



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 18, 2018 – 04:18 PM EST

PDB ID : 6EK0
EMDB ID: : EMD-3883
Title : High-resolution cryo-EM structure of the human 80S ribosome
Authors : Natchiar, S.K.; Myasnikov, A.G.; Kratzat, H.; Hazemann, I.; Klaholz, B.P.
Deposited on : 2017-09-24
Resolution : 2.90 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

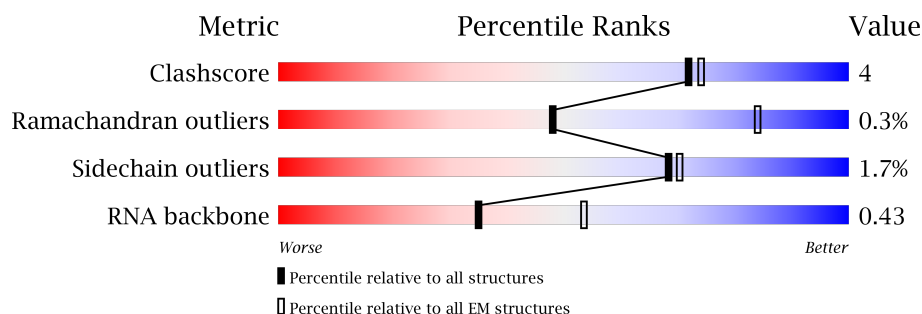
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.























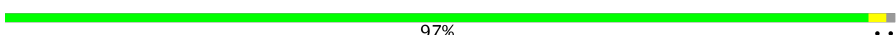




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	L5	5070	45% 24% 5% . 26%
2	L7	120	76% 23% .
3	L8	156	69% 24% 6% .
4	LA	257	81% 13% . .
5	LB	403	79% 20% .
6	LC	427	76% 10% 14%
7	LD	297	81% 18% .
8	LE	288	67% 15% 18%

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Mol	Chain	Length	Quality of chain
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	


















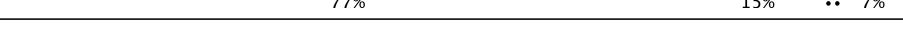


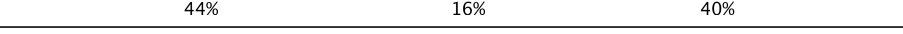
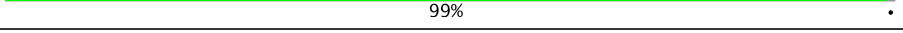
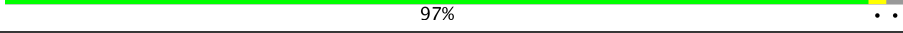
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Mol	Chain	Length	Quality of chain
34	Lf	110	95%
35	Lg	117	97%
36	Lh	123	98%
37	Li	105	95%
38	Lj	97	86%
39	Lk	70	99%
40	Ll	51	94%
41	Lm	128	41%
42	Ln	25	92%
43	Lo	106	99%
44	Lp	92	97%
45	Lr	137	90%
46	Lz	217	96%
47	S2	1869	59%
48	S6	75	47%
49	SA	295	61%
50	SB	264	72%
51	SD	243	78%
52	SE	263	87%
53	SF	204	75%
54	SH	194	77%
55	SI	208	75%
56	SK	165	52%
57	SL	158	84%
58	SP	145	78%

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Mol	Chain	Length	Quality of chain
59	SQ	146	 79% 21% .
60	SR	135	 86% 14%
61	SS	152	 75% 19% . 5%
62	ST	145	 90% 8% ..
63	SU	119	 76% 12% 13%
64	SV	83	 82% 17% .
65	SX	143	 81% 15% ..
66	Sa	115	 85% . 11%
67	Sc	69	 88% . 7%
68	Sd	56	 95% . .
69	Sg	317	 97% ..
70	SC	293	 63% 12% 24%
71	SG	249	 74% 21% 5%
72	SJ	194	 81% 12% . 5%
73	SM	132	 75% 15% . 8%
74	SN	151	 91% 8% ..
75	SO	151	 77% 15% .. 7%
76	SW	130	 86% 12% ..
77	SY	133	 89% 8% ..
78	SZ	125	 44% 16% 40%
79	Sb	84	 99% .
80	Se	59	 97% ..
81	Sf	156	 40% . 57%

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
1	B8Q	L5	1456	X	-	-	-
1	B9H	L5	2786	X	-	-	-
47	B8Q	S2	1219	X	-	-	-
47	E3C	S2	568	X	-	-	-

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 219596 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3773	Total	C	N	O	P	0	0
			80257	35772	14588	26125	3772		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L5	2113	C	G	conflict	GB 86475748

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	402	Total	C	N	O	S	1	0
			3244	2065	609	556	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	368	Total	C	N	O	S	0	0
			2928	1841	583	489	15		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

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

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

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	1	0
			870	547	178	139	6		

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

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

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

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

- Molecule 46 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S2	1740	Total	C	N	O	P	0	0
			36938	16495	6598	12106	1739		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	582	C	U	conflict	GB 36162
S2	583	C	A	conflict	GB 36162
S2	584	G	A	conflict	GB 36162
S2	798	A	G	conflict	GB 36162
S2	1095	U	C	conflict	GB 36162

- Molecule 48 is a RNA chain called Human initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S6	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 50 is a protein called 40S ribosomal protein S3a.

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

- Molecule 51 is a protein called 40S ribosomal protein S3.

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

- Molecule 52 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 54 is a protein called 40S ribosomal protein S7.

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

- Molecule 55 is a protein called 40S ribosomal protein S8.

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

- Molecule 56 is a protein called 40S ribosomal protein S10.

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

- Molecule 57 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 58 is a protein called 40S ribosomal protein S15.

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

- Molecule 59 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SQ	146	Total	C	N	O	S	0	0
			1158	736	218	200	4		

- Molecule 60 is a protein called 40S ribosomal protein S17.

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

- Molecule 61 is a protein called 40S ribosomal protein S18.

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

- Molecule 62 is a protein called 40S ribosomal protein S19.

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

- Molecule 63 is a protein called 40S ribosomal protein S20.

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

- Molecule 64 is a protein called 40S ribosomal protein S21.

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

- Molecule 65 is a protein called 40S ribosomal protein S23.

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

- Molecule 66 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sa	102	Total	C	N	O	S	1	0
			829	517	174	133	5		

- Molecule 67 is a protein called 40S ribosomal protein S28.

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

- Molecule 68 is a protein called 40S ribosomal protein S29.

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

- Molecule 69 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 70 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SC	222	Total	C	N	O	S	1	0
			1733	1120	301	302	10		

- Molecule 71 is a protein called 40S ribosomal protein S6.

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

- Molecule 72 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SJ	185	Total	C	N	O	S	1	0
			1533	974	309	248	2		

- Molecule 73 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SM	122	Total	C	N	O	S	0	0
			942	590	165	179	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P25398
SM	69	LEU	CYS	conflict	UNP P25398
SM	99	ASN	LYS	conflict	UNP P25398

- Molecule 74 is a protein called 40S ribosomal protein S13.

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

- Molecule 75 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SO	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 76 is a protein called 40S ribosomal protein S15a.

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

- Molecule 77 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SY	131	Total	C	N	O	S	1	0
			1073	678	212	178	5		

- Molecule 78 is a protein called 40S ribosomal protein S25.

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

- Molecule 79 is a protein called 40S ribosomal protein S27.

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

- Molecule 80 is a protein called 40S ribosomal protein S30.

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

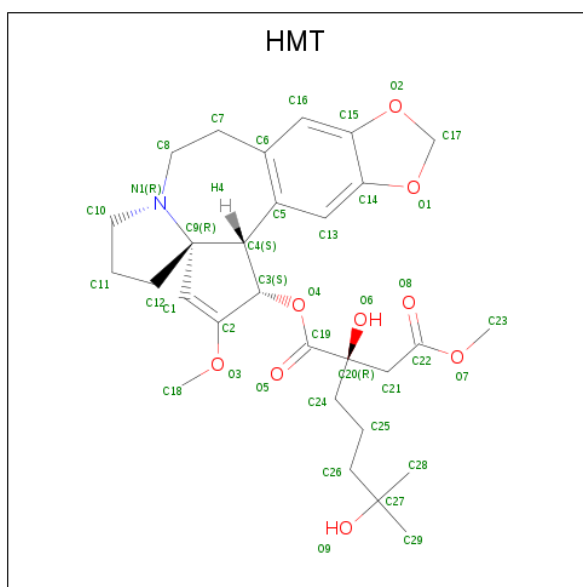
- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
82	L7	3	Total	Mg	0
			3	3	
82	LV	1	Total	Mg	0
			1	1	
82	Sd	1	Total	Mg	0
			1	1	
82	S2	134	Total	Mg	0
			134	134	
82	L8	6	Total	Mg	0
			6	6	
82	Le	1	Total	Mg	0
			1	1	
82	LN	1	Total	Mg	0
			1	1	
82	SF	1	Total	Mg	0
			1	1	
82	LP	1	Total	Mg	0
			1	1	
82	Lf	1	Total	Mg	0
			1	1	
82	L5	251	Total	Mg	0
			251	251	
82	LT	1	Total	Mg	0
			1	1	

- Molecule 83 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano
yl]cephalotaxine (three-letter code: HMT) (formula: C₂₉H₃₉NO₉).

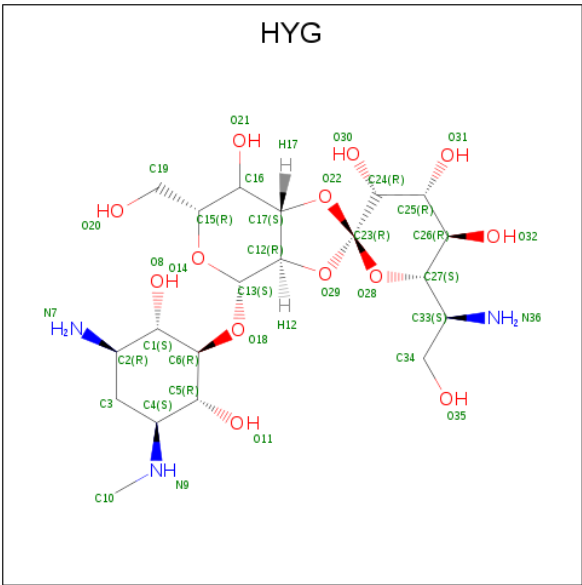


Mol	Chain	Residues	Atoms				AltConf
83	L5	1	Total	C	N	O	0
			39	29	1	9	

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 85 is HYGROMYCIN B (three-letter code: HYG) (formula: C₂₀H₃₇N₃O₁₃).



Mol	Chain	Residues	Atoms				AltConf
85	S2	1	Total	C	N	O	0
			36	20	3	13	

- Molecule 86 is water.

Mol	Chain	Residues	Atoms		AltConf
86	L5	16	Total	O	0
			16	16	
86	LA	1	Total	O	0
			1	1	
86	LB	1	Total	O	0
			1	1	
86	LC	1	Total	O	0
			1	1	
86	LF	1	Total	O	0
			1	1	
86	LG	1	Total	O	0
			1	1	
86	LH	1	Total	O	0
			1	1	
86	LI	2	Total	O	0
			2	2	
86	LN	1	Total	O	0
			1	1	
86	LS	2	Total	O	0
			2	2	
86	LY	1	Total	O	0
			1	1	

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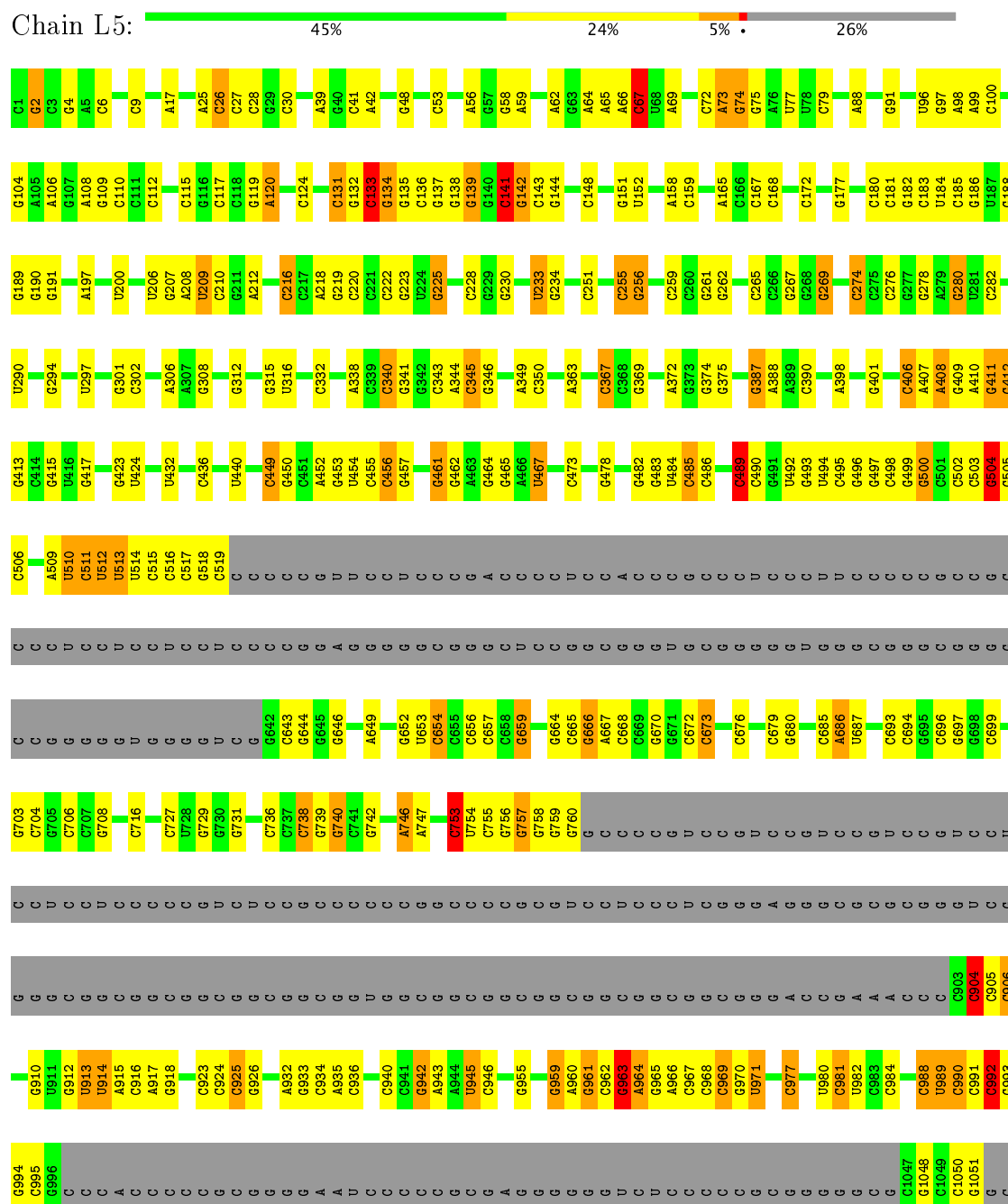
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Mol	Chain	Residues	Atoms		AltConf
86	La	2	Total 2	O 2	0
86	Lb	1	Total 1	O 1	0
86	Lf	1	Total 1	O 1	0
86	Lm	1	Total 1	O 1	0
86	S2	14	Total 14	O 14	0
86	SF	1	Total 1	O 1	0
86	SL	1	Total 1	O 1	0
86	SP	1	Total 1	O 1	0
86	SQ	2	Total 2	O 2	0
86	SR	1	Total 1	O 1	0
86	SS	2	Total 2	O 2	0
86	SV	1	Total 1	O 1	0
86	SC	1	Total 1	O 1	0
86	SG	1	Total 1	O 1	0
86	SJ	1	Total 1	O 1	0
86	SN	1	Total 1	O 1	0
86	Sf	1	Total 1	O 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

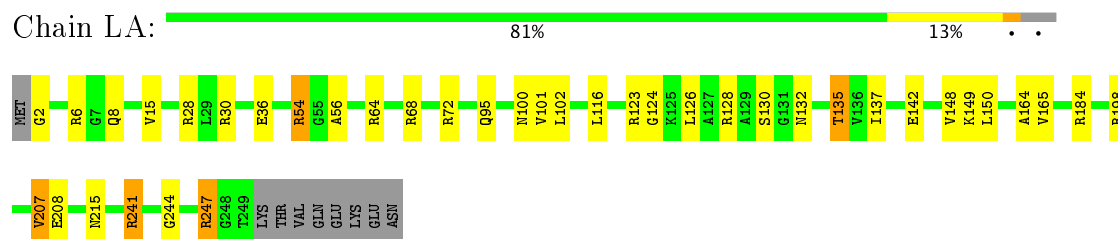
• Molecule 1: 28S ribosomal RNA



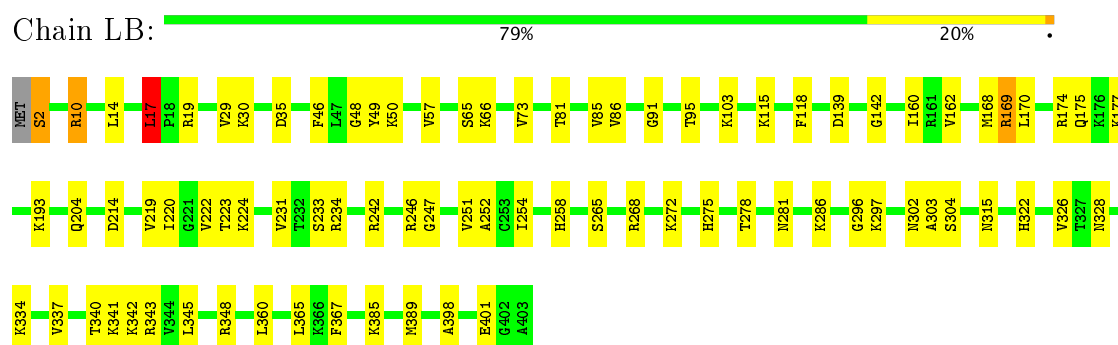
G2421	C2422	U2304	U2305	G2306	A2313	G2316	C2317	G2318	G2321	G2331	A2332	G2333	G2334	C2337	G2338	G2345	C2346	A2347	G2348	C2351	U2352	G2357	A2360	G2361	U2362	A2363	G2370	G2378	A2381	A2382	A2389	G2502	G2503	A2504	A2505	G2506	C2509	G2510	A2511	A2512	A2513	U2519	G2520	G2521	A2518				
C	U	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C				
C2091	G2092	A2093	G2094	A2095	G2096	U2097	G2098	G2099	A2100	C2101	G2102	G2106	C2107	C2110	G2111	G2112	C2113	G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C			
A1999	G2000	G2001	A2002	G2003	U2004	G2005	U2006	G2007	U2008	A2009	C2010	A2011	A2012	A2013	C2014	U2015	C2016	A2017	C2018	C2019	U2020	G2021	G2024	A2025	A2026	A2033	G2034	C2035	C2036	C2037	U2038	C2042	A2043	U2044	G2045	G2046	A2047	U2048	G2055	G2056	C2062	C2068	A2069	C2072	C2077	C2084	G2085	G2089	U2090
C1921	G1922	G1925	A1929	U1930	C1931	A1932	C1935	C1936	G1940	G1945	U1946	G1947	G1948	G1951	G1952	U1953	U1954	U1959	A1960	G1961	A1962	G1965	U1966	A1967	G1968	G1969	A1970	G1971	U1974	G1975	A1976	C1977	U1980	G1981	G1982	A1983	A1984	G1985	U1986	C1987	G1988	G1989	C1991	C1994	A1995	G1996	C1997	A1998	
G1821	U1822	G1823	U1824	U1834	G1835	G1836	A1837	G1842	A1850	G1851	U1852	G1853	G1854	G1855	G1864	G1865	U1866	G1869	A1870	A1871	G1872	U1876	C1881	U1882	G1883	G1884	G1885	U1886	U1888	G1890	A1891	A1892	C1893	C1894	A1897	C1898	U1906	A1907	U1908	?1909	C1913	C1914	A1915	G1916	A1917	U1918	G1919	C1920	
C1714	G1715	G1716	A1719	U1726	A1729	G1734	C1740	G1741	A1742	A1743	G1750	G1753	U1754	C1755	U1756	U1757	G1758	G1759	G1760	G1761	C1762	G1763	G1764	A1765	A1766	G1767	C1768	G1769	A1770	U1771	C1772	U1773	C1774	A1775	A1776	A1787	A1794	?1797	A1802	G1803	A1804	U1805	G1806	G1807	A1808	G1809	G1810	G1819	C1820
C1607	U1620	G1624	G1625	C1628	A1631	A1632	G1633	A1634	C1640	G1641	A1642	A1653	G1654	C1661	C1662	G1663	C1666	C1674	C1675	C1676	U1677	G1678	A1679	G1680	G1681	U1687	G1691	C1694	U1695	C1696	G1697	C1698	A1699	G1700	U1701	C1702	C1703	C1704	G1705	A1706	C1707	C1708	C1709	A	C	C	C		
A1497	G1498	G1502	A1503	G1504	C1505	A1508	C1509	U1513	U1514	A1515	A1518	C1519	C1520	A1521	A1522	A1525	A1534	C1535	C1540	A1547	G1549	G1550	C1551	G1552	C1556	G1559	C1566	U1571	G1577	U1578	C1579	U1582	G1586	C1590	U1591	U1596	G1597	A1600	A1601										
C1378	G1379	A1383	G1384	A1387	G1388	A1394	A1397	A1398	G1399	C1402	G1403	G1404	C1405	G1406	C1407	G1408	C1409	U1410	C1411	C1414	G1415	G1416	C1417	A1420	C1431	A1432	A1433	U1441	C1442	G1444	U1445	C1446	C1447	G1448	C1449	G1453	?1456	G1457	C1472	G1482	C1483	C1486	C1493						
A1270	G1271	C1272	G1273	A1274	G1275	C1276	G1277	A1278	C1280	G1281	G1284	G1287	G1293	A1294	C1295	G1296	C1301	U1302	A1303	C1304	C1305	C1312	C1313	A1322	A1323	A1324	C1325	A1326	A1337	C1340	C1344	A1345	C1346	G1353	A1354	G1358	G1359	G1360	C1365	G1366	C1367	G1370	C1376	G1377					
G1194	G1195	G1196	G1197	A1198	G1199	G1200	U1201	G1202	G1203	C1204	G1205	C1210	G1211	C1214	C1215	C1216	G1217	G1218	G1219	G1220	G1221	A1222	G	G	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U		
G	G	C	C	A	C	C	G	G	G	G	G1064	G1069	G1070	C1071	G1072	G1073	G1074	C1077	C1082	U1083	A1085	C1086	U1100	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C

C3937	C3938	C3939	C3940	C3941	C3942	C3943	C3944	C3945	C3946	C3947	C3948	C3949	C3950	C3951	C3952	C3953	C3954	C3955	C3956	C3957	C3958	C3959	C3960	C3961	C3962	C3963	C3964	C3965	C3966	C3967	C3968	C3969	C3970	C3971	C3972	C3973	C3974	C3975	C3976	C3977	C4034	C4035	C4036	C4037	C4038	C4039	C4040	C4041	C4042	C4043	C4044	C4045	C4046	C4047	C4048	C4049	C4050	C4051	C4052																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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C3605	C3606	C3607	C3608	C3609	C3610	C3611	C3612	C3613	C3614	C3615	C3616	C3617	C3618	C3619	C3620	C3621	C3622	C3623	C3624	C3625	C3626	C3627	C3628	C3629	C3630	C3631	C3632	C3633	C3634	C3635	C3636	C3637	C3638	C3639	C3640	C3641	C3642	C3643	C3644	C3645	C3646	C3647	C3648	C3649	C3650	C3651	C3652	C3653	C3654	C3655	C3656	C3657	C3658	C3659	C3660	C3661	C3662	C3663	C3664	C3665	C3666	C3667	C3668	C3669	C3670	C3671	C3672	C3673	C3674	C3675	C3676	C3677	C3678	C3679	C3680	C3681	C3682	C3683	C3684	C3685	C3686	C3687	C3688	C3689	C3690	C3691	C3692	C3693	C3694	C3695	C3696	C3697	C3698	C3699	C3700	C3701	C3702	C3703	C3704	C3705	C3706	C3707	C3708	C3709	C3710	C3711	C3712	C3713	C3714	C3715	C3716	C3717	C3718	C3719	C3720	C3721	C3722	C3723	C3724	C3725	C3726	C3727	C3728	C3729	C3730	C3731	C3732	C3733	C3734	C3735	C3736	C3737	C3738	C3739	C3740	C3741	C3742	C3743	C3744	C3745	C3746	C3747	C3748	C3749	C3750	C3751	C3752	C3753	C3754	C3755	C3756	C3757	C3758	C3759	C3760	C3761	C3762	C3763	C3764	C3765	C3766	C3767	C3768	C3769	C3770	C3771	C3772	C3773	C3774	C3775	C3776	C3777	C3778	C3779	C3780	C3781	C3782	C3783	C3784	C3785	C3786	C3787	C3788	C3789	C3790	C3791	C3792	C3793	C3794	C3795	C3796	C3797	C3798	C3799	C3800	C3801	C3802	C3803	C3804	C3805	C3806	C3807	C3808	C3809	C3810	C3811	C3812	C3813	C3814	C3815	C3816	C3817	C3818	C3819	C3820	C3821	C3822	C3823	C3824	C3825	C3826	C3827	C3828	C3829	C3830	C3831	C3832	C3833	C3834	C3835	C3836	C3837	C3838	C3839	C3840	C3841	C3842	C3843	C3844	C3845	C3846	C3847	C3848	C3849	C3850	C3851	C3852	C3853	C3854	C3855	C3856	C3857	C3858	C3859	C3860	C3861	C3862	C3863	C3864	C3865	C3866	C3867	C3868	C3869	C3870	C3871	C3872	C3873	C3874	C3875	C3876	C3877	C3878	C3879	C3880	C3881	C3882	C3883	C3884	C3885	C3886	C3887	C3888	C3889	C3890	C3891	C3892	C3893	C3894	C3895	C3896	C3897	C3898	C3899	C3900	C3901	C3902	C3903	C3904	C3905	C3906	C3907	C3908	C3909	C3910	C3911	C3912	C3913	C3914	C3915	C3916	C3917	C3918	C3919	C3920	C3921	C3922	C3923	C3924	C3925	C3926	C3927	C3928	C3929	C3930	C3931	C3932	C3933	C3934	C3935	C3936	C3937	C3938	C3939	C3940	C3941	C3942	C3943	C3944	C3945	C3946	C3947	C3948	C3949	C3950	C3951	C3952	C3953	C3954	C3955	C3956	C3957	C3958	C3959	C3960	C3961	C3962	C3963	C3964	C3965	C3966	C3967	C3968	C3969	C3970	C3971	C3972	C3973	C3974	C3975	C3976	C3977	C4034	C4035	C4036	C4037	C4038	C4039	C4040	C4041	C4042	C4043	C4044	C4045	C4046	C4047	C4048	C4049	C4050	C4051	C4052																																																																																																																																																																																																																																																																																																																																																															
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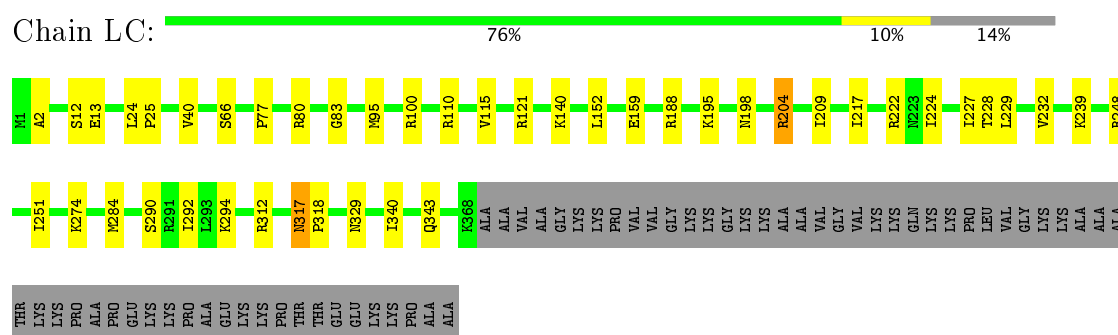
- Molecule 4: 60S ribosomal protein L8



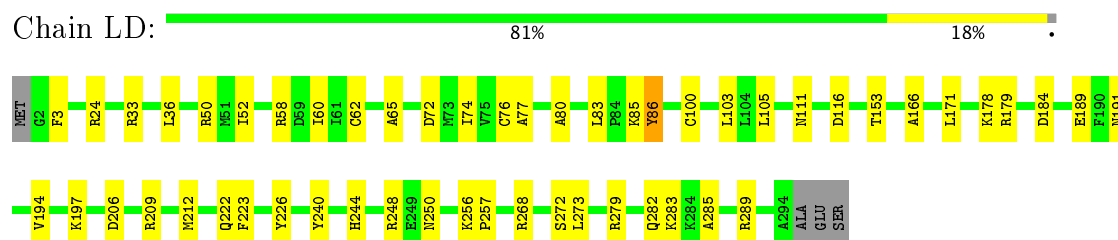
- Molecule 5: 60S ribosomal protein L3



- Molecule 6: 60S ribosomal protein L4




- Molecule 7: 60S ribosomal protein L5

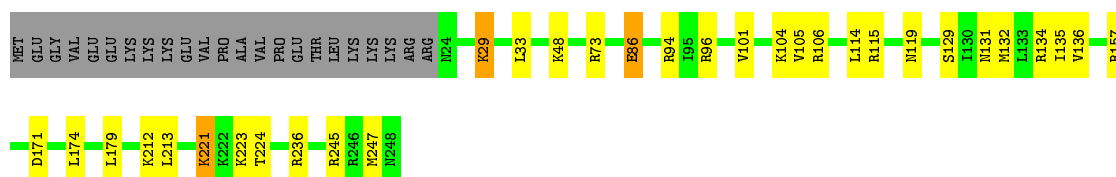


- Molecule 8: 60S ribosomal protein L6

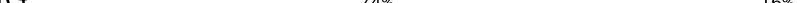


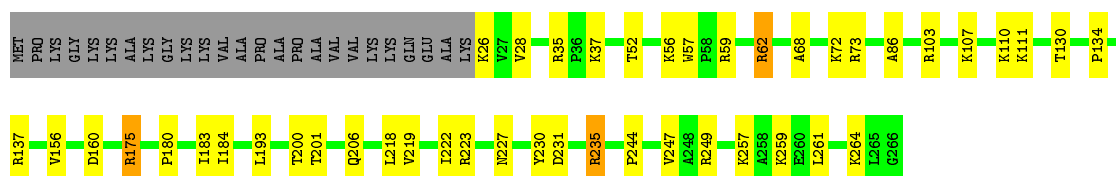
- Molecule 9: 60S ribosomal protein L7

Chain LF:  78% 12% 9%




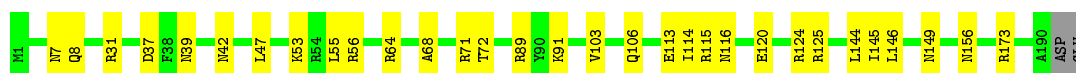
- Molecule 10: 60S ribosomal protein L7a

Chain LG:  74% 16% 9%

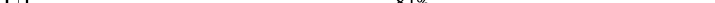


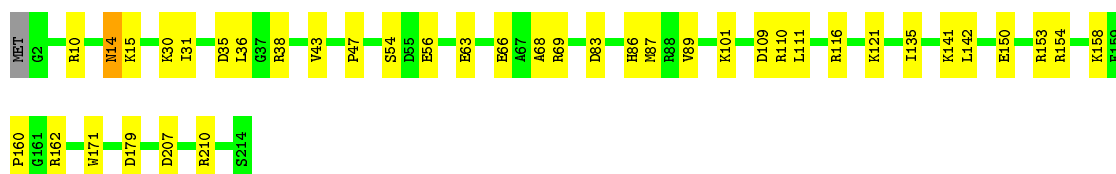
- Molecule 11: 60S ribosomal protein L9

Chain LH:  83% 16%

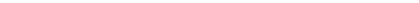


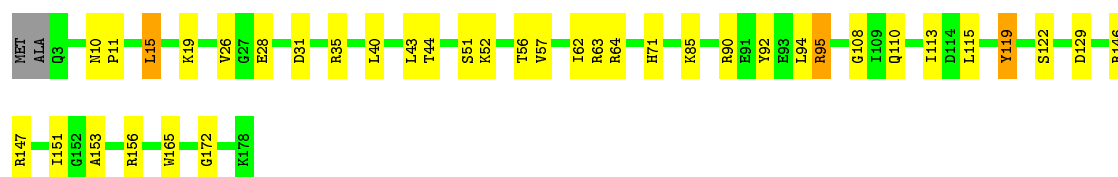
- Molecule 12: 60S ribosomal protein L10-like

Chain LI:  81% 18%



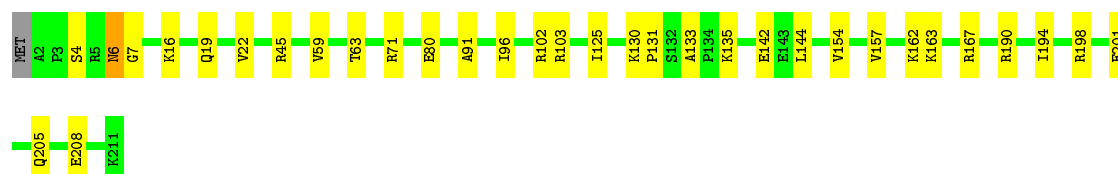
- Molecule 13: 60S ribosomal protein L11

Chain LJ:  78% 20% .



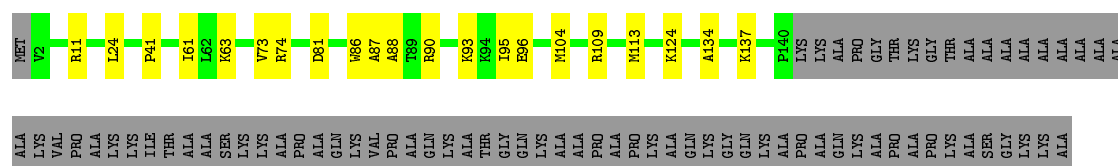
- Molecule 14: 60S ribosomal protein L13

Chain LL: 84% 15%



- Molecule 15: 60S ribosomal protein L14

Chain LM: 55% 10% 35%



- Molecule 16: 60S ribosomal protein L15

Chain LN: 86% 12%



- Molecule 17: 60S ribosomal protein L13a

Chain LO: 84% 15%




- Molecule 18: 60S ribosomal protein L17

Chain LP: 68% 15% 17%




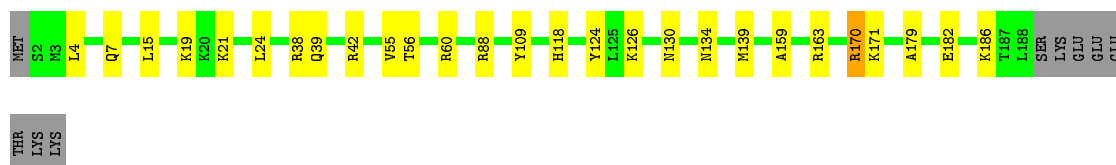
- Molecule 19: 60S ribosomal protein L18

Chain LQ:  89% 10% ..




- Molecule 20: 60S ribosomal protein L19

Chain LR:  82% 13% • 5%




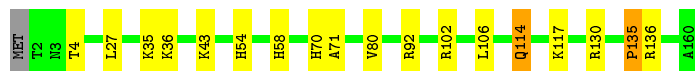
- Molecule 21: 60S ribosomal protein L18a

Chain LS:  84% 15% •



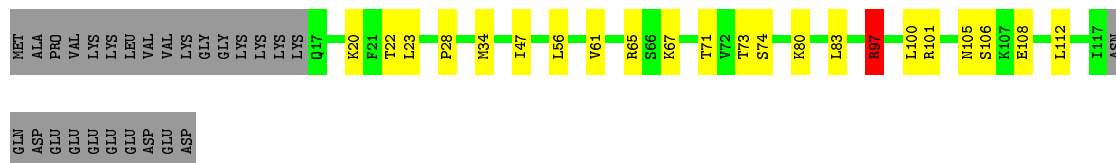
- Molecule 22: 60S ribosomal protein L21

Chain LT:  88% 10% ..




- Molecule 23: 60S ribosomal protein L22

Chain LU:  62% 16% • 21%



- Molecule 24: 60S ribosomal protein L23

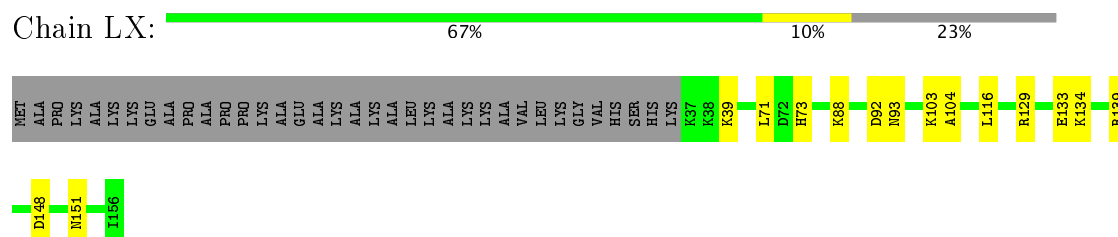
Chain LV:  79% 14% • 6%



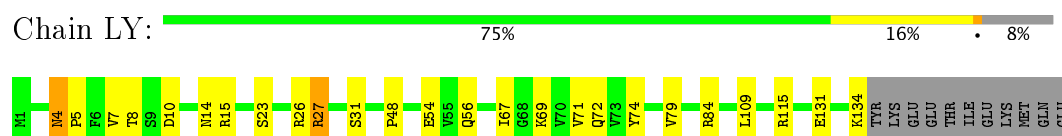
- Molecule 25: 60S ribosomal protein L24

Chain LW:  68% 10% • 21%

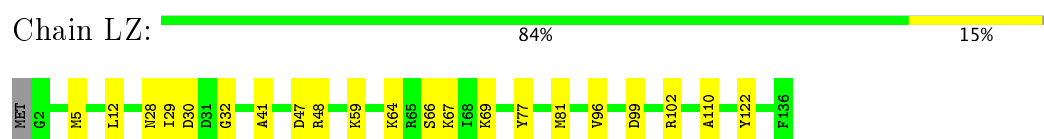
- Molecule 26: 60S ribosomal protein L23a



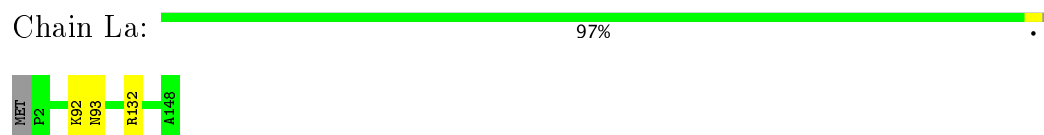
- Molecule 27: 60S ribosomal protein L26



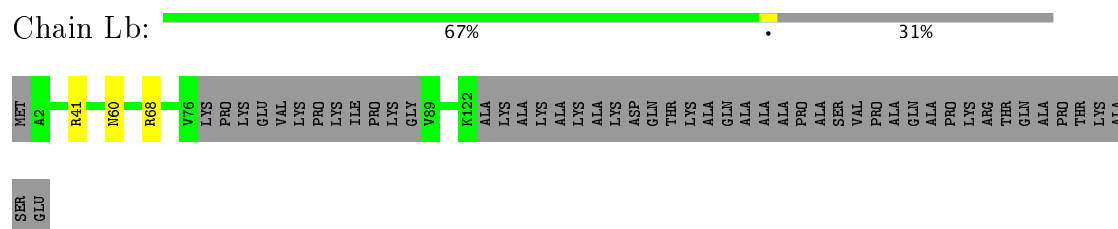
- Molecule 28: 60S ribosomal protein L27



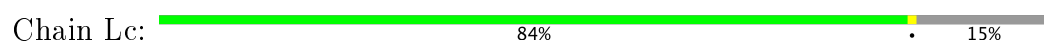
- Molecule 29: 60S ribosomal protein L27a



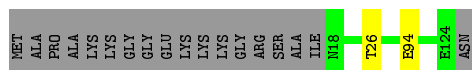
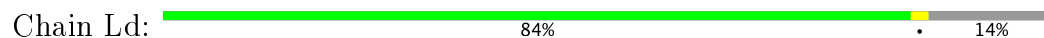
- Molecule 30: 60S ribosomal protein L29



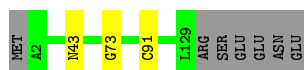
- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31



- Molecule 33: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L35a



- Molecule 35: 60S ribosomal protein L34



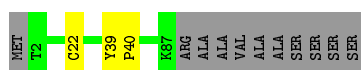
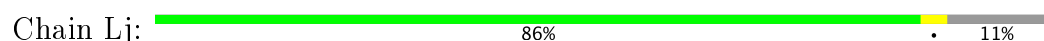
- Molecule 36: 60S ribosomal protein L35



- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37



- Molecule 39: 60S ribosomal protein L38

Chain Lk:  99%



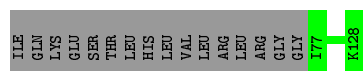
- Molecule 40: 60S ribosomal protein L39

Chain Ll:  94%



- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:  41%  59%



- Molecule 42: 60S ribosomal protein L41

Chain Ln:  92%



- Molecule 43: 60S ribosomal protein L36a

Chain Lo:  99%



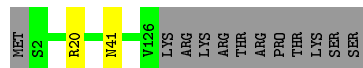
- Molecule 44: 60S ribosomal protein L37a

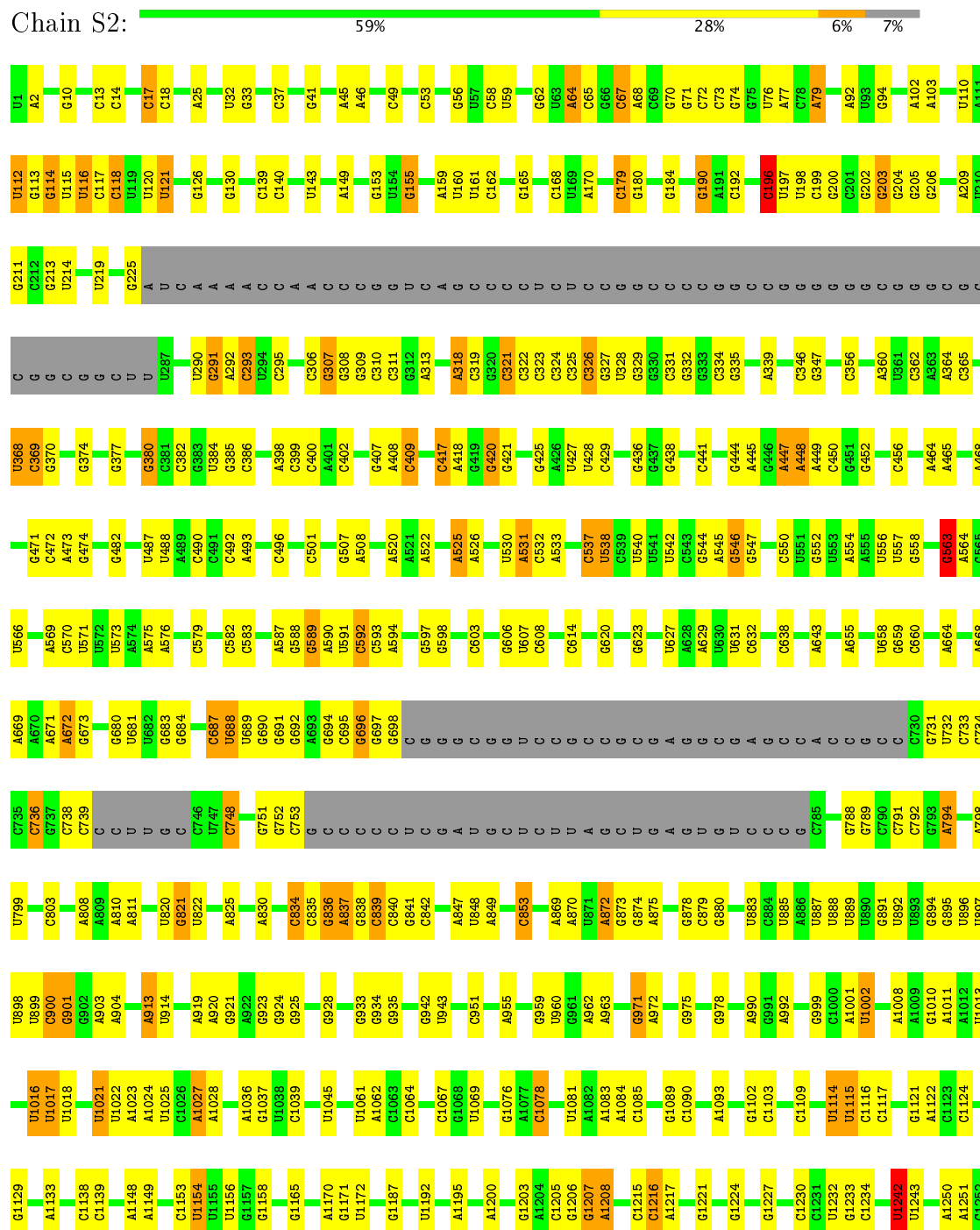
Chain Lp:  97%

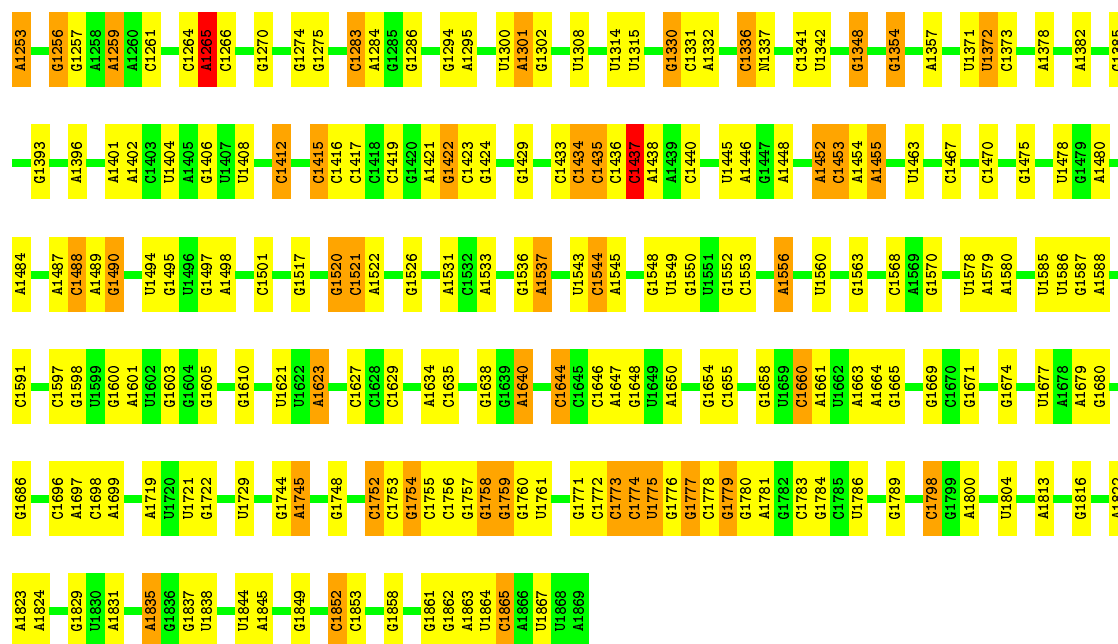


- Molecule 45: 60S ribosomal protein L28

Chain Lr:  90%  9%







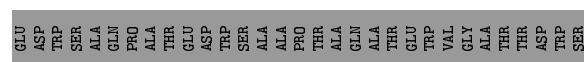
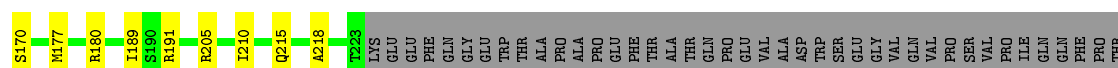
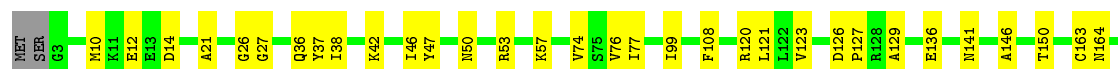
- Molecule 48: Human initiator Met-tRNA-i

Chain S6: 47% 40% 13%



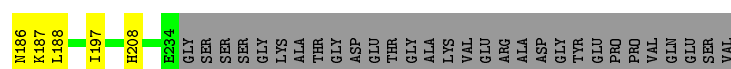
- Molecule 49: 40S ribosomal protein SA

Chain SA: 61% 14% 25%




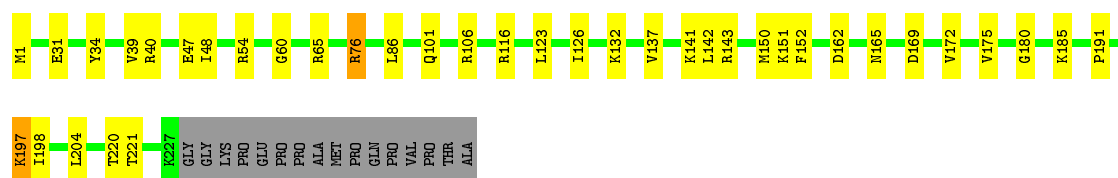
- Molecule 50: 40S ribosomal protein S3a

Chain SB: 72% 9% 19%




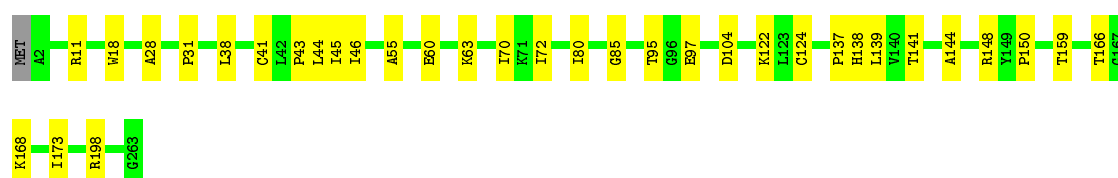
- Molecule 51: 40S ribosomal protein S3

Chain SD: 




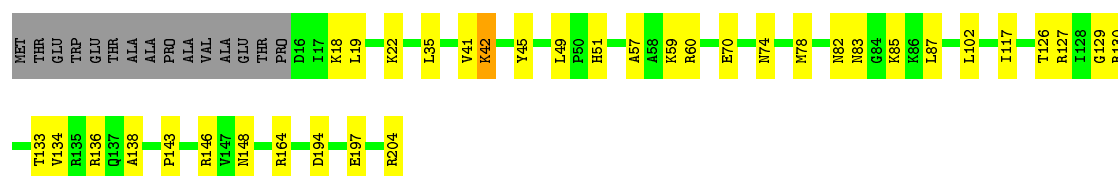
- Molecule 52: 40S ribosomal protein S4, X isoform

Chain SE: 




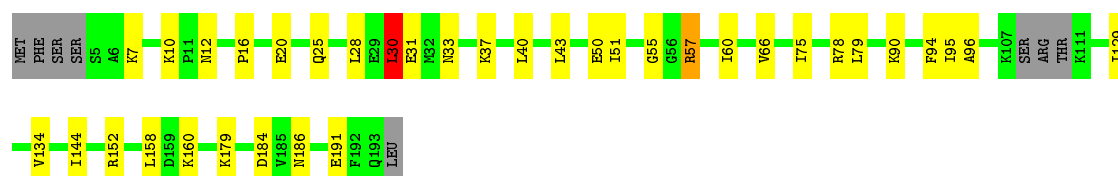
- Molecule 53: 40S ribosomal protein S5

Chain SF: 



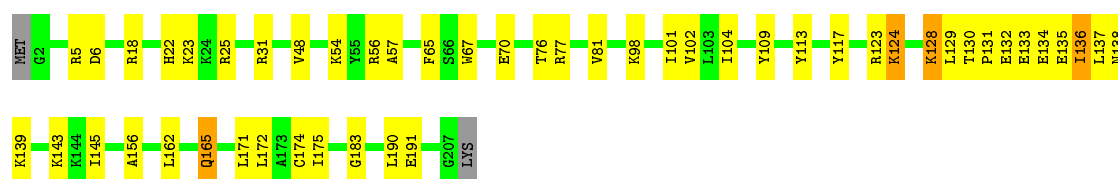
- Molecule 54: 40S ribosomal protein S7

Chain SH: 



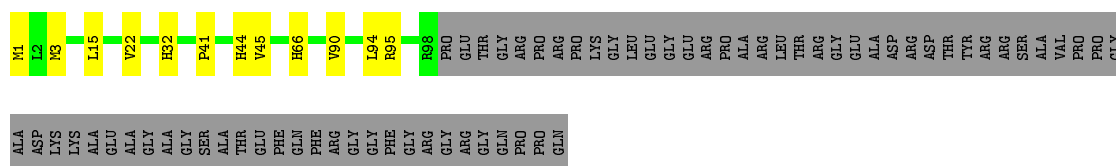
- Molecule 55: 40S ribosomal protein S8

Chain SI: 



- Molecule 56: 40S ribosomal protein S10

Chain SK: 



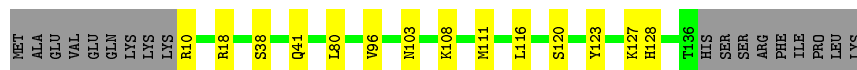
- Molecule 57: 40S ribosomal protein S11

Chain SL: 84% 11% ..



- Molecule 58: 40S ribosomal protein S15

Chain SP: 78% 10% 12%



- Molecule 59: 40S ribosomal protein S16

Chain SQ: 79% 21% .



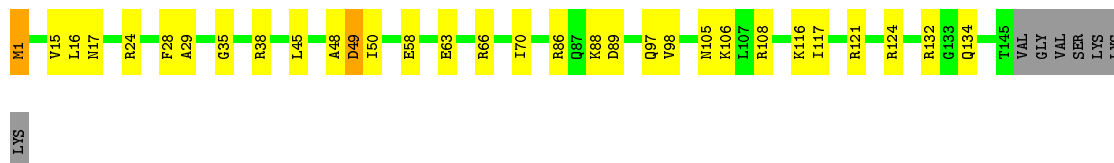
- Molecule 60: 40S ribosomal protein S17

Chain SR: 86% 14%



- Molecule 61: 40S ribosomal protein S18

Chain SS: 75% 19% 5%

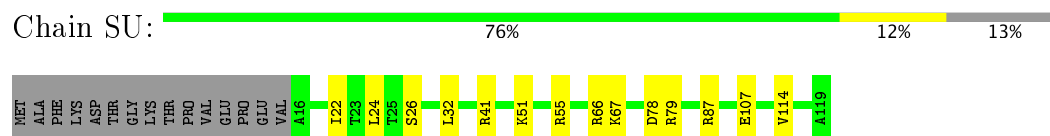


- Molecule 62: 40S ribosomal protein S19

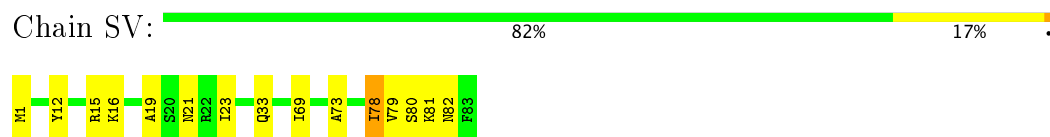
Chain ST: 90% 8% ..



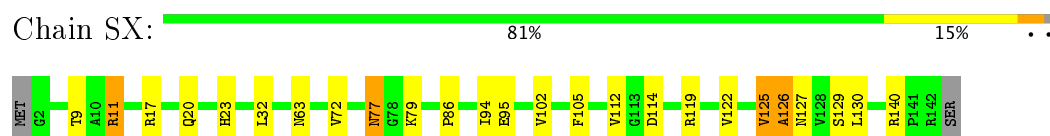
- Molecule 63: 40S ribosomal protein S20



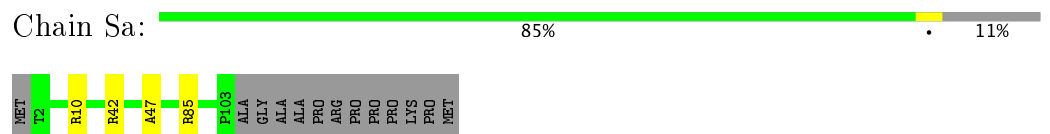
- Molecule 64: 40S ribosomal protein S21



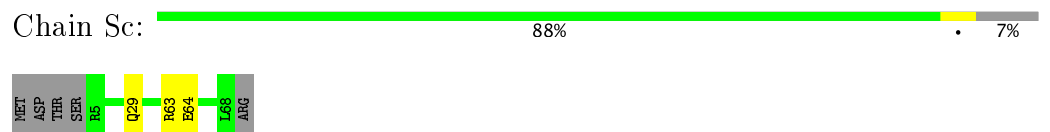
- Molecule 65: 40S ribosomal protein S23



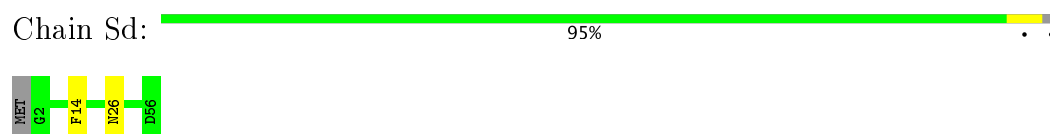
- Molecule 66: 40S ribosomal protein S26



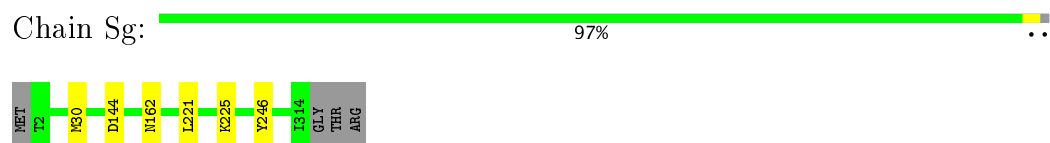
- Molecule 67: 40S ribosomal protein S28



- Molecule 68: 40S ribosomal protein S29

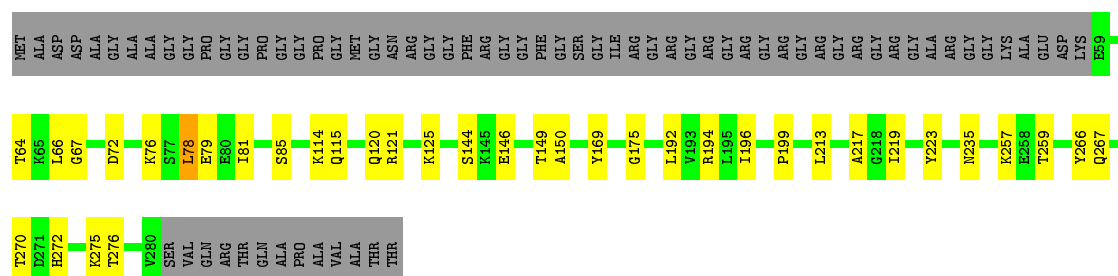


- Molecule 69: Receptor of activated protein C kinase 1



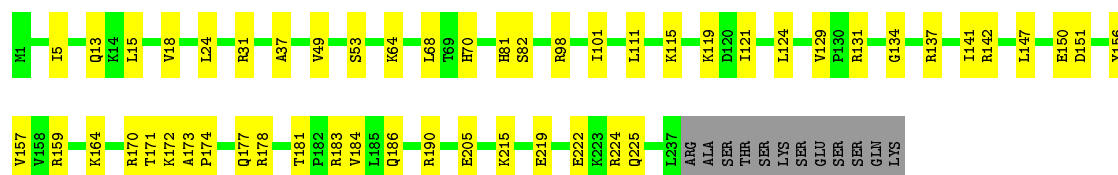
- Molecule 70: 40S ribosomal protein S2





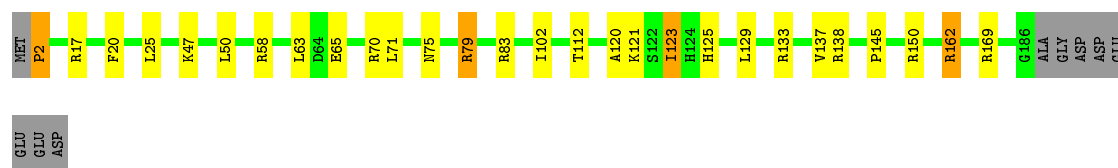
- Molecule 71: 40S ribosomal protein S6

Chain SG: 74% 21% 5%



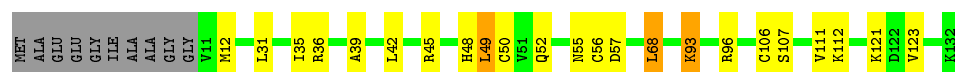
- Molecule 72: 40S ribosomal protein S9

Chain SJ: 81% 12% 5%



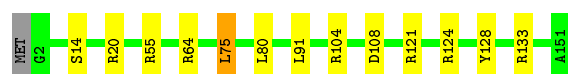
- Molecule 73: 40S ribosomal protein S12

Chain SM: 75% 15% 8%



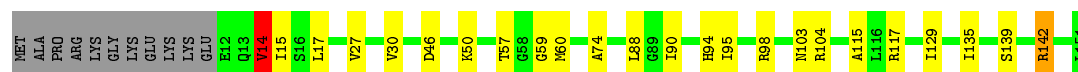
- Molecule 74: 40S ribosomal protein S13

Chain SN: 91% 8% 2%




- Molecule 75: 40S ribosomal protein S14

Chain SO: 77% 15% 7%



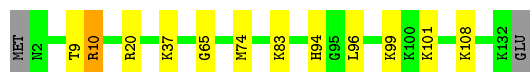
- Molecule 76: 40S ribosomal protein S15a

Chain SW:  86% 12% ..



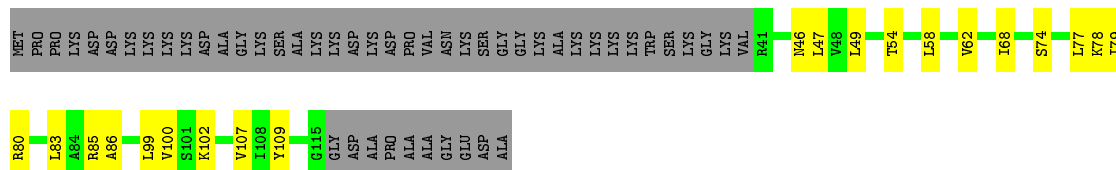
- Molecule 77: 40S ribosomal protein S24

Chain SY:  89% 8% ..



- Molecule 78: 40S ribosomal protein S25

Chain SZ:  44% 16% 40%



- Molecule 79: 40S ribosomal protein S27

Chain Sb:  99% .



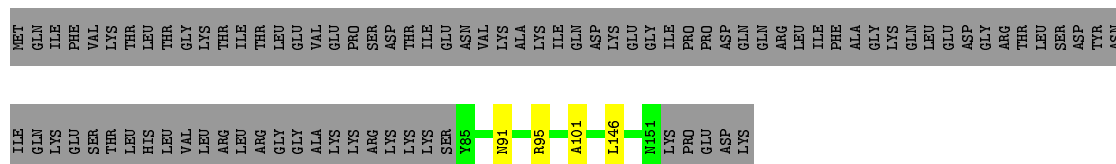
- Molecule 80: 40S ribosomal protein S30

Chain Se:  97% ..



- Molecule 81: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  40% . 57%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	138234	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	3.5	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HYG, BGH, 2MG, 4AC, 1MA, P4U, I4U, A2M, B9H, B8Q, MA6, B8T, B8W, E6G, B8H, B8K, UR3, 7MG, OMC, ZN, OMU, MHG, B8N, P7G, 6MZ, MLZ, 5MU, MG, OMG, E7G, HMT, M7A, E3C, 5MC, B9B, PSU

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 >2	RMSZ	# Z >2
1	L5	0.90	1/87128 (0.0%)	1.12	495/135765 (0.4%)
10	LG	0.45	0/1971	0.68	0/2651
11	LH	0.47	0/1537	0.63	1/2066 (0.0%)
12	LI	0.42	0/1751	0.62	1/2340 (0.0%)
13	LJ	0.37	0/1433	0.73	3/1915 (0.2%)
14	LL	0.47	0/1732	0.64	0/2315
15	LM	0.47	0/1161	0.63	0/1554
16	LN	0.57	0/1746	0.64	1/2338 (0.0%)
17	LO	0.51	0/1682	0.61	0/2250
18	LP	0.52	0/1268	0.66	0/1701
19	LQ	0.48	0/1537	0.64	0/2052
2	L7	0.80	0/2858	0.98	4/4455 (0.1%)
20	LR	0.41	0/1582	0.64	1/2091 (0.0%)
21	LS	0.52	0/1493	0.57	0/2003
22	LT	0.49	0/1326	0.64	0/1770
23	LU	0.38	0/839	0.66	0/1126
24	LV	0.49	0/993	0.64	0/1332
25	LW	0.40	0/1030	0.64	0/1364
26	LX	0.44	0/1002	0.62	0/1345
27	LY	0.44	0/1132	0.62	0/1504
28	LZ	0.45	0/1130	0.66	1/1507 (0.1%)
29	La	0.52	0/1191	0.64	0/1591
3	L8	0.91	0/3679	1.08	14/5732 (0.2%)
30	Lb	0.38	0/889	0.64	0/1175
31	Lc	0.44	0/774	0.68	0/1038
32	Ld	0.43	0/903	0.65	0/1216
33	Le	0.52	0/1071	0.61	0/1429
34	Lf	0.56	0/895	0.68	0/1198
35	Lg	0.46	0/916	0.62	0/1220
36	Lh	0.39	0/1023	0.58	0/1351

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
37	Li	0.37	0/843	0.57	0/1115
38	Lj	0.52	0/720	0.61	0/952
39	Lk	0.40	0/575	0.60	0/761
4	LA	0.54	0/1936	0.70	1/2596 (0.0%)
40	Ll	0.48	0/454	0.62	0/599
41	Lm	0.46	0/425	0.61	0/561
42	Ln	0.67	0/231	0.66	0/294
43	Lo	0.45	0/887	0.65	0/1170
44	Lp	0.46	0/718	0.60	0/953
45	Lr	0.47	0/1017	0.65	0/1364
46	Lz	0.30	0/1769	0.63	0/2371
47	S2	0.92	4/40440 (0.0%)	1.09	200/62994 (0.3%)
48	S6	0.35	0/1795	0.96	6/2798 (0.2%)
49	SA	0.44	0/1778	0.64	1/2416 (0.0%)
5	LB	0.51	0/3315	0.73	3/4435 (0.1%)
50	SB	0.42	0/1765	0.60	1/2362 (0.0%)
51	SD	0.43	0/1793	0.67	0/2414
52	SE	0.45	0/2118	0.64	2/2849 (0.1%)
53	SF	0.42	0/1516	0.67	1/2037 (0.0%)
54	SH	0.40	0/1519	0.68	1/2033 (0.0%)
55	SI	0.46	0/1715	0.67	1/2287 (0.0%)
56	SK	0.45	0/851	0.67	1/1147 (0.1%)
57	SL	0.56	1/1268 (0.1%)	0.67	0/1696
58	SP	0.42	0/1065	0.68	1/1423 (0.1%)
59	SQ	0.49	0/1176	0.70	1/1572 (0.1%)
6	LC	0.48	0/2971	0.65	1/3988 (0.0%)
60	SR	0.40	0/1105	0.63	0/1484
61	SS	0.41	0/1216	0.64	1/1628 (0.1%)
62	ST	0.43	0/1131	0.59	0/1515
63	SU	0.39	0/831	0.62	0/1115
64	SV	0.41	0/643	0.70	1/860 (0.1%)
65	SX	0.49	0/1116	0.70	0/1490
66	Sa	0.52	0/847	0.64	0/1135
67	Sc	0.45	0/508	0.76	0/680
68	Sd	0.54	0/470	0.71	0/623
69	Sg	0.39	0/2493	0.72	1/3394 (0.0%)
7	LD	0.41	0/2428	0.63	1/3252 (0.0%)
70	SC	0.51	0/1773	0.71	2/2395 (0.1%)
71	SG	0.39	0/1946	0.64	1/2590 (0.0%)
72	SJ	0.49	1/1561 (0.1%)	0.73	1/2083 (0.0%)
73	SM	0.34	0/952	0.60	0/1279
74	SN	0.45	0/1232	0.63	0/1656
75	SO	0.41	0/1062	0.65	1/1425 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
76	SW	0.50	0/1051	0.68	0/1406
77	SY	0.42	0/1094	0.63	0/1452
78	SZ	0.39	0/604	0.71	0/810
79	Sb	0.42	0/665	0.64	0/891
8	LE	0.40	0/1942	0.68	0/2606
80	Se	0.37	0/465	0.60	0/612
81	Sf	0.34	0/560	0.76	1/745 (0.1%)
9	LF	0.50	0/1916	0.69	2/2553 (0.1%)
All	All	0.75	7/231943 (0.0%)	0.96	754/340260 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L5	2	0
11	LH	0	2
12	LI	0	1
13	LJ	0	1
14	LL	0	2
15	LM	0	1
16	LN	0	1
17	LO	0	1
22	LT	0	2
23	LU	0	1
25	LW	0	1
27	LY	0	1
32	Ld	0	1
33	Le	0	1
34	Lf	0	3
36	Lh	0	1
38	Lj	0	1
4	LA	0	3
45	Lr	0	1
46	Lz	0	2
47	S2	2	0
5	LB	0	4
51	SD	0	2
53	SF	0	4
54	SH	0	2
55	SI	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
56	SK	0	1
57	SL	0	2
58	SP	0	1
59	SQ	0	1
62	ST	0	1
63	SU	0	1
64	SV	0	1
65	SX	0	5
66	Sa	0	1
67	Sc	0	2
7	LD	0	1
70	SC	0	1
72	SJ	0	4
73	SM	0	2
75	SO	0	1
77	SY	0	1
78	SZ	0	1
8	LE	0	1
81	Sf	0	1
9	LF	0	2
All	All	4	72

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	2465	C	N1-C6	-6.30	1.33	1.37
47	S2	1853	C	N3-C4	-5.44	1.30	1.33
57	SL	128	VAL	CB-CG1	-5.25	1.41	1.52
47	S2	1200	A	N9-C4	-5.21	1.34	1.37
47	S2	1697	A	N9-C4	-5.17	1.34	1.37

The worst 5 of 754 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	501	C	C2-N1-C1'	14.41	134.65	118.80
1	L5	485	C	N1-C2-O2	13.90	127.24	118.90
47	S2	501	C	N1-C2-O2	13.88	127.23	118.90
1	L5	485	C	C2-N1-C1'	12.47	132.52	118.80
47	S2	293	C	N1-C2-O2	11.94	126.06	118.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	L5	1456	B8Q	C4
1	L5	2786	B9H	C4
47	S2	568	E3C	C4
47	S2	1219	B8Q	C4

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	LA	142	GLU	Peptide
4	LA	241	ARG	Sidechain
4	LA	54	ARG	Peptide
5	LB	17	LEU	Peptide
5	LB	2	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L5	80257	0	40195	341	0
2	L7	2558	0	1296	12	0
3	L8	3315	0	1685	14	0
4	LA	1898	0	1992	25	0
5	LB	3244	0	3389	53	0
6	LC	2928	0	3105	26	0
7	LD	2382	0	2410	31	0
8	LE	1904	0	2055	28	0
9	LF	1878	0	2009	18	0
10	LG	1935	0	2087	23	0
11	LH	1518	0	1601	18	0
12	LI	1711	0	1748	22	0
13	LJ	1410	0	1440	24	0
14	LL	1701	0	1818	19	0
15	LM	1138	0	1204	11	0
16	LN	1701	0	1749	19	0
17	LO	1650	0	1794	18	0
18	LP	1242	0	1269	18	0
19	LQ	1513	0	1628	13	0
20	LR	1566	0	1728	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	LS	1453	0	1490	17	0
22	LT	1298	0	1366	13	0
23	LU	825	0	850	12	0
24	LV	979	0	1039	12	0
25	LW	1015	0	1079	15	0
26	LX	985	0	1066	9	0
27	LY	1115	0	1205	15	0
28	LZ	1107	0	1182	12	0
29	La	1162	0	1213	0	0
30	Lb	876	0	948	0	0
31	Lc	764	0	804	0	0
32	Ld	888	0	930	0	0
33	Le	1053	0	1147	0	0
34	Lf	876	0	912	0	0
35	Lg	906	0	1002	0	0
36	Lh	1015	0	1148	0	0
37	Li	832	0	917	0	0
38	Lj	705	0	737	0	0
39	Lk	569	0	637	0	0
40	Ll	444	0	483	0	0
41	Lm	430	0	466	0	0
42	Ln	230	0	276	0	0
43	Lo	870	0	945	0	0
44	Lp	708	0	756	0	0
45	Lr	1002	0	1068	0	0
46	Lz	1741	0	1854	0	0
47	S2	36938	0	18612	158	0
48	S6	1604	0	816	9	0
49	SA	1741	0	1746	21	0
50	SB	1738	0	1809	14	0
51	SD	1765	0	1865	20	0
52	SE	2076	0	2177	21	0
53	SF	1495	0	1549	19	0
54	SH	1497	0	1590	21	0
55	SI	1686	0	1772	53	0
56	SK	827	0	854	6	0
57	SL	1247	0	1323	9	0
58	SP	1045	0	1095	8	0
59	SQ	1158	0	1231	19	0
60	SR	1090	0	1149	13	0
61	SS	1198	0	1261	22	0
62	ST	1112	0	1146	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	SU	821	0	883	9	0
64	SV	636	0	637	9	0
65	SX	1098	0	1167	13	0
66	Sa	829	0	883	0	0
67	Sc	506	0	536	0	0
68	Sd	459	0	448	0	0
69	Sg	2436	0	2393	0	0
70	SC	1733	0	1826	23	0
71	SG	1923	0	2089	35	0
72	SJ	1533	0	1653	17	0
73	SM	942	0	961	11	0
74	SN	1208	0	1294	9	0
75	SO	1049	0	1073	14	0
76	SW	1034	0	1080	14	0
77	SY	1073	0	1155	8	0
78	SZ	598	0	656	12	0
79	Sb	651	0	672	0	0
80	Se	459	0	503	0	0
81	Sf	548	0	551	0	0
82	L5	251	0	0	0	0
82	L7	3	0	0	0	0
82	L8	6	0	0	0	0
82	LN	1	0	0	0	0
82	LP	1	0	0	0	0
82	LT	1	0	0	0	0
82	LV	1	0	0	0	0
82	Le	1	0	0	0	0
82	Lf	1	0	0	0	0
82	S2	134	0	0	0	0
82	SF	1	0	0	0	0
82	Sd	1	0	0	0	0
83	L5	39	0	39	3	0
84	Lg	1	0	0	0	0
84	Lj	1	0	0	0	0
84	Lm	1	0	0	0	0
84	Lo	1	0	0	0	0
84	Lp	1	0	0	0	0
84	Sa	1	0	0	0	0
84	Sd	1	0	0	0	0
84	Sf	1	0	0	0	0
85	S2	36	0	37	0	0
86	L5	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	LA	1	0	0	1	0
86	LB	1	0	0	0	0
86	LC	1	0	0	0	0
86	LF	1	0	0	0	0
86	LG	1	0	0	0	0
86	LH	1	0	0	0	0
86	LI	2	0	0	0	0
86	LN	1	0	0	0	0
86	LS	2	0	0	0	0
86	LY	1	0	0	0	0
86	La	2	0	0	0	0
86	Lb	1	0	0	0	0
86	Lf	1	0	0	0	0
86	Lm	1	0	0	0	0
86	S2	14	0	0	0	0
86	SC	1	0	0	0	0
86	SF	1	0	0	0	0
86	SG	1	0	0	0	0
86	SJ	1	0	0	0	0
86	SL	1	0	0	0	0
86	SN	1	0	0	0	0
86	SP	1	0	0	0	0
86	SQ	2	0	0	0	0
86	SR	1	0	0	0	0
86	SS	2	0	0	0	0
86	SV	1	0	0	1	0
86	Sf	1	0	0	0	0
All	All	219596	0	162253	1167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 1167 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SI:130:THR:OG1	55:SI:134:GLU:CB	1.69	1.40
55:SI:130:THR:CA	55:SI:134:GLU:HB3	1.49	1.33
55:SI:130:THR:CB	55:SI:134:GLU:HB3	1.67	1.24
55:SI:123:ARG:HD3	55:SI:129:LEU:CD1	1.69	1.22
55:SI:123:ARG:HD3	55:SI:129:LEU:HD12	1.31	1.08

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	221 (90%)	25 (10%)	0	100	100
5	LB	401/403 (100%)	377 (94%)	23 (6%)	1 (0%)	51	82
6	LC	365/427 (86%)	335 (92%)	29 (8%)	1 (0%)	44	77
7	LD	291/297 (98%)	269 (92%)	22 (8%)	0	100	100
8	LE	232/288 (81%)	204 (88%)	28 (12%)	0	100	100
9	LF	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
10	LG	240/266 (90%)	215 (90%)	24 (10%)	1 (0%)	38	72
11	LH	188/192 (98%)	171 (91%)	17 (9%)	0	100	100
12	LI	211/214 (99%)	186 (88%)	24 (11%)	1 (0%)	32	68
13	LJ	174/178 (98%)	154 (88%)	20 (12%)	0	100	100
14	LL	208/211 (99%)	182 (88%)	26 (12%)	0	100	100
15	LM	137/215 (64%)	123 (90%)	13 (10%)	1 (1%)	25	60
16	LN	201/204 (98%)	185 (92%)	13 (6%)	3 (2%)	12	39
17	LO	199/203 (98%)	188 (94%)	11 (6%)	0	100	100
18	LP	151/184 (82%)	141 (93%)	10 (7%)	0	100	100
19	LQ	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
20	LR	185/196 (94%)	175 (95%)	10 (5%)	0	100	100
21	LS	173/176 (98%)	161 (93%)	12 (7%)	0	100	100
22	LT	157/160 (98%)	144 (92%)	13 (8%)	0	100	100
23	LU	99/128 (77%)	85 (86%)	14 (14%)	0	100	100
24	LV	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
25	LW	122/157 (78%)	107 (88%)	15 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	LX	118/156 (76%)	108 (92%)	10 (8%)	0	100	100
27	LY	132/145 (91%)	125 (95%)	6 (4%)	1 (1%)	22	57
28	LZ	133/136 (98%)	118 (89%)	15 (11%)	0	100	100
29	La	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
30	Lb	105/159 (66%)	91 (87%)	14 (13%)	0	100	100
31	Lc	96/115 (84%)	82 (85%)	14 (15%)	0	100	100
32	Ld	105/125 (84%)	96 (91%)	9 (9%)	0	100	100
33	Le	126/135 (93%)	116 (92%)	9 (7%)	1 (1%)	22	57
34	Lf	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	9	33
35	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
36	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
38	Lj	84/97 (87%)	75 (89%)	8 (10%)	1 (1%)	15	46
39	Lk	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
40	Ll	48/51 (94%)	42 (88%)	6 (12%)	0	100	100
41	Lm	49/128 (38%)	49 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
44	Lp	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
45	Lr	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
46	Lz	215/217 (99%)	154 (72%)	61 (28%)	0	100	100
49	SA	219/295 (74%)	192 (88%)	26 (12%)	1 (0%)	32	68
50	SB	212/264 (80%)	198 (93%)	14 (7%)	0	100	100
51	SD	225/243 (93%)	198 (88%)	27 (12%)	0	100	100
52	SE	260/263 (99%)	241 (93%)	19 (7%)	0	100	100
53	SF	187/204 (92%)	167 (89%)	20 (11%)	0	100	100
54	SH	182/194 (94%)	159 (87%)	23 (13%)	0	100	100
55	SI	204/208 (98%)	189 (93%)	14 (7%)	1 (0%)	32	68
56	SK	96/165 (58%)	85 (88%)	11 (12%)	0	100	100
57	SL	151/158 (96%)	134 (89%)	17 (11%)	0	100	100
58	SP	125/145 (86%)	112 (90%)	12 (10%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	SQ	142/146 (97%)	124 (87%)	16 (11%)	2 (1%)	13	41
60	SR	133/135 (98%)	118 (89%)	15 (11%)	0	100	100
61	SS	143/152 (94%)	127 (89%)	16 (11%)	0	100	100
62	ST	141/145 (97%)	128 (91%)	12 (8%)	1 (1%)	25	60
63	SU	102/119 (86%)	90 (88%)	12 (12%)	0	100	100
64	SV	81/83 (98%)	71 (88%)	8 (10%)	2 (2%)	6	25
65	SX	139/143 (97%)	125 (90%)	12 (9%)	2 (1%)	13	41
66	Sa	101/115 (88%)	89 (88%)	11 (11%)	1 (1%)	18	51
67	Sc	62/69 (90%)	45 (73%)	16 (26%)	1 (2%)	11	37
68	Sd	53/56 (95%)	50 (94%)	2 (4%)	1 (2%)	9	33
69	Sg	311/317 (98%)	264 (85%)	46 (15%)	1 (0%)	44	77
70	SC	221/293 (75%)	198 (90%)	22 (10%)	1 (0%)	32	68
71	SG	235/249 (94%)	219 (93%)	16 (7%)	0	100	100
72	SJ	184/194 (95%)	165 (90%)	18 (10%)	1 (0%)	32	68
73	SM	120/132 (91%)	108 (90%)	12 (10%)	0	100	100
74	SN	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
75	SO	138/151 (91%)	122 (88%)	16 (12%)	0	100	100
76	SW	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
77	SY	130/133 (98%)	121 (93%)	9 (7%)	0	100	100
78	SZ	73/125 (58%)	61 (84%)	11 (15%)	1 (1%)	13	41
79	Sb	81/84 (96%)	69 (85%)	12 (15%)	0	100	100
80	Se	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
81	Sf	65/156 (42%)	47 (72%)	18 (28%)	0	100	100
All	All	11565/12905 (90%)	10453 (90%)	1082 (9%)	30 (0%)	48	77

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	LN	124	ASP
65	SX	127	ASN
15	LM	88	ALA
59	SQ	44	PRO
62	ST	41	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/199 (96%)	183 (96%)	7 (4%)	39	74
5	LB	349/349 (100%)	344 (99%)	5 (1%)	71	91
6	LC	305/347 (88%)	297 (97%)	8 (3%)	51	83
7	LD	246/250 (98%)	241 (98%)	5 (2%)	60	87
8	LE	209/252 (83%)	207 (99%)	2 (1%)	80	95
9	LF	195/215 (91%)	192 (98%)	3 (2%)	70	91
10	LG	204/223 (92%)	195 (96%)	9 (4%)	33	67
11	LH	169/171 (99%)	167 (99%)	2 (1%)	75	93
12	LI	180/181 (99%)	177 (98%)	3 (2%)	66	89
13	LJ	148/149 (99%)	144 (97%)	4 (3%)	50	82
14	LL	176/177 (99%)	171 (97%)	5 (3%)	49	82
15	LM	118/161 (73%)	117 (99%)	1 (1%)	85	96
16	LN	171/172 (99%)	169 (99%)	2 (1%)	75	93
17	LO	173/174 (99%)	168 (97%)	5 (3%)	48	81
18	LP	134/163 (82%)	133 (99%)	1 (1%)	87	97
19	LQ	164/165 (99%)	161 (98%)	3 (2%)	64	89
20	LR	166/175 (95%)	163 (98%)	3 (2%)	64	89
21	LS	156/157 (99%)	155 (99%)	1 (1%)	89	97
22	LT	139/140 (99%)	137 (99%)	2 (1%)	71	91
23	LU	91/115 (79%)	90 (99%)	1 (1%)	78	94
24	LV	101/107 (94%)	99 (98%)	2 (2%)	60	87
25	LW	103/126 (82%)	101 (98%)	2 (2%)	62	88
26	LX	108/133 (81%)	108 (100%)	0	100	100
27	LY	124/135 (92%)	120 (97%)	4 (3%)	44	78
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	120/121 (99%)	117 (98%)	3 (2%)	53	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Lb	88/126 (70%)	85 (97%)	3 (3%)	42	76
31	Lc	83/97 (86%)	82 (99%)	1 (1%)	75	93
32	Ld	98/110 (89%)	97 (99%)	1 (1%)	80	95
33	Le	114/121 (94%)	113 (99%)	1 (1%)	82	95
34	Lf	88/89 (99%)	87 (99%)	1 (1%)	78	94
35	Lg	98/100 (98%)	97 (99%)	1 (1%)	80	95
36	Lh	109/110 (99%)	108 (99%)	1 (1%)	82	95
37	Li	86/89 (97%)	84 (98%)	2 (2%)	56	85
38	Lj	73/80 (91%)	72 (99%)	1 (1%)	71	91
39	Lk	64/65 (98%)	64 (100%)	0	100	100
40	Ll	47/48 (98%)	45 (96%)	2 (4%)	33	68
41	Lm	47/115 (41%)	47 (100%)	0	100	100
42	Ln	23/24 (96%)	22 (96%)	1 (4%)	33	68
43	Lo	94/94 (100%)	94 (100%)	0	100	100
44	Lp	74/75 (99%)	72 (97%)	2 (3%)	50	82
45	Lr	109/121 (90%)	108 (99%)	1 (1%)	82	95
46	Lz	195/196 (100%)	188 (96%)	7 (4%)	40	75
49	SA	183/243 (75%)	181 (99%)	2 (1%)	78	94
50	SB	195/231 (84%)	194 (100%)	1 (0%)	91	97
51	SD	190/202 (94%)	187 (98%)	3 (2%)	68	90
52	SE	224/225 (100%)	223 (100%)	1 (0%)	93	98
53	SF	159/170 (94%)	155 (98%)	4 (2%)	53	83
54	SH	166/174 (95%)	163 (98%)	3 (2%)	64	89
55	SI	178/180 (99%)	173 (97%)	5 (3%)	49	82
56	SK	89/136 (65%)	88 (99%)	1 (1%)	78	94
57	SL	137/142 (96%)	133 (97%)	4 (3%)	48	81
58	SP	113/130 (87%)	113 (100%)	0	100	100
59	SQ	121/121 (100%)	120 (99%)	1 (1%)	85	96
60	SR	122/122 (100%)	122 (100%)	0	100	100
61	SS	126/132 (96%)	124 (98%)	2 (2%)	68	90
62	ST	113/115 (98%)	112 (99%)	1 (1%)	82	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	SU	94/107 (88%)	93 (99%)	1 (1%)	78	94
64	SV	67/67 (100%)	66 (98%)	1 (2%)	70	91
65	SX	113/115 (98%)	112 (99%)	1 (1%)	82	95
66	Sa	90/98 (92%)	87 (97%)	3 (3%)	43	77
67	Sc	57/62 (92%)	57 (100%)	0	100	100
68	Sd	48/49 (98%)	47 (98%)	1 (2%)	59	86
69	Sg	272/275 (99%)	268 (98%)	4 (2%)	70	91
70	SC	189/225 (84%)	188 (100%)	1 (0%)	91	97
71	SG	207/218 (95%)	203 (98%)	4 (2%)	62	88
72	SJ	162/168 (96%)	158 (98%)	4 (2%)	53	83
73	SM	102/108 (94%)	94 (92%)	8 (8%)	15	39
74	SN	130/131 (99%)	127 (98%)	3 (2%)	56	85
75	SO	110/119 (92%)	107 (97%)	3 (3%)	50	82
76	SW	112/113 (99%)	110 (98%)	2 (2%)	64	89
77	SY	114/115 (99%)	113 (99%)	1 (1%)	82	95
78	SZ	66/103 (64%)	64 (97%)	2 (3%)	46	80
79	Sb	75/76 (99%)	75 (100%)	0	100	100
80	Se	47/48 (98%)	46 (98%)	1 (2%)	59	86
81	Sf	60/140 (43%)	58 (97%)	2 (3%)	43	77
All	All	10077/10995 (92%)	9899 (98%)	178 (2%)	68	89

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	La	92	LYS
44	Lp	84	ARG
74	SN	75	LEU
29	La	132	ARG
35	Lg	54	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
33	Le	43	ASN

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Mol	Chain	Res	Type
46	Lz	96	ASN
71	SG	81	HIS
34	Lf	56	ASN
45	Lr	41	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3677/5070 (72%)	1083 (29%)	23 (0%)
2	L7	119/120 (99%)	16 (13%)	0
3	L8	155/156 (99%)	33 (21%)	1 (0%)
47	S2	1708/1869 (91%)	452 (26%)	7 (0%)
48	S6	74/75 (98%)	32 (43%)	1 (1%)
All	All	5733/7290 (78%)	1616 (28%)	32 (0%)

5 of 1616 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	2	G
1	L5	4	G
1	L5	6	C
1	L5	17	A
1	L5	25	A

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	3597	G
1	L5	3876	A
47	S2	688	U
1	L5	3673	C
1	L5	4378	A

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

138 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
1	OMG	L5	1316	1	18,26,27	1.24	3 (16%)	22,38,41	2.30	7 (31%)
1	1MA	L5	1322	1,82	16,25,26	1.55	4 (25%)	13,37,40	1.34	2 (15%)
1	A2M	L5	1326	1	18,25,26	0.91	1 (5%)	20,36,39	1.80	2 (10%)
1	P4U	L5	1348	1	18,24,25	1.03	1 (5%)	20,33,36	2.06	1 (5%)
1	B8Q	L5	1456	1	16,22,23	1.30	2 (12%)	19,32,35	1.08	2 (10%)
1	2MG	L5	1517	1	19,26,27	1.02	2 (10%)	20,38,41	2.48	8 (40%)
1	OMG	L5	1522	1	18,26,27	1.26	3 (16%)	22,38,41	2.18	6 (27%)
1	A2M	L5	1524	1	18,25,26	1.11	2 (11%)	20,36,39	1.73	3 (15%)
1	A2M	L5	1534	1,82	18,25,26	1.02	1 (5%)	20,36,39	1.75	2 (10%)
1	B9B	L5	1574	1	21,28,29	1.00	2 (9%)	23,40,43	1.80	5 (21%)
1	PSU	L5	1582	1	16,21,22	1.58	5 (31%)	20,30,33	3.34	5 (25%)
1	7MG	L5	1605	1	20,26,27	1.42	2 (10%)	22,39,42	2.57	5 (22%)
1	OMG	L5	1625	1	18,26,27	1.20	3 (16%)	22,38,41	2.06	6 (27%)
1	I4U	L5	1659	1,82	17,24,25	0.89	1 (5%)	19,34,37	2.62	3 (15%)
1	PSU	L5	1677	1	16,21,22	1.90	5 (31%)	20,30,33	3.51	7 (35%)
1	PSU	L5	1683	1	16,21,22	1.93	5 (31%)	20,30,33	3.31	6 (30%)
1	E7G	L5	1797	1	20,27,28	1.36	2 (10%)	24,40,43	2.63	6 (25%)
1	B8H	L5	1860	1	16,22,23	1.33	2 (12%)	21,32,35	2.33	3 (14%)
1	UR3	L5	1866	1	14,22,23	0.84	0	16,32,35	0.88	1 (6%)
1	A2M	L5	1871	1,82	18,25,26	1.01	2 (11%)	20,36,39	1.82	2 (10%)
1	OMG	L5	1883	1	18,26,27	1.18	3 (16%)	22,38,41	1.99	6 (27%)
1	P7G	L5	1909	1	21,28,29	1.28	2 (9%)	26,41,44	3.00	7 (26%)
1	OMG	L5	2050	1	18,26,27	1.08	2 (11%)	22,38,41	1.99	6 (27%)
1	E7G	L5	2297	1	20,27,28	1.33	2 (10%)	24,40,43	2.66	7 (29%)
1	A2M	L5	2363	1,82	18,25,26	1.06	2 (11%)	20,36,39	1.62	2 (10%)
1	OMG	L5	2364	1	18,26,27	1.06	2 (11%)	22,38,41	2.00	6 (27%)
1	OMC	L5	2365	1,82	15,22,23	1.01	0	19,31,34	1.09	1 (5%)
1	B9B	L5	237	1	21,28,29	1.24	3 (14%)	23,40,43	1.86	6 (26%)
1	B8W	L5	2380	1	18,26,27	0.97	1 (5%)	19,38,41	1.76	4 (21%)
1	A2M	L5	2401	1	18,25,26	1.01	2 (11%)	20,36,39	1.67	2 (10%)
1	OMC	L5	2422	1,82	15,22,23	1.14	2 (13%)	19,31,34	0.73	0
1	OMG	L5	2424	1	18,26,27	1.24	3 (16%)	22,38,41	2.04	7 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	2508	1	16,21,22	1.57	3 (18%)	20,30,33	3.37	6 (30%)
1	7MG	L5	2522	1	20,26,27	1.41	2 (10%)	22,39,42	2.68	4 (18%)
1	B9B	L5	2754	1	21,28,29	1.10	2 (9%)	23,40,43	2.04	6 (26%)
1	OMG	L5	2773	1	18,26,27	1.22	2 (11%)	22,38,41	2.14	6 (27%)
1	B9H	L5	2786	1	19,25,26	1.23	3 (15%)	20,35,38	1.87	4 (20%)
1	OMC	L5	2804	1	15,22,23	1.07	1 (6%)	19,31,34	0.96	0
1	OMC	L5	2861	1	15,22,23	1.03	1 (6%)	19,31,34	0.77	0
1	OMC	L5	3701	1,82	15,22,23	1.03	1 (6%)	19,31,34	0.97	0
1	PSU	L5	3715	1,82	16,21,22	1.41	4 (25%)	20,30,33	3.41	6 (30%)
1	A2M	L5	3718	1	18,25,26	0.93	1 (5%)	20,36,39	1.63	2 (10%)
1	A2M	L5	3723	1	18,25,26	1.08	1 (5%)	20,36,39	1.53	2 (10%)
1	PSU	L5	3729	1	16,21,22	1.59	4 (25%)	20,30,33	3.42	5 (25%)
1	OMG	L5	373	1	18,26,27	1.20	3 (16%)	22,38,41	2.22	6 (27%)
1	B8H	L5	3762	1	16,22,23	1.60	3 (18%)	21,32,35	2.46	6 (28%)
1	PSU	L5	3764	1	16,21,22	1.51	3 (18%)	20,30,33	3.45	5 (25%)
1	5MC	L5	3782	1,82	15,22,23	1.21	1 (6%)	17,32,35	0.94	1 (5%)
1	A2M	L5	3785	1	18,25,26	0.95	1 (5%)	20,36,39	1.67	3 (15%)
1	OMG	L5	3792	1	18,26,27	1.16	2 (11%)	22,38,41	2.10	6 (27%)
1	A2M	L5	3825	1	18,25,26	1.05	2 (11%)	20,36,39	1.83	2 (10%)
1	A2M	L5	3867	1	18,25,26	1.01	1 (5%)	20,36,39	1.65	3 (15%)
1	OMC	L5	3869	1	15,22,23	1.10	1 (6%)	19,31,34	1.19	1 (5%)
1	P7G	L5	3880	1	21,28,29	1.24	3 (14%)	26,41,44	3.18	8 (30%)
1	OMC	L5	3887	1	15,22,23	1.03	1 (6%)	19,31,34	1.12	1 (5%)
1	B8K	L5	3897	1	22,28,29	1.63	3 (13%)	25,42,45	2.44	5 (20%)
1	BGH	L5	3899	1	22,29,30	2.30	4 (18%)	24,43,46	2.76	10 (41%)
1	OMC	L5	3909	1	15,22,23	1.05	1 (6%)	19,31,34	0.82	0
1	A2M	L5	398	1	18,25,26	1.06	1 (5%)	20,36,39	1.81	2 (10%)
1	5MU	L5	4083	1	14,22,23	0.89	1 (7%)	16,32,35	2.28	2 (12%)
1	B8W	L5	4129	1	18,26,27	1.07	1 (5%)	19,38,41	1.95	4 (21%)
1	B8W	L5	4185	1	18,26,27	0.97	2 (11%)	19,38,41	1.92	4 (21%)
1	I4U	L5	4194	1	17,24,25	0.82	0	19,34,37	3.08	3 (15%)
1	OMG	L5	4196	1,82	18,26,27	1.16	2 (11%)	22,38,41	2.04	6 (27%)
1	6MZ	L5	4220	1	18,25,26	0.97	2 (11%)	16,36,39	2.61	4 (25%)
1	PSU	L5	4293	1	16,21,22	1.62	3 (18%)	20,30,33	3.41	6 (30%)
1	B8H	L5	4296	1	16,22,23	1.54	3 (18%)	21,32,35	2.25	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	L5	4306	1	14,22,23	1.14	2 (14%)	18,31,34	2.29	2 (11%)
1	5MC	L5	4335	1	15,22,23	1.46	2 (13%)	17,32,35	0.97	2 (11%)
1	E6G	L5	4355	1	20,27,28	1.25	3 (15%)	22,39,42	1.97	6 (27%)
1	OMG	L5	4370	1	18,26,27	1.08	2 (11%)	22,38,41	1.99	5 (22%)
1	MHG	L5	4371	1	25,32,33	1.19	2 (8%)	29,46,49	2.79	8 (27%)
1	PSU	L5	4403	1	16,21,22	1.56	5 (31%)	20,30,33	3.61	8 (40%)
1	1MA	L5	4415	1	16,25,26	1.67	5 (31%)	13,37,40	1.34	2 (15%)
1	PSU	L5	4442	1	16,21,22	1.64	4 (25%)	20,30,33	3.37	7 (35%)
1	5MC	L5	4447	1,82	15,22,23	1.34	3 (20%)	17,32,35	1.99	4 (23%)
1	PSU	L5	4450	1,82	16,21,22	2.02	4 (25%)	20,30,33	3.39	6 (30%)
1	B8W	L5	4472	1	18,26,27	1.07	1 (5%)	19,38,41	2.04	4 (21%)
1	B8T	L5	4483	1	16,22,23	0.91	0	16,31,34	1.12	2 (12%)
1	OMG	L5	4494	1	18,26,27	1.19	3 (16%)	22,38,41	2.21	6 (27%)
1	PSU	L5	4500	1	16,21,22	1.74	5 (31%)	20,30,33	3.33	5 (25%)
1	A2M	L5	4523	1,82	18,25,26	0.96	1 (5%)	20,36,39	1.78	2 (10%)
1	B8W	L5	4529	1,82	18,26,27	1.03	2 (11%)	19,38,41	2.04	4 (21%)
1	UR3	L5	4530	1	14,22,23	0.93	1 (7%)	16,32,35	0.76	0
1	PSU	L5	4531	1	16,21,22	1.77	4 (25%)	20,30,33	3.41	6 (30%)
1	OMC	L5	4536	1	15,22,23	1.15	1 (6%)	19,31,34	1.21	2 (10%)
1	7MG	L5	4550	1	20,26,27	1.30	2 (10%)	22,39,42	2.53	5 (22%)
1	M7A	L5	4564	1	20,25,26	1.01	2 (10%)	23,37,40	2.26	5 (21%)
1	A2M	L5	4571	1	18,25,26	1.04	2 (11%)	20,36,39	1.73	2 (10%)
1	UR3	L5	4597	1	14,22,23	0.68	0	16,32,35	0.73	0
1	OMU	L5	4620	1	14,22,23	1.06	2 (14%)	18,31,34	2.54	4 (22%)
1	OMG	L5	4623	1	18,26,27	1.15	3 (16%)	22,38,41	2.13	6 (27%)
1	PSU	L5	4628	1	16,21,22	1.57	4 (25%)	20,30,33	3.35	7 (35%)
1	PSU	L5	4636	1	16,21,22	1.77	4 (25%)	20,30,33	3.38	6 (30%)
1	OMG	L5	4637	1	18,26,27	1.23	3 (16%)	22,38,41	2.19	7 (31%)
1	B8T	L5	4671	1	16,22,23	0.93	1 (6%)	16,31,34	1.11	2 (12%)
1	B8K	L5	4690	1	22,28,29	1.75	3 (13%)	25,42,45	2.71	6 (24%)
1	OMG	L5	4870	1	18,26,27	1.29	3 (16%)	22,38,41	2.08	6 (27%)
1	2MG	L5	4872	1	19,26,27	1.22	2 (10%)	20,38,41	3.29	10 (50%)
1	2MG	L5	729	1	19,26,27	1.06	2 (10%)	20,38,41	2.27	7 (35%)
1	2MG	L5	978	1	19,26,27	1.11	2 (10%)	20,38,41	2.43	8 (40%)
3	OMU	L8	14	1,3	14,22,23	1.15	2 (14%)	18,31,34	1.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MLZ	LC	333	6	9,9,10	1.30	1 (11%)	6,9,11	1.34	1 (16%)
41	MLZ	Lm	98	41	9,9,10	1.81	1 (11%)	6,9,11	1.61	2 (33%)
47	A2M	S2	1031	47	18,25,26	1.04	1 (5%)	20,36,39	1.76	3 (15%)
47	PSU	S2	1081	47	16,21,22	1.51	5 (31%)	20,30,33	3.71	8 (40%)
47	OMU	S2	116	47	14,22,23	1.09	1 (7%)	18,31,34	2.39	2 (11%)
47	PSU	S2	119	47	16,21,22	1.54	4 (25%)	20,30,33	3.27	5 (25%)
47	OMU	S2	121	47	14,22,23	1.32	2 (14%)	18,31,34	2.33	2 (11%)
47	B8Q	S2	1219	82,47	16,22,23	1.27	2 (12%)	19,32,35	0.97	2 (10%)
47	PSU	S2	1243	47	16,21,22	1.71	5 (31%)	20,30,33	3.49	6 (30%)
47	B8N	S2	1248	47	16,29,30	1.34	2 (12%)	20,42,45	0.83	1 (5%)
47	4AC	S2	1337	47	18,24,25	1.23	5 (27%)	20,34,37	1.41	3 (15%)
47	5MC	S2	1374	47	15,22,23	1.34	1 (6%)	17,32,35	1.00	1 (5%)
47	A2M	S2	159	47	18,25,26	1.07	1 (5%)	20,36,39	1.50	2 (10%)
47	A2M	S2	166	47	18,25,26	1.20	2 (11%)	20,36,39	1.70	2 (10%)
47	A2M	S2	1678	47	18,25,26	0.97	1 (5%)	20,36,39	1.68	2 (10%)
47	OMC	S2	1703	47	15,22,23	1.01	0	19,31,34	0.91	0
47	OMC	S2	1710	47	15,22,23	1.12	1 (6%)	19,31,34	0.85	0
47	OMC	S2	174	82,47	15,22,23	0.98	0	19,31,34	0.87	1 (5%)
47	M7A	S2	1806	47	20,25,26	1.07	2 (10%)	23,37,40	2.22	5 (21%)
47	UR3	S2	1830	47	14,22,23	0.82	0	16,32,35	0.78	0
47	6MZ	S2	1832	82,47	18,25,26	0.99	1 (5%)	16,36,39	2.47	3 (18%)
47	4AC	S2	1842	47	18,24,25	1.38	4 (22%)	20,34,37	1.54	5 (25%)
47	MA6	S2	1850	47	16,26,27	0.88	1 (6%)	18,38,41	2.35	3 (16%)
47	MA6	S2	1851	47	16,26,27	0.84	1 (6%)	18,38,41	2.24	3 (16%)
47	A2M	S2	27	82,47	18,25,26	1.04	1 (5%)	20,36,39	1.81	3 (15%)
47	A2M	S2	484	47	18,25,26	1.00	1 (5%)	20,36,39	1.58	2 (10%)
47	OMG	S2	509	82,47	18,26,27	1.16	2 (11%)	22,38,41	2.06	6 (27%)
47	OMC	S2	517	47	15,22,23	1.03	0	19,31,34	0.97	0
47	E3C	S2	568	47	17,23,24	1.30	3 (17%)	19,33,36	1.58	3 (15%)
47	PSU	S2	612	47	16,21,22	1.72	4 (25%)	20,30,33	3.27	7 (35%)
47	OMG	S2	644	47	18,26,27	1.13	2 (11%)	22,38,41	2.15	6 (27%)
47	A2M	S2	668	82,47	18,25,26	1.06	2 (11%)	20,36,39	1.74	2 (10%)
47	OMG	S2	683	47	18,26,27	1.19	3 (16%)	22,38,41	2.25	6 (27%)
47	5MU	S2	814	47	14,22,23	0.90	1 (7%)	16,32,35	2.27	2 (12%)
47	PSU	S2	822	47	16,21,22	1.74	4 (25%)	20,30,33	3.39	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	PSU	S2	823	47	16,21,22	1.62	4 (25%)	20,30,33	3.28	7 (35%)

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
1	OMG	L5	1316	1	-	0/5/27/28	0/3/3/3
1	1MA	L5	1322	1,82	-	0/3/25/26	0/3/3/3
1	A2M	L5	1326	1	-	0/5/27/28	0/3/3/3
1	P4U	L5	1348	1	-	0/7/29/30	0/2/2/2
1	B8Q	L5	1456	1	1/1/9/11	0/7/42/43	0/2/2/2
1	2MG	L5	1517	1	-	0/5/27/28	0/3/3/3
1	OMG	L5	1522	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	1524	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	1534	1,82	-	0/5/27/28	0/3/3/3
1	B9B	L5	1574	1	-	2/7/29/30	0/3/3/3
1	PSU	L5	1582	1	-	0/7/25/26	0/2/2/2
1	7MG	L5	1605	1	-	0/7/37/38	0/3/3/3
1	OMG	L5	1625	1	-	0/5/27/28	0/3/3/3
1	I4U	L5	1659	1,82	-	1/7/29/30	0/2/2/2
1	PSU	L5	1677	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1683	1	-	0/7/25/26	0/2/2/2
1	E7G	L5	1797	1	-	0/9/39/40	0/3/3/3
1	B8H	L5	1860	1	-	0/7/25/26	0/2/2/2
1	UR3	L5	1866	1	-	0/3/25/26	0/2/2/2
1	A2M	L5	1871	1,82	-	0/5/27/28	0/3/3/3
1	OMG	L5	1883	1	-	0/5/27/28	0/3/3/3
1	P7G	L5	1909	1	-	0/10/40/41	0/3/3/3
1	OMG	L5	2050	1	-	0/5/27/28	0/3/3/3
1	E7G	L5	2297	1	-	0/9/39/40	0/3/3/3
1	A2M	L5	2363	1,82	-	0/5/27/28	0/3/3/3
1	OMG	L5	2364	1	-	0/5/27/28	0/3/3/3
1	OMC	L5	2365	1,82	-	0/5/27/28	0/2/2/2
1	B9B	L5	237	1	-	1/7/29/30	0/3/3/3
1	B8W	L5	2380	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	2401	1	-	0/5/27/28	0/3/3/3
1	OMC	L5	2422	1,82	-	0/5/27/28	0/2/2/2
1	OMG	L5	2424	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	2508	1	-	0/7/25/26	0/2/2/2
1	7MG	L5	2522	1	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B9B	L5	2754	1	-	0/7/29/30	0/3/3/3
1	OMG	L5	2773	1	-	0/5/27/28	0/3/3/3
1	B9H	L5	2786	1	1/1/9/11	0/12/47/48	0/2/2/2
1	OMC	L5	2804	1	-	0/5/27/28	0/2/2/2
1	OMC	L5	2861	1	-	0/5/27/28	0/2/2/2
1	OMC	L5	3701	1,82	-	0/5/27/28	0/2/2/2
1	PSU	L5	3715	1,82	-	0/7/25/26	0/2/2/2
1	A2M	L5	3718	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	3723	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	3729	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	373	1	-	0/5/27/28	0/3/3/3
1	B8H	L5	3762	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3764	1	-	0/7/25/26	0/2/2/2
1	5MC	L5	3782	1,82	-	0/3/25/26	0/2/2/2
1	A2M	L5	3785	1	-	0/5/27/28	0/3/3/3
1	OMG	L5	3792	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	3825	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	3867	1	-	0/5/27/28	0/3/3/3
1	OMC	L5	3869	1	-	0/5/27/28	0/2/2/2
1	P7G	L5	3880	1	-	0/10/40/41	0/3/3/3
1	OMC	L5	3887	1	-	0/5/27/28	0/2/2/2
1	B8K	L5	3897	1	-	0/11/41/42	0/3/3/3
1	BGH	L5	3899	1	-	0/13/43/44	0/3/3/3
1	OMC	L5	3909	1	-	0/5/27/28	0/2/2/2
1	A2M	L5	398	1	-	0/5/27/28	0/3/3/3
1	5MU	L5	4083	1	-	0/3/25/26	0/2/2/2
1	B8W	L5	4129	1	-	2/5/27/28	0/3/3/3
1	B8W	L5	4185	1	-	2/5/27/28	0/3/3/3
1	I4U	L5	4194	1	-	1/7/29/30	0/2/2/2
1	OMG	L5	4196	1,82	-	0/5/27/28	0/3/3/3
1	6MZ	L5	4220	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	4293	1	-	0/7/25/26	0/2/2/2
1	B8H	L5	4296	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	4306	1	-	0/5/27/28	0/2/2/2
1	5MC	L5	4335	1	-	0/3/25/26	0/2/2/2
1	E6G	L5	4355	1	-	2/6/28/29	0/3/3/3
1	OMG	L5	4370	1	-	0/5/27/28	0/3/3/3
1	MHG	L5	4371	1	-	0/16/46/47	0/3/3/3
1	PSU	L5	4403	1	-	0/7/25/26	0/2/2/2
1	1MA	L5	4415	1	-	0/3/25/26	0/3/3/3
1	PSU	L5	4442	1	-	0/7/25/26	0/2/2/2
1	5MC	L5	4447	1,82	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	4450	1,82	-	0/7/25/26	0/2/2/2
1	B8W	L5	4472	1	-	2/5/27/28	0/3/3/3
1	B8T	L5	4483	1	-	0/5/27/28	0/2/2/2
1	OMG	L5	4494	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	4500	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	4523	1,82	-	0/5/27/28	0/3/3/3
1	B8W	L5	4529	1,82	-	2/5/27/28	0/3/3/3
1	UR3	L5	4530	1	-	0/3/25/26	0/2/2/2
1	PSU	L5	4531	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	4536	1	-	0/5/27/28	0/2/2/2
1	7MG	L5	4550	1	-	0/7/37/38	0/3/3/3
1	M7A	L5	4564	1	-	0/7/37/38	0/3/3/3
1	A2M	L5	4571	1	-	0/5/27/28	0/3/3/3
1	UR3	L5	4597	1	-	0/3/25/26	0/2/2/2
1	OMU	L5	4620	1	-	0/5/27/28	0/2/2/2
1	OMG	L5	4623	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	4628	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4636	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4637	1	-	0/5/27/28	0/3/3/3
1	B8T	L5	4671	1	-	0/5/27/28	0/2/2/2
1	B8K	L5	4690	1	-	0/11/41/42	0/3/3/3
1	OMG	L5	4870	1	-	0/5/27/28	0/3/3/3
1	2MG	L5	4872	1	-	0/5/27/28	0/3/3/3
1	2MG	L5	729	1	-	0/5/27/28	0/3/3/3
1	2MG	L5	978	1	-	0/5/27/28	0/3/3/3
3	OMU	L8	14	1,3	-	0/5/27/28	0/2/2/2
6	MLZ	LC	333	6	-	0/6/8/10	0/0/0/0
41	MLZ	Lm	98	41	-	0/6/8/10	0/0/0/0
47	A2M	S2	1031	47	-	0/5/27/28	0/3/3/3
47	PSU	S2	1081	47	-	0/7/25/26	0/2/2/2
47	OMU	S2	116	47	-	0/5/27/28	0/2/2/2
47	PSU	S2	119	47	-	0/7/25/26	0/2/2/2
47	OMU	S2	121	47	-	0/5/27/28	0/2/2/2
47	B8Q	S2	1219	82,47	1/1/9/11	0/7/42/43	0/2/2/2
47	PSU	S2	1243	47	-	0/7/25/26	0/2/2/2
47	B8N	S2	1248	47	-	0/12/34/35	0/2/2/2
47	4AC	S2	1337	47	-	2/7/29/30	0/2/2/2
47	5MC	S2	1374	47	-	0/3/25/26	0/2/2/2
47	A2M	S2	159	47	-	0/5/27/28	0/3/3/3
47	A2M	S2	166	47	-	0/5/27/28	0/3/3/3
47	A2M	S2	1678	47	-	0/5/27/28	0/3/3/3
47	OMC	S2	1703	47	-	0/5/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	OMC	S2	1710	47	-	0/5/27/28	0/2/2/2
47	OMC	S2	174	82,47	-	0/5/27/28	0/2/2/2
47	M7A	S2	1806	47	-	0/7/37/38	0/3/3/3
47	UR3	S2	1830	47	-	0/3/25/26	0/2/2/2
47	6MZ	S2	1832	82,47	-	0/5/27/28	0/3/3/3
47	4AC	S2	1842	47	-	0/7/29/30	0/2/2/2
47	MA6	S2	1850	47	-	0/7/29/30	0/3/3/3
47	MA6	S2	1851	47	-	0/7/29/30	0/3/3/3
47	A2M	S2	27	82,47	-	0/5/27/28	0/3/3/3
47	A2M	S2	484	47	-	0/5/27/28	0/3/3/3
47	OMG	S2	509	82,47	-	0/5/27/28	0/3/3/3
47	OMC	S2	517	47	-	0/5/27/28	0/2/2/2
47	E3C	S2	568	47	1/1/9/11	0/9/44/45	0/2/2/2
47	PSU	S2	612	47	-	0/7/25/26	0/2/2/2
47	OMG	S2	644	47	-	0/5/27/28	0/3/3/3
47	A2M	S2	668	82,47	-	0/5/27/28	0/3/3/3
47	OMG	S2	683	47	-	0/5/27/28	0/3/3/3
47	5MU	S2	814	47	-	0/3/25/26	0/2/2/2
47	PSU	S2	822	47	-	0/7/25/26	0/2/2/2
47	PSU	S2	823	47	-	0/7/25/26	0/2/2/2

The worst 5 of 299 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4450	PSU	C5-C1'	-6.22	1.46	1.52
1	L5	1677	PSU	C5-C1'	-5.65	1.47	1.52
1	L5	1683	PSU	C5-C1'	-5.59	1.47	1.52
1	L5	4690	B8K	C5-N7	-5.52	1.32	1.40
1	L5	4531	PSU	C5-C1'	-5.33	1.47	1.52

The worst 5 of 543 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1081	PSU	N1-C2-N3	-9.71	121.41	128.40
1	L5	3715	PSU	N1-C2-N3	-9.58	121.51	128.40
1	L5	4403	PSU	N1-C2-N3	-9.18	121.79	128.40
1	L5	1677	PSU	C5-C4-N3	-9.08	117.98	125.43
1	L5	3764	PSU	N1-C2-N3	-9.08	121.87	128.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	L5	2786	B9H	C4
47	S2	1219	B8Q	C4
1	L5	1456	B8Q	C4
47	S2	568	E3C	C4

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	S2	1337	4AC	CM7-C7-N4-C4
1	L5	237	B9B	C61-O6-C6-C5
47	S2	1337	4AC	O7-C7-N4-C4
1	L5	4185	B8W	C61-O6-C6-N1
1	L5	1574	B9B	C61-O6-C6-N1

There are no ring outliers.

25 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	1322	1MA	1	0
1	L5	1326	A2M	1	0
1	L5	1456	B8Q	1	0
1	L5	1522	OMG	1	0
1	L5	1625	OMG	1	0
1	L5	1797	E7G	1	0
1	L5	1871	A2M	1	0
1	L5	1909	P7G	1	0
1	L5	2363	A2M	1	0
1	L5	2422	OMC	1	0
1	L5	2522	7MG	1	0
1	L5	3723	A2M	1	0
1	L5	4194	I4U	1	0
1	L5	4220	6MZ	1	0
1	L5	4415	1MA	1	0
1	L5	4523	A2M	1	0
1	L5	4571	A2M	1	0
1	L5	4623	OMG	1	0
1	L5	4671	B8T	1	0
1	L5	729	2MG	1	0
3	L8	14	OMU	1	0
47	S2	116	OMU	1	0
47	S2	121	OMU	1	0
47	S2	1337	4AC	1	0
47	S2	159	A2M	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 412 ligands modelled in this entry, 410 are monoatomic - leaving 2 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
83	HMT	L5	5348	-	37,43,43	1.89	6 (16%)	47,66,66	1.61	10 (21%)
85	HYG	S2	2034	-	35,39,39	0.85	1 (2%)	41,60,60	1.59	7 (17%)

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
83	HMT	L5	5348	-	-	0/27/74/74	0/5/5/5
85	HYG	S2	2034	-	-	0/12/87/87	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	L5	5348	HMT	C5-C4	-6.68	1.39	1.51
83	L5	5348	HMT	C7-C6	-5.86	1.38	1.51
83	L5	5348	HMT	C3-C2	-3.45	1.40	1.50
83	L5	5348	HMT	C13-C14	-2.83	1.33	1.38
83	L5	5348	HMT	C16-C15	-2.80	1.33	1.38

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	2034	HYG	O22-C17-C12	-4.78	96.03	103.60
83	L5	5348	HMT	C25-C24-C20	-4.31	109.68	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	L5	5348	HMT	C7-C6-C16	-3.45	111.77	119.29
83	L5	5348	HMT	C13-C5-C4	-3.37	109.43	119.08
85	S2	2034	HYG	O8-C1-C2	-3.06	104.17	109.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	L5	5348	HMT	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
59	SQ	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SQ	2:PRO	C	3:SER	N	8.50