



wwPDB EM Validation Summary Report ⓘ

May 7, 2026 – 08:20 pm BST

PDB ID : 9RU7 / pdb_00009ru7
EMDB ID : EMD-54265
Title : WT-HEK 80S ribosome bound to Kozak mRNA (WT-Kozak)
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.
Deposited on : 2025-07-03
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

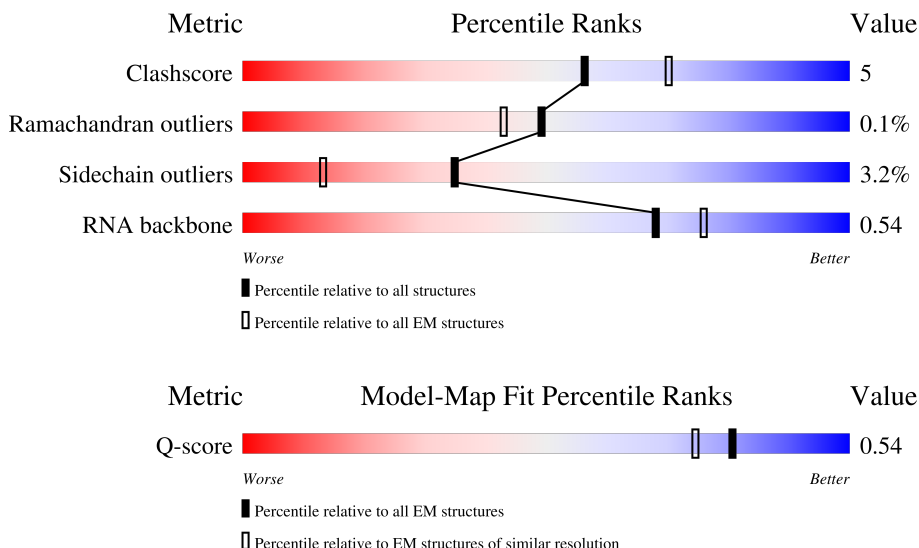
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.











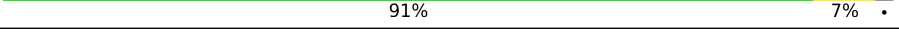

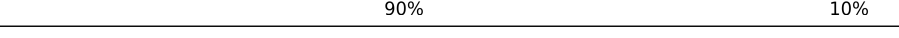
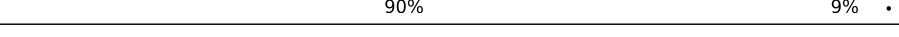

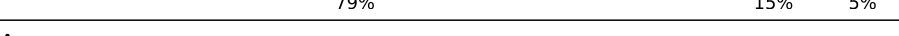


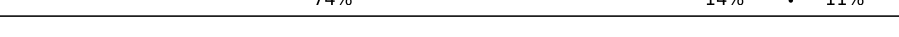

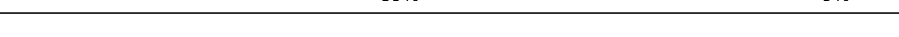






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	SP	145	
2	L8	156	
3	L5	5069	



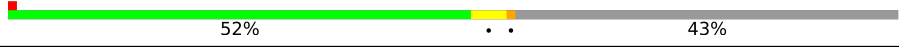



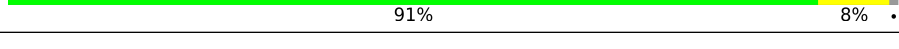
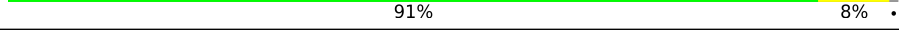
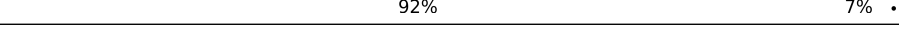
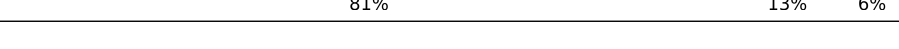
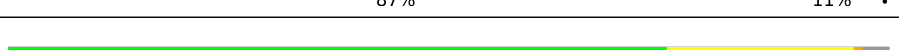



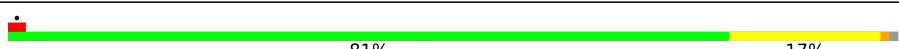





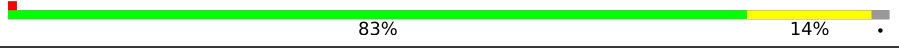
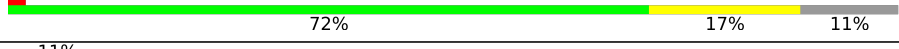



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	LA	252	
5	LB	396	
6	LC	427	
7	LJ	178	
8	LH	192	
9	LE	288	
10	LG	266	
11	LO	203	
12	LL	211	
13	LV	140	
14	LM	136	
15	La	148	
16	LN	204	
17	LI	214	
18	LD	297	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LP	154	
24	LU	128	
25	LX	156	
26	LY	145	
27	LW	157	
28	LZ	136	

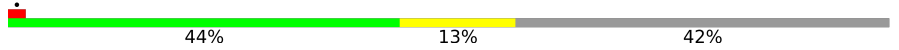





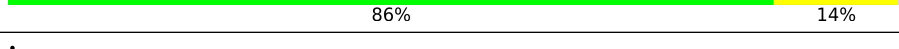
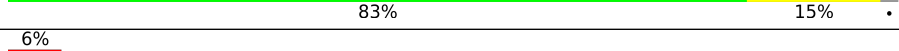
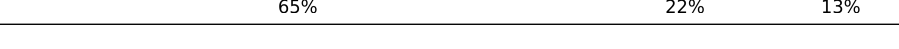
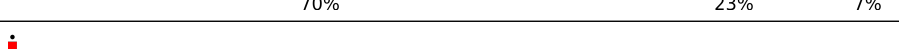
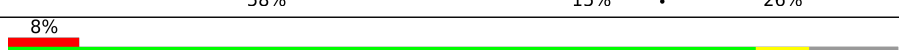

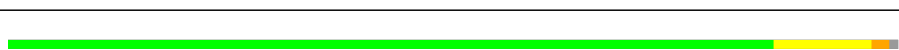

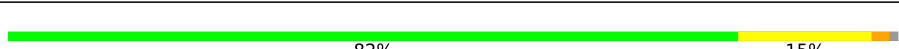

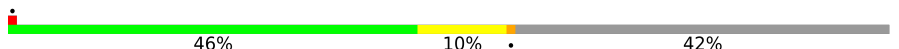








Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Lr	137	
30	Lh	123	
31	Lb	159	
32	LF	248	
33	Lc	115	
34	Ld	125	
35	Le	129	
36	Lf	110	
37	Lg	109	
38	Li	105	
39	Lj	87	
40	Lk	70	
41	Ll	51	
42	Lm	128	
43	Ln	25	
44	Lo	106	
45	Lp	89	
46	Pt	77	
47	L7	120	
48	SA	295	
49	SB	264	
50	SE	263	
51	SF	204	
52	SH	194	
53	SI	208	

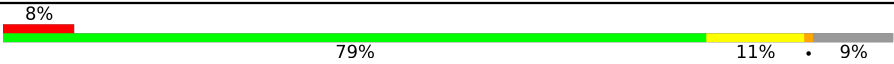

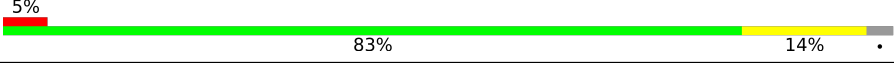

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	SK	165	
55	SL	158	
56	SQ	146	
57	SS	152	
58	ST	145	
59	SU	119	
60	SV	83	
61	SX	143	
62	Sc	69	
63	Sd	56	
64	SC	293	
65	SG	249	
66	SJ	194	
67	SN	151	
68	SO	151	
69	SW	130	
70	SY	133	
71	SZ	125	
72	Sb	84	
73	Se	133	
74	Sa	115	
75	S2	1868	
76	mR	27	
77	S6	74	
78	Sg	317	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	SD	243	
80	SM	132	
81	SR	135	
82	Sf	156	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 199163 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 protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	SP	129	Total	C	N	O	S	0	0
			814	505	163	144	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L8	151	Total	C	N	O	P	0	0
			3215	1434	570	1060	151		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3376	Total	C	N	O	P	1	0
			72477	32309	13259	23532	3377		

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	251	Total	C	N	O	S	0	0
			1895	1188	391	310	6		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	395	Total	C	N	O	S	0	0
			2719	1725	544	442	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	365	Total	C	N	O	S	0	0
			2836	1786	570	467	13		

- Molecule 7 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LJ	168	Total	C	N	O	S	0	0
			1207	773	230	199	5		

- Molecule 8 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LH	190	Total	C	N	O	S	0	0
			1435	911	275	243	6		

- Molecule 9 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LE	208	Total	C	N	O	S	0	0
			1584	1018	302	260	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	230	Total	C	N	O	S	1	0
			1696	1082	326	285	3		

- Molecule 11 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LO	199	Total	C	N	O	S	0	0
			1605	1036	317	248	4		

- Molecule 12 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LL	206	Total	C	N	O	S	0	0
			1583	992	335	252	4		

- Molecule 13 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LV	132	Total	C	N	O	S	0	0
			943	596	178	164	5		

- Molecule 14 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LM	136	Total	C	N	O	S	0	0
			1089	700	212	170	7		

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	La	147	Total	C	N	O	S	1	0
			1157	731	239	184	3		

- 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
			1694	1069	356	265	4		

- Molecule 17 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	203	Total	C	N	O	S	0	0
			1610	1024	313	261	12		

- Molecule 18 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LD	293	Total	C	N	O	S	0	0
			2232	1417	416	387	12		

- 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
			1497	936	312	244	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	175	Total	C	N	O	S	0	0
			1391	864	298	220	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	176	Total	C	N	O	S	0	0
			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
			1221	773	241	202	5		

- Molecule 23 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 24 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	99	Total	C	N	O	S	0	0
			781	504	139	136	2		

- Molecule 25 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LX	118	Total	C	N	O	S	0	0
			955	612	180	162	1		

- Molecule 26 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LY	130	Total	C	N	O	S	0	0
			1057	665	215	174	3		

- Molecule 27 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	61	Total	C	N	O	S	0	0
			515	330	100	82	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
			1088	703	205	177	3		

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lr	122	Total	C	N	O	S	0	0
			973	603	202	164	4		

- Molecule 30 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lh	122	Total	C	N	O	S	0	0
			954	604	197	152	1		

- Molecule 31 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lb	91	Total	C	N	O	S	0	0
			700	437	150	111	2		

- Molecule 32 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LF	225	Total	C	N	O	S	0	0
			1756	1123	337	289	7		

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lc	98	Total	C	N	O	S	0	0
			740	469	132	134	5		

- Molecule 34 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ld	107	Total	C	N	O	S	0	0
			877	554	170	151	2		

- Molecule 35 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Le	128	Total	C	N	O	S	0	0
			1045	661	214	165	5		

- Molecule 36 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lf	109	Total	C	N	O	S	0	0
			860	546	174	137	3		

- Molecule 37 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lg	108	Total	C	N	O	S	0	0
			838	522	175	135	6		

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Li	99	Total	C	N	O	S	0	0
			756	474	159	119	4		

- Molecule 39 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lj	86	Total	C	N	O	S	0	0
			695	427	153	110	5		

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lk	68	Total	C	N	O	S	0	0
			545	350	98	96	1		

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ll	50	Total	C	N	O	S	0	0
			433	275	94	63	1		

- Molecule 42 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lm	51	Total	C	N	O	S	0	0
			408	253	87	63	5		

- Molecule 43 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ln	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 44 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lo	105	Total	C	N	O	S	1	0
			849	535	170	138	6		

- Molecule 45 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lp	88	Total	C	N	O	S	1	0
			682	429	133	113	7		

- Molecule 46 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	Pt	76	Total	C	N	O	P	S	0	0
			1624	724	296	527	76	1		

- Molecule 47 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L7	119	Total	C	N	O	P	0	0
			2542	1132	454	837	119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SA	217	Total	C	N	O	S	0	0
			1624	1035	290	292	7		

- Molecule 49 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SB	214	Total	C	N	O	S	0	0
			1708	1086	307	301	14		

- Molecule 50 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SE	258	Total	C	N	O	S	0	0
			1914	1220	363	324	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SF	182	Total	C	N	O	S	0	0
			1350	843	261	240	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SH	178	Total	C	N	O	S	0	0
			1173	743	221	209			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SI	186	Total	C	N	O	S	0	0
			1446	906	287	248	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SK	95	Total	C	N	O	S	0	0
			690	451	125	111	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SL	138	Total	C	N	O	S	0	0
			1071	687	201	177	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SQ	140	Total	C	N	O	S	0	0
			1019	639	197	181	2		

- Molecule 57 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SS	140	Total	C	N	O		1	0
			956	594	202	160			

- Molecule 58 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	ST	141	Total	C	N	O	S	0	0
			1000	626	193	179	2		

- Molecule 59 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SU	97	Total	C	N	O		0	0
			487	291	97	99			

- Molecule 60 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SV	83	Total	C	N	O	S	1	0
			587	362	110	110	5		

- Molecule 61 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SX	140	Total	C	N	O	S	0	0
			1065	675	214	173	3		

- Molecule 62 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Sc	60	Total	C	N	O	S	0	0
			447	274	90	81	2		

- Molecule 63 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sd	52	Total	C	N	O	S	0	0
			425	266	87	67	5		

- Molecule 64 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SC	216	Total	C	N	O	S	0	0
			1608	1044	274	280	10		

- Molecule 65 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SG	224	Total	C	N	O	S	0	0
			1325	806	271	247	1		

- Molecule 66 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SJ	178	Total	C	N	O	S	0	0
			1427	912	286	227	2		

- Molecule 67 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SN	150	Total	C	N	O	S	0	0
			1163	748	219	195	1		

- Molecule 68 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SO	136	Total	C	N	O	S	0	0
			995	610	195	184	6		

- Molecule 69 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SW	129	Total	C	N	O	S	0	0
			1021	654	193	168	6		

- Molecule 70 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SY	124	Total	C	N	O	S	0	0
			966	612	187	163	4		

- Molecule 71 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	SZ	72	Total	C	N	O	0	0
			474	293	95	86		

- Molecule 72 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Sb	81	Total	C	N	O	S	0	0
			542	337	108	96	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Sb	82	ARG	LYS	conflict	UNP P42677

- Molecule 73 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Se	49	Total	C	N	O	S	0	0
			386	236	87	62	1		

- Molecule 74 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sa	106	Total	C	N	O	S	0	0
			811	503	168	135	5		

- Molecule 75 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	S2	1563	Total	C	N	O	P	0	0
			33366	14900	6003	10901	1562		

- Molecule 76 is a RNA chain called Kozak mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	mR	14	Total	C	N	O	P	0	0
			304	135	58	97	14		

- Molecule 77 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	S6	72	Total	C	N	O	P	0	0
			1542	687	282	500	72	1	

- Molecule 78 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sg	309	Total	C	N	O	S	0	0
			2064	1297	379	381	7		

- Molecule 79 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SD	221	Total	C	N	O	S	0	0
			1457	932	268	253	4		

- Molecule 80 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SM	106	Total	C	N	O	S	0	0
			534	318	106	107	3		

- Molecule 81 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	SR	131	Total	C	N	O	S	0	0
			858	538	165	153	2		

- Molecule 82 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	Sf	45	Total	C	N	O	0	0
			224	134	45	45		

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
83	SP	1	Total 1	K 1	0
83	L5	9	Total 9	K 9	0
83	Lf	1	Total 1	K 1	0
83	SQ	1	Total 1	K 1	0
83	S2	5	Total 5	K 5	0

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

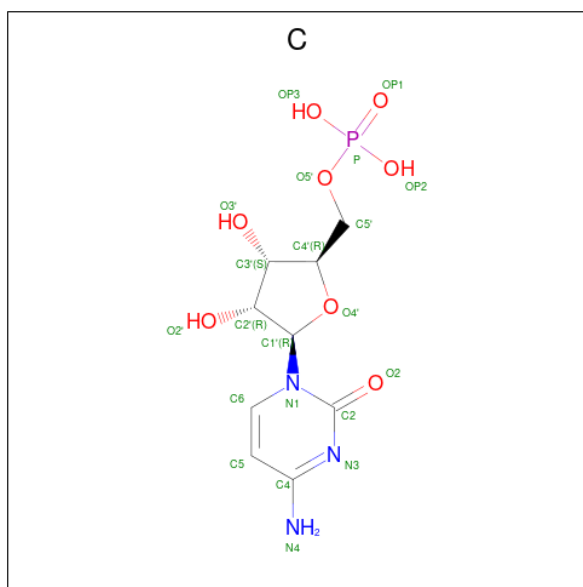
Mol	Chain	Residues	Atoms		AltConf
84	L8	4	Total 4	Mg 4	0
84	L5	43	Total 43	Mg 43	0
84	LA	1	Total 1	Mg 1	0
84	LB	1	Total 1	Mg 1	0
84	LH	1	Total 1	Mg 1	0
84	LV	1	Total 1	Mg 1	0
84	LN	1	Total 1	Mg 1	0
84	LI	2	Total 2	Mg 2	0
84	LQ	1	Total 1	Mg 1	0
84	LS	1	Total 1	Mg 1	0
84	LP	1	Total 1	Mg 1	0
84	Le	1	Total 1	Mg 1	0
84	Lg	1	Total 1	Mg 1	0
84	Lj	1	Total 1	Mg 1	0
84	Pt	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
84	L7	3	Total	Mg	0
			3	3	
84	S2	10	Total	Mg	0
			10	10	

- Molecule 85 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C) (formula: $C_9H_{14}N_3O_8P$).



Mol	Chain	Residues	Atoms					AltConf
85	L5	1	Total	C	N	O	P	0
			20	9	3	7	1	
85	Lo	1	Total	C	N	O	P	0
			20	9	3	7	1	

- Molecule 86 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
86	L5	3	Total	Na	0
			3	3	
86	S2	4	Total	Na	0
			4	4	

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

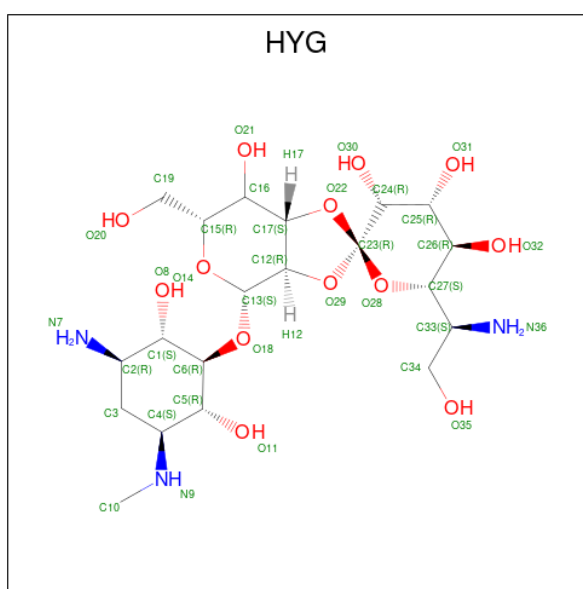
Mol	Chain	Residues	Atoms		AltConf
87	Lg	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

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

- Molecule 88 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



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

- Molecule 89 is water.

Mol	Chain	Residues	Atoms		AltConf
89	L8	8	Total	O	0
			8	8	
89	L5	273	Total	O	0
			273	273	
89	LA	6	Total	O	0
			6	6	
89	LB	3	Total	O	0
			3	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
89	LC	2	Total 2	O 2	0
89	LJ	1	Total 1	O 1	0
89	LH	2	Total 2	O 2	0
89	LO	1	Total 1	O 1	0
89	LV	1	Total 1	O 1	0
89	La	2	Total 2	O 2	0
89	LI	2	Total 2	O 2	0
89	LQ	1	Total 1	O 1	0
89	LR	5	Total 5	O 5	0
89	LW	2	Total 2	O 2	0
89	Lr	2	Total 2	O 2	0
89	LF	1	Total 1	O 1	0
89	Lc	4	Total 4	O 4	0
89	Lg	1	Total 1	O 1	0
89	Li	1	Total 1	O 1	0
89	Lm	1	Total 1	O 1	0
89	Ln	1	Total 1	O 1	0
89	Lp	3	Total 3	O 3	0
89	Pt	9	Total 9	O 9	0
89	L7	9	Total 9	O 9	0
89	SB	1	Total 1	O 1	0

Continued on next page...

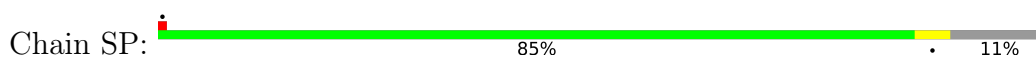
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
89	SF	1	Total 1	O 1	0
89	SS	1	Total 1	O 1	0
89	Sd	2	Total 2	O 2	0
89	SC	1	Total 1	O 1	0
89	SG	2	Total 2	O 2	0
89	SJ	2	Total 2	O 2	0
89	SO	2	Total 2	O 2	0
89	Sa	1	Total 1	O 1	0
89	S2	92	Total 92	O 92	0
89	S6	1	Total 1	O 1	0
89	Sg	1	Total 1	O 1	0

3 Residue-property plots

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

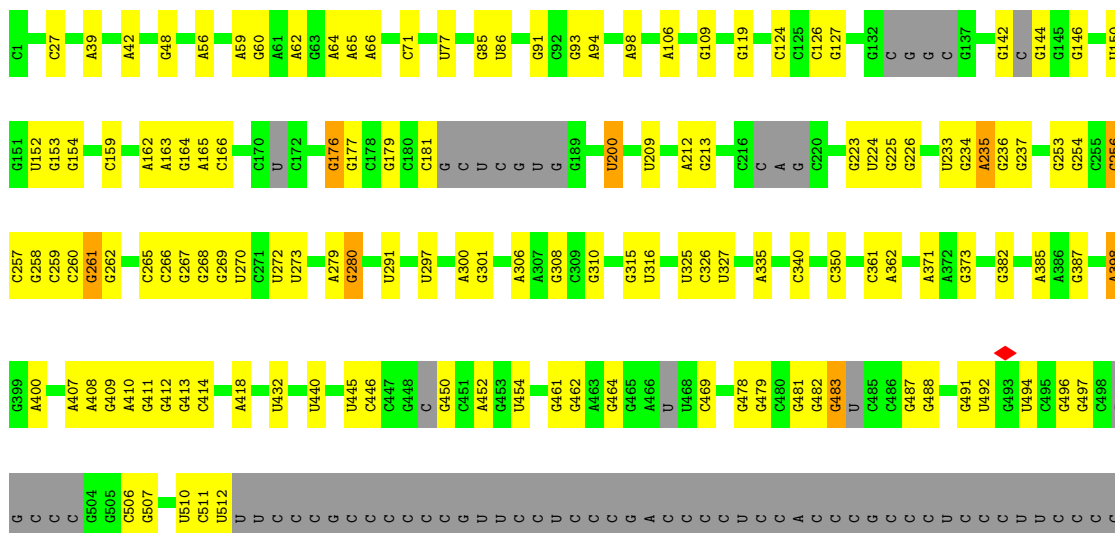
- Molecule 1: 40S ribosomal protein S15

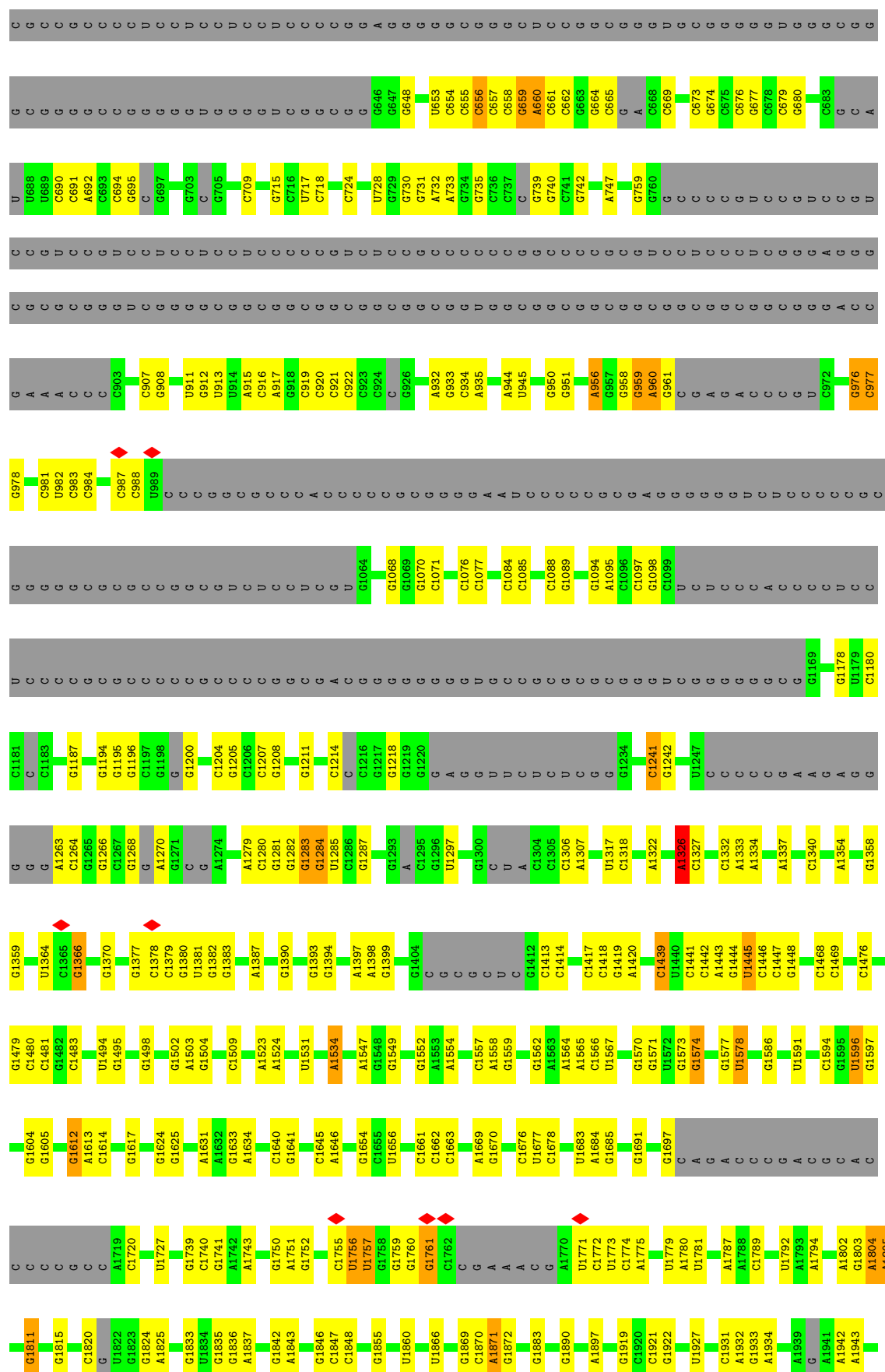


- Molecule 2: 5.8S rRNA



- Molecule 3: 28S rRNA





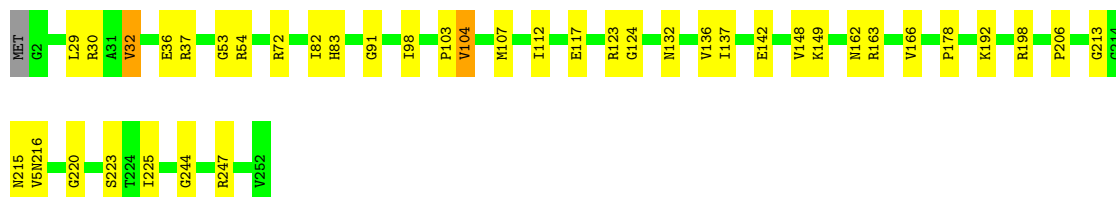


G4870	C4741	G4509	G4254	G4136	U	C3924	A3825	U3721	C	G
C4871	C4742	A4610	C4258	C	A	U3925	A3826	G3722	U	C
G4872	G4743	G4618	C4263	C	C	C3926	A3830	A3723	A	C
A4874	A4744	U4619	G4264	C	U	G3934	G3838	A3724	G3597	C
C	C	U4620	U4265	C	U	G	U3839	A3727	C3602	C
G4877	C4749	U4521	U4266	C	U	G	U3840	A3728	G3603	C
U4882	U4627	G4522	G4267	C	A	G	C3841	U3729	A3610	C
C4883	U4628	A4523	G4268	C	U	G	C3842	A3732	A3611	C
G4884	C4636	G4524	A4268	C	U	G	C3843	A3733	G3615	C
C	U4637	A4525	A4273	C	U	G	U3844	U3734	G3616	C
C	G4637	U4530	A4274	G	G4065	A3946	G	G3735	G3617	C
C	C4757	U4531	G4275	G	U4067	C3947	U3848	A3736	C3618	C
C	U4758	U4532	C	G4149	U4068	U	A3849	A3737	G3626	C
G	G4643	G4537	A4280	C4162	U4070	G	C3850	A3746	A3645	C
C	G4644	G4538	A4281	U4163	U4071	G	U3851	A3747	A3647	C
C	C4645	U4539	A4282	C4170	G4076	A	U3852	A3748	A3648	C
C	U4646	U4540	G4291	C4171	C4080	G	U3853	G3749	A3630	C
C	A4656	G4541	U4295	C4183	G4081	G	C3854	C3750	A3635	C
C	U4657	C4542	U4296	C4184	G4084	G	A3856	G3753	U3641	C
C	C4670	A4544	G4297	U4188	G	U	A3861	U3758	A3646	C
C	A4671	G4545	U4298	U4189	C4088	G	A3862	A3759	A3647	C
C	U4672	C4546	U4299	U4190	G4089	U	A3867	A3760	A3648	C
C	U4673	C4547	G4305	C4191	G4090	A	C3870	U3762	G3661	C
G	G4680	A4548	U4306	A4192	G4093	G	C3871	A3763	A3662	C
C	A4681	G4550	C4312	C4193	G4094	C	A3871	U3764	A3663	C
C	C4688	U4551	U4313	U4194	G4095	A	A3877	G3765	G3664	C
C	U4689	U4552	A4314	C4195	C4096	G	C3878	A3766	G3665	C
C	G4690	C4560	C4314	C4203	G4097	G	G3879	G3767	G3669	C
C	A4691	G4567	C4318	A4202	A4098	U	C3893	U3768	G3672	C
C	U4699	A4568	C4319	U4208	G4099	G	A3894	U3770	C3673	C
C	A4700	U4569	G4320	C4209	C4100	A	G3895	G3776	U3680	C
C	C	G4570	U4321	A4212	C	G	C3896	G3777	A3687	C
C	A4708	A4571	G4322	C4219	C	G	G3897	G3778	U3688	C
C	U4709	U4572	A4323	A4219	G	C	G3898	A3783	A3687	C
C	C4710	G4573	A4324	A4220	C	C	G3899	A3784	G3689	C
C	C4711	U4574	U4324	C4221	A	C	G3900	A3785	U3690	C
C	C	G4575	U4329	G4330	G	C	A3901	U3786	G3691	C
C	C	U4576	G4331	C4332	C	C	G3906	C3787	A3692	C
C	A4717	U4577	C4336	U4225	G4109	G	G3907	C3788	U3707	C
C	C	U4578	U4336	U4227	C4110	C	A3908	C3807	C3708	C
C	G4721	G4579	A4336	G4228	U4111	C	G3909	C3808	U3709	C
C	U4722	U4580	U4339	U4229	C4112	C	C3910	C3710	G3710	C
C	A4723	G4581	U4344	A4233	G4115	C	C3911	A3711	A3711	C
C	A4724	C4585	C4345	C4237	C4119	C	U3915	U3715	U3715	C
C	C	U4488	U4346	U4238	C4122	C	A3916	G3716	G3716	C
C	G	U4493	U4353	A4239	G4123	C	A3917	A3717	A3717	C
C	C	U4498	U4361	G4240	C4126	C	G3918	A3816	A3816	C
C	C	C4499	A4362	A4251	A4127	C	U3919	A3817	A3817	C
C	U4500	U4500	A4363	A4251	A4128	A	U3920	A3719	A3719	C
C	C4508	C4508	A4608	A4251	A4128	G	G	G3819	G3819	C



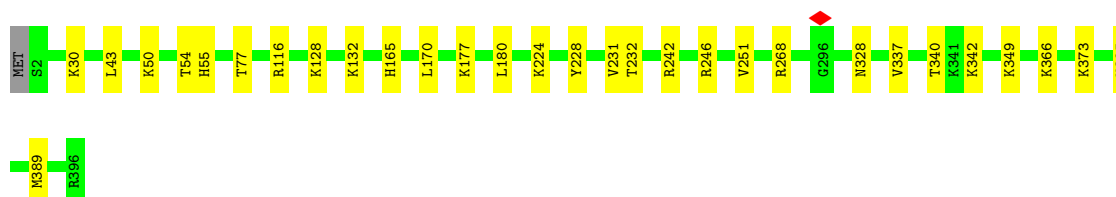
- Molecule 4: Large ribosomal subunit protein uL2

Chain LA: 84% 15% .



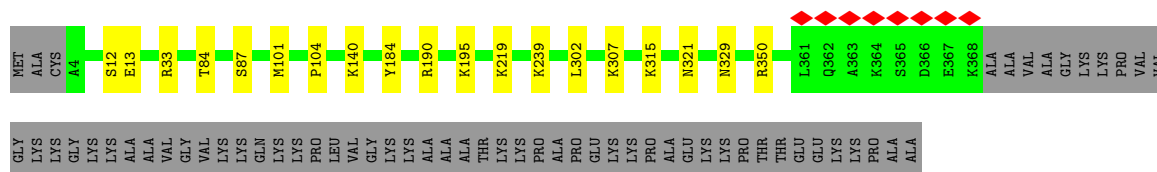
- Molecule 5: Large ribosomal subunit protein uL3

Chain LB: 92% 8%



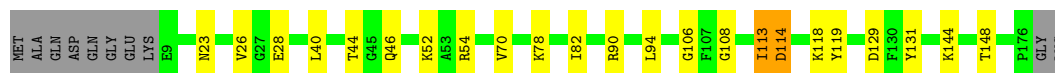
- Molecule 6: 60S ribosomal protein L4

Chain LC: 81% 15%



- Molecule 7: 60S ribosomal protein L11

Chain LJ: 81% 12% 6%



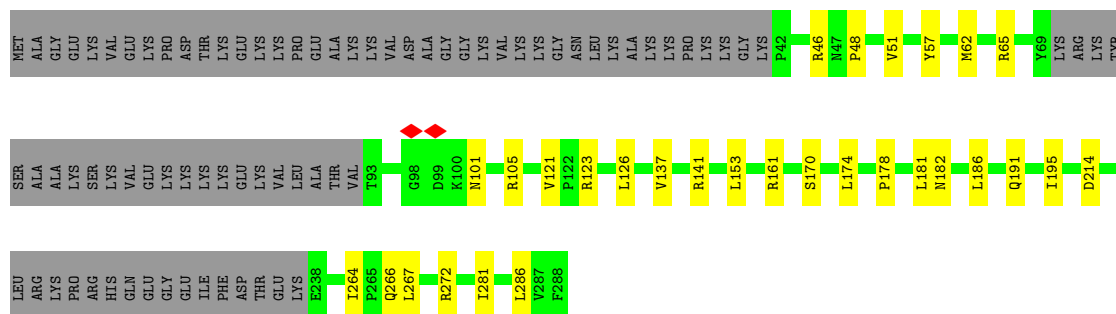
- Molecule 8: 60S ribosomal protein L9

Chain LH: 87% 12%




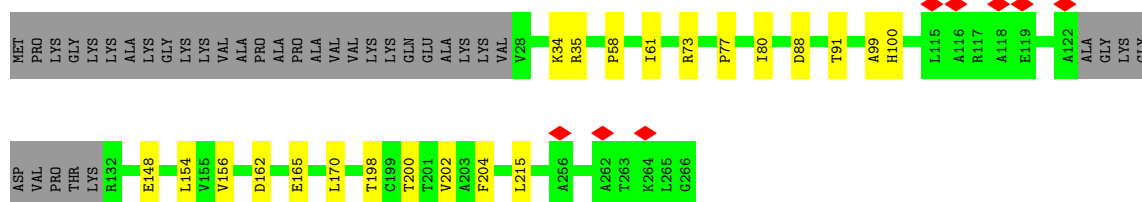
- Molecule 9: Large ribosomal subunit protein eL6

Chain LE:  62% 10% 28%




- Molecule 10: 60S ribosomal protein L7a

Chain LG:  78% 8% 14%



- Molecule 11: 60S ribosomal protein L13a

Chain LO:  85% 13% .




- Molecule 12: 60S ribosomal protein L13

Chain LL:  91% 7% .



- Molecule 13: 60S ribosomal protein L23

Chain LV:  86% 8% . 6%



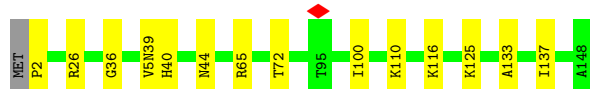
- Molecule 14: Large ribosomal subunit protein eL14

Chain LM:  90% 10%



- Molecule 15: Large ribosomal subunit protein uL15

Chain La: 90% 9%



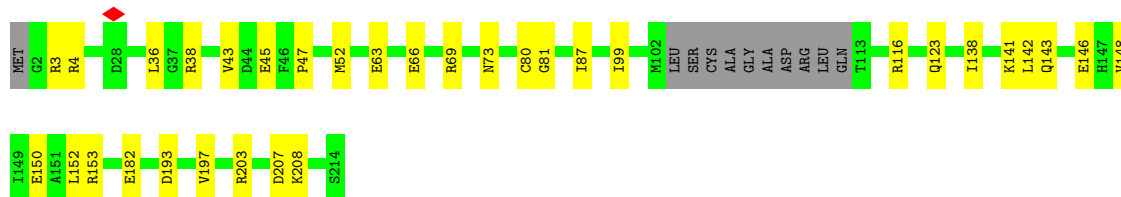
- Molecule 16: 60S ribosomal protein L15

Chain LN: 91% 8%



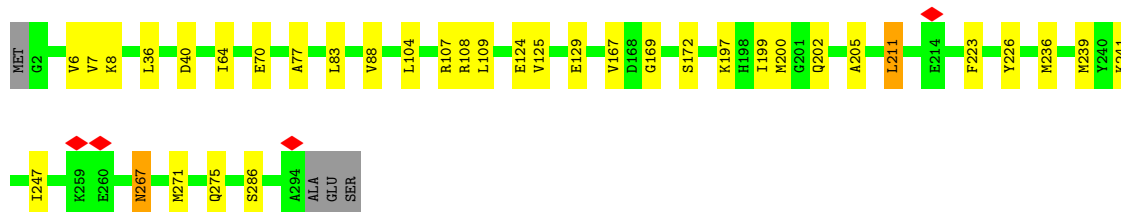
- Molecule 17: 60S ribosomal protein L10

Chain LI: 79% 15% 5%



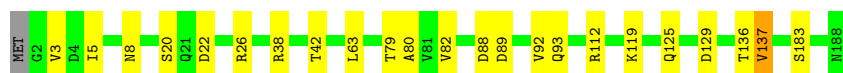
- Molecule 18: 60S ribosomal protein L5

Chain LD: 87% 11% 2%



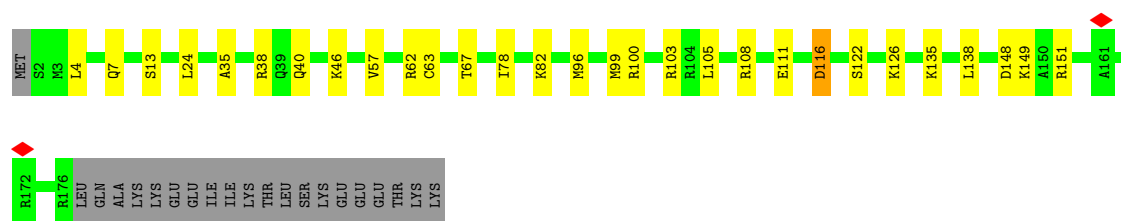
- Molecule 19: 60S ribosomal protein L18

Chain LQ: 87% 12% 1%



- Molecule 20: 60S ribosomal protein L19

Chain LR: 74% 14% 11%



- Molecule 21: 60S ribosomal protein L18a

Chain LS: 85% 14% .



- Molecule 22: 60S ribosomal protein L21

Chain LT: 89% 9% ..



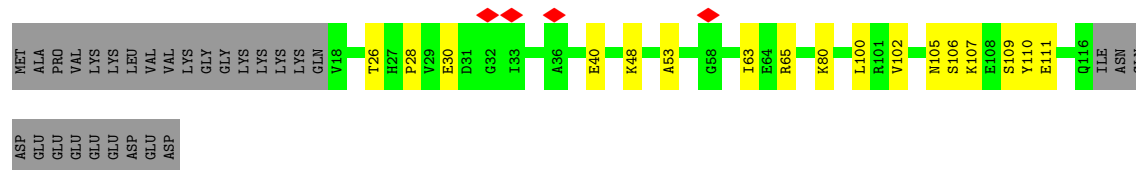
- Molecule 23: Large ribosomal subunit protein uL22

Chain LP: 92% 7% .



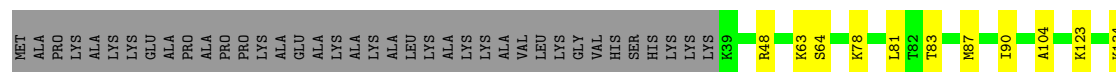
- Molecule 24: 60S ribosomal protein L22

Chain LU: 64% 13% 23%




- Molecule 25: 60S ribosomal protein L23a

Chain LX: 65% 10% 24%



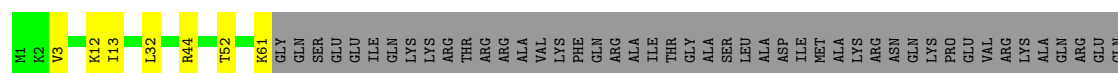
- Molecule 26: 60S ribosomal protein L26

Chain LY:  73% 17% 10%




- Molecule 27: 60S ribosomal protein L24

Chain LW:  34% 61%



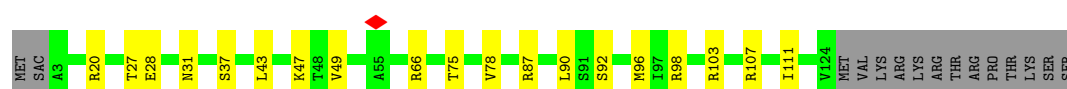
- Molecule 28: 60S ribosomal protein L27

Chain LZ:  76% 21% ..




- Molecule 29: 60S ribosomal protein L28

Chain Lr:  75% 14% 11%



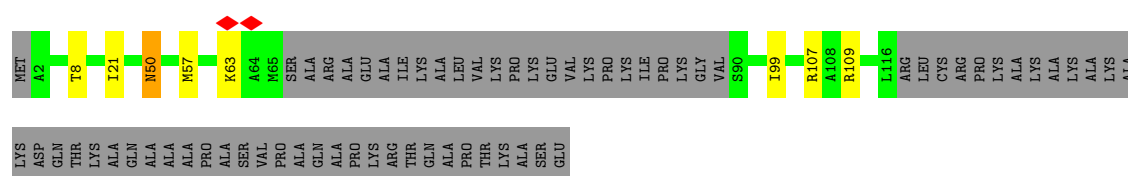
- Molecule 30: 60S ribosomal protein L35

Chain Lh:  89% 10% .




- Molecule 31: Large ribosomal subunit protein eL29

Chain Lb:  52% 43%



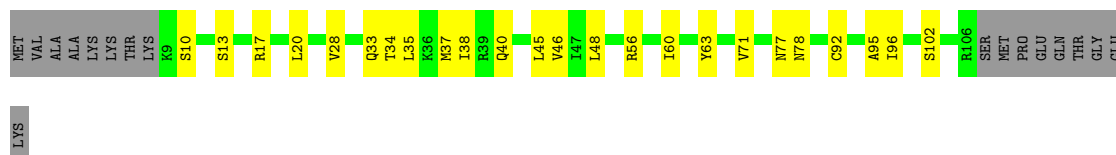
- Molecule 32: Large ribosomal subunit protein uL30

Chain LF:  85% 6% 9%



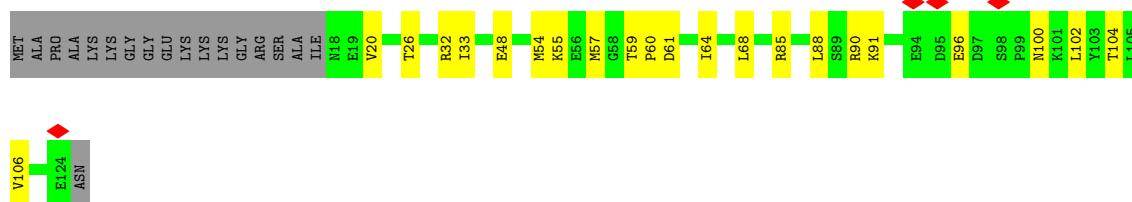
- Molecule 33: 60S ribosomal protein L30

Chain Lc:  64% 21% 15%



- Molecule 34: 60S ribosomal protein L31

Chain Ld:  68% 18% 14%



- Molecule 35: Large ribosomal subunit protein eL32

Chain Le:  91% 8% 1%



- Molecule 36: Large ribosomal subunit protein eL33

Chain Lf:  91% 8% 1%




- Molecule 37: Large ribosomal subunit protein eL34

Chain Lg:  92% 7% 1%




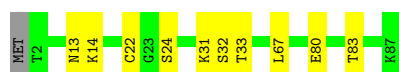
- Molecule 38: 60S ribosomal protein L36

Chain Li:  81% 13% 6%




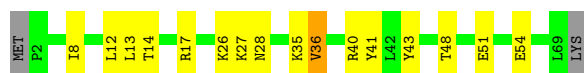
- Molecule 39: Large ribosomal subunit protein eL37

Chain Lj:  87% 11% .



- Molecule 40: 60S ribosomal protein L38

Chain Lk:  74% 21% ..



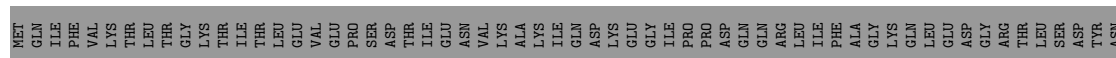
- Molecule 41: 60S ribosomal protein L39

Chain Ll:  86% 12% .



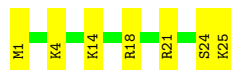
- Molecule 42: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:  31% 9% 60%




- Molecule 43: 60S ribosomal protein L41

Chain Ln:  72% 28%

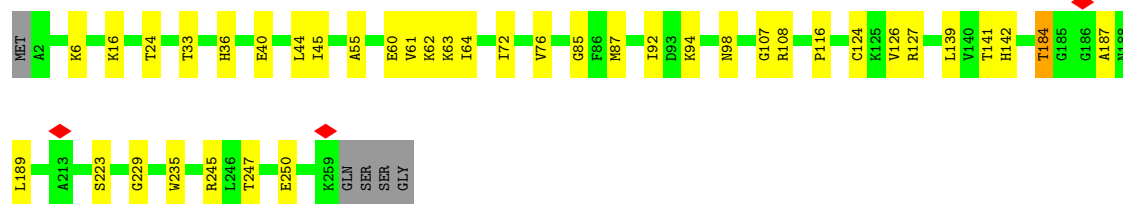
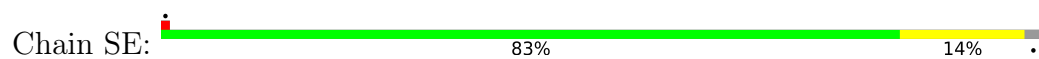


- Molecule 44: Large ribosomal subunit protein eL42

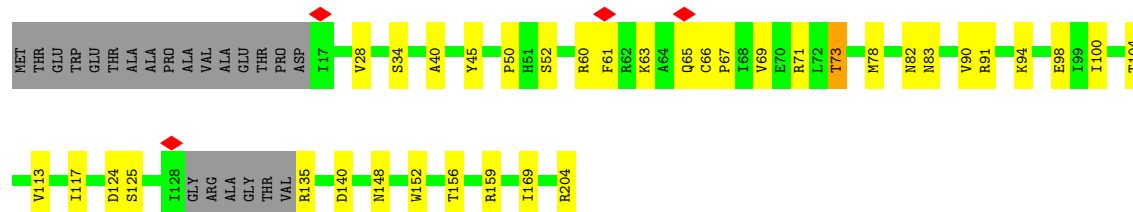
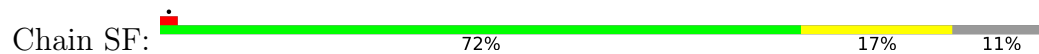
Chain Lo:  81% 17% ..



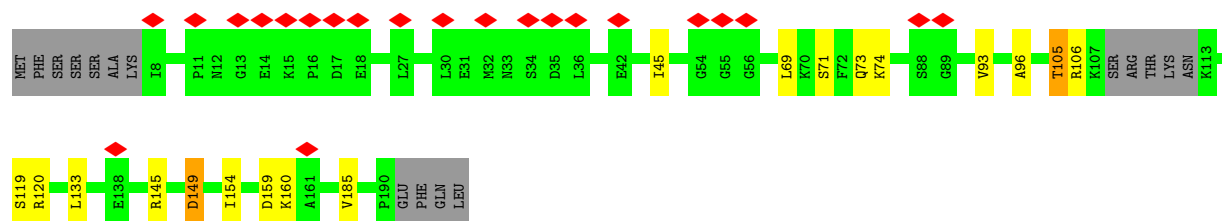
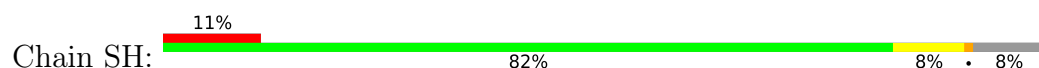
- Molecule 50: Small ribosomal subunit protein eS4, X isoform



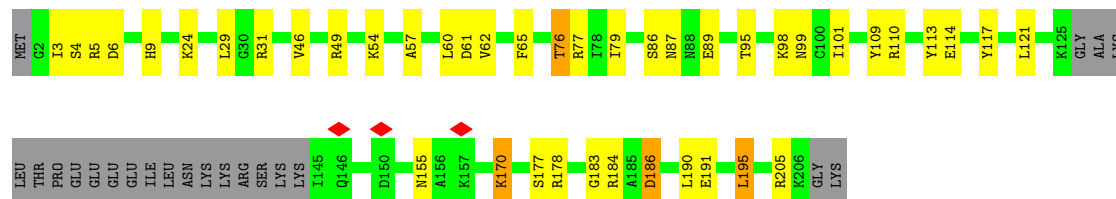
- Molecule 51: 40S ribosomal protein S5



- Molecule 52: 40S ribosomal protein S7



- Molecule 53: 40S ribosomal protein S8




- Molecule 54: 40S ribosomal protein S10




PRO ALA ARG LEU THR ARG GLY GLU
ALA ASP ARG ASP THR TYR ARG ARG SER ALA VAL
PRO PRO GLY ALA ASP LYS LYS ALA GLU GLY GLY ALA
GLY SER THR THR ARG GLU ALA VAL PRO PRO GLN

- Molecule 55: 40S ribosomal protein S11

Chain SL:  76% 10% 13%


MET R2 Q13 I16 R22 VAL LEU ARG GLY THR LYS LYS GLU K32 I40 T54 F62 S67 I72 M90 K81 M82 T85 K104 S114 F115 C116 D119 T127 E130 C131 S135 K136 A148 ALA GLY THR LYS LYS GLN PHE PHE GLN
LYS PHE

- Molecule 56: 40S ribosomal protein S16

Chain SQ:  76% 18% 6%


MET PRO SER LYS PRO LYS L7 Q8 S9 V10 Q11 V12 F13 G14 T20 H24 R27 R37 L51 R69 V72 Q75 I81 R85 Q86 S87 I88 A91 Y95 Y96 Q97 D101 K105 K106 E107 I108 K109 D110 I111 I112 I113 Q114 R117 L120
C127 Q142 R146

- Molecule 57: 40S ribosomal protein S18

Chain SS:  79% 12% 8%


MET SER L3 Q10 L13 R14 V15 L16 N17 G22 K25 V34 I26 A27 F28 T31 A32 I33 R38 A56 H125 R130 V131 R132 G133 T136 R142 GLY ARG THR VAL VAL VAL SER LYS LYS LYS

- Molecule 58: 40S ribosomal protein S19

Chain ST:  80% 16% 4%

MET P2 V6 Q11 F14 S25 L28 K29 W33 V34 D35 T36 V37 K38 L39 A40 K43 R62 H63 L64 S74 I78 Q83 R84 N85 M88 G95 S96 K97 D118 R121 V138 A141 A142 LYS LYS HIS

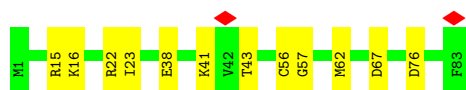
- Molecule 59: 40S ribosomal protein S20

Chain SU:  6% 78% 18%

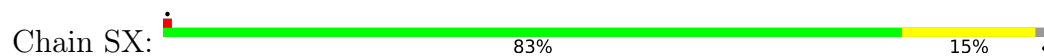
MET ALA PHE LYS ASP THR GLY LYS THR PRO VAL GLU PRO GLU VAL I17 R41 W47 E72 G73 P94 K99 GLN ILE THR SER ILE S105 P108 I116 A117 D118 ALA

- Molecule 60: 40S ribosomal protein S21

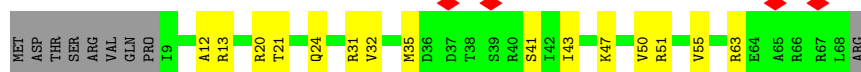
Chain SV:  86% 14%



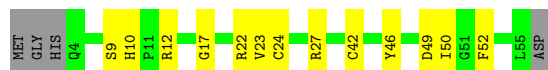
- Molecule 61: 40S ribosomal protein S23



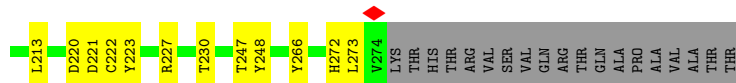
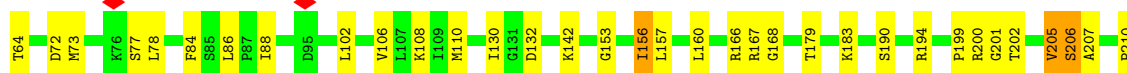
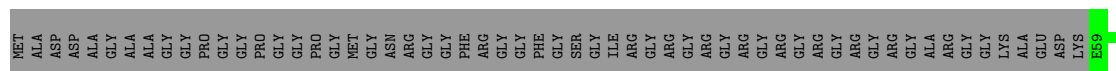
- Molecule 62: 40S ribosomal protein S28



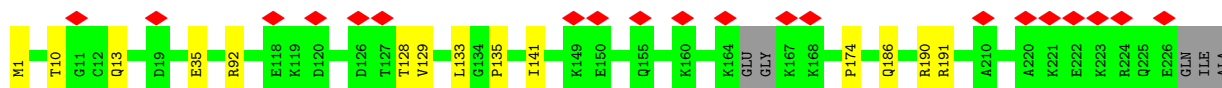
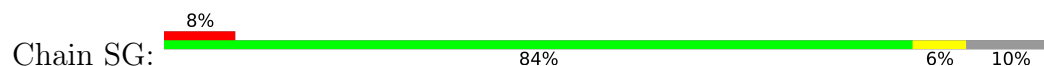
- Molecule 63: 40S ribosomal protein S29



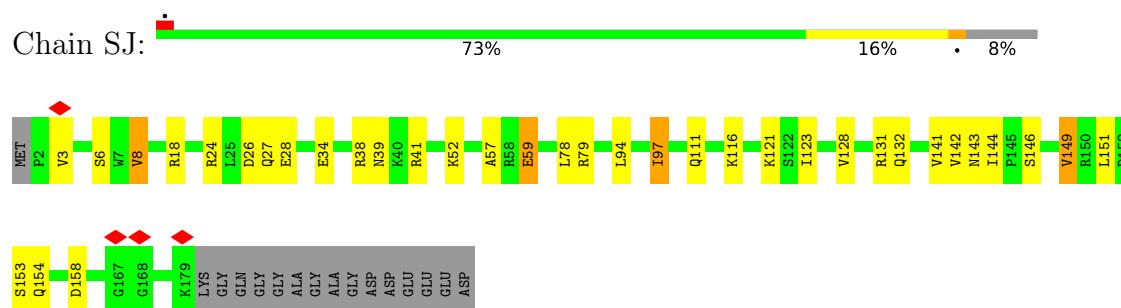
- Molecule 64: 40S ribosomal protein S2



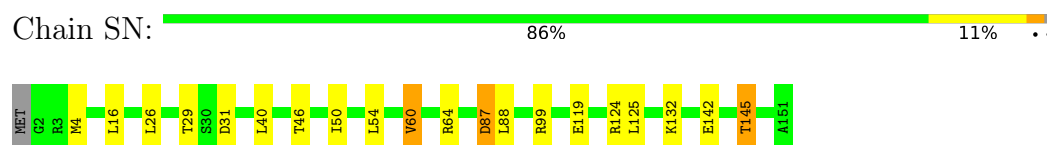
- Molecule 65: 40S ribosomal protein S6



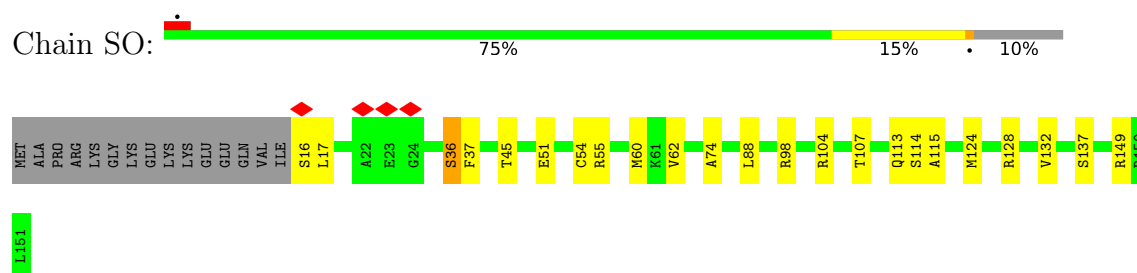
- Molecule 66: 40S ribosomal protein S9



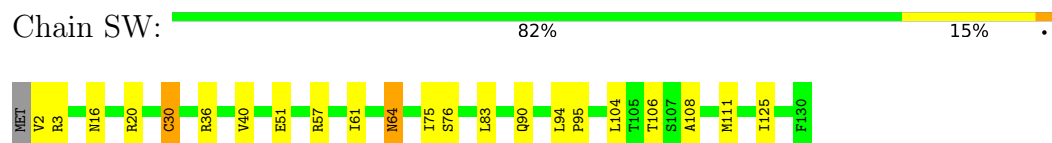
- Molecule 67: 40S ribosomal protein S13



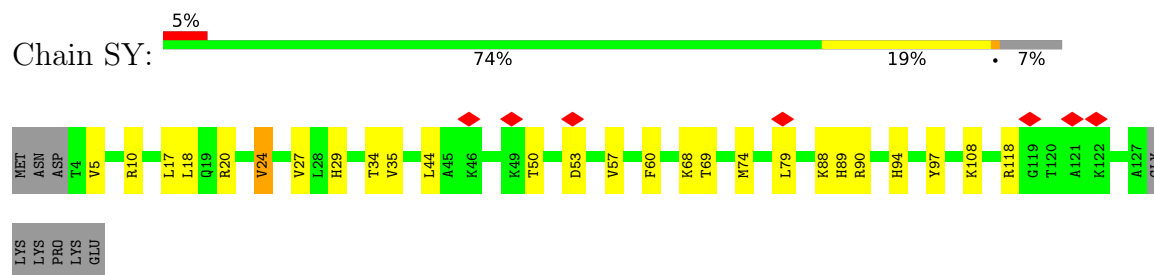
- Molecule 68: 40S ribosomal protein S14



- Molecule 69: 40S ribosomal protein S15a

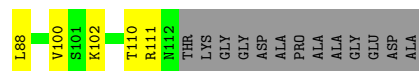


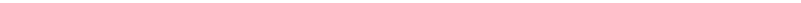
- Molecule 70: 40S ribosomal protein S24

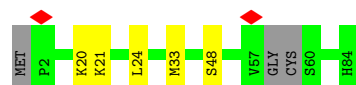


- Molecule 71: 40S ribosomal protein S25

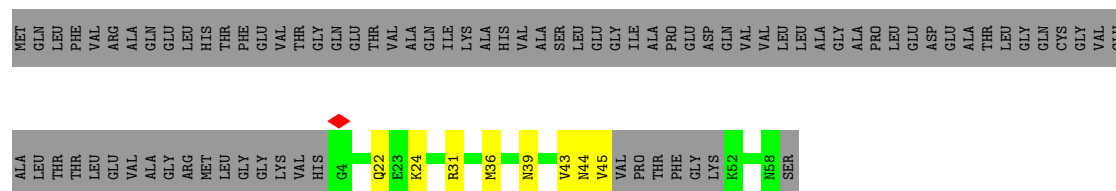





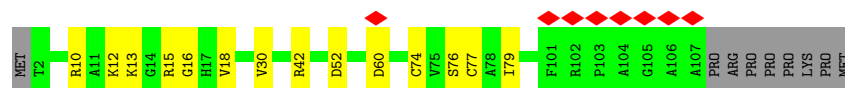
- Chain Sb:  90% 6%



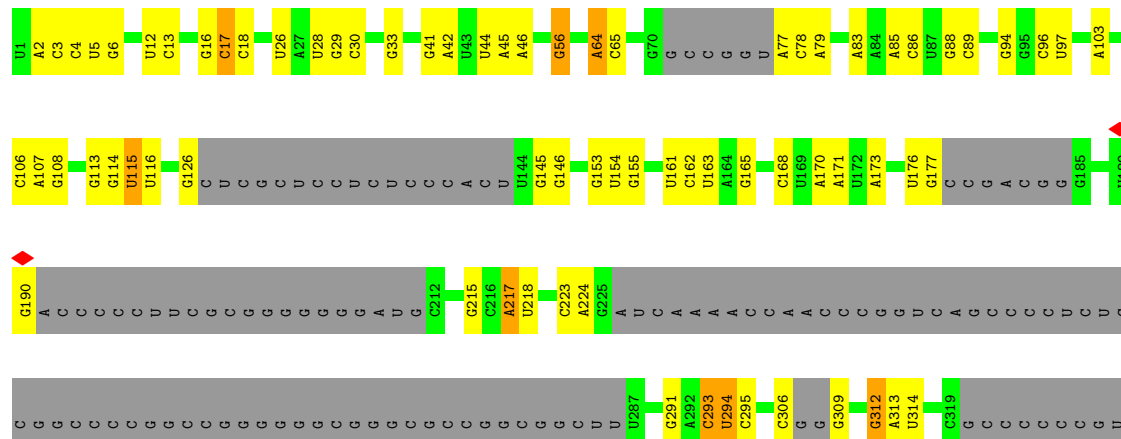
- Chain Se: 



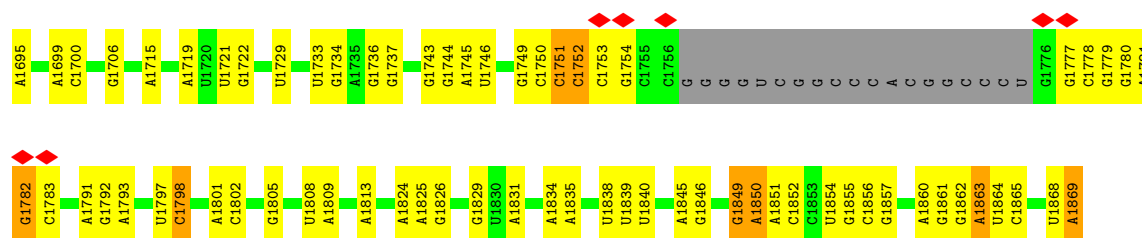
- Chain Sa: 



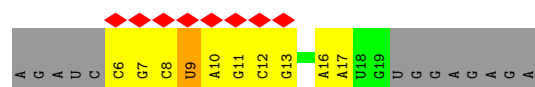
- Chain S2: 



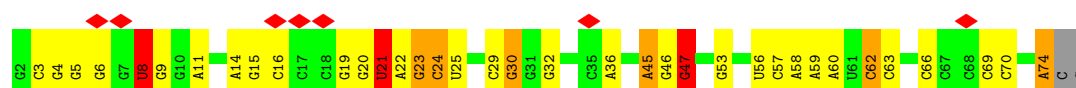




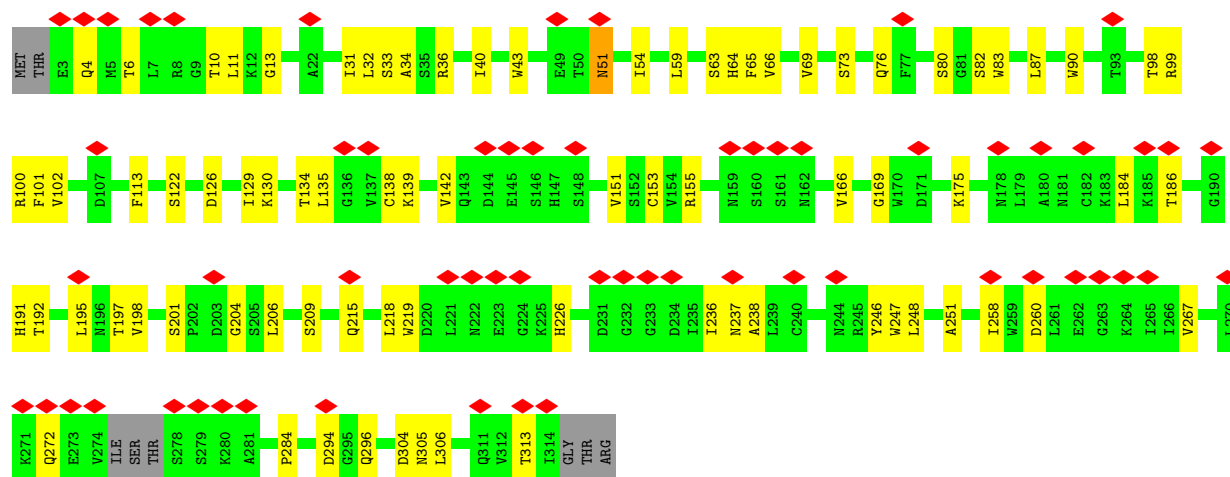
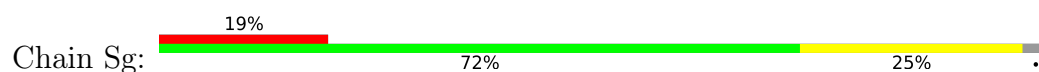
• Molecule 76: Kozak mRNA



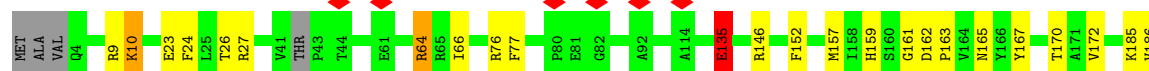
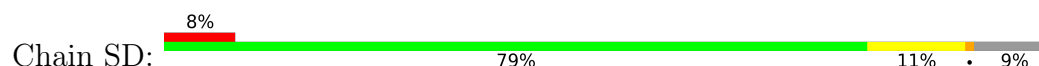
• Molecule 77: E-site tRNA



• Molecule 78: Receptor of activated protein C kinase 1



• Molecule 79: 40S ribosomal protein S3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55958	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	404.16, 404.16, 404.16	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.842, 0.842, 0.842	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, ZN, H2U, A2M, OMC, NA, MG, 5MC, 6MZ, 4SU, MLZ, HYG, OMU, 1MA, M3L, PSU, K, V5N, G7M, UR3, HIC

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	SP	0.08	0/824	0.24	0/1121
2	L8	0.14	0/3589	0.28	0/5587
3	L5	0.16	1/78615 (0.0%)	0.28	0/122538
4	LA	0.14	0/1920	0.29	0/2576
5	LB	0.12	0/2768	0.27	0/3754
6	LC	0.12	0/2890	0.25	0/3891
7	LJ	0.11	0/1227	0.29	0/1655
8	LH	0.11	0/1454	0.26	0/1964
9	LE	0.11	0/1616	0.26	0/2180
10	LG	0.12	0/1727	0.26	0/2353
11	LO	0.13	0/1637	0.28	0/2193
12	LL	0.30	0/1614	0.44	0/2177
13	LV	0.13	0/957	0.28	0/1293
14	LM	0.13	0/1111	0.25	0/1491
15	La	0.13	0/1173	0.28	0/1566
16	LN	0.14	0/1739	0.28	0/2331
17	LI	0.15	0/1648	0.33	0/2206
18	LD	0.11	0/2276	0.27	0/3072
19	LQ	0.13	0/1521	0.29	0/2034
20	LR	0.13	0/1407	0.28	0/1871
21	LS	0.13	0/1492	0.29	0/2003
22	LT	0.13	0/1246	0.28	0/1674
23	LP	0.13	0/1268	0.31	0/1701
24	LU	0.11	0/795	0.26	0/1071
25	LX	0.12	0/972	0.28	0/1307
26	LY	0.12	0/1074	0.28	0/1434
27	LW	0.11	0/528	0.23	0/703
28	LZ	0.12	0/1111	0.30	0/1487
29	Lr	0.12	0/988	0.28	0/1328
30	Lh	0.10	0/962	0.23	0/1282
31	Lb	0.12	0/701	0.28	0/929

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LF	0.13	0/1789	0.26	0/2402
33	Lc	0.12	0/750	0.25	0/1011
34	Ld	0.13	0/892	0.28	0/1203
35	Le	0.13	0/1063	0.28	0/1421
36	Lf	0.14	0/879	0.28	0/1179
37	Lg	0.13	0/848	0.29	0/1132
38	Li	0.10	0/767	0.24	0/1025
39	Lj	0.13	0/710	0.30	0/941
40	Lk	0.14	0/549	0.32	0/728
41	Ll	0.13	0/443	0.38	0/588
42	Lm	0.11	0/402	0.28	0/536
43	Ln	0.11	0/240	0.18	0/305
44	Lo	0.15	0/856	0.32	0/1133
45	Lp	0.17	0/695	0.31	0/925
46	Pt	0.17	0/1720	0.27	0/2675
47	L7	0.15	0/2840	0.28	0/4425
48	SA	0.13	0/1660	0.33	0/2266
49	SB	0.15	0/1735	0.40	0/2327
50	SE	0.12	0/1956	0.31	0/2654
51	SF	0.12	0/1369	0.36	0/1851
52	SH	0.12	0/1189	0.28	0/1622
53	SI	0.14	0/1472	0.34	0/1977
54	SK	0.18	0/711	0.43	0/973
55	SL	0.12	0/1091	0.29	0/1471
56	SQ	0.13	0/1034	0.38	0/1395
57	SS	0.10	0/970	0.29	0/1312
58	ST	0.12	0/1017	0.36	0/1374
59	SU	0.07	0/485	0.26	0/672
60	SV	0.12	0/592	0.33	0/797
61	SX	0.13	0/1083	0.34	0/1450
62	Sc	0.11	0/448	0.29	0/601
63	Sd	0.12	0/435	0.31	0/579
64	SC	0.14	0/1644	0.36	0/2232
65	SG	0.10	0/1332	0.27	0/1823
66	SJ	0.13	0/1452	0.34	0/1952
67	SN	0.12	0/1187	0.27	0/1604
68	SO	0.14	0/1008	0.39	0/1355
69	SW	0.13	0/1038	0.29	0/1389
70	SY	0.12	0/983	0.34	0/1316
71	SZ	0.10	0/477	0.33	0/652
72	Sb	0.11	0/550	0.33	0/742
73	Se	0.10	0/388	0.28	0/508
74	Sa	0.11	0/823	0.27	0/1106

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	S2	0.14	0/37306	0.29	0/58113
76	mR	0.13	0/340	0.30	0/529
77	S6	0.25	0/1629	0.44	0/2537
78	Sg	0.27	0/2110	0.71	0/2905
79	SD	0.31	0/1474	0.87	3/2003 (0.1%)
80	SM	0.19	0/532	0.54	0/737
81	SR	0.25	0/869	0.71	0/1187
82	Sf	0.13	0/220	0.32	0/301
All	All	0.15	1/210902 (0.0%)	0.31	3/310713 (0.0%)

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
12	LL	0	1
79	SD	0	5
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4523	A2M	O3'-P	5.05	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	SD	189	MET	CA-C-N	8.87	132.72	120.39
79	SD	189	MET	C-N-CA	8.87	132.72	120.39
79	SD	135	GLU	CB-CG-CD	5.99	122.78	112.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	LL	49	ARG	Sidechain
79	SD	135	GLU	Sidechain
79	SD	146	ARG	Sidechain
79	SD	24	PHE	Sidechain
79	SD	64	ARG	Sidechain

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	SP	814	0	628	5	0
2	L8	3215	0	1631	20	0
3	L5	72477	0	36733	490	0
4	LA	1895	0	1967	29	0
5	LB	2719	0	2344	22	0
6	LC	2836	0	2954	16	0
7	LJ	1207	0	1138	15	0
8	LH	1435	0	1457	15	0
9	LE	1584	0	1620	21	0
10	LG	1696	0	1649	15	0
11	LO	1605	0	1726	19	0
12	LL	1583	0	1613	9	0
13	LV	943	0	959	8	0
14	LM	1089	0	1128	18	0
15	La	1157	0	1177	10	0
16	LN	1694	0	1738	12	0
17	LI	1610	0	1629	26	0
18	LD	2232	0	2145	23	0
19	LQ	1497	0	1605	14	0
20	LR	1391	0	1469	23	0
21	LS	1453	0	1482	18	0
22	LT	1221	0	1222	11	0
23	LP	1242	0	1269	6	0
24	LU	781	0	790	11	0
25	LX	955	0	1023	12	0
26	LY	1057	0	1119	18	0
27	LW	515	0	530	4	0
28	LZ	1088	0	1145	22	0
29	Lr	973	0	1023	11	0
30	Lh	954	0	1034	8	0
31	Lb	700	0	710	6	0
32	LF	1756	0	1765	10	0
33	Lc	740	0	751	15	0
34	Ld	877	0	913	11	0
35	Le	1045	0	1125	9	0
36	Lf	860	0	890	6	0
37	Lg	838	0	895	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Li	756	0	772	10	0
39	Lj	695	0	710	6	0
40	Lk	545	0	589	7	0
41	Ll	433	0	461	5	0
42	Lm	408	0	423	8	0
43	Ln	239	0	289	4	0
44	Lo	849	0	888	12	0
45	Lp	682	0	724	9	0
46	Pt	1624	0	833	13	0
47	L7	2542	0	1285	7	0
48	SA	1624	0	1568	17	0
49	SB	1708	0	1760	53	0
50	SE	1914	0	1860	32	0
51	SF	1350	0	1291	25	0
52	SH	1173	0	998	10	0
53	SI	1446	0	1426	28	0
54	SK	690	0	603	19	0
55	SL	1071	0	1073	9	0
56	SQ	1019	0	976	20	0
57	SS	956	0	826	16	0
58	ST	1000	0	931	18	0
59	SU	487	0	214	2	0
60	SV	587	0	553	8	0
61	SX	1065	0	1112	10	0
62	Sc	447	0	448	11	0
63	Sd	425	0	412	9	0
64	SC	1608	0	1628	28	0
65	SG	1325	0	977	10	0
66	SJ	1427	0	1490	27	0
67	SN	1163	0	1208	13	0
68	SO	995	0	1007	15	0
69	SW	1021	0	1070	16	0
70	SY	966	0	986	18	0
71	SZ	474	0	407	11	0
72	Sb	542	0	433	4	0
73	Se	386	0	422	6	0
74	Sa	811	0	835	8	0
75	S2	33366	0	16861	309	0
76	mR	304	0	153	3	0
77	S6	1542	0	789	19	0
78	Sg	2064	0	1698	40	0
79	SD	1457	0	1310	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	SM	534	0	281	2	0
81	SR	858	0	703	13	0
82	Sf	224	0	92	3	0
83	L5	9	0	0	0	0
83	Lf	1	0	0	0	0
83	S2	5	0	0	0	0
83	SP	1	0	0	0	0
83	SQ	1	0	0	0	0
84	L5	43	0	0	0	0
84	L7	3	0	0	0	0
84	L8	4	0	0	0	0
84	LA	1	0	0	0	0
84	LB	1	0	0	0	0
84	LH	1	0	0	0	0
84	LI	2	0	0	0	0
84	LN	1	0	0	0	0
84	LP	1	0	0	0	0
84	LQ	1	0	0	0	0
84	LS	1	0	0	0	0
84	LV	1	0	0	0	0
84	Le	1	0	0	0	0
84	Lg	1	0	0	0	0
84	Lj	1	0	0	0	0
84	Pt	1	0	0	0	0
84	S2	10	0	0	0	0
85	L5	20	0	12	0	0
85	Lo	20	0	11	1	0
86	L5	3	0	0	0	0
86	S2	4	0	0	0	0
87	Lg	1	0	0	0	0
87	Lj	1	0	0	0	0
87	Lm	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
88	S2	36	0	37	0	0
89	L5	273	0	0	1	0
89	L7	9	0	0	0	0
89	L8	8	0	0	0	0
89	LA	6	0	0	0	0
89	LB	3	0	0	0	0
89	LC	2	0	0	0	0
89	LF	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	LH	2	0	0	0	0
89	LI	2	0	0	1	0
89	LJ	1	0	0	0	0
89	LO	1	0	0	0	0
89	LQ	1	0	0	0	0
89	LR	5	0	0	0	0
89	LV	1	0	0	0	0
89	LW	2	0	0	0	0
89	La	2	0	0	0	0
89	Lc	4	0	0	1	0
89	Lg	1	0	0	0	0
89	Li	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Ln	1	0	0	0	0
89	Lp	3	0	0	0	0
89	Lr	2	0	0	0	0
89	Pt	9	0	0	0	0
89	S2	92	0	0	3	0
89	S6	1	0	0	0	0
89	SB	1	0	0	0	0
89	SC	1	0	0	0	0
89	SF	1	0	0	0	0
89	SG	2	0	0	0	0
89	SJ	2	0	0	0	0
89	SO	2	0	0	0	0
89	SS	1	0	0	0	0
89	Sa	1	0	0	0	0
89	Sd	2	0	0	1	0
89	Sg	1	0	0	0	0
All	All	199163	0	140431	1625	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 5.

The worst 5 of 1625 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)
50:SE:16:LYS:CE	75:S2:812:A:H5'	1.51	1.38
50:SE:16:LYS:NZ	75:S2:812:A:H5'	1.55	1.21
50:SE:16:LYS:NZ	75:S2:812:A:C5'	2.13	1.11
50:SE:16:LYS:HE2	75:S2:812:A:H5'	1.12	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Lk:54:GLU:OE1	40:Lk:54:GLU:N	1.86	1.08

There are no symmetry-related clashes.

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	
1	SP	127/145 (88%)	118 (93%)	9 (7%)	0	100	100
4	LA	248/252 (98%)	238 (96%)	10 (4%)	0	100	100
5	LB	392/396 (99%)	386 (98%)	6 (2%)	0	100	100
6	LC	363/427 (85%)	356 (98%)	7 (2%)	0	100	100
7	LJ	166/178 (93%)	160 (96%)	6 (4%)	0	100	100
8	LH	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
9	LE	202/288 (70%)	193 (96%)	9 (4%)	0	100	100
10	LG	227/266 (85%)	221 (97%)	6 (3%)	0	100	100
11	LO	197/203 (97%)	194 (98%)	3 (2%)	0	100	100
12	LL	204/211 (97%)	198 (97%)	6 (3%)	0	100	100
13	LV	130/140 (93%)	129 (99%)	1 (1%)	0	100	100
14	LM	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
15	La	145/148 (98%)	140 (97%)	5 (3%)	0	100	100
16	LN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
17	LI	199/214 (93%)	195 (98%)	4 (2%)	0	100	100
18	LD	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
19	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
20	LR	173/196 (88%)	171 (99%)	2 (1%)	0	100	100
21	LS	174/176 (99%)	168 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	LT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
23	LP	151/154 (98%)	146 (97%)	5 (3%)	0	100	100
24	LU	97/128 (76%)	93 (96%)	4 (4%)	0	100	100
25	LX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
26	LY	128/145 (88%)	125 (98%)	3 (2%)	0	100	100
27	LW	59/157 (38%)	57 (97%)	2 (3%)	0	100	100
28	LZ	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
29	Lr	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
30	Lh	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
31	Lb	86/159 (54%)	84 (98%)	2 (2%)	0	100	100
32	LF	223/248 (90%)	220 (99%)	3 (1%)	0	100	100
33	Lc	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
34	Ld	105/125 (84%)	99 (94%)	6 (6%)	0	100	100
35	Le	126/129 (98%)	126 (100%)	0	0	100	100
36	Lf	107/110 (97%)	107 (100%)	0	0	100	100
37	Lg	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
38	Li	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
39	Lj	84/87 (97%)	84 (100%)	0	0	100	100
40	Lk	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
41	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
42	Lm	48/128 (38%)	48 (100%)	0	0	100	100
43	Ln	23/25 (92%)	23 (100%)	0	0	100	100
44	Lo	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
45	Lp	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
48	SA	215/295 (73%)	194 (90%)	21 (10%)	0	100	100
49	SB	212/264 (80%)	197 (93%)	15 (7%)	0	100	100
50	SE	256/263 (97%)	238 (93%)	18 (7%)	0	100	100
51	SF	178/204 (87%)	154 (86%)	24 (14%)	0	100	100
52	SH	174/194 (90%)	167 (96%)	7 (4%)	0	100	100
53	SI	182/208 (88%)	168 (92%)	13 (7%)	1 (0%)	24	60
54	SK	93/165 (56%)	80 (86%)	13 (14%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	SL	134/158 (85%)	129 (96%)	5 (4%)	0	100	100
56	SQ	138/146 (94%)	122 (88%)	16 (12%)	0	100	100
57	SS	139/152 (91%)	121 (87%)	18 (13%)	0	100	100
58	ST	139/145 (96%)	134 (96%)	5 (4%)	0	100	100
59	SU	93/119 (78%)	88 (95%)	5 (5%)	0	100	100
60	SV	82/83 (99%)	79 (96%)	3 (4%)	0	100	100
61	SX	138/143 (96%)	127 (92%)	11 (8%)	0	100	100
62	Sc	58/69 (84%)	49 (84%)	9 (16%)	0	100	100
63	Sd	50/56 (89%)	44 (88%)	6 (12%)	0	100	100
64	SC	214/293 (73%)	199 (93%)	15 (7%)	0	100	100
65	SG	220/249 (88%)	211 (96%)	9 (4%)	0	100	100
66	SJ	176/194 (91%)	168 (96%)	8 (4%)	0	100	100
67	SN	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
68	SO	134/151 (89%)	114 (85%)	20 (15%)	0	100	100
69	SW	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
70	SY	122/133 (92%)	115 (94%)	7 (6%)	0	100	100
71	SZ	70/125 (56%)	60 (86%)	10 (14%)	0	100	100
72	Sb	77/84 (92%)	66 (86%)	11 (14%)	0	100	100
73	Se	45/133 (34%)	44 (98%)	1 (2%)	0	100	100
74	Sa	104/115 (90%)	103 (99%)	1 (1%)	0	100	100
78	Sg	305/317 (96%)	254 (83%)	42 (14%)	9 (3%)	3	19
79	SD	217/243 (89%)	198 (91%)	19 (9%)	0	100	100
80	SM	102/132 (77%)	89 (87%)	13 (13%)	0	100	100
81	SR	129/135 (96%)	115 (89%)	13 (10%)	1 (1%)	16	50
82	Sf	37/156 (24%)	28 (76%)	6 (16%)	3 (8%)	1	3
All	All	10940/12614 (87%)	10372 (95%)	554 (5%)	14 (0%)	49	80

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
78	Sg	139	LYS
81	SR	131	PRO
82	Sf	121	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
82	Sf	122	PRO
78	Sg	51	ASN

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	
1	SP	47/130 (36%)	46 (98%)	1 (2%)	47	75
4	LA	184/193 (95%)	181 (98%)	3 (2%)	55	79
5	LB	192/344 (56%)	191 (100%)	1 (0%)	81	89
6	LC	285/348 (82%)	285 (100%)	0	100	100
7	LJ	101/149 (68%)	98 (97%)	3 (3%)	36	69
8	LH	143/171 (84%)	143 (100%)	0	100	100
9	LE	158/252 (63%)	155 (98%)	3 (2%)	50	76
10	LG	152/223 (68%)	148 (97%)	4 (3%)	40	72
11	LO	162/174 (93%)	160 (99%)	2 (1%)	63	82
12	LL	148/177 (84%)	147 (99%)	1 (1%)	76	86
13	LV	90/107 (84%)	88 (98%)	2 (2%)	45	74
14	LM	107/116 (92%)	106 (99%)	1 (1%)	70	85
15	La	114/120 (95%)	114 (100%)	0	100	100
16	LN	170/172 (99%)	169 (99%)	1 (1%)	78	88
17	LI	163/181 (90%)	163 (100%)	0	100	100
18	LD	205/250 (82%)	197 (96%)	8 (4%)	28	62
19	LQ	160/165 (97%)	154 (96%)	6 (4%)	29	63
20	LR	137/175 (78%)	133 (97%)	4 (3%)	37	70
21	LS	154/157 (98%)	151 (98%)	3 (2%)	50	76
22	LT	119/140 (85%)	117 (98%)	2 (2%)	53	78
23	LP	134/135 (99%)	130 (97%)	4 (3%)	36	69
24	LU	81/115 (70%)	79 (98%)	2 (2%)	42	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	LX	102/133 (77%)	100 (98%)	2 (2%)	48	76
26	LY	114/135 (84%)	113 (99%)	1 (1%)	70	85
27	LW	54/126 (43%)	53 (98%)	1 (2%)	50	76
28	LZ	112/118 (95%)	105 (94%)	7 (6%)	16	48
29	Lr	104/120 (87%)	100 (96%)	4 (4%)	29	63
30	Lh	93/110 (84%)	91 (98%)	2 (2%)	45	74
31	Lb	63/125 (50%)	61 (97%)	2 (3%)	34	67
32	LF	166/215 (77%)	165 (99%)	1 (1%)	78	88
33	Lc	76/97 (78%)	72 (95%)	4 (5%)	20	54
34	Ld	95/110 (86%)	90 (95%)	5 (5%)	20	54
35	Le	112/115 (97%)	111 (99%)	1 (1%)	70	85
36	Lf	84/89 (94%)	82 (98%)	2 (2%)	43	73
37	Lg	86/94 (92%)	86 (100%)	0	100	100
38	Li	70/89 (79%)	67 (96%)	3 (4%)	26	60
39	Lj	70/74 (95%)	68 (97%)	2 (3%)	37	70
40	Lk	58/65 (89%)	52 (90%)	6 (10%)	7	28
41	Ll	45/48 (94%)	44 (98%)	1 (2%)	45	74
42	Lm	41/115 (36%)	40 (98%)	1 (2%)	43	73
43	Ln	24/24 (100%)	22 (92%)	2 (8%)	10	37
44	Lo	88/93 (95%)	85 (97%)	3 (3%)	32	66
45	Lp	70/72 (97%)	65 (93%)	5 (7%)	13	43
48	SA	157/243 (65%)	146 (93%)	11 (7%)	14	44
49	SB	187/231 (81%)	171 (91%)	16 (9%)	10	36
50	SE	182/225 (81%)	175 (96%)	7 (4%)	29	63
51	SF	123/170 (72%)	120 (98%)	3 (2%)	43	73
52	SH	86/174 (49%)	82 (95%)	4 (5%)	23	58
53	SI	139/180 (77%)	131 (94%)	8 (6%)	18	51
54	SK	55/136 (40%)	53 (96%)	2 (4%)	31	65
55	SL	108/142 (76%)	102 (94%)	6 (6%)	19	52
56	SQ	90/121 (74%)	84 (93%)	6 (7%)	15	46
57	SS	65/132 (49%)	63 (97%)	2 (3%)	35	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	ST	84/115 (73%)	80 (95%)	4 (5%)	23	57
59	SU	2/107 (2%)	2 (100%)	0	100	100
60	SV	53/67 (79%)	50 (94%)	3 (6%)	18	52
61	SX	104/115 (90%)	98 (94%)	6 (6%)	18	51
62	Sc	44/62 (71%)	41 (93%)	3 (7%)	14	45
63	Sd	43/49 (88%)	41 (95%)	2 (5%)	23	58
64	SC	164/225 (73%)	154 (94%)	10 (6%)	17	49
65	SG	63/218 (29%)	61 (97%)	2 (3%)	34	67
66	SJ	144/168 (86%)	138 (96%)	6 (4%)	26	61
67	SN	118/131 (90%)	112 (95%)	6 (5%)	21	55
68	SO	101/119 (85%)	93 (92%)	8 (8%)	11	39
69	SW	108/113 (96%)	103 (95%)	5 (5%)	24	58
70	SY	96/115 (84%)	92 (96%)	4 (4%)	26	61
71	SZ	34/103 (33%)	32 (94%)	2 (6%)	18	50
72	Sb	37/76 (49%)	37 (100%)	0	100	100
73	Se	38/104 (36%)	37 (97%)	1 (3%)	40	72
74	Sa	82/98 (84%)	79 (96%)	3 (4%)	30	64
78	Sg	163/275 (59%)	154 (94%)	9 (6%)	19	53
79	SD	109/202 (54%)	108 (99%)	1 (1%)	70	85
80	SM	7/108 (6%)	6 (86%)	1 (14%)	3	16
81	SR	59/122 (48%)	58 (98%)	1 (2%)	53	78
All	All	7778/10607 (73%)	7530 (97%)	248 (3%)	35	67

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	SA	193	HIS
69	SW	2	VAL
52	SH	45	ILE
68	SO	114	SER
78	Sg	10	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
48	SA	113	GLN
60	SV	35	ASN
49	SB	92	GLN
50	SE	67	GLN
74	Sa	72	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L8	148/156 (94%)	14 (9%)	0
3	L5	3322/5069 (65%)	465 (13%)	5 (0%)
46	Pt	74/77 (96%)	8 (10%)	0
47	L7	118/120 (98%)	17 (14%)	0
75	S2	1544/1868 (82%)	362 (23%)	7 (0%)
76	mR	13/27 (48%)	8 (61%)	0
77	S6	70/74 (94%)	21 (30%)	1 (1%)
All	All	5289/7391 (71%)	895 (16%)	13 (0%)

5 of 895 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L8	23	C
2	L8	25	G
2	L8	34	U
2	L8	35	C
2	L8	39	G

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
75	S2	604	A
75	S2	980	A
77	S6	59	A
75	S2	1395	C
75	S2	1679	A

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

115 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	A2M	L5	3825	3	22,25,26	3.94	10 (45%)	31,36,39	3.63	14 (45%)
3	PSU	L5	4403	3	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
31	MLZ	Lb	5	31	8,9,10	0.79	0	4,9,11	0.64	0
3	PSU	L5	4493	3	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
3	OMC	L5	4456	3	19,22,23	0.58	0	26,31,34	0.79	1 (3%)
3	OMG	L5	3899	3	23,26,27	0.51	0	33,38,41	0.51	0
3	A2M	L5	2363	3	22,25,26	3.94	11 (50%)	31,36,39	3.78	14 (45%)
3	A2M	L5	4590	3	22,25,26	3.94	9 (40%)	31,36,39	3.80	16 (51%)
3	OMC	L5	2804	3	19,22,23	0.55	0	26,31,34	0.62	0
77	H2U	S6	21	77	18,21,22	0.48	0	21,30,33	1.00	1 (4%)
3	OMG	L5	3744	3	23,26,27	0.49	0	33,38,41	0.49	0
3	PSU	L5	3853	3	18,21,22	1.03	1 (5%)	22,30,33	1.72	4 (18%)
44	MLZ	Lo	53	44	8,9,10	0.77	0	4,9,11	0.62	0
3	OMG	L5	4494	3	23,26,27	0.51	0	33,38,41	0.49	0
3	OMU	L5	3925	3	19,22,23	3.01	8 (42%)	26,31,34	1.70	5 (19%)
3	OMG	L5	3944	3	23,26,27	0.50	0	33,38,41	0.60	0
3	PSU	L5	4353	3	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
42	M3L	Lm	98	42	10,11,12	0.42	0	9,14,16	0.37	0
4	V5N	LA	216	4	9,11,12	2.67	2 (22%)	9,14,16	1.21	0
3	PSU	L5	4576	3	18,21,22	1.05	1 (5%)	22,30,33	1.75	4 (18%)
3	OMG	L5	3627	3	23,26,27	0.50	0	33,38,41	0.60	0
3	PSU	L5	4471	3	18,21,22	1.05	1 (5%)	22,30,33	1.63	4 (18%)
3	OMG	L5	3792	3	23,26,27	0.50	0	33,38,41	0.49	0
3	OMG	L5	4637	3	23,26,27	0.51	0	33,38,41	0.49	0
3	A2M	L5	4571	3	22,25,26	3.90	10 (45%)	31,36,39	3.68	14 (45%)
3	PSU	L5	1792	3	18,21,22	1.04	1 (5%)	22,30,33	1.61	4 (18%)
3	A2M	L5	1871	3	22,25,26	3.93	10 (45%)	31,36,39	3.69	15 (48%)
3	OMC	L5	3887	3	19,22,23	0.54	0	26,31,34	0.71	0
3	OMG	L5	4228	3	23,26,27	0.49	0	33,38,41	0.54	0
3	A2M	L5	3830	3	22,25,26	3.94	10 (45%)	31,36,39	3.70	13 (41%)
3	PSU	L5	3851	3	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
3	OMG	L5	1316	3	23,26,27	0.51	0	33,38,41	0.52	0
3	A2M	L5	2815	3	22,25,26	3.95	10 (45%)	31,36,39	3.85	16 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	2365	3	19,22,23	0.53	0	26,31,34	0.64	0
3	A2M	L5	398	3	22,25,26	3.90	10 (45%)	31,36,39	3.66	13 (41%)
3	A2M	L5	3723	3	22,25,26	3.93	10 (45%)	31,36,39	3.72	15 (48%)
3	OMC	L5	3808	3	19,22,23	0.60	0	26,31,34	0.86	2 (7%)
3	PSU	L5	4361	3	18,21,22	1.03	1 (5%)	22,30,33	1.68	4 (18%)
3	OMC	L5	1340	3	19,22,23	0.53	0	26,31,34	0.64	0
3	OMG	L5	4499	3	23,26,27	0.50	0	33,38,41	0.45	0
3	A2M	L5	1326	3	22,25,26	3.93	10 (45%)	31,36,39	3.74	15 (48%)
77	PSU	S6	56	77	18,21,22	1.06	1 (5%)	22,30,33	1.71	3 (13%)
3	OMG	L5	2424	3	23,26,27	0.50	0	33,38,41	0.44	0
3	PSU	L5	4972	3	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
3	5MC	L5	3782	3	18,22,23	0.57	0	26,32,35	0.68	0
46	H2U	Pt	21	46	18,21,22	0.59	0	21,30,33	1.54	4 (19%)
3	OMG	L5	2364	3	23,26,27	0.49	0	33,38,41	0.46	0
3	OMC	L5	1881	3	19,22,23	0.57	0	26,31,34	0.65	0
3	OMG	L5	4370	3	23,26,27	0.50	0	33,38,41	0.55	0
3	PSU	L5	4531	3	18,21,22	1.06	1 (5%)	22,30,33	1.88	5 (22%)
3	PSU	L5	5010	3	18,21,22	1.06	1 (5%)	22,30,33	1.71	4 (18%)
3	OMC	L5	2422	3	19,22,23	0.59	0	26,31,34	0.78	1 (3%)
3	PSU	L5	4569	3	18,21,22	1.08	1 (5%)	22,30,33	1.70	4 (18%)
3	PSU	L5	3764	3	18,21,22	1.04	1 (5%)	22,30,33	1.67	4 (18%)
3	PSU	L5	4636	3	18,21,22	1.06	1 (5%)	22,30,33	1.84	5 (22%)
3	PSU	L5	4442	3	18,21,22	1.09	1 (5%)	22,30,33	1.79	5 (22%)
3	UR3	L5	4530	3	19,22,23	2.78	8 (42%)	26,32,35	1.29	2 (7%)
77	4SU	S6	8	77	18,21,22	3.78	8 (44%)	26,30,33	2.20	5 (19%)
3	PSU	L5	4579	3	18,21,22	1.04	1 (5%)	22,30,33	1.72	4 (18%)
3	A2M	L5	1524	3	22,25,26	3.98	10 (45%)	31,36,39	3.97	14 (45%)
3	OMC	L5	4536	3	19,22,23	0.55	0	26,31,34	0.69	0
3	PSU	L5	4420	3	18,21,22	1.04	1 (5%)	22,30,33	1.59	4 (18%)
3	PSU	L5	4552	3	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
3	OMC	L5	2351	3	19,22,23	0.58	0	26,31,34	1.07	2 (7%)
3	OMU	L5	4227	3	19,22,23	3.02	8 (42%)	26,31,34	1.73	4 (15%)
3	A2M	L5	3724	3	22,25,26	3.93	10 (45%)	31,36,39	3.71	14 (45%)
3	5MC	L5	4447	3	18,22,23	0.72	0	26,32,35	0.73	0
3	OMG	L5	4618	3	23,26,27	0.50	0	33,38,41	0.53	0
3	PSU	L5	4457	3	18,21,22	1.05	1 (5%)	22,30,33	1.76	5 (22%)
3	PSU	L5	3920	3	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	G7M	Pt	47	46	23,26,27	2.77	8 (34%)	35,39,42	2.33	10 (28%)
3	PSU	L5	3729	3	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)
3	1MA	L5	1322	3	21,25,26	0.50	0	31,37,40	0.75	1 (3%)
3	PSU	L5	4689	3	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	L5	3844	3	18,21,22	1.02	1 (5%)	22,30,33	1.74	4 (18%)
3	PSU	L5	4500	3	18,21,22	1.12	1 (5%)	22,30,33	1.79	4 (18%)
3	OMG	L5	4392	3	23,26,27	0.51	0	33,38,41	0.45	0
3	PSU	L5	3734	3	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	L5	3758	3	18,21,22	1.04	1 (5%)	22,30,33	1.71	4 (18%)
15	V5N	La	39	15	9,11,12	2.63	2 (22%)	9,14,16	1.19	1 (11%)
3	PSU	L5	3768	3	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	L5	1860	3	18,21,22	1.07	1 (5%)	22,30,33	1.71	4 (18%)
3	OMG	L5	4196	46,3	23,26,27	0.49	0	33,38,41	0.50	0
3	OMG	L5	1522	3	23,26,27	0.52	0	33,38,41	0.56	0
3	PSU	L5	3715	3	18,21,22	1.03	1 (5%)	22,30,33	1.70	4 (18%)
3	PSU	L5	1781	3	18,21,22	1.04	1 (5%)	22,30,33	1.63	4 (18%)
3	A2M	L5	1534	84,3	22,25,26	3.93	10 (45%)	31,36,39	3.77	14 (45%)
3	PSU	L5	4423	3	18,21,22	1.09	1 (5%)	22,30,33	1.73	4 (18%)
5	HIC	LB	245	5	10,11,12	0.57	0	8,14,16	0.62	0
3	PSU	L5	3762	3	18,21,22	1.04	1 (5%)	22,30,33	1.66	4 (18%)
3	OMG	L5	4623	3	23,26,27	0.50	0	33,38,41	0.52	0
46	PSU	Pt	56	46	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
3	PSU	L5	4299	3	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
46	4SU	Pt	8	46	18,21,22	3.76	8 (44%)	26,30,33	2.23	4 (15%)
3	A2M	L5	400	3	22,25,26	3.91	10 (45%)	31,36,39	3.71	15 (48%)
77	G7M	S6	47	77	23,26,27	2.78	8 (34%)	35,39,42	2.29	10 (28%)
3	A2M	L5	2401	3	22,25,26	3.92	11 (50%)	31,36,39	3.74	16 (51%)
3	OMG	L5	2876	3	23,26,27	0.55	0	33,38,41	0.48	0
3	PSU	L5	4431	3	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
3	PSU	L5	4673	3	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
3	A2M	L5	3718	3	22,25,26	3.91	10 (45%)	31,36,39	3.69	15 (48%)
3	PSU	L5	4628	3	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	L5	4532	3	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
3	OMU	L5	4306	3	19,22,23	2.98	8 (42%)	26,31,34	1.72	5 (19%)
3	6MZ	L5	4220	3	22,25,26	2.69	4 (18%)	30,36,39	3.58	12 (40%)
3	OMC	L5	3841	3	19,22,23	0.53	0	26,31,34	0.71	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4521	3	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
3	OMC	L5	3869	3	19,22,23	0.55	0	26,31,34	0.66	0
3	OMC	L5	3701	3	19,22,23	0.56	0	26,31,34	0.55	0
3	PSU	L5	5001	3	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
3	A2M	L5	4523	3	22,25,26	3.90	11 (50%)	31,36,39	3.68	14 (45%)
3	PSU	L5	3770	3	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
3	A2M	L5	3867	3	22,25,26	3.94	10 (45%)	31,36,39	3.77	15 (48%)
3	PSU	L5	4296	3	18,21,22	1.05	1 (5%)	22,30,33	1.69	4 (18%)
3	OMU	L5	4498	3	19,22,23	3.02	8 (42%)	26,31,34	1.71	5 (19%)

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	A2M	L5	3825	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
31	MLZ	Lb	5	31	-	0/7/8/10	-
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3899	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	2363	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
77	H2U	S6	21	77	-	1/7/38/39	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3853	3	-	0/7/25/26	0/2/2/2
44	MLZ	Lo	53	44	-	5/7/8/10	-
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	2/9/27/28	0/2/2/2
3	OMG	L5	3944	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
42	M3L	Lm	98	42	-	1/9/10/12	-
4	V5N	LA	216	4	-	3/9/10/12	0/1/1/1
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2815	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
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	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	2/9/27/28	0/3/3/3
77	PSU	S6	56	77	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	3	-	1/7/25/26	0/2/2/2
46	H2U	Pt	21	46	-	3/7/38/39	0/2/2/2
3	OMG	L5	2364	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	1881	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2422	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4569	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3764	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4636	3	-	3/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
77	4SU	S6	8	77	-	3/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4420	3	-	5/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	3	-	2/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	4227	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	3	-	0/7/25/26	0/2/2/2
46	G7M	Pt	47	46	-	0/7/25/26	0/3/3/3
3	PSU	L5	3729	3	-	2/7/25/26	0/2/2/2
3	1MA	L5	1322	3	-	0/7/25/26	0/3/3/3
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	3/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
15	V5N	La	39	15	-	0/9/10/12	0/1/1/1
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	46,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	84,3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
5	HIC	LB	245	5	-	0/5/6/8	0/1/1/1
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
46	PSU	Pt	56	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
46	4SU	Pt	8	46	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
77	G7M	S6	47	77	-	3/7/25/26	0/3/3/3
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	2876	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	1/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	3841	3	-	2/9/27/28	0/2/2/2
3	PSU	L5	4521	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3701	3	-	4/9/27/28	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4296	3	-	1/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2

The worst 5 of 306 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3830	A2M	C3'-C2'	-12.74	1.24	1.52
3	L5	1524	A2M	C3'-C2'	-12.68	1.24	1.52
3	L5	4590	A2M	C3'-C2'	-12.67	1.24	1.52
3	L5	3825	A2M	C3'-C2'	-12.67	1.24	1.52
3	L5	3867	A2M	C3'-C2'	-12.66	1.24	1.52

The worst 5 of 517 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1524	A2M	C1'-N9-C8	-12.74	98.36	127.14
3	L5	1534	A2M	C1'-N9-C8	-11.48	101.21	127.14
3	L5	3867	A2M	C1'-N9-C8	-11.42	101.36	127.14
3	L5	4220	6MZ	C1'-N9-C8	-11.39	101.42	127.14
3	L5	2815	A2M	C1'-N9-C8	-11.31	101.59	127.14

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	LA	216	V5N	O-C-CA-CB
4	LA	216	V5N	C-CA-CB-CG
44	Lo	53	MLZ	N-CA-CB-CG
44	Lo	53	MLZ	C-CA-CB-CG
3	L5	398	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

28 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3899	OMG	1	0
3	L5	2804	OMC	1	0
77	S6	21	H2U	1	0
3	L5	3925	OMU	1	0
3	L5	3944	OMG	1	0
3	L5	4637	OMG	1	0
3	L5	1871	A2M	1	0
3	L5	398	A2M	1	0
3	L5	3723	A2M	3	0
3	L5	1340	OMC	1	0
3	L5	1326	A2M	2	0
46	Pt	21	H2U	3	0
3	L5	2422	OMC	1	0
3	L5	4442	PSU	1	0
77	S6	8	4SU	2	0
3	L5	4579	PSU	2	0
3	L5	4420	PSU	1	0
3	L5	2351	OMC	1	0
3	L5	4227	OMU	2	0
3	L5	3724	A2M	1	0
3	L5	4618	OMG	2	0
46	Pt	47	G7M	1	0
3	L5	4689	PSU	1	0
77	S6	47	G7M	2	0
3	L5	4431	PSU	1	0
3	L5	3718	A2M	3	0
3	L5	4220	6MZ	1	0
3	L5	4523	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 106 ligands modelled in this entry, 103 are monoatomic - leaving 3 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
85	C	Lo	202	-	18,21,22	0.45	0	26,30,33	1.32	3 (11%)
88	HYG	S2	1901	-	35,39,39	3.11	11 (31%)	43,60,60	1.88	9 (20%)
85	C	L5	5102	-	18,21,22	0.43	0	26,30,33	0.51	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
85	C	Lo	202	-	-	4/7/25/26	0/2/2/2
88	HYG	S2	1901	-	-	5/12/87/87	0/4/4/4
85	C	L5	5102	-	-	1/7/25/26	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	S2	1901	HYG	O29-C12	11.06	1.61	1.43
88	S2	1901	HYG	O14-C13	6.54	1.58	1.41
88	S2	1901	HYG	O22-C17	6.54	1.53	1.43
88	S2	1901	HYG	O28-C23	5.92	1.47	1.40
88	S2	1901	HYG	C16-C15	4.52	1.62	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	S2	1901	HYG	O29-C12-C13	5.41	125.05	110.86
88	S2	1901	HYG	O22-C17-C16	4.92	123.19	111.22
88	S2	1901	HYG	O28-C27-C26	4.32	114.66	108.52
85	Lo	202	C	C1'-N1-C2	4.13	127.65	118.42
88	S2	1901	HYG	O14-C15-C16	3.50	116.04	109.69

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

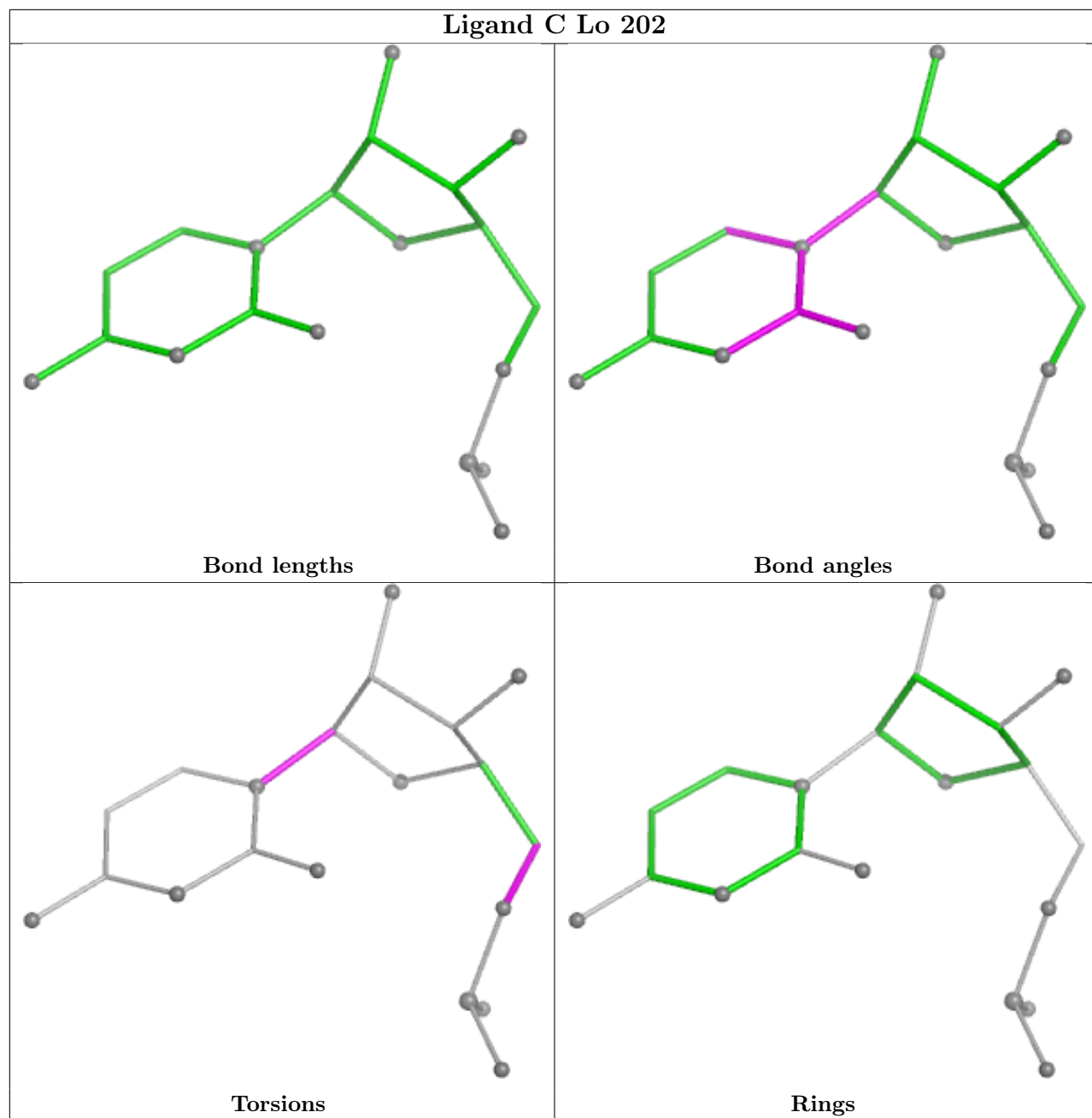
Mol	Chain	Res	Type	Atoms
88	S2	1901	HYG	O28-C27-C33-C34
88	S2	1901	HYG	C27-C33-C34-O35
88	S2	1901	HYG	N36-C33-C34-O35
88	S2	1901	HYG	O14-C13-O18-C6
85	Lo	202	C	O4'-C1'-N1-C6

There are no ring outliers.

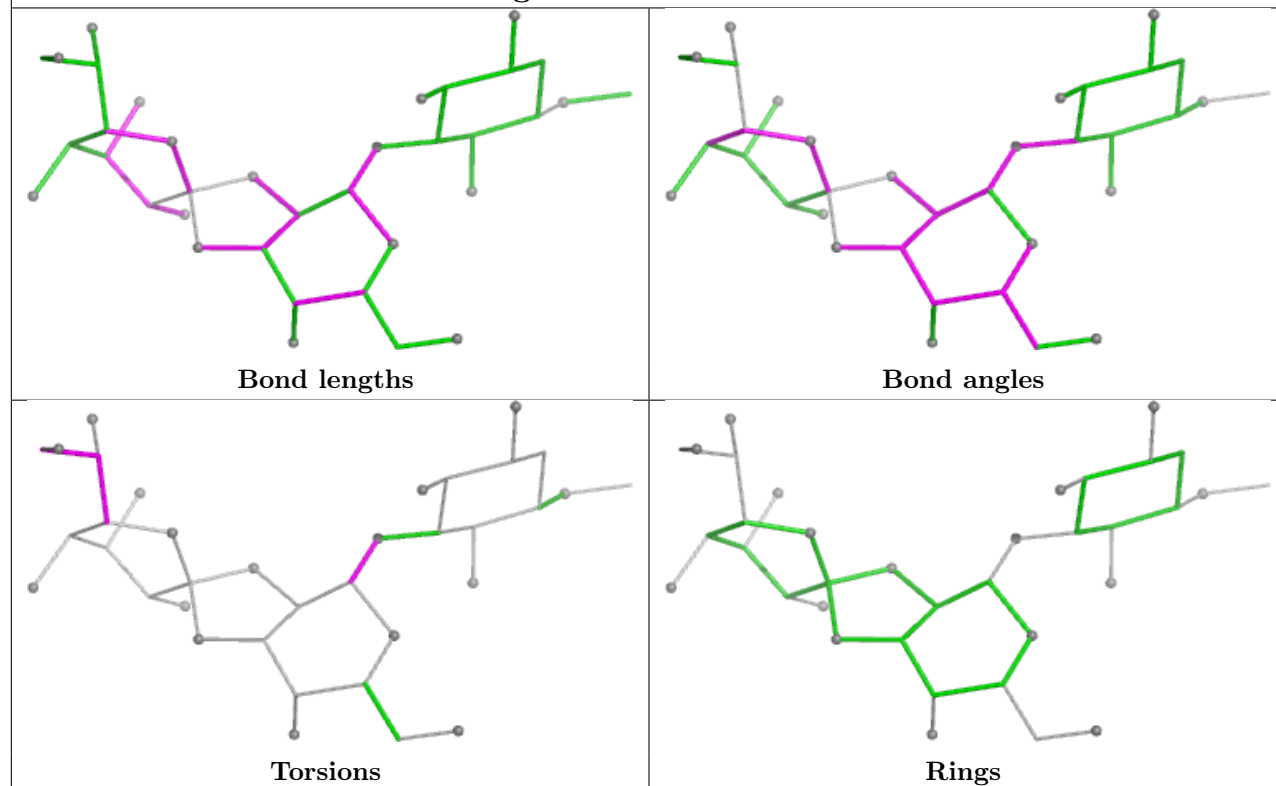
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	Lo	202	C	1	0

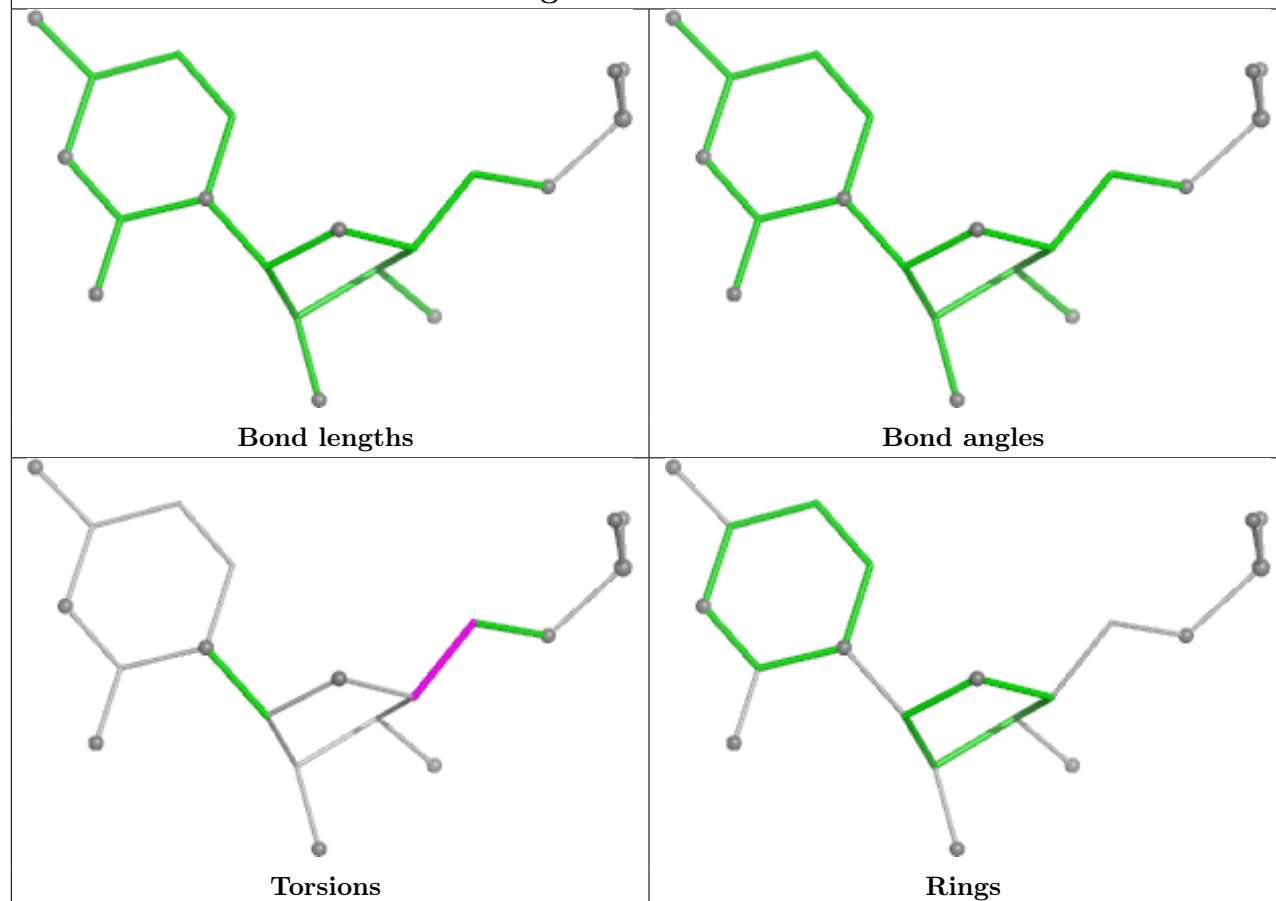
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand HYG S2 1901



Ligand C L5 5102



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
77	S6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S6	47:G7M	O3'	49:C	P	4.81

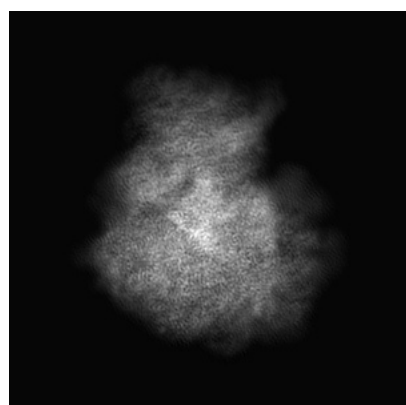
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54265. These allow visual inspection of the internal detail of the map and identification of artifacts.

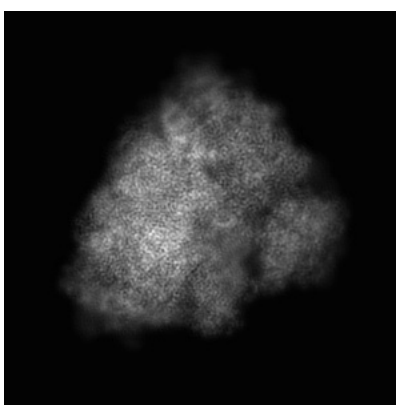
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

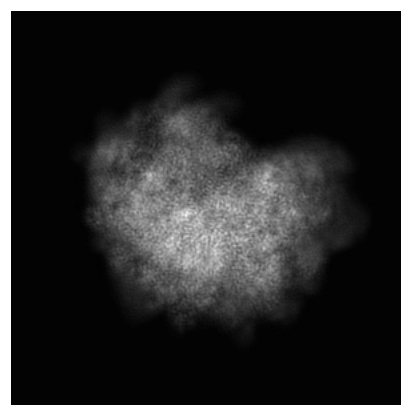
6.1.1 Primary map



X



Y

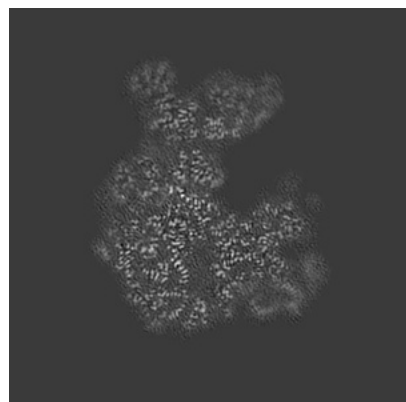


Z

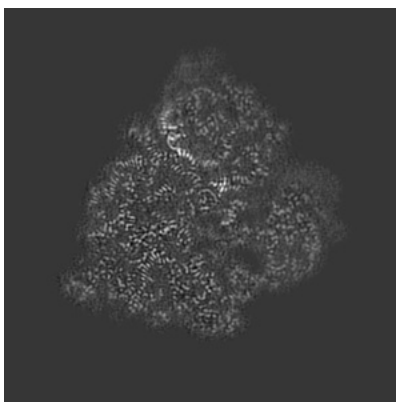
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

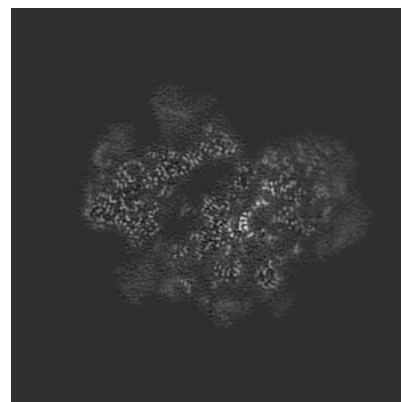
6.2.1 Primary map



X Index: 240



Y Index: 240

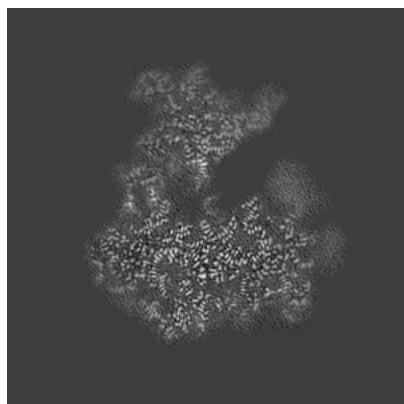


Z Index: 240

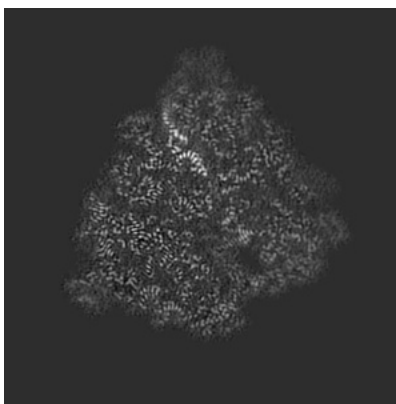
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

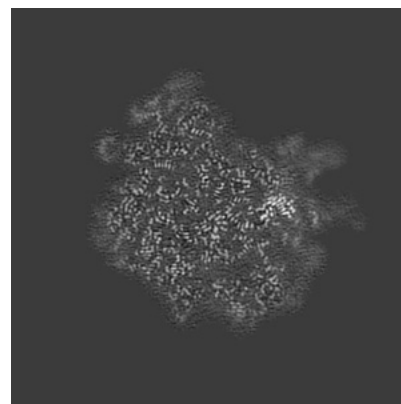
6.3.1 Primary map



X Index: 210



Y Index: 233

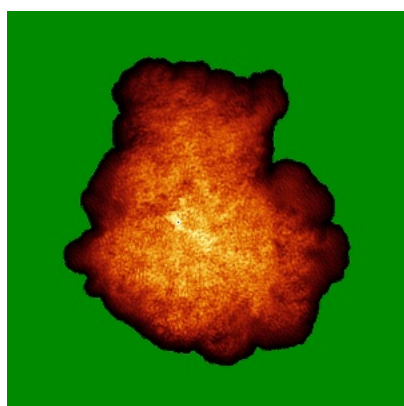


Z Index: 205

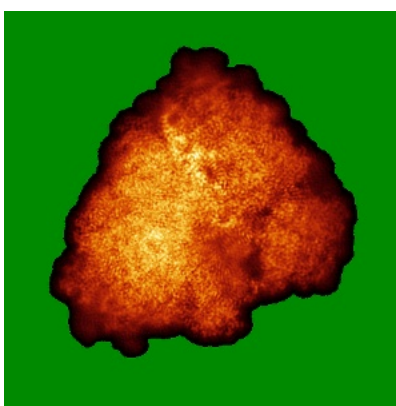
The images above show the largest variance slices of the map in three orthogonal directions.

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

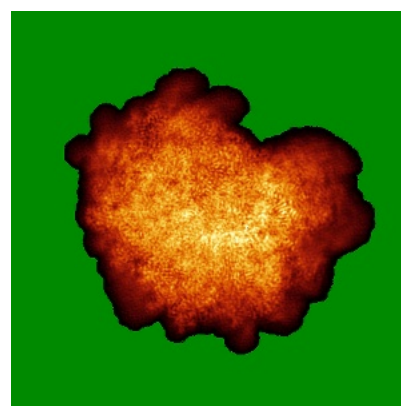
6.4.1 Primary map



X



Y

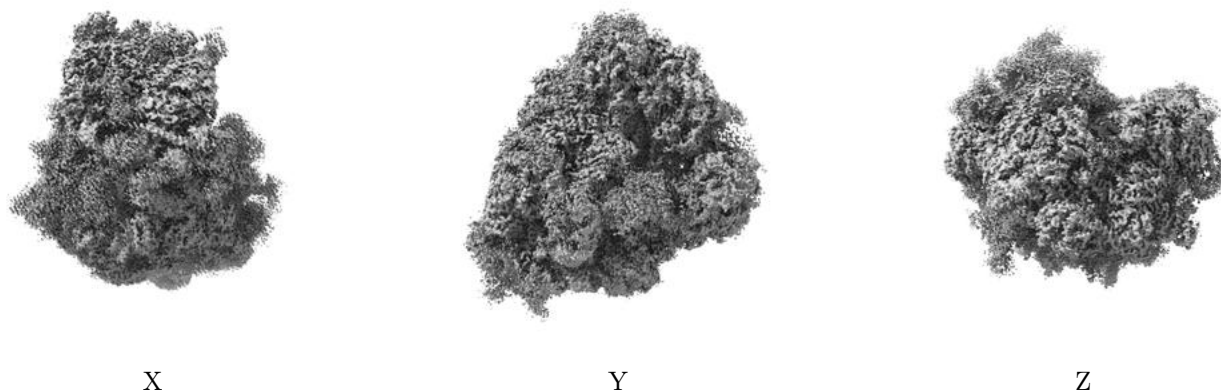


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

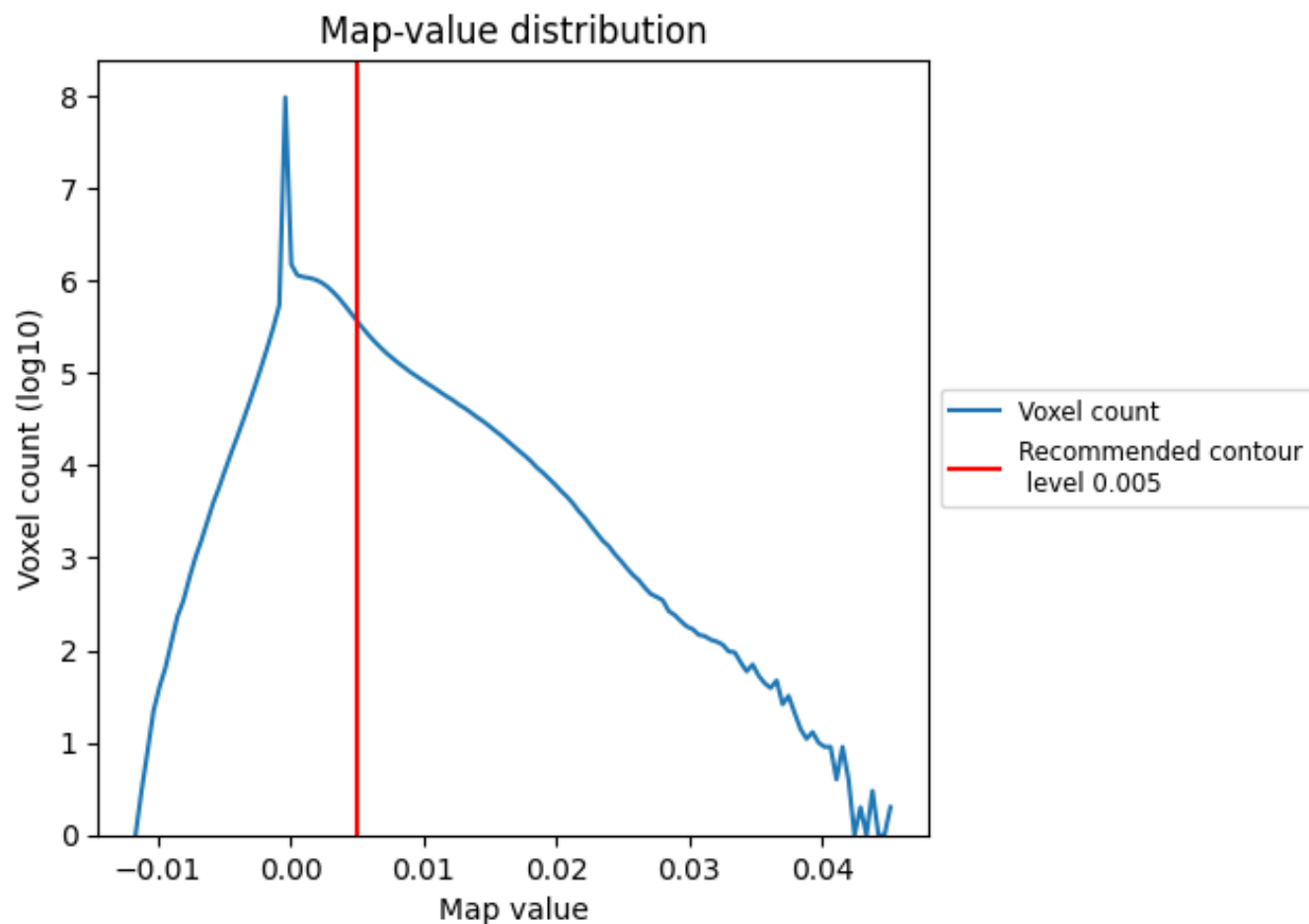
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

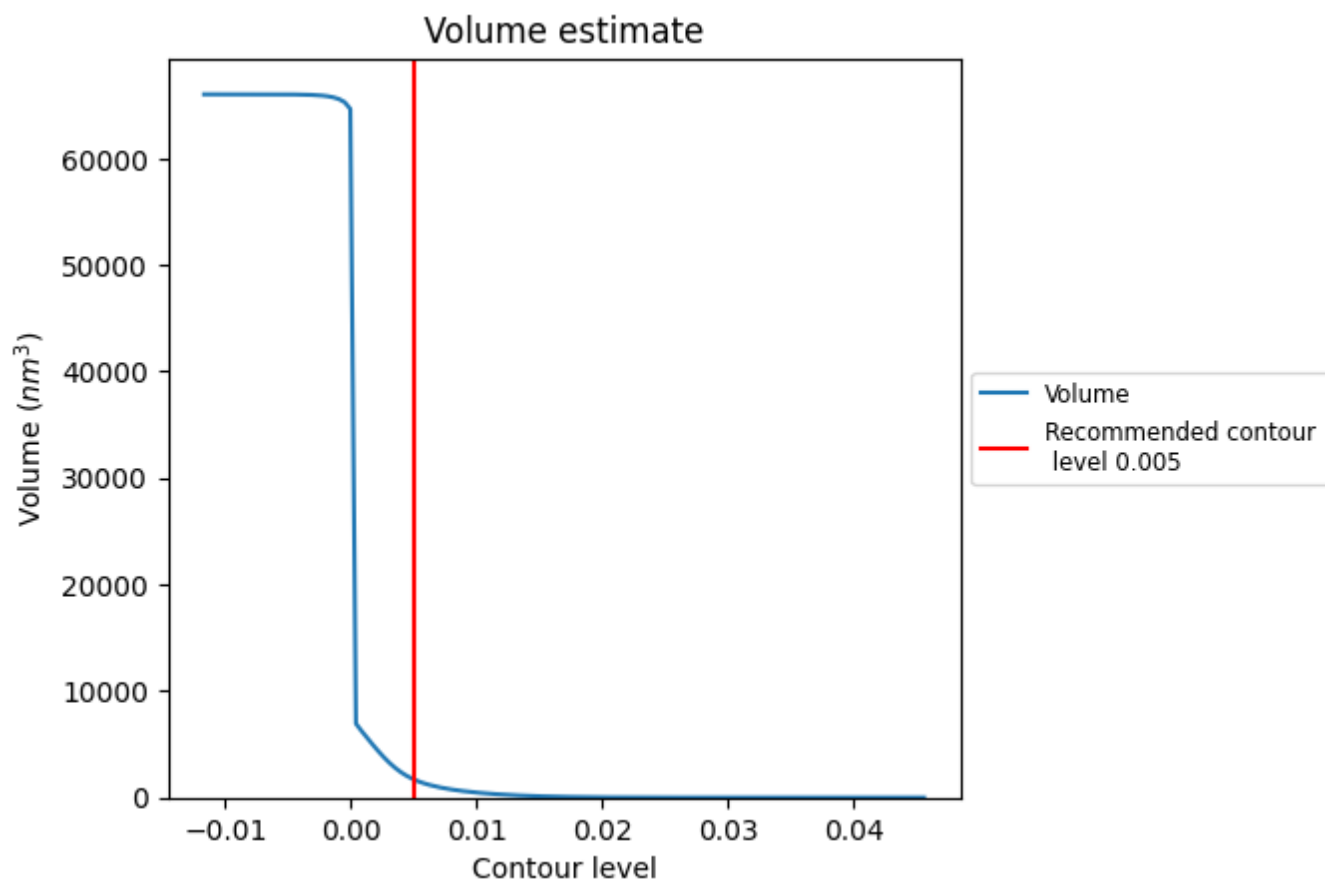
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

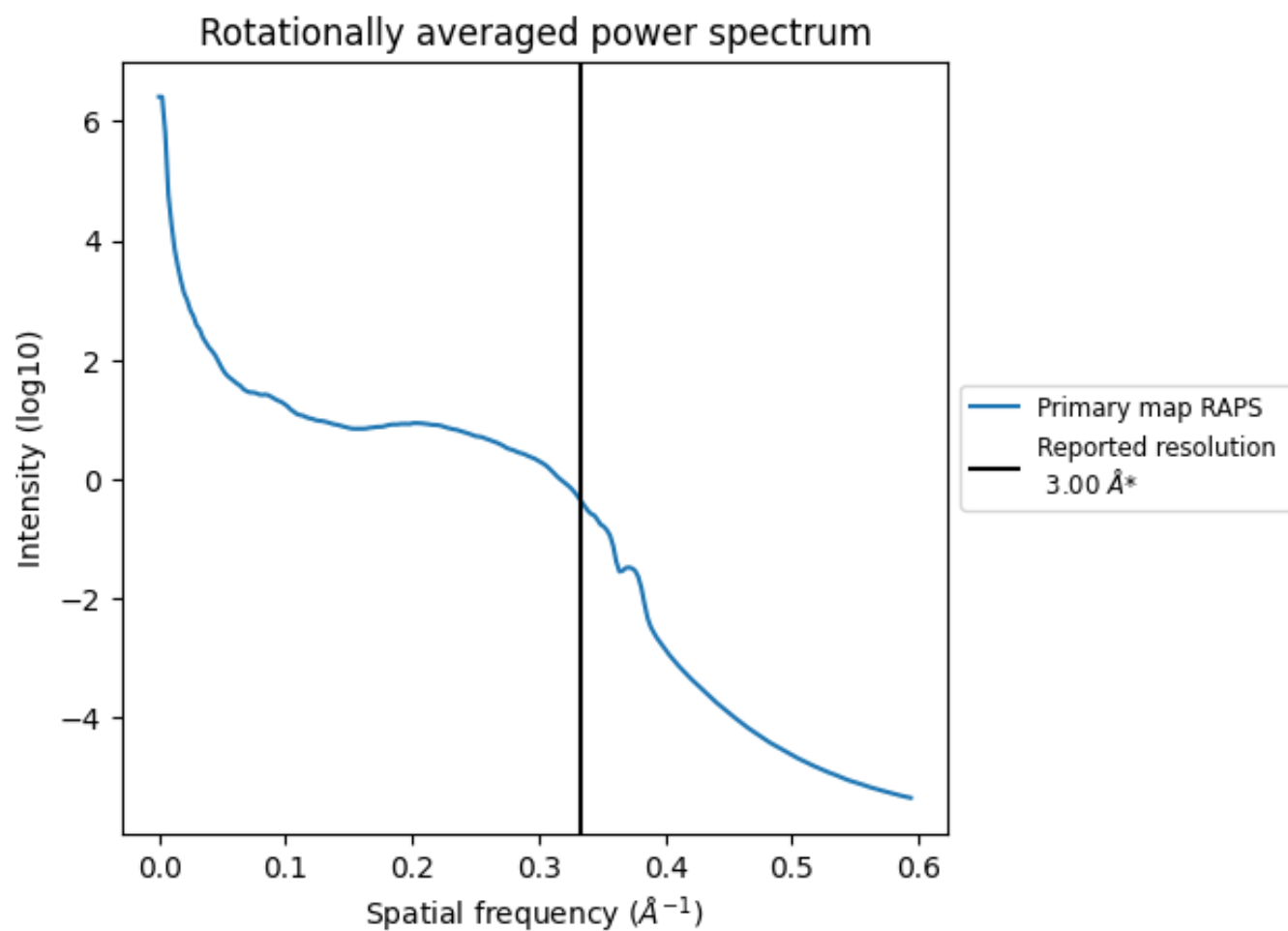
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1714 nm³; this corresponds to an approximate mass of 1549 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

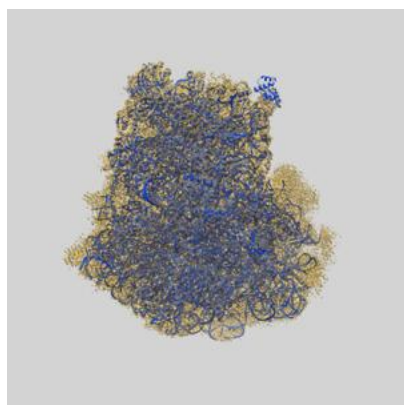
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

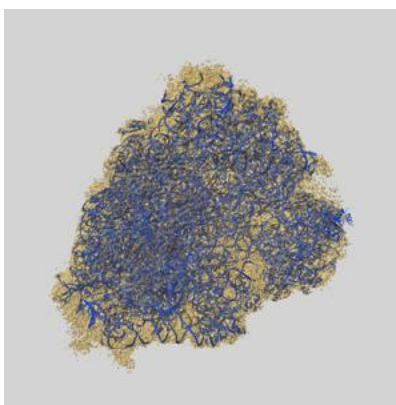
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54265 and PDB model 9RU7. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

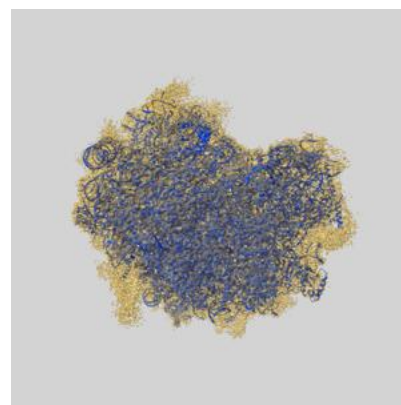
9.1 Map-model overlay [i](#)



X



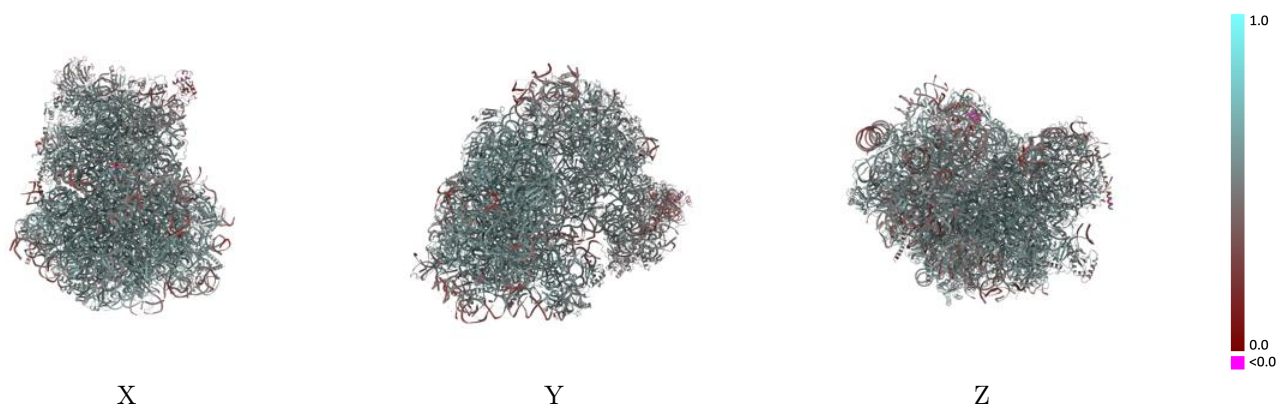
Y



Z

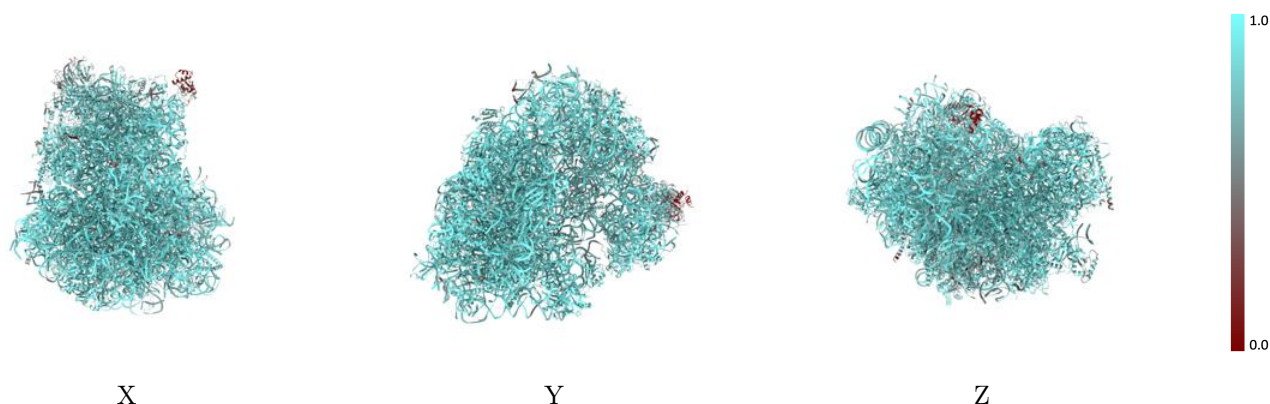
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



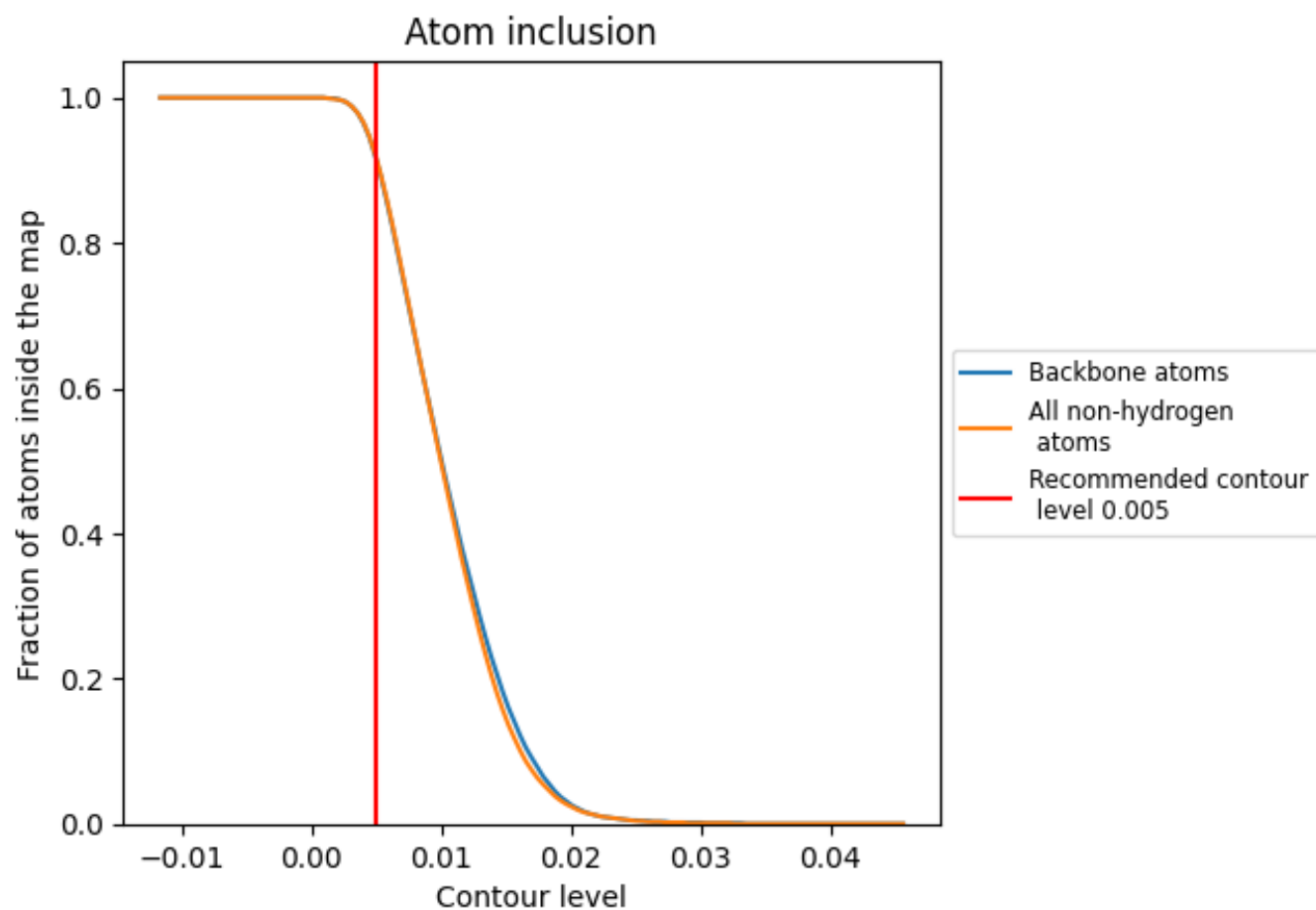
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.5400
L5	 0.9470	 0.5450
L7	 0.9750	 0.5630
L8	 0.9580	 0.5540
LA	 0.9650	 0.5940
LB	 0.9750	 0.5980
LC	 0.9160	 0.5790
LD	 0.9130	 0.5560
LE	 0.8960	 0.5550
LF	 0.9350	 0.5830
LG	 0.8820	 0.5440
LH	 0.9270	 0.5710
LI	 0.9240	 0.5770
LJ	 0.9180	 0.5420
LL	 0.8900	 0.5640
LM	 0.9300	 0.5680
LN	 0.9650	 0.6030
LO	 0.9370	 0.5860
LP	 0.9250	 0.5920
LQ	 0.9430	 0.5940
LR	 0.9420	 0.5700
LS	 0.9360	 0.5920
LT	 0.9170	 0.5730
LU	 0.8190	 0.5140
LV	 0.9470	 0.5880
LW	 0.9820	 0.5840
LX	 0.8980	 0.5720
LY	 0.8970	 0.5730
LZ	 0.9260	 0.5550
La	 0.9450	 0.5950
Lb	 0.8840	 0.5500
Lc	 0.9740	 0.5560
Ld	 0.8940	 0.5690
Le	 0.9250	 0.5940
Lf	 0.9520	 0.6080















Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lg	 0.9640	 0.5840
Lh	 0.8950	 0.5640
Li	 0.9130	 0.5660
Lj	 0.9740	 0.6020
Lk	 0.8300	 0.5240
Ll	 0.9470	 0.5820
Lm	 0.9490	 0.5800
Ln	 0.9500	 0.5720
Lo	 0.8960	 0.5760
Lp	 0.9800	 0.5780
Lr	 0.9210	 0.5820
Pt	 0.7710	 0.4530
S2	 0.9410	 0.5170
S6	 0.7340	 0.2550
SA	 0.8070	 0.5400
SB	 0.8670	 0.5320
SC	 0.8490	 0.5540
SD	 0.7700	 0.5060
SE	 0.8520	 0.5280
SF	 0.8410	 0.5020
SG	 0.7970	 0.4640
SH	 0.7400	 0.5060
SI	 0.9260	 0.5370
SJ	 0.8550	 0.5180
SK	 0.8090	 0.4600
SL	 0.9150	 0.5630
SM	 0.2490	 0.2880
SN	 0.9200	 0.5520
SO	 0.8640	 0.5270
SP	 0.8820	 0.4830
SQ	 0.8390	 0.5210
SR	 0.7660	 0.5160
SS	 0.9140	 0.5020
ST	 0.8580	 0.4930
SU	 0.8320	 0.5010
SV	 0.7840	 0.5400
SW	 0.8930	 0.5640
SX	 0.8840	 0.5540
SY	 0.7990	 0.4940
SZ	 0.8420	 0.4810
Sa	 0.8680	 0.5450
Sb	 0.8710	 0.5610

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Sc	 0.8120	 0.5020
Sd	 0.9110	 0.5400
Se	 0.8280	 0.5230
Sf	 0.5580	 0.3090
Sg	 0.6510	 0.4570
mR	 0.4510	 0.3870