	7.04	122.63	116.59
83	At	8	4SU	C4-N3-C2	-6.95	120.59	127.34
3	L5	4636	PSU	N1-C2-N3	6.82	122.86	115.13
1	S2	109	PSU	N1-C2-N3	6.80	122.83	115.13
29	SV	1	AME	OT-CT1-CT2	-6.80	109.44	122.06
3	L5	4531	PSU	N1-C2-N3	6.79	122.82	115.13
84	Pt	8	4SU	C4-N3-C2	-6.76	120.77	127.34
64	Lr	2	SAC	OAC-C1A-C2A	-6.75	109.53	122.06
64	Lr	2	SAC	OAC-C1A-N	-6.72	109.59	121.95
6	SA	2	SAC	CA-N-C1A	-6.70	110.79	123.15
3	L5	4442	PSU	N1-C2-N3	6.61	122.62	115.13
1	S2	1692	PSU	N1-C2-N3	6.58	122.59	115.13
3	L5	1862	PSU	N1-C2-N3	6.57	122.58	115.13
3	L5	4220	6MZ	C2-N1-C6	6.57	122.22	116.59
3	L5	3768	PSU	N1-C2-N3	6.55	122.55	115.13
6	SA	2	SAC	OAC-C1A-N	-6.50	110.00	121.95
3	L5	4673	PSU	N1-C2-N3	6.44	122.43	115.13
3	L5	1582	PSU	N1-C2-N3	6.43	122.42	115.13
3	L5	3758	PSU	N1-C2-N3	6.42	122.41	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	3764	PSU	N1-C2-N3	6.41	122.40	115.13
1	S2	1004	PSU	N1-C2-N3	6.39	122.37	115.13
1	S2	572	PSU	N1-C2-N3	6.36	122.34	115.13
1	S2	918	PSU	N1-C2-N3	6.36	122.33	115.13
3	L5	3920	PSU	N1-C2-N3	6.34	122.31	115.13
3	L5	3884	PSU	N1-C2-N3	6.34	122.31	115.13
1	S2	1232	PSU	N1-C2-N3	6.34	122.31	115.13
3	L5	3639	PSU	N1-C2-N3	6.32	122.28	115.13
3	L5	2508	PSU	N1-C2-N3	6.30	122.27	115.13
3	L5	4579	PSU	N1-C2-N3	6.28	122.24	115.13
83	At	8	4SU	C5-C4-N3	6.27	120.50	114.69
1	S2	681	PSU	N1-C2-N3	6.26	122.22	115.13
3	L5	4403	PSU	N1-C2-N3	6.24	122.20	115.13
3	L5	4361	PSU	N1-C2-N3	6.24	122.20	115.13
3	L5	1677	PSU	N1-C2-N3	6.24	122.20	115.13
3	L5	4423	PSU	N1-C2-N3	6.23	122.19	115.13
3	L5	4299	PSU	N1-C2-N3	6.23	122.19	115.13
3	L5	5001	PSU	N1-C2-N3	6.22	122.17	115.13
3	L5	4552	PSU	N1-C2-N3	6.20	122.15	115.13
3	L5	4628	PSU	N1-C2-N3	6.19	122.14	115.13
3	L5	4532	PSU	N1-C2-N3	6.19	122.14	115.13
1	S2	651	PSU	N1-C2-N3	6.18	122.14	115.13
3	L5	3818	UY1	N1-C2-N3	6.18	122.13	115.13
1	S2	966	PSU	N1-C2-N3	6.17	122.12	115.13
3	L5	4500	PSU	N1-C2-N3	6.17	122.12	115.13
3	L5	3853	PSU	N1-C2-N3	6.16	122.11	115.13
3	L5	3762	PSU	N1-C2-N3	6.16	122.11	115.13
3	L5	4569	PSU	N1-C2-N3	6.16	122.11	115.13
1	S2	34	PSU	N1-C2-N3	6.15	122.10	115.13
3	L5	3637	PSU	N1-C2-N3	6.14	122.09	115.13
3	L5	4296	PSU	N1-C2-N3	6.14	122.09	115.13
1	S2	1081	PSU	N1-C2-N3	6.13	122.08	115.13
3	L5	1683	PSU	N1-C2-N3	6.13	122.08	115.13
3	L5	4312	PSU	N1-C2-N3	6.13	122.08	115.13
3	L5	4457	PSU	N1-C2-N3	6.12	122.06	115.13
3	L5	1782	PSU	N1-C2-N3	6.11	122.06	115.13
3	L5	1744	PSU	N1-C2-N3	6.11	122.05	115.13
3	L5	1860	PSU	N1-C2-N3	6.10	122.04	115.13
3	L5	4353	PSU	N1-C2-N3	6.10	122.04	115.13
2	L8	55	PSU	N1-C2-N3	6.09	122.03	115.13
2	L8	69	PSU	N1-C2-N3	6.09	122.03	115.13
1	S2	1177	PSU	N1-C2-N3	6.09	122.03	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	801	PSU	N1-C2-N3	6.09	122.03	115.13
83	At	39	PSU	N1-C2-N3	6.08	122.02	115.13
3	L5	4521	PSU	N1-C2-N3	6.08	122.02	115.13
1	S2	815	PSU	N1-C2-N3	6.08	122.02	115.13
3	L5	1779	PSU	N1-C2-N3	6.08	122.02	115.13
3	L5	3695	PSU	N1-C2-N3	6.08	122.02	115.13
1	S2	1326	UY1	N1-C2-N3	6.08	122.01	115.13
3	L5	4431	PSU	N1-C2-N3	6.07	122.01	115.13
3	L5	5010	PSU	N1-C2-N3	6.06	122.00	115.13
1	S2	649	PSU	N1-C2-N3	6.05	121.99	115.13
3	L5	1781	PSU	N1-C2-N3	6.05	121.99	115.13
1	S2	1244	PSU	N1-C2-N3	6.05	121.98	115.13
3	L5	4689	PSU	N1-C2-N3	6.05	121.98	115.13
1	S2	822	PSU	N1-C2-N3	6.04	121.97	115.13
3	L5	3734	PSU	N1-C2-N3	6.03	121.96	115.13
1	S2	866	PSU	N1-C2-N3	6.01	121.94	115.13
1	S2	1056	PSU	N1-C2-N3	6.01	121.94	115.13
1	S2	609	PSU	N1-C2-N3	6.00	121.93	115.13
1	S2	1136	PSU	N1-C2-N3	6.00	121.93	115.13
3	L5	3851	PSU	N1-C2-N3	6.00	121.93	115.13
1	S2	1367	PSU	N1-C2-N3	5.99	121.92	115.13
3	L5	2843	PSU	N1-C2-N3	5.98	121.91	115.13
1	S2	1243	PSU	N1-C2-N3	5.96	121.88	115.13
3	L5	1792	PSU	N1-C2-N3	5.95	121.88	115.13
3	L5	4493	PSU	N1-C2-N3	5.95	121.87	115.13
1	S2	686	PSU	N1-C2-N3	5.94	121.86	115.13
3	L5	4293	PSU	N1-C2-N3	5.94	121.86	115.13
1	S2	1239	PSU	N1-C2-N3	5.93	121.85	115.13
3	L5	4576	PSU	N1-C2-N3	5.93	121.84	115.13
1	S2	296	PSU	N1-C2-N3	5.92	121.84	115.13
1	S2	1238	PSU	N1-C2-N3	5.92	121.83	115.13
84	Pt	56	PSU	N1-C2-N3	5.89	121.80	115.13
1	S2	93	PSU	N1-C2-N3	5.89	121.80	115.13
1	S2	105	PSU	N1-C2-N3	5.89	121.80	115.13
3	L5	3844	PSU	N1-C2-N3	5.88	121.79	115.13
3	L5	3715	PSU	N1-C2-N3	5.88	121.79	115.13
3	L5	2839	PSU	N1-C2-N3	5.87	121.78	115.13
1	S2	814	PSU	N1-C2-N3	5.87	121.78	115.13
1	S2	1174	PSU	N1-C2-N3	5.87	121.78	115.13
1	S2	573	PSU	N1-C2-N3	5.86	121.78	115.13
1	S2	863	PSU	N1-C2-N3	5.86	121.77	115.13
1	S2	1445	PSU	N1-C2-N3	5.86	121.77	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	406	PSU	N1-C2-N3	5.86	121.77	115.13
1	S2	1625	PSU	N1-C2-N3	5.86	121.76	115.13
84	Pt	8	4SU	C5-C4-N3	5.85	120.11	114.69
3	L5	4471	PSU	N1-C2-N3	5.85	121.75	115.13
83	At	32	PSU	N1-C2-N3	5.85	121.75	115.13
3	L5	4972	PSU	N1-C2-N3	5.83	121.74	115.13
3	L5	3770	PSU	N1-C2-N3	5.83	121.73	115.13
1	S2	36	PSU	N1-C2-N3	5.81	121.71	115.13
3	L5	3729	PSU	N1-C2-N3	5.80	121.70	115.13
1	S2	1643	PSU	N1-C2-N3	5.80	121.70	115.13
83	At	16	H2U	C4-N3-C2	-5.79	120.99	125.79
3	L5	1536	PSU	N1-C2-N3	5.75	121.64	115.13
1	S2	1347	PSU	N1-C2-N3	5.75	121.64	115.13
1	S2	218	PSU	N1-C2-N3	5.73	121.63	115.13
3	L5	2632	PSU	N1-C2-N3	5.71	121.60	115.13
3	L5	4530	UR3	C4-N3-C2	-5.68	119.21	124.56
83	At	46	7MG	C5-C4-N3	-5.48	117.69	128.13
83	At	46	7MG	N9-C8-N7	-5.47	95.56	103.38
3	L5	4420	PSU	N1-C2-N3	5.46	121.32	115.13
1	S2	1248	B8N	C4-N3-C2	-5.38	118.66	125.46
1	S2	119	PSU	N1-C2-N3	5.32	121.16	115.13
81	5A	50	5CT	C4-C3-C2	-4.80	103.37	113.47
3	L5	3925	OMU	C4-N3-C2	-4.75	120.32	126.58
3	L5	4498	OMU	C4-N3-C2	-4.71	120.36	126.58
3	L5	2837	OMU	C4-N3-C2	-4.68	120.41	126.58
3	L5	4636	PSU	C4-N3-C2	-4.67	119.62	126.34
1	S2	172	OMU	C4-N3-C2	-4.63	120.47	126.58
3	L5	4620	OMU	N3-C2-N1	4.63	121.04	114.89
1	S2	428	OMU	C4-N3-C2	-4.59	120.52	126.58
1	S2	354	OMU	C4-N3-C2	-4.58	120.54	126.58
2	L8	14	OMU	C4-N3-C2	-4.57	120.55	126.58
3	L5	3925	OMU	N3-C2-N1	4.55	120.94	114.89
1	S2	627	OMU	C4-N3-C2	-4.54	120.60	126.58
3	L5	2837	OMU	N3-C2-N1	4.52	120.89	114.89
3	L5	4620	OMU	C4-N3-C2	-4.51	120.63	126.58
3	L5	3768	PSU	C4-N3-C2	-4.50	119.86	126.34
3	L5	4227	OMU	C4-N3-C2	-4.48	120.67	126.58
1	S2	1081	PSU	C4-N3-C2	-4.48	119.88	126.34
3	L5	4531	PSU	C4-N3-C2	-4.47	119.90	126.34
3	L5	4442	PSU	C4-N3-C2	-4.46	119.91	126.34
1	S2	109	PSU	C4-N3-C2	-4.44	119.94	126.34
3	L5	3764	PSU	C4-N3-C2	-4.43	119.95	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	2843	PSU	C4-N3-C2	-4.43	119.96	126.34
1	S2	1442	OMU	C4-N3-C2	-4.41	120.76	126.58
1	S2	1692	PSU	C4-N3-C2	-4.39	120.01	126.34
1	S2	121	OMU	C4-N3-C2	-4.38	120.80	126.58
1	S2	1804	OMU	C4-N3-C2	-4.36	120.83	126.58
1	S2	1288	OMU	C4-N3-C2	-4.34	120.86	126.58
83	At	20	H2U	C4-N3-C2	-4.34	122.20	125.79
83	At	46	7MG	C2-N3-C4	4.33	120.02	112.30
84	Pt	21	H2U	C4-N3-C2	-4.33	122.20	125.79
3	L5	3920	PSU	C4-N3-C2	-4.32	120.11	126.34
3	L5	4306	OMU	N3-C2-N1	4.32	120.62	114.89
3	L5	4498	OMU	N3-C2-N1	4.32	120.62	114.89
3	L5	3818	UY1	C4-N3-C2	-4.30	120.14	126.34
3	L5	4673	PSU	C4-N3-C2	-4.30	120.14	126.34
3	L5	2415	OMU	C4-N3-C2	-4.27	120.94	126.58
3	L5	1582	PSU	C4-N3-C2	-4.27	120.19	126.34
1	S2	1804	OMU	N3-C2-N1	4.26	120.55	114.89
1	S2	116	OMU	C4-N3-C2	-4.26	120.97	126.58
1	S2	572	PSU	C4-N3-C2	-4.24	120.22	126.34
3	L5	1862	PSU	C4-N3-C2	-4.22	120.26	126.34
3	L5	4296	PSU	C4-N3-C2	-4.21	120.28	126.34
3	L5	4552	PSU	O2-C2-N1	-4.20	118.17	122.79
1	S2	1442	OMU	N3-C2-N1	4.19	120.45	114.89
3	L5	2839	PSU	O2-C2-N1	-4.19	118.18	122.79
1	S2	172	OMU	N3-C2-N1	4.18	120.44	114.89
1	S2	1004	PSU	C4-N3-C2	-4.17	120.33	126.34
1	S2	428	OMU	N3-C2-N1	4.17	120.42	114.89
3	L5	2415	OMU	N3-C2-N1	4.16	120.41	114.89
3	L5	4579	PSU	C4-N3-C2	-4.16	120.34	126.34
3	L5	4457	PSU	C4-N3-C2	-4.15	120.36	126.34
1	S2	1326	UY1	C4-N3-C2	-4.15	120.36	126.34
1	S2	116	OMU	N3-C2-N1	4.14	120.38	114.89
3	L5	4521	PSU	C4-N3-C2	-4.13	120.38	126.34
1	S2	681	PSU	C4-N3-C2	-4.13	120.39	126.34
3	L5	3637	PSU	C4-N3-C2	-4.12	120.40	126.34
3	L5	1677	PSU	C4-N3-C2	-4.11	120.41	126.34
3	L5	4312	PSU	C4-N3-C2	-4.11	120.41	126.34
1	S2	105	PSU	C4-N3-C2	-4.11	120.42	126.34
1	S2	822	PSU	C4-N3-C2	-4.11	120.42	126.34
1	S2	354	OMU	N3-C2-N1	4.10	120.34	114.89
3	L5	4306	OMU	C4-N3-C2	-4.10	121.17	126.58
1	S2	1232	PSU	C4-N3-C2	-4.09	120.44	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	Lr	2	SAC	C2A-C1A-N	-4.09	109.18	116.10
1	S2	918	PSU	C4-N3-C2	-4.08	120.46	126.34
3	L5	5001	PSU	C4-N3-C2	-4.08	120.46	126.34
1	S2	966	PSU	C4-N3-C2	-4.08	120.47	126.34
3	L5	4403	PSU	C4-N3-C2	-4.08	120.47	126.34
1	S2	34	PSU	C4-N3-C2	-4.06	120.48	126.34
3	L5	3758	PSU	C4-N3-C2	-4.06	120.48	126.34
3	L5	1744	PSU	C4-N3-C2	-4.06	120.48	126.34
3	L5	2508	PSU	C4-N3-C2	-4.06	120.49	126.34
3	L5	4447	5MC	C5-C6-N1	-4.06	119.17	123.34
84	Pt	8	4SU	N3-C2-N1	4.06	120.27	114.89
3	L5	4500	PSU	C4-N3-C2	-4.05	120.50	126.34
3	L5	3734	PSU	C4-N3-C2	-4.05	120.50	126.34
3	L5	2839	PSU	C4-N3-C2	-4.05	120.50	126.34
3	L5	4569	PSU	C4-N3-C2	-4.03	120.53	126.34
1	S2	1244	PSU	C4-N3-C2	-4.03	120.53	126.34
29	SV	1	AME	CT2-CT1-N	-4.03	109.28	116.10
3	L5	3853	PSU	O2-C2-N1	-4.03	118.36	122.79
3	L5	4299	PSU	C4-N3-C2	-4.02	120.54	126.34
3	L5	4353	PSU	C4-N3-C2	-4.02	120.55	126.34
6	SA	2	SAC	C2A-C1A-N	-4.02	109.30	116.10
1	S2	573	PSU	C4-N3-C2	-4.01	120.56	126.34
3	L5	3695	PSU	C4-N3-C2	-4.01	120.56	126.34
83	At	39	PSU	C4-N3-C2	-4.01	120.56	126.34
1	S2	801	PSU	C4-N3-C2	-4.01	120.57	126.34
1	S2	1347	PSU	C4-N3-C2	-4.01	120.57	126.34
3	L5	4361	PSU	C4-N3-C2	-4.01	120.57	126.34
3	L5	1862	PSU	O2-C2-N1	-4.00	118.39	122.79
1	S2	814	PSU	C4-N3-C2	-4.00	120.58	126.34
1	S2	651	PSU	C4-N3-C2	-3.99	120.58	126.34
1	S2	866	PSU	C4-N3-C2	-3.99	120.58	126.34
3	L5	4423	PSU	C4-N3-C2	-3.99	120.58	126.34
3	L5	3851	PSU	C4-N3-C2	-3.99	120.59	126.34
3	L5	4552	PSU	C4-N3-C2	-3.98	120.60	126.34
1	S2	1056	PSU	C4-N3-C2	-3.97	120.61	126.34
2	L8	14	OMU	C5-C4-N3	3.97	120.77	114.84
3	L5	1779	PSU	C4-N3-C2	-3.96	120.63	126.34
3	L5	4972	PSU	C4-N3-C2	-3.96	120.63	126.34
1	S2	121	OMU	N3-C2-N1	3.96	120.14	114.89
1	S2	815	PSU	C4-N3-C2	-3.96	120.64	126.34
3	L5	3715	PSU	C4-N3-C2	-3.95	120.64	126.34
1	S2	1239	PSU	C4-N3-C2	-3.95	120.65	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	At	8	4SU	N3-C2-N1	3.95	120.13	114.89
1	S2	627	OMU	N3-C2-N1	3.95	120.13	114.89
3	L5	1782	PSU	C4-N3-C2	-3.95	120.65	126.34
3	L5	3844	PSU	C4-N3-C2	-3.95	120.65	126.34
3	L5	4431	PSU	C4-N3-C2	-3.94	120.66	126.34
3	L5	1536	PSU	C4-N3-C2	-3.94	120.66	126.34
1	S2	1639	G7M	C3'-C2'-C1'	3.94	106.91	100.98
1	S2	1288	OMU	N3-C2-N1	3.94	120.12	114.89
3	L5	3853	PSU	C4-N3-C2	-3.93	120.68	126.34
3	L5	5010	PSU	C4-N3-C2	-3.93	120.68	126.34
3	L5	4227	OMU	N3-C2-N1	3.92	120.09	114.89
2	L8	55	PSU	C4-N3-C2	-3.92	120.70	126.34
3	L5	1860	PSU	C4-N3-C2	-3.91	120.71	126.34
1	S2	296	PSU	C4-N3-C2	-3.91	120.71	126.34
3	L5	3770	PSU	C4-N3-C2	-3.91	120.71	126.34
3	L5	3729	PSU	C4-N3-C2	-3.90	120.72	126.34
1	S2	406	PSU	C4-N3-C2	-3.90	120.72	126.34
1	S2	1174	PSU	C4-N3-C2	-3.90	120.73	126.34
1	S2	1177	PSU	C4-N3-C2	-3.90	120.73	126.34
3	L5	1792	PSU	C4-N3-C2	-3.89	120.73	126.34
3	L5	3762	PSU	C4-N3-C2	-3.89	120.73	126.34
1	S2	1238	PSU	C4-N3-C2	-3.89	120.73	126.34
1	S2	1367	PSU	C4-N3-C2	-3.89	120.73	126.34
3	L5	4471	PSU	C4-N3-C2	-3.89	120.73	126.34
2	L8	14	OMU	N3-C2-N1	3.88	120.05	114.89
2	L8	69	PSU	C4-N3-C2	-3.88	120.74	126.34
1	S2	1643	PSU	C4-N3-C2	-3.88	120.74	126.34
3	L5	3639	PSU	C4-N3-C2	-3.88	120.75	126.34
1	S2	649	PSU	C4-N3-C2	-3.87	120.76	126.34
1	S2	863	PSU	C4-N3-C2	-3.87	120.77	126.34
3	L5	4689	PSU	C4-N3-C2	-3.86	120.77	126.34
1	S2	1243	PSU	C4-N3-C2	-3.86	120.78	126.34
3	L5	4431	PSU	O2-C2-N1	-3.86	118.54	122.79
1	S2	93	PSU	C4-N3-C2	-3.85	120.79	126.34
1	S2	609	PSU	C4-N3-C2	-3.85	120.79	126.34
1	S2	109	PSU	O2-C2-N1	-3.84	118.56	122.79
84	Pt	56	PSU	C4-N3-C2	-3.84	120.80	126.34
1	S2	1445	PSU	C4-N3-C2	-3.84	120.81	126.34
3	L5	4532	PSU	C4-N3-C2	-3.84	120.81	126.34
1	S2	218	PSU	C4-N3-C2	-3.83	120.81	126.34
1	S2	1136	PSU	C4-N3-C2	-3.83	120.82	126.34
3	L5	4403	PSU	O2-C2-N1	-3.83	118.58	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	36	PSU	C4-N3-C2	-3.82	120.83	126.34
1	S2	1625	PSU	C4-N3-C2	-3.82	120.84	126.34
1	S2	686	PSU	C4-N3-C2	-3.81	120.85	126.34
84	Pt	8	4SU	C5-C4-S4	-3.80	119.57	124.47
3	L5	3884	PSU	C4-N3-C2	-3.80	120.87	126.34
3	L5	4220	6MZ	C9-N6-C6	-3.79	119.61	122.87
3	L5	4498	OMU	C5-C4-N3	3.79	120.51	114.84
3	L5	1781	PSU	C4-N3-C2	-3.78	120.90	126.34
3	L5	4628	PSU	C4-N3-C2	-3.77	120.91	126.34
3	L5	4576	PSU	C4-N3-C2	-3.76	120.92	126.34
3	L5	4493	PSU	C4-N3-C2	-3.74	120.94	126.34
3	L5	4293	PSU	C4-N3-C2	-3.74	120.95	126.34
3	L5	4227	OMU	C5-C4-N3	3.71	120.39	114.84
3	L5	4442	PSU	O2-C2-N1	-3.71	118.70	122.79
1	S2	428	OMU	C5-C4-N3	3.71	120.39	114.84
3	L5	3925	OMU	C5-C4-N3	3.71	120.39	114.84
1	S2	354	OMU	C5-C4-N3	3.71	120.39	114.84
1	S2	651	PSU	O2-C2-N1	-3.71	118.71	122.79
1	S2	1367	PSU	O2-C2-N1	-3.71	118.71	122.79
83	At	32	PSU	C4-N3-C2	-3.70	121.01	126.34
2	L8	69	PSU	O2-C2-N1	-3.69	118.73	122.79
1	S2	627	OMU	C5-C4-N3	3.69	120.35	114.84
1	S2	918	PSU	C3'-C2'-C1'	3.68	105.92	101.64
3	L5	4628	PSU	O2-C2-N1	-3.68	118.74	122.79
83	At	8	4SU	C5-C4-S4	-3.67	119.74	124.47
3	L5	3762	PSU	O2-C2-N1	-3.67	118.75	122.79
3	L5	1860	PSU	O2-C2-N1	-3.67	118.75	122.79
1	S2	121	OMU	C5-C4-N3	3.65	120.31	114.84
1	S2	866	PSU	O2-C2-N1	-3.61	118.81	122.79
3	L5	4689	PSU	O2-C2-N1	-3.61	118.81	122.79
1	S2	119	PSU	C4-N3-C2	-3.60	121.15	126.34
3	L5	2632	PSU	C4-N3-C2	-3.60	121.15	126.34
3	L5	2415	OMU	C1'-N1-C2	3.60	124.08	117.57
1	S2	1442	OMU	C5-C4-N3	3.58	120.20	114.84
3	L5	4500	PSU	O2-C2-N1	-3.58	118.85	122.79
3	L5	4312	PSU	O2-C2-N1	-3.57	118.86	122.79
1	S2	1804	OMU	C5-C4-N3	3.57	120.18	114.84
1	S2	172	OMU	C5-C4-N3	3.57	120.18	114.84
3	L5	2401	A2M	N3-C2-N1	-3.57	123.10	128.68
1	S2	1288	OMU	C5-C4-N3	3.56	120.16	114.84
3	L5	5001	PSU	O2-C2-N1	-3.56	118.87	122.79
3	L5	3729	PSU	O2-C2-N1	-3.56	118.88	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	93	PSU	O2-C2-N1	-3.54	118.89	122.79
1	S2	649	PSU	O2-C2-N1	-3.54	118.90	122.79
1	S2	1136	PSU	O2-C2-N1	-3.52	118.92	122.79
1	S2	1445	PSU	O2-C2-N1	-3.52	118.92	122.79
1	S2	1692	PSU	O2-C2-N1	-3.52	118.92	122.79
3	L5	4569	PSU	O2-C2-N1	-3.52	118.92	122.79
1	S2	1643	PSU	O2-C2-N1	-3.51	118.92	122.79
3	L5	1683	PSU	C4-N3-C2	-3.51	121.28	126.34
3	L5	2837	OMU	C5-C4-N3	3.51	120.09	114.84
1	S2	406	PSU	O2-C2-N1	-3.51	118.93	122.79
1	S2	1248	B8N	C31-N3-C2	3.50	122.92	117.67
1	S2	918	PSU	O2-C2-N1	-3.50	118.93	122.79
3	L5	2508	PSU	O2-C2-N1	-3.50	118.94	122.79
3	L5	2415	OMU	C5-C4-N3	3.49	120.07	114.84
1	S2	36	PSU	O2-C2-N1	-3.46	118.98	122.79
1	S2	1243	PSU	O2-C2-N1	-3.46	118.99	122.79
3	L5	4620	OMU	C5-C4-N3	3.45	120.01	114.84
84	Pt	56	PSU	O2-C2-N1	-3.45	118.99	122.79
1	S2	686	PSU	O2-C2-N1	-3.45	118.99	122.79
1	S2	863	PSU	O2-C2-N1	-3.45	118.99	122.79
3	L5	2787	A2M	N3-C2-N1	-3.45	123.29	128.68
83	At	39	PSU	O2-C2-N1	-3.45	119.00	122.79
1	S2	1244	PSU	O2-C2-N1	-3.45	119.00	122.79
1	S2	609	PSU	O2-C2-N1	-3.44	119.00	122.79
1	S2	1625	PSU	O2-C2-N1	-3.44	119.00	122.79
3	L5	5010	PSU	O2-C2-N1	-3.44	119.00	122.79
1	S2	116	OMU	C5-C4-N3	3.44	119.99	114.84
1	S2	1056	PSU	O2-C2-N1	-3.44	119.01	122.79
3	L5	4442	PSU	C3'-C2'-C1'	3.44	105.64	101.64
1	S2	34	PSU	O2-C2-N1	-3.42	119.02	122.79
3	L5	3734	PSU	O2-C2-N1	-3.42	119.02	122.79
1	S2	512	A2M	N3-C2-N1	-3.40	123.36	128.68
1	S2	296	PSU	O2-C2-N1	-3.39	119.05	122.79
1	S2	166	A2M	N3-C2-N1	-3.39	123.38	128.68
1	S2	105	PSU	O2-C2-N1	-3.38	119.07	122.79
1	S2	1177	PSU	O2-C2-N1	-3.38	119.07	122.79
1	S2	966	PSU	O2-C2-N1	-3.38	119.07	122.79
1	S2	801	PSU	O2-C2-N1	-3.37	119.08	122.79
1	S2	1832	6MZ	N3-C2-N1	-3.37	123.41	128.68
3	L5	1677	PSU	O2-C2-N1	-3.37	119.08	122.79
3	L5	3764	PSU	C3'-C2'-C1'	3.36	105.55	101.64
3	L5	1782	PSU	O2-C2-N1	-3.36	119.09	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	4220	6MZ	N3-C2-N1	-3.35	123.44	128.68
3	L5	4523	A2M	N3-C2-N1	-3.34	123.45	128.68
3	L5	4306	OMU	C5-C4-N3	3.34	119.84	114.84
3	L5	4576	PSU	O2-C2-N1	-3.34	119.11	122.79
83	At	32	PSU	O2-C2-N1	-3.34	119.11	122.79
1	S2	822	PSU	O2-C2-N1	-3.34	119.11	122.79
3	L5	4420	PSU	C4-N3-C2	-3.34	121.53	126.34
1	S2	681	PSU	O2-C2-N1	-3.34	119.12	122.79
3	L5	3782	5MC	C5-C6-N1	-3.34	119.91	123.34
1	S2	1174	PSU	O2-C2-N1	-3.33	119.12	122.79
3	L5	4531	PSU	O2-C2-N1	-3.33	119.13	122.79
1	S2	1239	PSU	O2-C2-N1	-3.32	119.13	122.79
3	L5	3920	PSU	O2-C2-N1	-3.31	119.14	122.79
1	S2	1383	A2M	N3-C2-N1	-3.30	123.51	128.68
1	S2	822	PSU	C3'-C2'-C1'	3.30	105.48	101.64
1	S2	1238	PSU	O2-C2-N1	-3.29	119.16	122.79
3	L5	3851	PSU	O2-C2-N1	-3.29	119.17	122.79
3	L5	4353	PSU	O2-C2-N1	-3.28	119.18	122.79
3	L5	3830	A2M	N3-C2-N1	-3.28	123.55	128.68
3	L5	3758	PSU	O2-C2-N1	-3.28	119.18	122.79
1	S2	814	PSU	O2-C2-N1	-3.27	119.19	122.79
3	L5	1534	A2M	N3-C2-N1	-3.27	123.57	128.68
3	L5	3785	A2M	N3-C2-N1	-3.26	123.58	128.68
1	S2	573	PSU	O2-C2-N1	-3.26	119.20	122.79
1	S2	1004	PSU	O2-C2-N1	-3.26	119.20	122.79
3	L5	3770	PSU	O2-C2-N1	-3.26	119.21	122.79
3	L5	4227	OMU	O4-C4-C5	-3.25	119.44	125.16
3	L5	1779	PSU	O2-C2-N1	-3.25	119.22	122.79
3	L5	3760	A2M	N3-C2-N1	-3.25	123.60	128.68
3	L5	3764	PSU	O2-C2-N1	-3.25	119.22	122.79
3	L5	1781	PSU	O2-C2-N1	-3.24	119.22	122.79
1	S2	1678	A2M	N3-C2-N1	-3.24	123.61	128.68
3	L5	1871	A2M	N3-C2-N1	-3.24	123.61	128.68
3	L5	3695	PSU	O2-C2-N1	-3.24	119.22	122.79
3	L5	4498	OMU	O4-C4-C5	-3.24	119.46	125.16
2	L8	55	PSU	O2-C2-N1	-3.24	119.23	122.79
1	S2	172	OMU	O4-C4-C5	-3.24	119.47	125.16
1	S2	1232	PSU	O2-C2-N1	-3.23	119.23	122.79
1	S2	99	A2M	N3-C2-N1	-3.23	123.63	128.68
3	L5	4420	PSU	O2-C2-N1	-3.23	119.24	122.79
1	S2	1850	MA6	C4-C5-N7	-3.22	106.04	109.40
1	S2	468	A2M	N3-C2-N1	-3.22	123.64	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	218	PSU	O2-C2-N1	-3.22	119.25	122.79
3	L5	400	A2M	N3-C2-N1	-3.22	123.65	128.68
1	S2	27	A2M	N3-C2-N1	-3.21	123.66	128.68
3	L5	4636	PSU	O2-C2-N1	-3.21	119.25	122.79
3	L5	3825	A2M	N3-C2-N1	-3.20	123.67	128.68
3	L5	3884	PSU	O2-C2-N1	-3.20	119.27	122.79
81	5A	50	5CT	C3-C2-C1	-3.19	104.87	112.16
3	L5	4423	PSU	O2-C2-N1	-3.19	119.27	122.79
1	S2	1347	PSU	O2-C2-N1	-3.19	119.28	122.79
1	S2	1031	A2M	N3-C2-N1	-3.19	123.70	128.68
1	S2	815	PSU	O2-C2-N1	-3.19	119.28	122.79
2	L8	14	OMU	O4-C4-C5	-3.18	119.57	125.16
3	L5	3723	A2M	N3-C2-N1	-3.18	123.71	128.68
3	L5	4471	PSU	O2-C2-N1	-3.18	119.29	122.79
3	L5	1744	PSU	O2-C2-N1	-3.17	119.30	122.79
3	L5	3715	PSU	O2-C2-N1	-3.17	119.30	122.79
1	S2	572	PSU	O2-C2-N1	-3.17	119.30	122.79
1	S2	1326	UY1	O2-C2-N1	-3.17	119.30	122.79
3	L5	2363	A2M	N3-C2-N1	-3.17	123.72	128.68
1	S2	354	OMU	O4-C4-C5	-3.16	119.60	125.16
1	S2	119	PSU	O2-C2-N1	-3.16	119.31	122.79
3	L5	2843	PSU	O2-C2-N1	-3.15	119.32	122.79
3	L5	3768	PSU	O2-C2-N1	-3.14	119.33	122.79
3	L5	398	A2M	N3-C2-N1	-3.12	123.81	128.68
3	L5	3724	A2M	N3-C2-N1	-3.10	123.83	128.68
3	L5	2415	OMU	O4-C4-C5	-3.10	119.72	125.16
1	S2	590	A2M	N3-C2-N1	-3.09	123.86	128.68
1	S2	428	OMU	O4-C4-C5	-3.09	119.73	125.16
81	5A	50	5CT	C1-NZ-CE	-3.08	106.53	113.42
1	S2	627	OMU	O4-C4-C5	-3.08	119.75	125.16
3	L5	4361	PSU	O2-C2-N1	-3.07	119.41	122.79
3	L5	4521	PSU	O2-C2-N1	-3.07	119.41	122.79
1	S2	1442	OMU	O4-C4-C5	-3.07	119.77	125.16
1	S2	1004	PSU	C3'-C2'-C1'	3.06	105.20	101.64
3	L5	4590	A2M	N3-C2-N1	-3.05	123.91	128.68
3	L5	4579	PSU	O2-C2-N1	-3.04	119.44	122.79
1	S2	1850	MA6	N3-C2-N1	-3.03	123.94	128.68
3	L5	2815	A2M	N3-C2-N1	-3.03	123.95	128.68
3	L5	3639	PSU	O2-C2-N1	-3.03	119.46	122.79
1	S2	668	A2M	N3-C2-N1	-3.02	123.95	128.68
3	L5	1792	PSU	O2-C2-N1	-3.02	119.46	122.79
1	S2	1851	MA6	N3-C2-N1	-3.02	123.96	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	3818	UY1	O2-C2-N1	-3.01	119.47	122.79
3	L5	4620	OMU	O4-C4-C5	-3.01	119.86	125.16
1	S2	1288	OMU	O4-C4-C5	-3.01	119.87	125.16
1	S2	484	A2M	N3-C2-N1	-3.01	123.98	128.68
3	L5	1326	A2M	N3-C2-N1	-3.00	123.99	128.68
1	S2	116	OMU	O4-C4-C5	-3.00	119.89	125.16
3	L5	1582	PSU	O2-C2-N1	-2.99	119.50	122.79
1	S2	1081	PSU	O2-C2-N1	-2.98	119.51	122.79
3	L5	4673	PSU	O2-C2-N1	-2.97	119.52	122.79
1	S2	668	A2M	C4-C5-N7	-2.97	106.30	109.40
3	L5	2815	A2M	C4-C5-N7	-2.97	106.30	109.40
3	L5	1534	A2M	C4-C5-N7	-2.97	106.31	109.40
1	S2	1842	4AC	N4-C4-N3	2.96	118.81	113.85
1	S2	576	A2M	N3-C2-N1	-2.95	124.06	128.68
3	L5	4306	OMU	O4-C4-C5	-2.95	119.97	125.16
1	S2	1851	MA6	C4-C5-N7	-2.95	106.32	109.40
3	L5	4296	PSU	O2-C2-N1	-2.95	119.55	122.79
3	L5	2632	PSU	O2-C2-N1	-2.94	119.55	122.79
3	L5	3925	OMU	O4-C4-C5	-2.90	120.06	125.16
3	L5	4571	A2M	N3-C2-N1	-2.90	124.15	128.68
3	L5	3782	5MC	C5-C4-N3	-2.90	118.55	121.67
3	L5	4493	PSU	O2-C2-N1	-2.89	119.61	122.79
3	L5	1683	PSU	O2-C2-N1	-2.89	119.61	122.79
1	S2	121	OMU	O4-C4-C5	-2.89	120.08	125.16
3	L5	4447	5MC	C5-C4-N3	-2.87	118.57	121.67
3	L5	1536	PSU	O2-C2-N1	-2.87	119.63	122.79
1	S2	159	A2M	N3-C2-N1	-2.87	124.20	128.68
3	L5	4590	A2M	C4-C5-N7	-2.87	106.41	109.40
3	L5	3718	A2M	N3-C2-N1	-2.84	124.24	128.68
3	L5	3867	A2M	N3-C2-N1	-2.84	124.24	128.68
1	S2	1337	4AC	N4-C4-N3	2.84	118.61	113.85
1	S2	27	A2M	C4-C5-N7	-2.83	106.45	109.40
3	L5	1524	A2M	N3-C2-N1	-2.82	124.27	128.68
3	L5	4293	PSU	O2-C2-N1	-2.82	119.69	122.79
3	L5	2401	A2M	C4-C5-N7	-2.81	106.47	109.40
3	L5	4636	PSU	C3'-C2'-C1'	2.78	104.87	101.64
3	L5	4299	PSU	O2-C2-N1	-2.77	119.74	122.79
1	S2	159	A2M	C4-C5-N7	-2.73	106.56	109.40
83	At	46	7MG	C5-C6-N1	2.73	115.80	110.99
1	S2	99	A2M	C4-C5-N7	-2.73	106.56	109.40
3	L5	1326	A2M	C4-C5-N7	-2.72	106.56	109.40
1	S2	1804	OMU	O4-C4-C5	-2.72	120.38	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1031	A2M	C4-C5-N7	-2.72	106.57	109.40
3	L5	3844	PSU	O2-C2-N1	-2.71	119.80	122.79
3	L5	1534	A2M	O3'-C3'-C4'	-2.70	103.24	111.05
3	L5	4420	PSU	C6-C5-C4	-2.69	116.32	118.20
1	S2	576	A2M	C4-C5-N7	-2.68	106.60	109.40
1	S2	1248	B8N	N3-C2-N1	2.67	120.53	116.76
3	L5	4457	PSU	O2-C2-N1	-2.66	119.86	122.79
1	S2	1842	4AC	C6-C5-C4	2.66	120.22	116.96
1	S2	1081	PSU	C5-C6-N1	-2.66	118.11	122.11
3	L5	3899	OMG	C8-N7-C5	2.66	108.06	102.99
1	S2	484	A2M	C4-C5-N7	-2.66	106.63	109.40
83	At	46	7MG	O4'-C1'-N9	2.66	112.92	109.30
1	S2	166	A2M	C4-C5-N7	-2.65	106.63	109.40
84	Pt	21	H2U	C5-C6-N1	-2.65	102.88	111.61
29	SV	1	AME	CE-SD-CG	2.65	109.50	100.40
3	L5	1871	A2M	C4-C5-N7	-2.64	106.64	109.40
3	L5	3760	A2M	C4-C5-N7	-2.64	106.65	109.40
84	Pt	33	OMC	O2-C2-N3	-2.64	118.04	122.33
3	L5	400	A2M	C4-C5-N7	-2.64	106.65	109.40
3	L5	1582	PSU	C3'-C2'-C1'	2.62	104.69	101.64
50	La	39	V5N	O-C-CA	-2.61	117.93	124.78
3	L5	3830	A2M	C4-C5-N7	-2.61	106.68	109.40
1	S2	1383	A2M	C4-C5-N7	-2.60	106.69	109.40
3	L5	3637	PSU	C5-C6-N1	-2.59	118.22	122.11
1	S2	172	OMU	O2'-C2'-C1'	2.59	114.13	109.08
1	S2	468	A2M	C4-C5-N7	-2.58	106.71	109.40
3	L5	3627	OMG	C8-N7-C5	2.58	107.91	102.99
1	S2	1639	G7M	CN7-N7-C8	-2.57	113.06	125.43
1	S2	512	A2M	C4-C5-N7	-2.57	106.72	109.40
3	L5	3723	A2M	C4-C5-N7	-2.57	106.72	109.40
1	S2	1832	6MZ	C4-C5-N7	-2.56	106.73	109.40
1	S2	590	A2M	C4-C5-N7	-2.56	106.74	109.40
3	L5	1524	A2M	C4-C5-N7	-2.55	106.74	109.40
1	S2	428	OMU	O2-C2-N1	-2.55	119.39	122.79
2	L8	75	OMG	C5-C6-N1	2.55	118.45	113.95
3	L5	4447	5MC	O2-C2-N3	-2.54	118.19	122.33
3	L5	398	A2M	C4-C5-N7	-2.54	106.75	109.40
3	L5	2837	OMU	O4-C4-C5	-2.54	120.70	125.16
3	L5	4636	PSU	C5-C6-N1	-2.54	118.31	122.11
3	L5	4618	OMG	C5-C6-N1	2.53	118.42	113.95
3	L5	4220	6MZ	C4-C5-N7	-2.53	106.76	109.40
3	L5	4196	OMG	C5-C6-N1	2.53	118.42	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	3764	PSU	C5-C6-N1	-2.53	118.32	122.11
3	L5	4637	OMG	C5-C6-N1	2.52	118.40	113.95
3	L5	3724	A2M	C4-C5-N7	-2.52	106.78	109.40
3	L5	4531	PSU	C5-C6-N1	-2.50	118.37	122.11
3	L5	2843	PSU	C5-C6-N1	-2.49	118.37	122.11
83	At	20	H2U	C5-C6-N1	-2.48	103.44	111.61
3	L5	3718	A2M	C4-C5-N7	-2.48	106.81	109.40
3	L5	3867	A2M	C4-C5-N7	-2.47	106.82	109.40
3	L5	4972	PSU	O2-C2-N1	-2.47	120.07	122.79
3	L5	3818	UY1	C5-C6-N1	-2.47	118.41	122.11
3	L5	2876	OMG	C8-N7-C5	2.44	107.65	102.99
3	L5	1522	OMG	C8-N7-C5	2.44	107.64	102.99
3	L5	2787	A2M	C4-C5-N7	-2.43	106.86	109.40
1	S2	119	PSU	C6-C5-C4	-2.43	116.50	118.20
3	L5	3744	OMG	C5-C6-N1	2.42	118.22	113.95
3	L5	1322	1MA	C8-N7-C5	2.42	107.60	102.99
3	L5	4637	OMG	C8-N7-C5	2.41	107.59	102.99
3	L5	2363	A2M	C4-C5-N7	-2.41	106.89	109.40
1	S2	1692	PSU	C5-C6-N1	-2.41	118.49	122.11
3	L5	3627	OMG	C5-C6-N1	2.41	118.20	113.95
3	L5	3925	OMU	O2-C2-N1	-2.40	119.59	122.79
39	LA	216	V5N	O-C-CA	-2.40	118.49	124.78
3	L5	3808	OMC	O2-C2-N3	-2.40	118.43	122.33
1	S2	683	OMG	C8-N7-C5	2.40	107.56	102.99
3	L5	4571	A2M	C4-C5-N7	-2.39	106.90	109.40
1	S2	867	OMG	C5-C6-N1	2.39	118.18	113.95
3	L5	4494	OMG	C5-C6-N1	2.39	118.17	113.95
1	S2	644	OMG	C8-N7-C5	2.39	107.54	102.99
3	L5	4499	OMG	C5-C6-N1	2.39	118.17	113.95
3	L5	1522	OMG	C5-C6-N1	2.39	118.17	113.95
3	L5	4618	OMG	C8-N7-C5	2.38	107.53	102.99
3	L5	4673	PSU	C5-C6-N1	-2.38	118.55	122.11
2	L8	75	OMG	C8-N7-C5	2.37	107.51	102.99
3	L5	4623	OMG	C5-C6-N1	2.36	118.13	113.95
3	L5	3785	A2M	C4-C5-N7	-2.36	106.94	109.40
3	L5	4227	OMU	C1'-N1-C2	2.36	121.84	117.57
1	S2	436	OMG	C5-C6-N1	2.36	118.12	113.95
3	L5	1625	OMG	C8-N7-C5	2.36	107.48	102.99
1	S2	1678	A2M	C4-C5-N7	-2.36	106.94	109.40
3	L5	3744	OMG	C8-N7-C5	2.36	107.48	102.99
3	L5	3944	OMG	C8-N7-C5	2.35	107.46	102.99
1	S2	1328	OMG	C5-C6-N1	2.35	118.09	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	4392	OMG	C8-N7-C5	2.34	107.46	102.99
1	S2	644	OMG	C5-C6-N1	2.34	118.09	113.95
3	L5	3944	OMG	C5-C6-N1	2.33	118.07	113.95
3	L5	1625	OMG	C5-C6-N1	2.33	118.06	113.95
83	At	46	7MG	C3'-C2'-C1'	2.33	105.85	101.43
3	L5	4370	OMG	C8-N7-C5	2.33	107.42	102.99
3	L5	3825	A2M	C4-C5-N7	-2.32	106.98	109.40
3	L5	4306	OMU	C1'-N1-C2	2.32	121.78	117.57
3	L5	1316	OMG	C5-C6-N1	2.32	118.06	113.95
3	L5	4530	UR3	C6-N1-C2	-2.32	119.71	121.79
1	S2	1004	PSU	C5-C6-N1	-2.32	118.62	122.11
3	L5	3637	PSU	O2-C2-N1	-2.32	120.23	122.79
1	S2	1447	OMG	C8-N7-C5	2.32	107.41	102.99
2	L8	69	PSU	O4'-C1'-C2'	2.32	108.41	105.14
3	L5	2364	OMG	C8-N7-C5	2.31	107.40	102.99
1	S2	1328	OMG	C8-N7-C5	2.31	107.39	102.99
1	S2	867	OMG	C8-N7-C5	2.31	107.39	102.99
3	L5	4521	PSU	C5-C6-N1	-2.31	118.65	122.11
6	SA	2	SAC	O-C-CA	-2.31	118.73	124.78
1	S2	509	OMG	C5-C6-N1	2.31	118.03	113.95
1	S2	601	OMG	C5-C6-N1	2.31	118.02	113.95
1	S2	109	PSU	C5-C6-N1	-2.30	118.66	122.11
83	At	46	7MG	C5-C4-N9	-2.30	103.36	106.35
3	L5	4499	OMG	C8-N7-C5	2.30	107.36	102.99
3	L5	3758	PSU	C5-C6-N1	-2.29	118.67	122.11
3	L5	3899	OMG	C5-C6-N1	2.29	117.99	113.95
39	LA	216	V5N	CG-CD2-NE2	-2.29	104.69	108.67
3	L5	4532	PSU	O2-C2-N3	-2.28	117.52	121.82
1	S2	1490	OMG	C5-C6-N1	2.28	117.98	113.95
1	S2	1337	4AC	C2'-C1'-N1	-2.28	106.76	113.22
3	L5	3768	PSU	C3'-C2'-C1'	2.28	104.29	101.64
1	S2	509	OMG	C8-N7-C5	2.27	107.32	102.99
1	S2	1337	4AC	C6-C5-C4	2.27	119.74	116.96
1	S2	1447	OMG	C5-C6-N1	2.26	117.95	113.95
3	L5	4296	PSU	C5-C6-N1	-2.26	118.71	122.11
3	L5	4370	OMG	C5-C6-N1	2.26	117.95	113.95
3	L5	4623	OMG	C8-N7-C5	2.26	107.30	102.99
83	At	46	7MG	O6-C6-C5	-2.26	122.00	127.54
3	L5	2364	OMG	C5-C6-N1	2.25	117.93	113.95
3	L5	3768	PSU	C5-C6-N1	-2.25	118.73	122.11
3	L5	4228	OMG	C5-C6-N1	2.24	117.91	113.95
1	S2	436	OMG	C8-N7-C5	2.24	107.25	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1248	B8N	O4'-C1'-C2'	2.23	108.30	105.14
3	L5	3920	PSU	C5-C6-N1	-2.23	118.76	122.11
3	L5	1582	PSU	C5-C6-N1	-2.23	118.76	122.11
3	L5	2876	OMG	C5-C6-N1	2.23	117.89	113.95
81	5A	50	5CT	CD-CG-CB	-2.23	105.74	113.62
3	L5	4532	PSU	O2-C2-N1	-2.23	120.34	122.79
1	S2	1081	PSU	C3'-C2'-C1'	2.22	104.23	101.64
1	S2	1490	OMG	C8-N7-C5	2.22	107.22	102.99
3	L5	3782	5MC	O2-C2-N3	-2.22	118.72	122.33
1	S2	601	OMG	C8-N7-C5	2.22	107.22	102.99
1	S2	683	OMG	C5-C6-N1	2.22	117.87	113.95
3	L5	1536	PSU	C5-C6-N1	-2.21	118.79	122.11
3	L5	3639	PSU	C5-C6-N1	-2.21	118.79	122.11
3	L5	4457	PSU	C5-C6-N1	-2.21	118.79	122.11
1	S2	572	PSU	C3'-C2'-C1'	2.21	104.21	101.64
1	S2	1326	UY1	C5-C6-N1	-2.21	118.80	122.11
3	L5	4196	OMG	C8-N7-C5	2.21	107.19	102.99
1	S2	1445	PSU	O4'-C1'-C2'	2.20	108.25	105.14
3	L5	4523	A2M	C4-C5-N7	-2.20	107.11	109.40
3	L5	3637	PSU	O2-C2-N3	-2.20	117.67	121.82
3	L5	4498	OMU	O2-C2-N1	-2.20	119.87	122.79
3	L5	4392	OMG	C5-C6-N1	2.20	117.83	113.95
3	L5	3792	OMG	C5-C6-N1	2.18	117.81	113.95
84	Pt	33	OMC	C1'-N1-C2	2.17	123.27	118.42
3	L5	4442	PSU	C5-C6-N1	-2.16	118.87	122.11
3	L5	4579	PSU	C5-C6-N1	-2.16	118.87	122.11
3	L5	4228	OMG	C8-N7-C5	2.16	107.10	102.99
3	L5	4299	PSU	C5-C6-N1	-2.16	118.87	122.11
3	L5	4196	OMG	O6-C6-C5	-2.15	120.17	124.37
83	At	16	H2U	C5-C6-N1	-2.15	104.53	111.61
1	S2	815	PSU	C5-C6-N1	-2.15	118.89	122.11
1	S2	572	PSU	C5-C6-N1	-2.15	118.89	122.11
1	S2	966	PSU	C5-C6-N1	-2.14	118.89	122.11
3	L5	1316	OMG	C8-N7-C5	2.14	107.07	102.99
1	S2	172	OMU	O2-C2-N1	-2.14	119.94	122.79
1	S2	822	PSU	C5-C6-N1	-2.14	118.90	122.11
1	S2	354	OMU	O2-C2-N1	-2.13	119.95	122.79
3	L5	4447	5MC	N1-C2-N3	2.13	122.69	118.81
3	L5	4423	PSU	C5-C6-N1	-2.13	118.92	122.11
1	S2	1248	B8N	O36-C34-O35	-2.13	119.26	124.09
3	L5	1322	1MA	C5-C6-N1	2.13	117.07	113.90
39	LA	216	V5N	CD2-NE2-CE1	2.12	109.09	105.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	2424	OMG	C5-C6-N1	2.12	117.70	113.95
1	S2	1643	PSU	O4'-C1'-C2'	2.12	108.13	105.14
3	L5	1862	PSU	C5-C6-N1	-2.12	118.93	122.11
1	S2	1842	4AC	C5-C4-N3	-2.10	119.21	122.59
1	S2	627	OMU	O2-C2-N1	-2.10	119.99	122.79
3	L5	4536	OMC	O2-C2-N3	-2.10	118.92	122.33
3	L5	2401	A2M	C2-N1-C6	2.10	122.34	118.75
3	L5	2424	OMG	C8-N7-C5	2.10	106.98	102.99
1	S2	1248	B8N	O36-C34-C33	2.10	120.52	113.38
1	S2	1244	PSU	C5-C6-N1	-2.10	118.97	122.11
3	L5	3792	OMG	C8-N7-C5	2.09	106.98	102.99
3	L5	2787	A2M	O4'-C4'-C5'	2.09	116.25	109.37
3	L5	4636	PSU	O2-C2-N3	-2.09	117.89	121.82
50	La	39	V5N	O2-CB-CA	2.07	111.66	107.28
3	L5	3758	PSU	C3'-C2'-C1'	2.07	104.05	101.64
3	L5	3785	A2M	CM'-O2'-C2'	-2.07	109.09	114.52
3	L5	3851	PSU	C5-C6-N1	-2.07	119.01	122.11
3	L5	4420	PSU	O4'-C1'-C2'	2.07	108.06	105.14
3	L5	1524	A2M	C2-N1-C6	2.06	122.28	118.75
3	L5	4456	OMC	O2-C2-N3	-2.06	118.98	122.33
3	L5	2508	PSU	C5-C6-N1	-2.06	119.02	122.11
3	L5	1744	PSU	C5-C6-N1	-2.05	119.03	122.11
3	L5	3853	PSU	O4'-C1'-C2'	2.05	108.03	105.14
83	At	16	H2U	O2-C2-N1	-2.04	120.54	123.11
1	S2	1851	MA6	N1-C6-N6	2.04	119.21	117.06
1	S2	105	PSU	C5-C6-N1	-2.04	119.04	122.11
1	S2	681	PSU	C5-C6-N1	-2.04	119.05	122.11
1	S2	218	PSU	O4'-C1'-C2'	2.04	108.02	105.14
3	L5	4471	PSU	C5-C6-N1	-2.04	119.06	122.11
3	L5	3695	PSU	C5-C6-N1	-2.03	119.06	122.11
1	S2	814	PSU	C5-C6-N1	-2.03	119.06	122.11
3	L5	3792	OMG	O6-C6-C5	-2.03	120.41	124.37
3	L5	5001	PSU	C5-C6-N1	-2.03	119.07	122.11
83	At	8	4SU	O2-C2-N1	-2.03	120.09	122.79
1	S2	116	OMU	O2-C2-N1	-2.03	120.09	122.79
1	S2	1347	PSU	C5-C6-N1	-2.02	119.08	122.11
1	S2	651	PSU	C5-C6-N1	-2.01	119.09	122.11
3	L5	1522	OMG	O6-C6-C5	-2.01	120.45	124.37
1	S2	1842	4AC	O2-C2-N3	-2.01	119.06	122.33
3	L5	4494	OMG	C8-N7-C5	2.01	106.81	102.99
1	S2	116	OMU	C1'-N1-C2	2.00	121.20	117.57
3	L5	4521	PSU	O4'-C1'-C2'	2.00	107.97	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	4403	PSU	C5-C6-N1	-2.00	119.11	122.11
2	L8	55	PSU	C5-C6-N1	-2.00	119.11	122.11

There are no chirality outliers.

All (199) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L8	14	OMU	C1'-C2'-O2'-CM2
6	SA	2	SAC	C-CA-N-C1A
6	SA	2	SAC	C-CA-CB-OG
29	SV	1	AME	OT-CT1-N-CA
40	LB	245	HIC	CA-CB-CG-ND1
66	Lb	5	MLZ	N-CA-CB-CG
66	Lb	5	MLZ	C-CA-CB-CG
83	At	46	7MG	O4'-C4'-C5'-O5'
83	At	46	7MG	C3'-C4'-C5'-O5'
84	Pt	21	H2U	O4'-C4'-C5'-O5'
84	Pt	21	H2U	O4'-C1'-N1-C6
84	Pt	21	H2U	C2'-C1'-N1-C2
84	Pt	21	H2U	C2'-C1'-N1-C6
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	121	OMU	C1'-C2'-O2'-CM2
1	S2	166	A2M	C1'-C2'-O2'-CM'
1	S2	354	OMU	C3'-C4'-C5'-O5'
1	S2	354	OMU	O4'-C4'-C5'-O5'
1	S2	428	OMU	C2'-C1'-N1-C6
1	S2	468	A2M	C1'-C2'-O2'-CM'
1	S2	576	A2M	C3'-C4'-C5'-O5'
1	S2	644	OMG	O4'-C4'-C5'-O5'
1	S2	644	OMG	C3'-C4'-C5'-O5'
1	S2	644	OMG	C1'-C2'-O2'-CM2
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	C1'-C2'-O2'-CM'
1	S2	1337	4AC	O7-C7-N4-C4
1	S2	1337	4AC	CM7-C7-N4-C4
1	S2	1383	A2M	C1'-C2'-O2'-CM'
1	S2	1391	OMC	C1'-C2'-O2'-CM2
1	S2	1442	OMU	O4'-C4'-C5'-O5'
1	S2	1447	OMG	C1'-C2'-O2'-CM2
1	S2	1678	A2M	C1'-C2'-O2'-CM'
1	S2	1804	OMU	C1'-C2'-O2'-CM2
1	S2	1832	6MZ	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
1	S2	1832	6MZ	N1-C6-N6-C9
1	S2	1842	4AC	N3-C4-N4-C7
1	S2	1842	4AC	C5-C4-N4-C7
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1326	A2M	C3'-C4'-C5'-O5'
3	L5	1582	PSU	C3'-C4'-C5'-O5'
3	L5	2415	OMU	C1'-C2'-O2'-CM2
3	L5	2422	OMC	C1'-C2'-O2'-CM2
3	L5	2424	OMG	O4'-C4'-C5'-O5'
3	L5	2424	OMG	C3'-C4'-C5'-O5'
3	L5	2424	OMG	C1'-C2'-O2'-CM2
3	L5	2632	PSU	C2'-C1'-C5-C4
3	L5	2632	PSU	C3'-C4'-C5'-O5'
3	L5	2632	PSU	O4'-C4'-C5'-O5'
3	L5	2815	A2M	C1'-C2'-O2'-CM'
3	L5	3723	A2M	C1'-C2'-O2'-CM'
3	L5	3724	A2M	C1'-C2'-O2'-CM'
3	L5	3785	A2M	C3'-C4'-C5'-O5'
3	L5	3818	UY1	C2'-C1'-C5-C6
3	L5	3867	A2M	C3'-C4'-C5'-O5'
3	L5	3887	OMC	C3'-C4'-C5'-O5'
3	L5	3887	OMC	O4'-C4'-C5'-O5'
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4227	OMU	C1'-C2'-O2'-CM2
3	L5	4420	PSU	C2'-C1'-C5-C4
3	L5	4420	PSU	C2'-C1'-C5-C6
3	L5	4471	PSU	C3'-C4'-C5'-O5'
3	L5	4471	PSU	O4'-C4'-C5'-O5'
3	L5	4523	A2M	C1'-C2'-O2'-CM'
3	L5	4531	PSU	O4'-C4'-C5'-O5'
3	L5	4571	A2M	C1'-C2'-O2'-CM'
3	L5	4590	A2M	C4'-C5'-O5'-P
3	L5	4618	OMG	C1'-C2'-O2'-CM2
3	L5	4636	PSU	C2'-C1'-C5-C6
3	L5	4637	OMG	C1'-C2'-O2'-CM2
81	5A	50	5CT	NZ-C1-C2-C3
81	5A	50	5CT	NZ-C1-C2-O1
81	5A	50	5CT	C2-C3-C4-N1
64	Lr	2	SAC	OAC-C1A-N-CA
81	5A	50	5CT	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
81	5A	50	5CT	CG-CD-CE-NZ
1	S2	428	OMU	C2'-C1'-N1-C2
84	Pt	21	H2U	C3'-C4'-C5'-O5'
1	S2	159	A2M	C3'-C4'-C5'-O5'
1	S2	627	OMU	O4'-C4'-C5'-O5'
1	S2	867	OMG	C3'-C4'-C5'-O5'
1	S2	1678	A2M	C3'-C4'-C5'-O5'
3	L5	1781	PSU	C3'-C4'-C5'-O5'
6	SA	2	SAC	OAC-C1A-N-CA
1	S2	159	A2M	O4'-C4'-C5'-O5'
1	S2	576	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
1	S2	867	OMG	O4'-C4'-C5'-O5'
1	S2	1639	G7M	O4'-C4'-C5'-O5'
1	S2	1639	G7M	C3'-C4'-C5'-O5'
3	L5	1781	PSU	O4'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	4228	OMG	C3'-C4'-C5'-O5'
3	L5	4531	PSU	C3'-C4'-C5'-O5'
66	Lb	5	MLZ	CA-CB-CG-CD
3	L5	1625	OMG	C3'-C2'-O2'-CM2
79	Lo	53	MLZ	CA-CB-CG-CD
3	L5	3701	OMC	C2'-C1'-N1-C6
1	S2	1248	B8N	C32-C31-N3-C4
1	S2	867	OMG	C4'-C5'-O5'-P
3	L5	4228	OMG	O4'-C4'-C5'-O5'
3	L5	4420	PSU	C3'-C4'-C5'-O5'
6	SA	2	SAC	N-CA-CB-OG
6	SA	2	SAC	C2A-C1A-N-CA
3	L5	4447	5MC	C2'-C1'-N1-C6
83	At	16	H2U	C4'-C5'-O5'-P
3	L5	3818	UY1	C4'-C5'-O5'-P
84	Pt	47	G7M	O4'-C4'-C5'-O5'
1	S2	218	PSU	C3'-C4'-C5'-O5'
1	S2	218	PSU	O4'-C4'-C5'-O5'
1	S2	1243	PSU	O4'-C4'-C5'-O5'
1	S2	1678	A2M	O4'-C4'-C5'-O5'
3	L5	1582	PSU	O4'-C4'-C5'-O5'
3	L5	2839	PSU	C3'-C4'-C5'-O5'
3	L5	2839	PSU	O4'-C4'-C5'-O5'
3	L5	3867	A2M	O4'-C4'-C5'-O5'
1	S2	1851	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	3729	PSU	O4'-C4'-C5'-O5'
3	L5	3782	5MC	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C2
1	S2	428	OMU	O4'-C4'-C5'-O5'
81	5A	50	5CT	C1-C2-C3-C4
84	Pt	33	OMC	C1'-C2'-O2'-CM2
1	S2	159	A2M	C1'-C2'-O2'-CM'
1	S2	512	A2M	C1'-C2'-O2'-CM'
3	L5	1340	OMC	C1'-C2'-O2'-CM2
3	L5	2364	OMG	C1'-C2'-O2'-CM2
3	L5	3744	OMG	C1'-C2'-O2'-CM2
3	L5	3867	A2M	C1'-C2'-O2'-CM'
3	L5	4620	OMU	C1'-C2'-O2'-CM2
1	S2	1248	B8N	C32-C31-N3-C2
83	At	46	7MG	C4'-C5'-O5'-P
1	S2	644	OMG	C4'-C5'-O5'-P
3	L5	1326	A2M	C4'-C5'-O5'-P
81	5A	50	5CT	CD-CE-NZ-C1
3	L5	4420	PSU	O4'-C4'-C5'-O5'
29	SV	1	AME	C-CA-N-CT1
1	S2	428	OMU	O4'-C1'-N1-C2
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	4447	5MC	O4'-C1'-N1-C6
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	3785	A2M	C4'-C5'-O5'-P
84	Pt	47	G7M	C3'-C4'-C5'-O5'
1	S2	1851	MA6	C4'-C5'-O5'-P
1	S2	428	OMU	O4'-C1'-N1-C6
3	L5	4447	5MC	O4'-C1'-N1-C2
3	L5	4500	PSU	C4'-C5'-O5'-P
1	S2	683	OMG	O4'-C4'-C5'-O5'
1	S2	1447	OMG	C3'-C4'-C5'-O5'
3	L5	4637	OMG	O4'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C2
3	L5	3701	OMC	O4'-C1'-N1-C2
1	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	3844	PSU	C4'-C5'-O5'-P
1	S2	428	OMU	C3'-C4'-C5'-O5'
40	LB	245	HIC	CA-CB-CG-CD2
3	L5	2422	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S2	863	PSU	O4'-C1'-C5-C4
1	S2	918	PSU	O4'-C1'-C5-C4
3	L5	3818	UY1	O4'-C1'-C5-C4
84	Pt	21	H2U	O4'-C1'-N1-C2
1	S2	1243	PSU	C3'-C4'-C5'-O5'
3	L5	1534	A2M	O4'-C4'-C5'-O5'
3	L5	2364	OMG	C3'-C4'-C5'-O5'
77	Lm	98	M3L	CD-CE-NZ-CM3
3	L5	3729	PSU	C3'-C4'-C5'-O5'
3	L5	3782	5MC	C3'-C4'-C5'-O5'
1	S2	116	OMU	C1'-C2'-O2'-CM2
1	S2	462	OMC	C1'-C2'-O2'-CM2
1	S2	683	OMG	C1'-C2'-O2'-CM2
3	L5	3830	A2M	C1'-C2'-O2'-CM'
20	SX	62	HY3	O-C-CA-C3
81	5A	50	5CT	C2-C1-NZ-CE
77	Lm	98	M3L	CD-CE-NZ-CM2
1	S2	1248	B8N	N34-C33-C34-O36
1	S2	863	PSU	O4'-C1'-C5-C6
1	S2	918	PSU	O4'-C1'-C5-C6
1	S2	1326	UY1	O4'-C1'-C5-C6
3	L5	3818	UY1	O4'-C1'-C5-C6
3	L5	4636	PSU	O4'-C1'-C5-C6
84	Pt	33	OMC	C2'-C1'-N1-C2
1	S2	590	A2M	C3'-C4'-C5'-O5'
1	S2	683	OMG	C3'-C4'-C5'-O5'
1	S2	1288	OMU	C3'-C4'-C5'-O5'
3	L5	2351	OMC	O4'-C4'-C5'-O5'
1	S2	822	PSU	O4'-C4'-C5'-O5'
3	L5	4636	PSU	O4'-C4'-C5'-O5'
3	L5	4637	OMG	C3'-C4'-C5'-O5'
77	Lm	98	M3L	CE-CD-CG-CB
40	LB	245	HIC	C-CA-CB-CG
39	LA	216	V5N	O-C-CA-CB
1	S2	218	PSU	C4'-C5'-O5'-P
1	S2	1081	PSU	C4'-C5'-O5'-P
77	Lm	98	M3L	N-CA-CB-CG
84	Pt	33	OMC	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 362 ligands modelled in this entry, 350 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
89	SPD	L5	5307	-	9,9,9	0.32	0	8,8,8	0.66	0
85	PUT	L5	5305	-	5,5,5	0.12	0	4,4,4	0.15	0
89	SPD	L5	5303	-	9,9,9	0.39	0	8,8,8	0.87	0
85	PUT	L5	5308	-	5,5,5	0.16	0	4,4,4	0.22	0
85	PUT	S2	1901	-	5,5,5	0.11	0	4,4,4	0.14	0
88	ANM	L5	5301	86	20,20,20	1.13	1 (5%)	22,27,27	1.50	4 (18%)
89	SPD	L5	5302	-	9,9,9	0.37	0	8,8,8	0.90	0
92	MET	Pt	78	84	6,7,8	0.52	0	2,7,9	2.25	1 (50%)
89	SPD	L5	5306	-	9,9,9	0.16	0	8,8,8	0.24	0
90	3H3	L5	5310	-	33,34,34	3.43	12 (36%)	34,45,45	4.07	16 (47%)
89	SPD	L5	5304	-	9,9,9	0.20	0	8,8,8	0.22	0
85	PUT	L5	5309	-	5,5,5	0.17	0	4,4,4	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5307	-	-	0/7/7/7	-
85	PUT	L5	5305	-	-	1/3/3/3	-
89	SPD	L5	5303	-	-	3/7/7/7	-
85	PUT	L5	5308	-	-	1/3/3/3	-
85	PUT	S2	1901	-	-	1/3/3/3	-
88	ANM	L5	5301	86	-	4/10/23/23	0/2/2/2
89	SPD	L5	5302	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	MET	Pt	78	84	-	1/5/6/8	-
89	SPD	L5	5306	-	-	1/7/7/7	-
90	3H3	L5	5310	-	-	17/39/51/51	0/1/2/2
89	SPD	L5	5304	-	-	5/7/7/7	-
85	PUT	L5	5309	-	-	3/3/3/3	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	L5	5310	3H3	C13-C12	9.48	1.53	1.33
90	L5	5310	3H3	O3-C22	7.98	1.39	1.23
90	L5	5310	3H3	O4-C23	7.51	1.38	1.23
90	L5	5310	3H3	C23-N	6.64	1.48	1.37
90	L5	5310	3H3	C22-N	6.41	1.48	1.37
90	L5	5310	3H3	C3-C2	5.17	1.54	1.33
88	L5	5301	ANM	O2-C5	4.57	1.45	1.35
90	L5	5310	3H3	C4-C3	3.12	1.53	1.44
90	L5	5310	3H3	C19-C20	3.06	1.57	1.53
90	L5	5310	3H3	O1-C10	2.85	1.40	1.34
90	L5	5310	3H3	O1-C11	-2.66	1.39	1.44
90	L5	5310	3H3	C24-C20	-2.30	1.49	1.53
90	L5	5310	3H3	O2-C16	-2.12	1.18	1.21

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
90	L5	5310	3H3	C22-N-C23	-11.50	111.83	125.78
90	L5	5310	3H3	O4-C23-N	-8.54	106.75	120.28
90	L5	5310	3H3	O3-C22-N	-7.61	108.22	120.28
90	L5	5310	3H3	O3-C22-C21	-7.02	108.95	122.62
90	L5	5310	3H3	O4-C23-C24	-6.86	109.26	122.62
90	L5	5310	3H3	C1-C2-C3	-6.11	113.30	126.16
90	L5	5310	3H3	C25-C12-C13	-4.77	110.90	123.45
90	L5	5310	3H3	O1-C11-C1	4.48	112.17	106.31
90	L5	5310	3H3	C24-C23-N	-4.34	110.63	115.95
88	L5	5301	ANM	O2-C5-C6	4.15	118.72	111.09
90	L5	5310	3H3	C1-C11-C12	-4.01	105.89	113.89
90	L5	5310	3H3	C8-C9-C10	-3.81	113.20	122.92
90	L5	5310	3H3	C21-C22-N	-3.81	111.28	115.95
90	L5	5310	3H3	C19-C18-C17	-3.56	106.09	113.19
92	Pt	78	MET	CE-SD-CG	3.17	111.30	100.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
90	L5	5310	3H3	C11-C12-C13	-2.86	112.19	120.93
90	L5	5310	3H3	C25-C12-C11	-2.80	110.84	115.68
88	L5	5301	ANM	O2-C5-O3	-2.34	118.31	122.96
90	L5	5310	3H3	C6-C7-C8	-2.26	107.00	112.92
88	L5	5301	ANM	C3-C2-C16	-2.24	101.06	104.29
88	L5	5301	ANM	C14-O1-C9	2.01	121.87	117.51

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	L5	5310	3H3	C2-C1-C11-O1
90	L5	5310	3H3	C2-C1-C11-C12
90	L5	5310	3H3	C-C1-C11-O1
90	L5	5310	3H3	C-C1-C11-C12
90	L5	5310	3H3	C9-C10-O1-C11
90	L5	5310	3H3	C25-C12-C13-C14
90	L5	5310	3H3	C1-C11-C12-C25
90	L5	5310	3H3	O1-C11-C12-C25
92	Pt	78	MET	CA-CB-CG-SD
90	L5	5310	3H3	C2-C3-C4-C5
90	L5	5310	3H3	O-C10-O1-C11
89	L5	5303	SPD	N6-C7-C8-C9
89	L5	5303	SPD	C4-C5-N6-C7
89	L5	5304	SPD	C4-C5-N6-C7
85	S2	1901	PUT	C1-C2-C3-C4
85	L5	5308	PUT	C1-C2-C3-C4
85	L5	5309	PUT	C1-C2-C3-C4
89	L5	5304	SPD	N6-C7-C8-C9
85	L5	5309	PUT	C2-C3-C4-N2
88	L5	5301	ANM	C11-C12-C15-C16
88	L5	5301	ANM	C13-C12-C15-C16
89	L5	5304	SPD	C7-C8-C9-N10
89	L5	5303	SPD	C8-C7-N6-C5
90	L5	5310	3H3	C12-C11-O1-C10
90	L5	5310	3H3	C12-C13-C14-C15
89	L5	5304	SPD	C2-C3-C4-C5
89	L5	5306	SPD	N1-C2-C3-C4
90	L5	5310	3H3	C16-C17-C18-O5
90	L5	5310	3H3	C-C1-C2-C3
88	L5	5301	ANM	C1-C9-O1-C14
85	L5	5309	PUT	N1-C1-C2-C3

Continued on next page...

Continued from previous page...

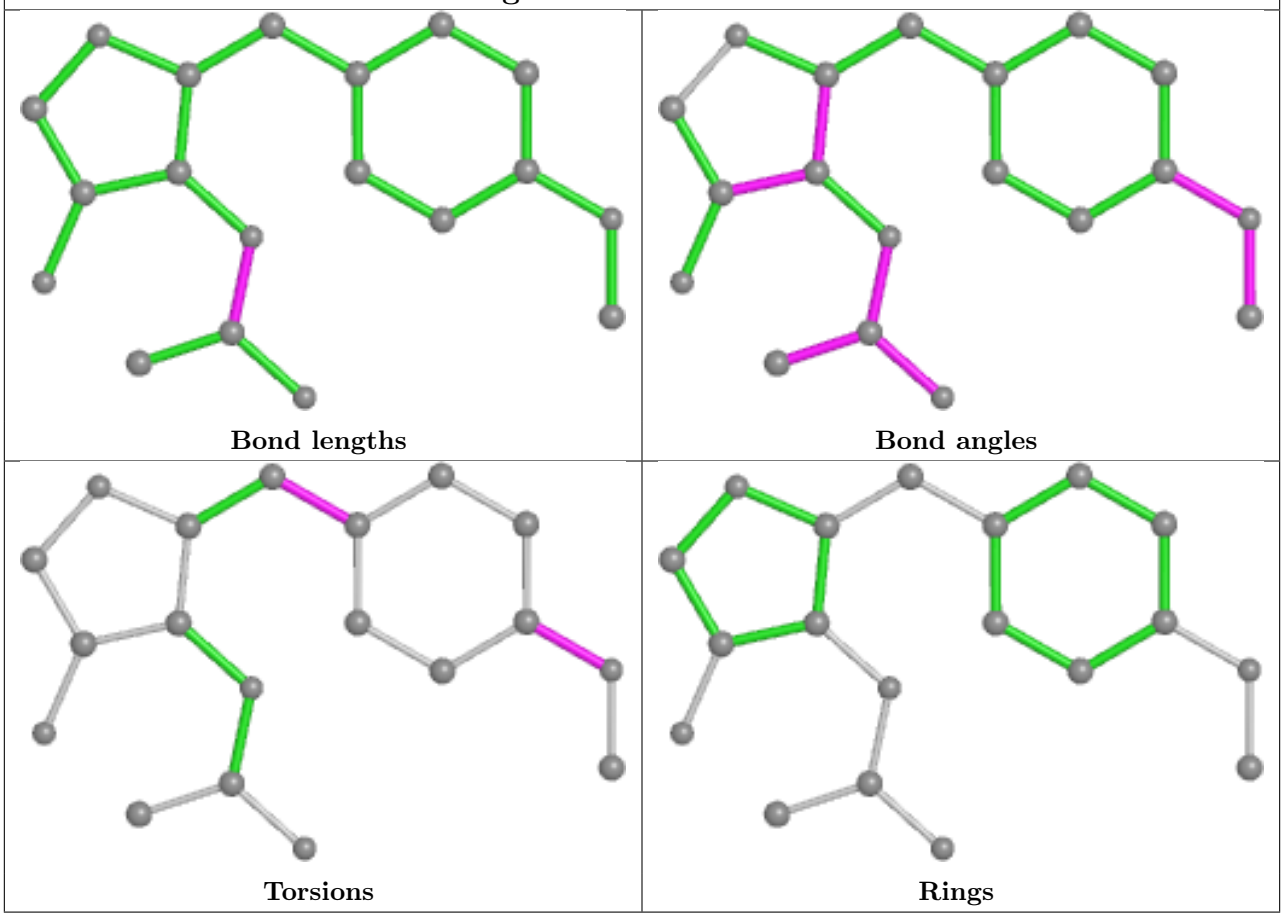
Mol	Chain	Res	Type	Atoms
89	L5	5304	SPD	N1-C2-C3-C4
88	L5	5301	ANM	C10-C9-O1-C14
90	L5	5310	3H3	C15-C14-C16-C17
90	L5	5310	3H3	C15-C14-C16-O2
85	L5	5305	PUT	C1-C2-C3-C4
90	L5	5310	3H3	C12-C13-C14-C16

There are no ring outliers.

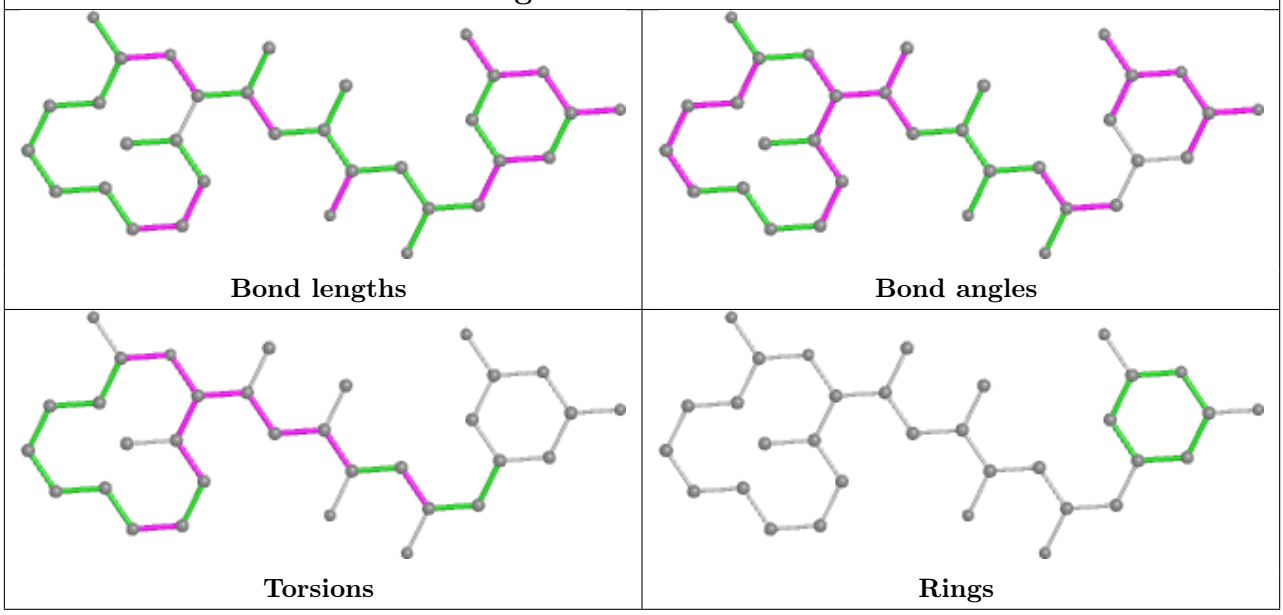
No monomer is involved in short contacts.

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

Ligand ANM L5 5301



Ligand 3H3 L5 5310



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.

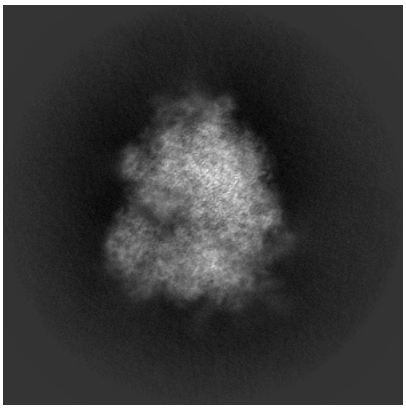
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-29760. These allow visual inspection of the internal detail of the map and identification of artifacts.

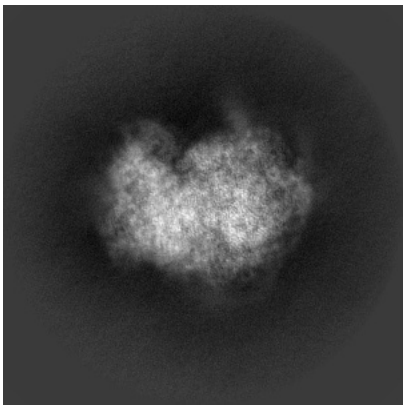
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

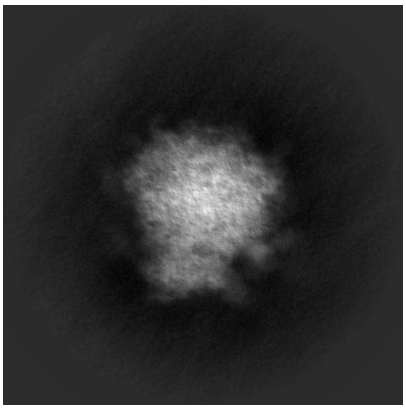
6.1.1 Primary map



X

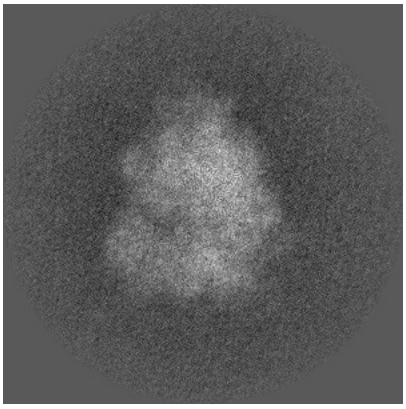


Y

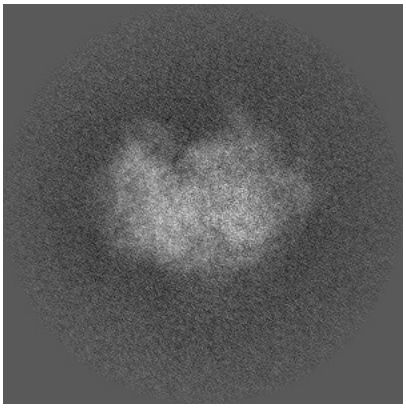


Z

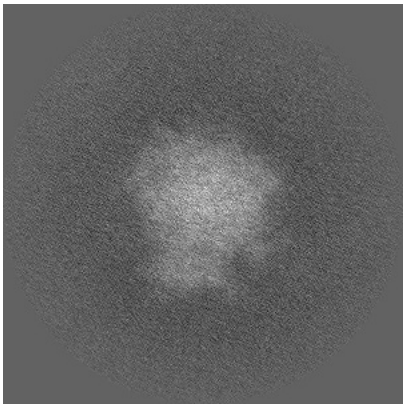
6.1.2 Raw map



X



Y

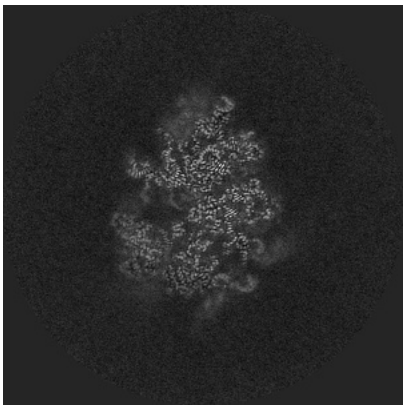


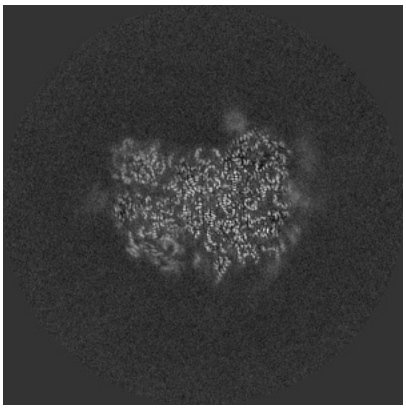
Z

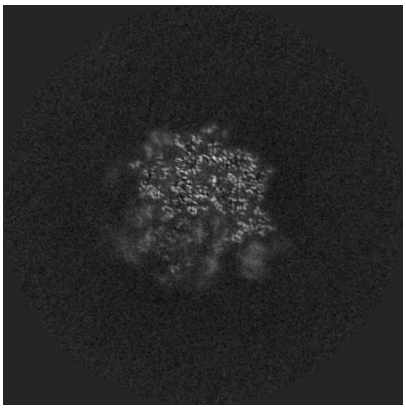
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

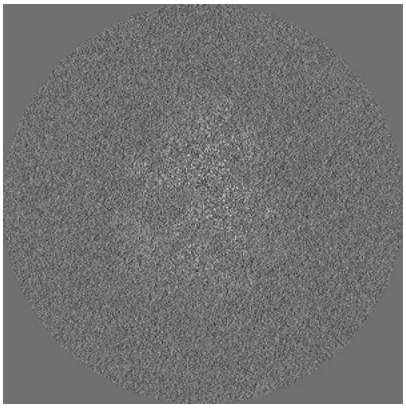
6.2.1 Primary map

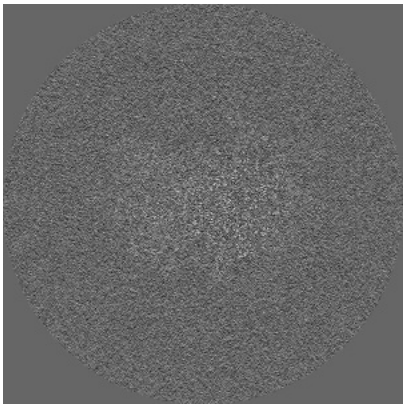

X Index: 320

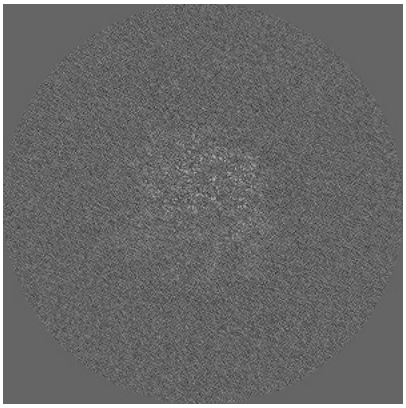

Y Index: 320


Z Index: 320

6.2.2 Raw map


X Index: 320

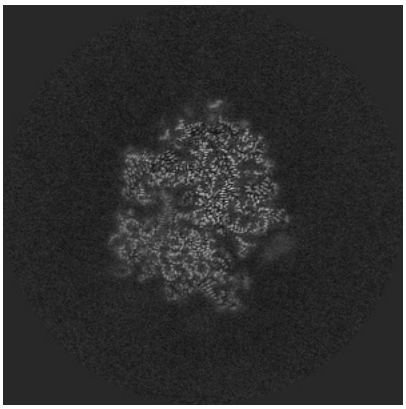

Y Index: 320

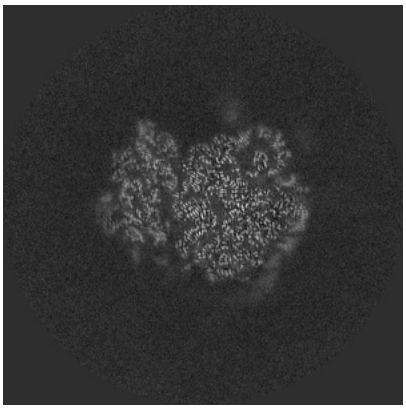

Z Index: 320

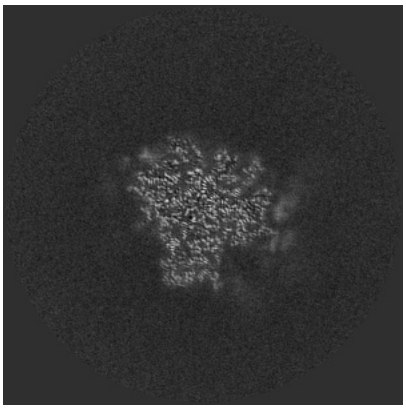
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

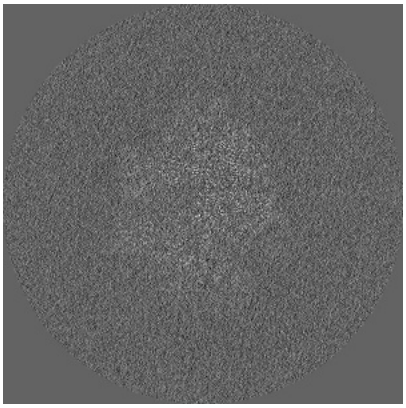
6.3.1 Primary map

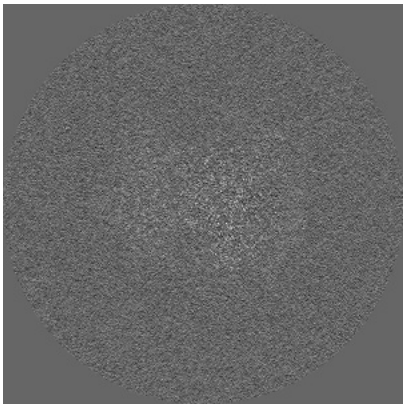

X Index: 298

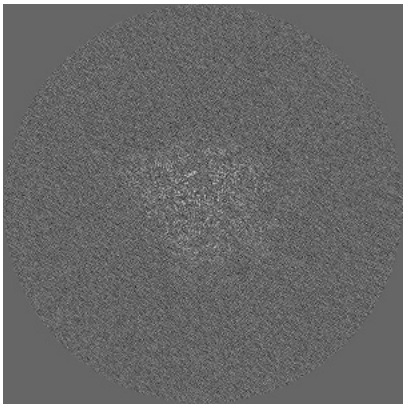

Y Index: 341


Z Index: 376

6.3.2 Raw map


X Index: 304

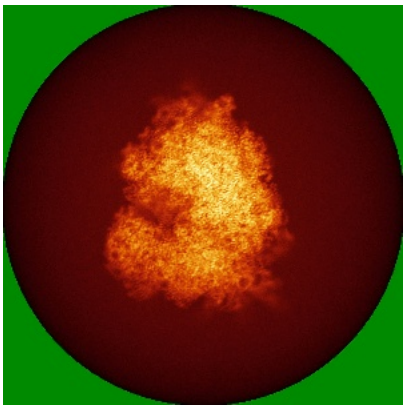

Y Index: 332

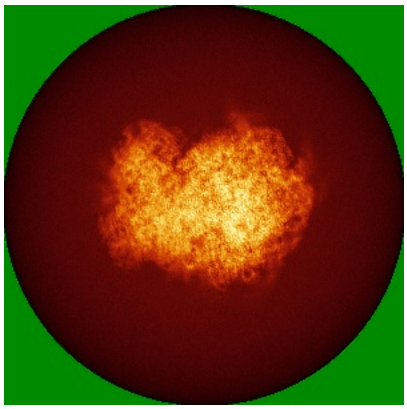

Z Index: 355

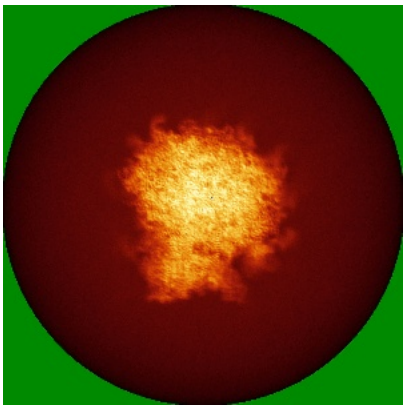
The images above show the largest variance slices of the map in three orthogonal directions.

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

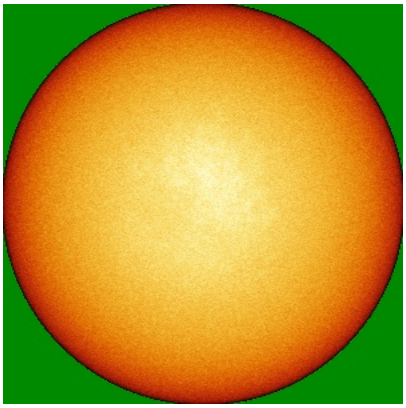
6.4.1 Primary map

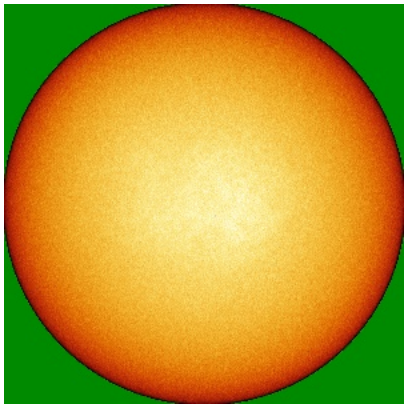

X

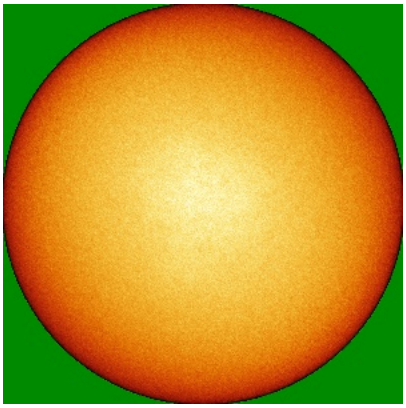

Y


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.

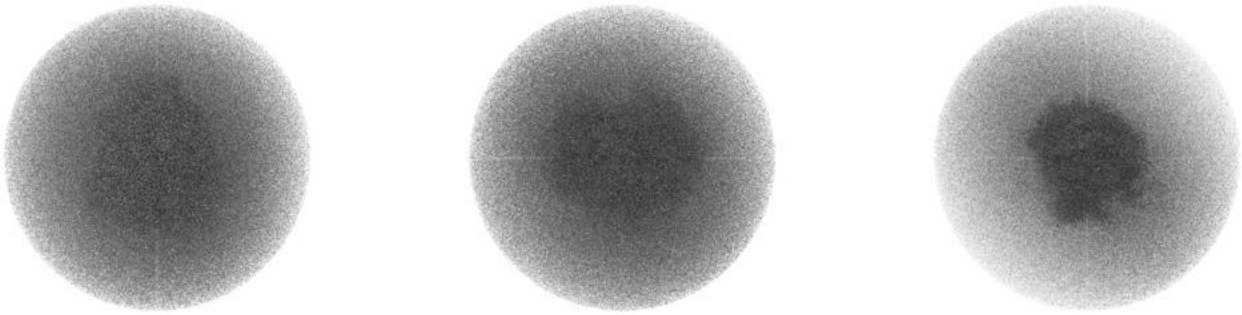
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

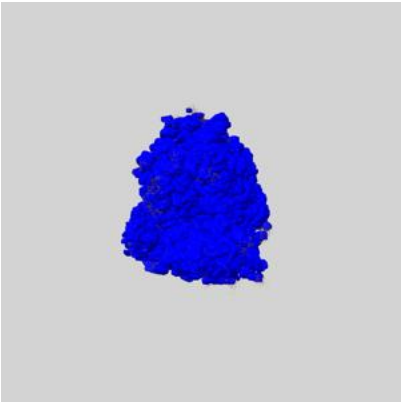
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

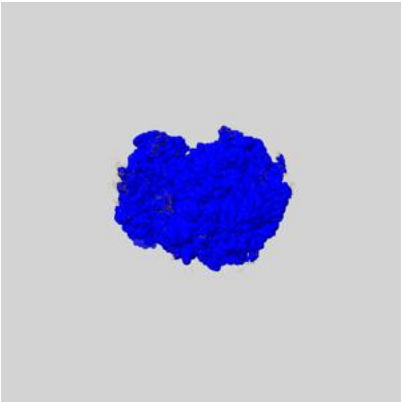
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

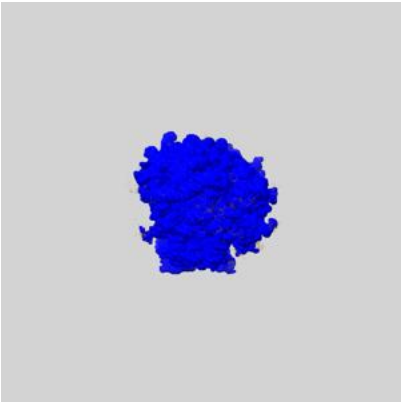
6.6.1 emd_29760_msk_1.map (i)



X



Y

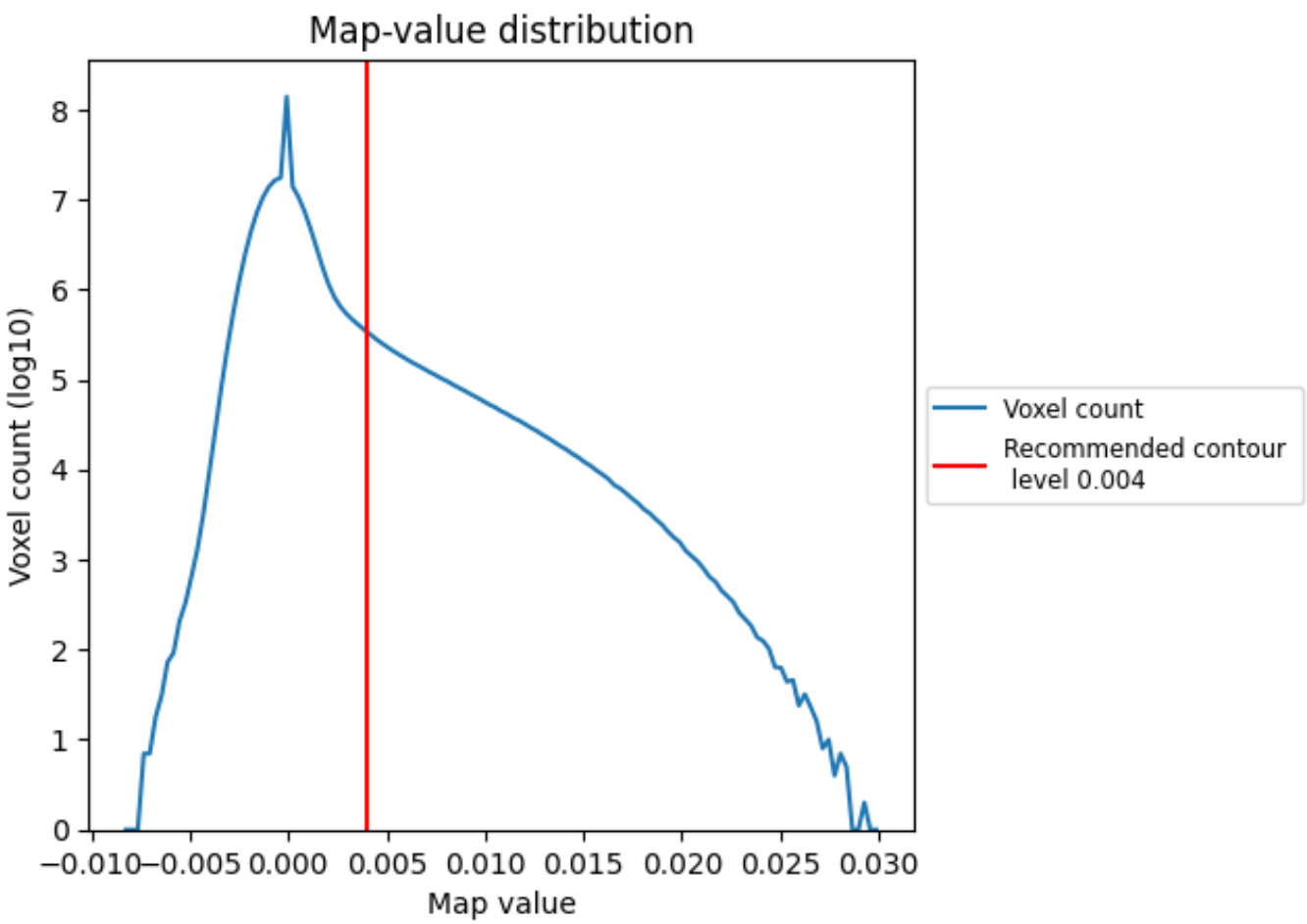


Z

7 Map analysis (i)

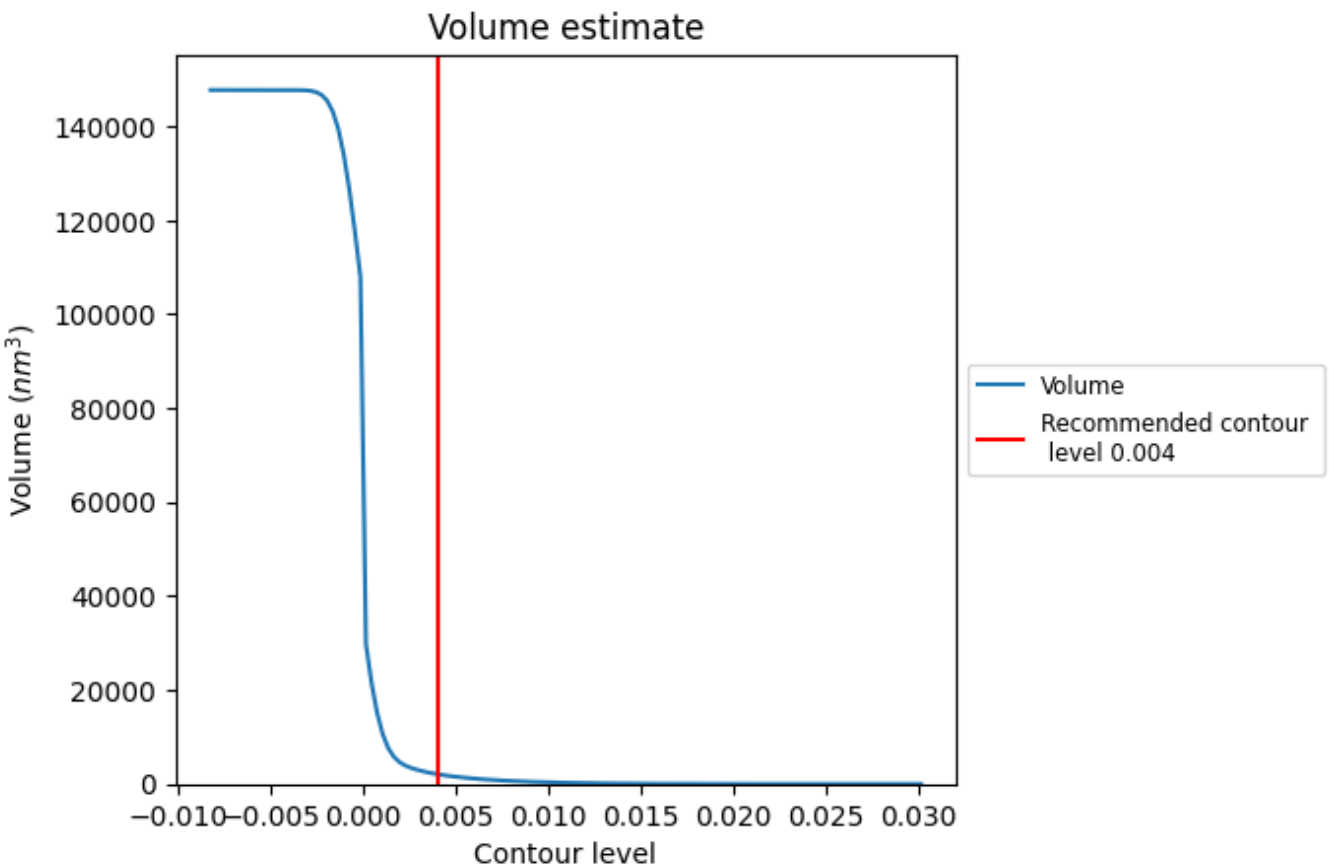
This section contains the results of statistical analysis of the map.

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.

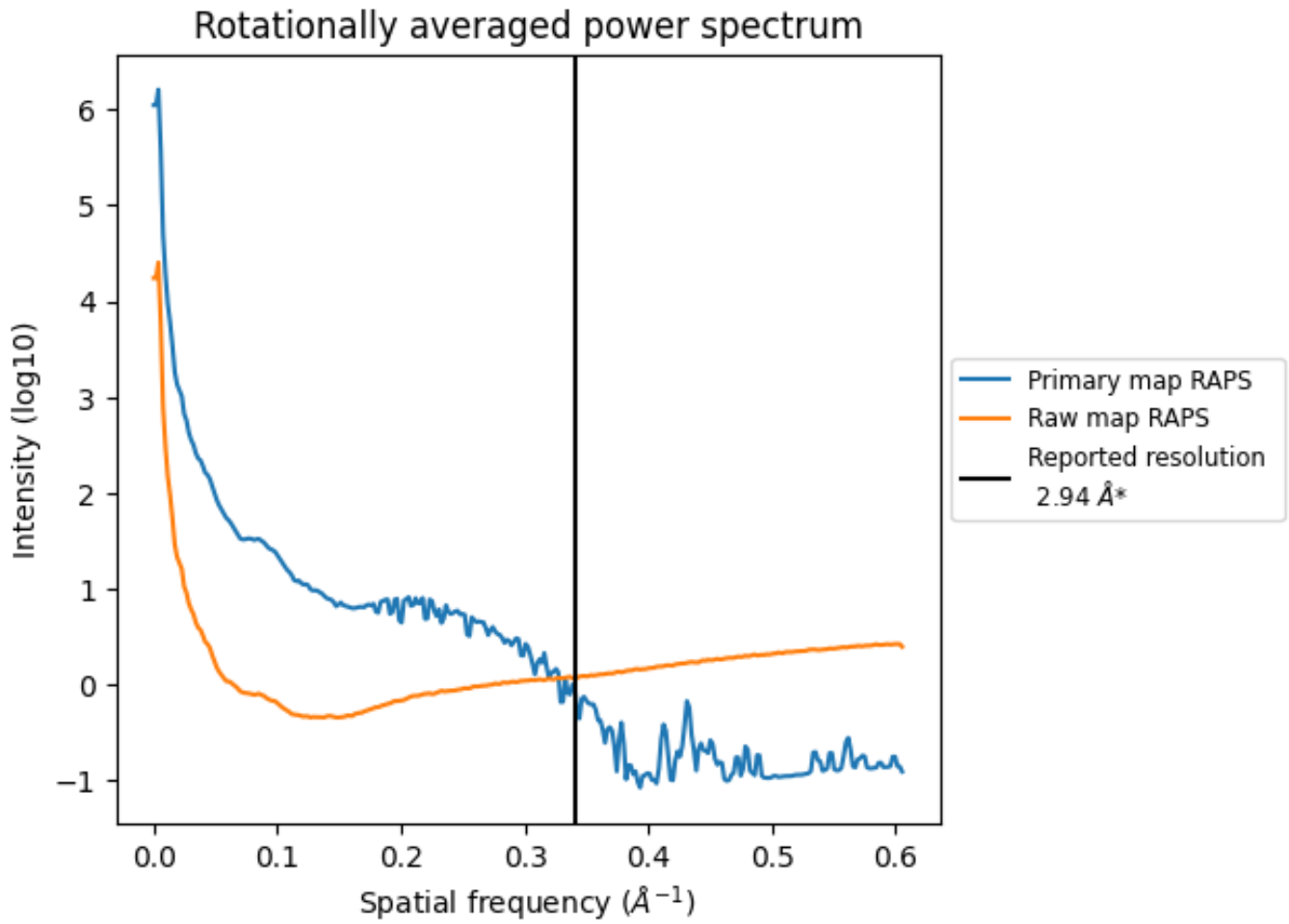
7.2 Volume estimate (i)



The volume at the recommended contour level is 2088 nm^3; this corresponds to an approximate mass of 1886 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)

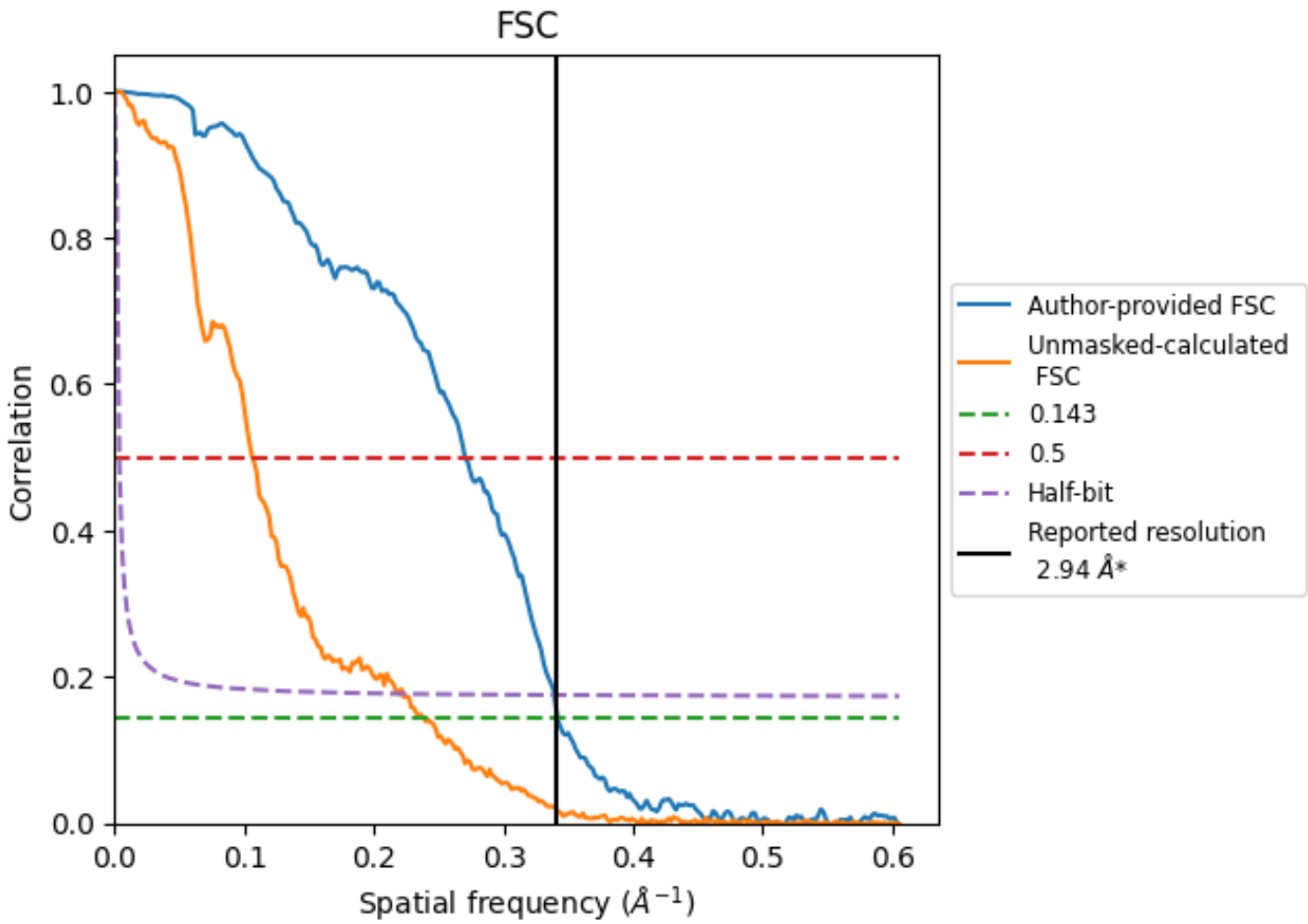


*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

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 0.340 Å^{-1}

8.2 Resolution estimates (i)

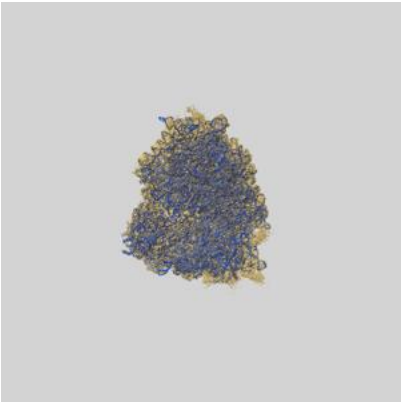
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.92	3.70	2.95
Unmasked-calculated*	4.19	9.40	4.56

*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 4.19 differs from the reported value 2.94 by more than 10 %

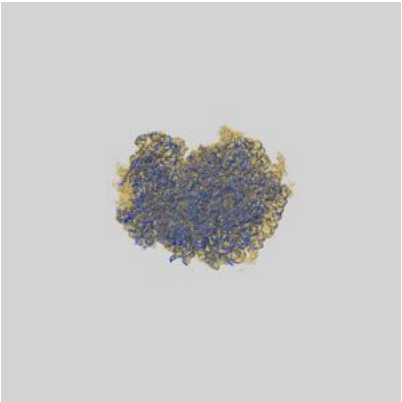
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-29760 and PDB model 8G61. Per-residue inclusion information can be found in section 3 on page 24.

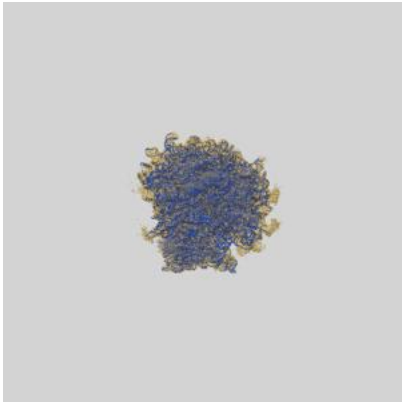
9.1 Map-model overlay (i)



X



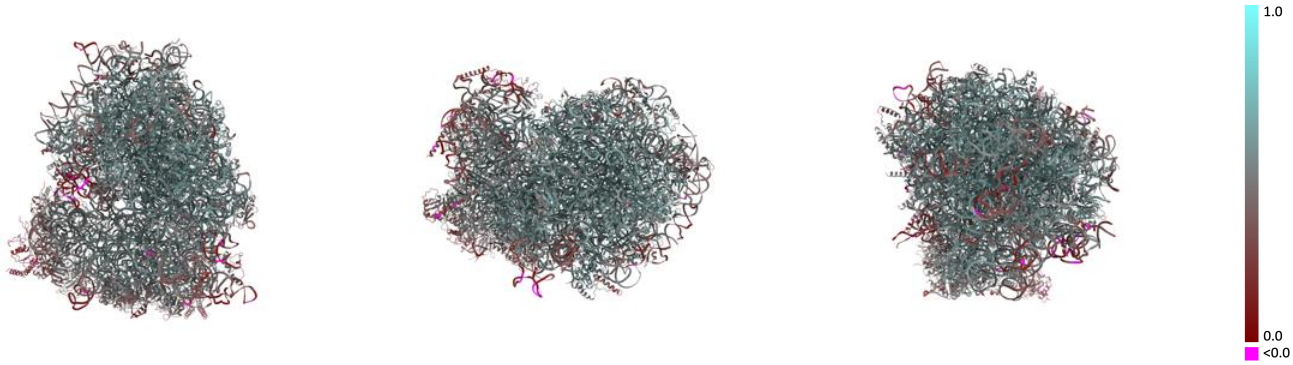
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

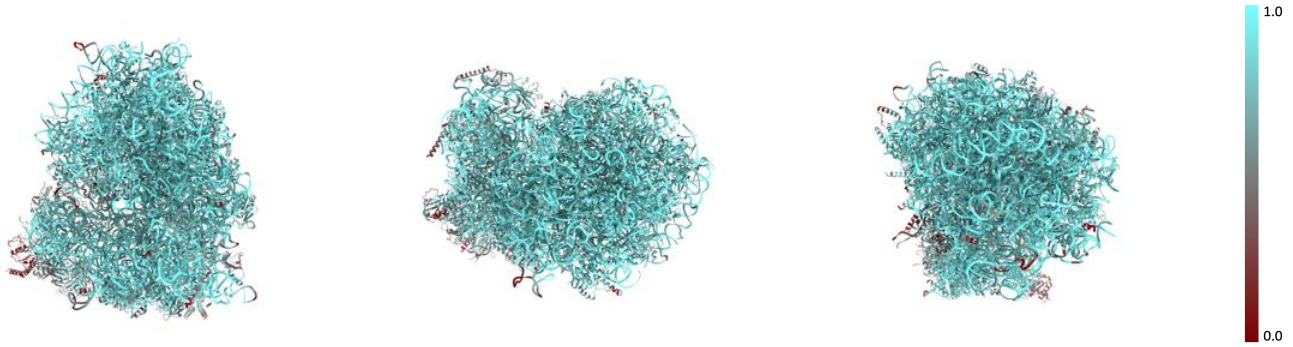
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

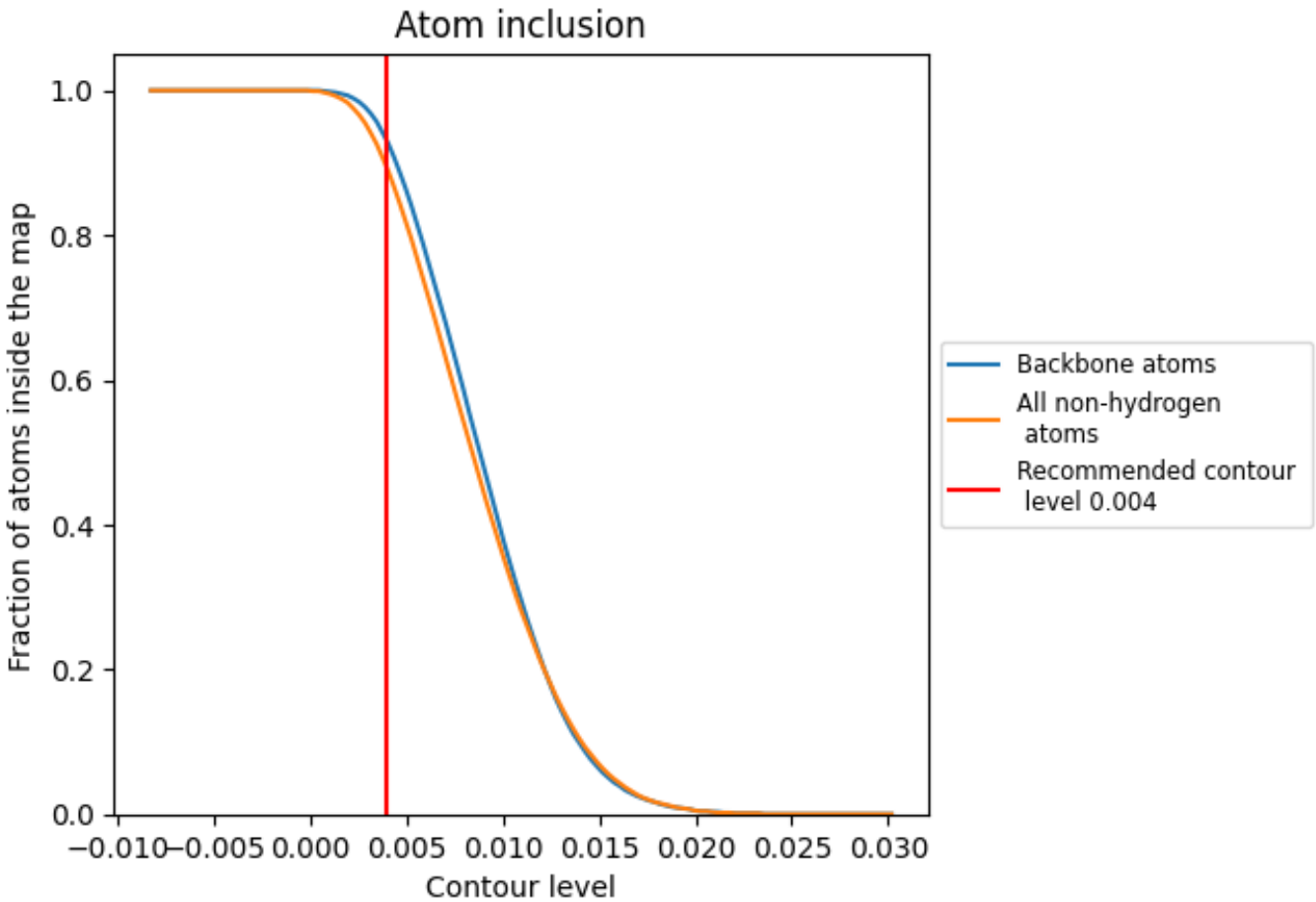
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.5100
5A	0.5460	0.4450
At	0.7180	0.4270
L5	0.9520	0.5290
L7	0.9880	0.5760
L8	0.9810	0.5630
LA	0.9410	0.6010
LB	0.9020	0.5770
LC	0.9140	0.5770
LD	0.8790	0.5230
LE	0.8720	0.5410
LF	0.9250	0.5730
LG	0.8020	0.5020
LH	0.8690	0.5390
LI	0.9030	0.5570
LJ	0.8250	0.4720
LL	0.8800	0.5470
LM	0.9020	0.5500
LN	0.9780	0.6100
LO	0.9230	0.5770
LP	0.9300	0.5920
LQ	0.9490	0.6050
LR	0.8470	0.5160
LS	0.9470	0.5870
LT	0.9130	0.5760
LU	0.8020	0.4820
LV	0.9250	0.5810
LW	0.6940	0.4220
LX	0.9190	0.5650
LY	0.9030	0.5590
LZ	0.8770	0.5340
La	0.9510	0.6000
Lb	0.8060	0.4950
Lc	0.8410	0.5400
Ld	0.8890	0.5550

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Chain	Atom inclusion	Q-score
Le	0.9630	0.6070
Lf	0.9530	0.6030
Lg	0.8900	0.5680
Lh	0.8860	0.5450
Li	0.8860	0.5270
Lj	0.9670	0.6080
Lk	0.8060	0.5110
Ll	0.9310	0.5630
Lm	0.8990	0.5580
Ln	0.9380	0.5690
Lo	0.9010	0.5670
Lp	0.9000	0.5740
Lr	0.9190	0.5810
Lz	0.3610	0.3050
Pt	0.8110	0.4480
S2	0.9560	0.4870
SA	0.7540	0.4380
SB	0.7030	0.3990
SC	0.8190	0.4990
SD	0.7200	0.4450
SE	0.8250	0.4810
SF	0.7770	0.4490
SG	0.7270	0.4140
SH	0.6270	0.3820
SI	0.8160	0.4800
SJ	0.7940	0.4410
SK	0.7110	0.4050
SL	0.8550	0.5270
SM	0.1570	0.1880
SN	0.8120	0.4880
SO	0.7690	0.4310
SP	0.7300	0.3990
SQ	0.8200	0.4540
SR	0.6540	0.3790
SS	0.7660	0.4380
ST	0.8360	0.4680
SU	0.7440	0.4190
SV	0.7760	0.4720
SW	0.8770	0.5250
SX	0.9010	0.5380
SY	0.7510	0.4040
SZ	0.6240	0.4100

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Chain	Atom inclusion	Q-score
Sa	0.8520	0.4810
Sb	0.7210	0.4450
Sc	0.7030	0.4220
Sd	0.9220	0.5000
Se	0.7780	0.4480
Sf	0.4000	0.2380
Sg	0.5670	0.3550
mR	0.9710	0.5440