



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 09:49 PM EDT

PDB ID : 6XA1 / pdb_00006xa1
EMDB ID : EMD-22085
Title : Structure of a drug-like compound stalled human translation termination complex
Authors : Li, W.; Cate, J.
Deposited on : 2020-06-03
Resolution : 2.80 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

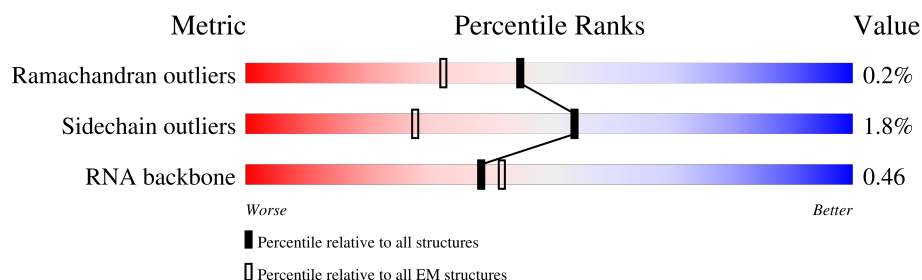
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	LA	248	
2	LB	396	
3	L5	3510	
4	L7	120	
5	L8	155	
6	LC	358	
7	LD	290	
8	LE	247	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	LF	225	7% 99%
10	LG	241	36% 98%
11	LH	190	24% 97%
12	LI	213	19% 97%
13	LJ	176	48% 97%
14	LL	204	21% 97%
15	LM	139	17% 99%
16	LN	203	97%
17	LO	201	10% 98%
18	LP	153	9% 99%
19	LQ	187	99%
20	LR	187	25% 94% 6%
21	LS	175	5% 97%
22	LT	159	20% 99%
23	LU	101	72% 99%
24	LV	131	11% 97%
25	LW	124	58% 99%
26	LX	120	23% 99%
27	LY	134	19% 97%
28	LZ	135	30% 96%
29	La	147	7% 98%
30	Lb	121	38% 88% 10%
31	Lc	98	20% 100%
32	Ld	107	16% 98%
33	Le	128	95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	Lf	109	
35	Lg	114	
36	Lh	122	
37	Li	102	
38	Lj	86	
39	Lk	69	
40	Ll	50	
41	Lm	52	
42	Ln	24	
43	Lo	105	
44	Lp	91	
45	Lr	125	
46	S2	1590	
47	SA	216	
48	SB	211	
49	SD	224	
50	SE	258	
51	SF	189	
52	SH	189	
53	SI	205	
54	SK	95	
55	SL	150	
56	SP	131	
57	SQ	140	
58	SR	131	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	SS	143	75% 99%
60	ST	141	71% 99%
61	SU	100	77% 99%
62	SV	84	63% 99%
63	SX	139	19% 99%
64	Sa	99	29% 98%
65	Sc	61	80% 98%
66	Sd	55	42% 100%
67	Sg	313	99% 98%
68	SC	220	34% 100%
69	SG	228	82% 98%
70	SJ	180	53% 99%
71	SM	120	93% 92% 7%
72	SN	150	37% 99%
73	SO	135	38% 97%
74	SW	129	19% 98%
75	SY	122	84% 99%
76	SZ	70	93% 99%
77	Sb	82	62% 100%
78	Se	54	52% 94% 6%
79	Sf	63	100% 97%
80	Bv	76	70% 38% 50% 11%
81	j	411	80% 78% 12% 9%
82	k	13	31% 46% 54%
83	NC	25	48% 92% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	B8N	S2	1248	X	-	-	-

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 211887 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 60S ribosomal protein L8.

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

- Molecule 2 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	LB	396	Total	C	N	O	S	0	0
			3197	2036	601	546	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3510	Total	C	N	O	P	0	0
			75317	33580	13769	24459	3509		

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

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

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	155	Total	C	N	O	P	0	0
			3298	1472	582	1089	155		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	358	Total	C	N	O	S	0	0
			2855	1797	570	473	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	290	Total	C	N	O	S	0	0
			2357	1493	428	422	14		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	207	Total	C	N	O	S	0	0
			1677	1064	323	276	14		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	204	Total	C	N	O	S	0	0
			1649	1032	343	270	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a protein called Heparin-binding protein HBp15.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	109	Total	C	N	O	S	0	0
			882	549	192	137	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lb	89	ALA	VAL	conflict	UNP P47914

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lj	86	Total	C	N	O	S	1	0
			713	439	158	111	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S2	1590	Total	C	N	O	P	0	0
			34012	15211	6116	11096	1589		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SA	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SB	211	Total	C	N	O	S	0	0
			1718	1091	307	306	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SD	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SE	258	Total	C	N	O	S	0	0
			2050	1311	381	350	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SH	185	Total	C	N	O	S	0	0
			1490	953	272	264	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SI	197	Total	C	N	O	S	0	0
			1624	1019	321	279	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
			799	524	139	130	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SL	140	Total	C	N	O	S	0	0
			1144	729	214	195	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SP	131	Total	C	N	O	S	0	0
			1075	682	204	182	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SQ	140	Total	C	N	O	S	0	0
			1117	710	211	193	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SR	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SS	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	ST	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SU	100	Total	C	N	O	S	0	0
			798	501	152	141	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SV	84	Total	C	N	O	S	0	0
			639	395	117	122	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SV	0	ACE	-	acetylation	UNP P63220

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SX	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Sc	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SC	220	Total	C	N	O	S	1	0
			1715	1109	296	300	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SG	228	Total	C	N	O	S	0	0
			1848	1155	368	318	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SJ	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SM	112	Total	C	N	O	S	0	0
			860	540	149	163	8		

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SO	138	IAS	ASP	conflict	UNP P62263

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SY	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SZ	70	Total	C	N	O	S	0	0
			559	360	102	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sb	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Se	51	Total	C	N	O	S	0	0
			407	251	90	65	1		

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

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

- Molecule 80 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bv	75	Total	C	N	O	P	0	0
			1621	725	289	532	75		

- Molecule 81 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	j	373	Total	C	N	O	S	0	0
			2930	1874	500	547	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	63	UXY	LYS	conflict	UNP P62495

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	k	13	Total	C	N	O	P	0	0
			270	122	44	91	13		

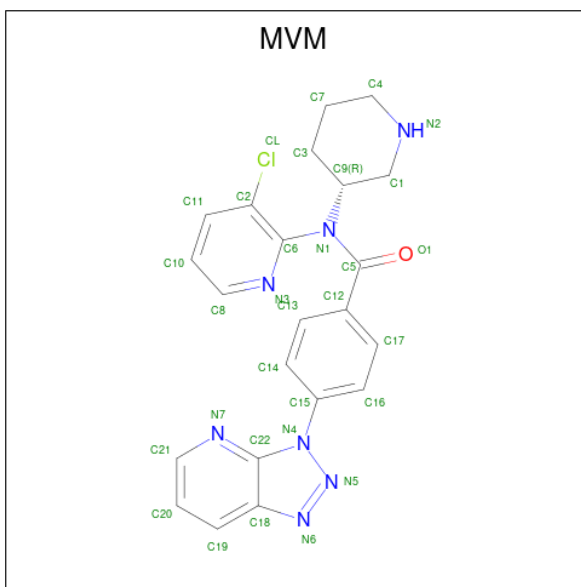
- Molecule 83 is a protein called Stalled Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	NC	25	Total	C	N	O	0	0
			177	121	28	28		

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

Mol	Chain	Residues	Atoms		AltConf
84	L5	145	Total	Mg	0
			145	145	
84	L7	5	Total	Mg	0
			5	5	
84	L8	2	Total	Mg	0
			2	2	
84	S2	35	Total	Mg	0
			35	35	
84	Bv	2	Total	Mg	0
			2	2	
84	k	1	Total	Mg	0
			1	1	

- Molecule 85 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (CCD ID: MVM) (formula: C₂₂H₂₀ClN₇O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
85	L5	1	Total	C	Cl	N	O	0
			31	22	1	7	1	

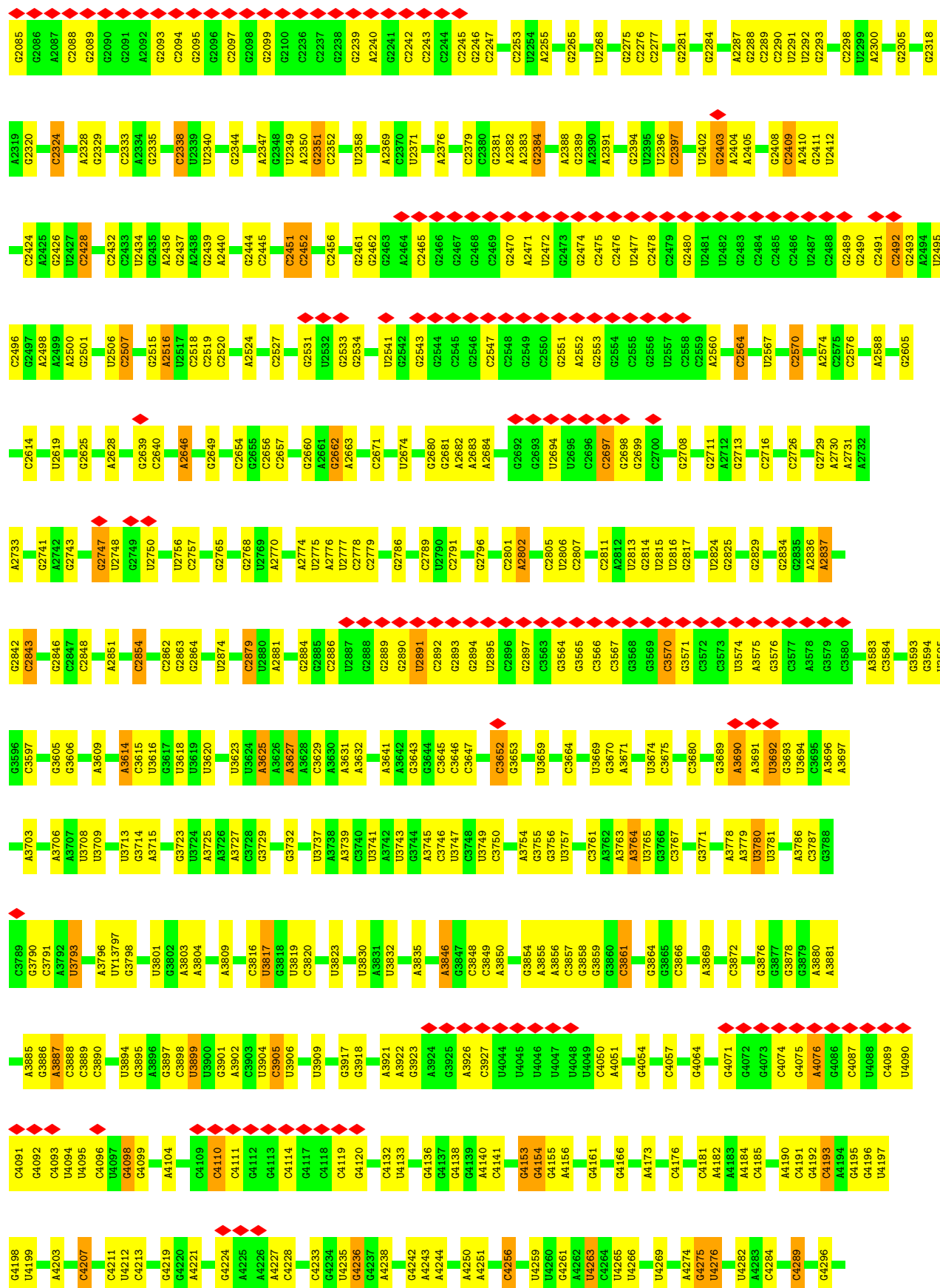
- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

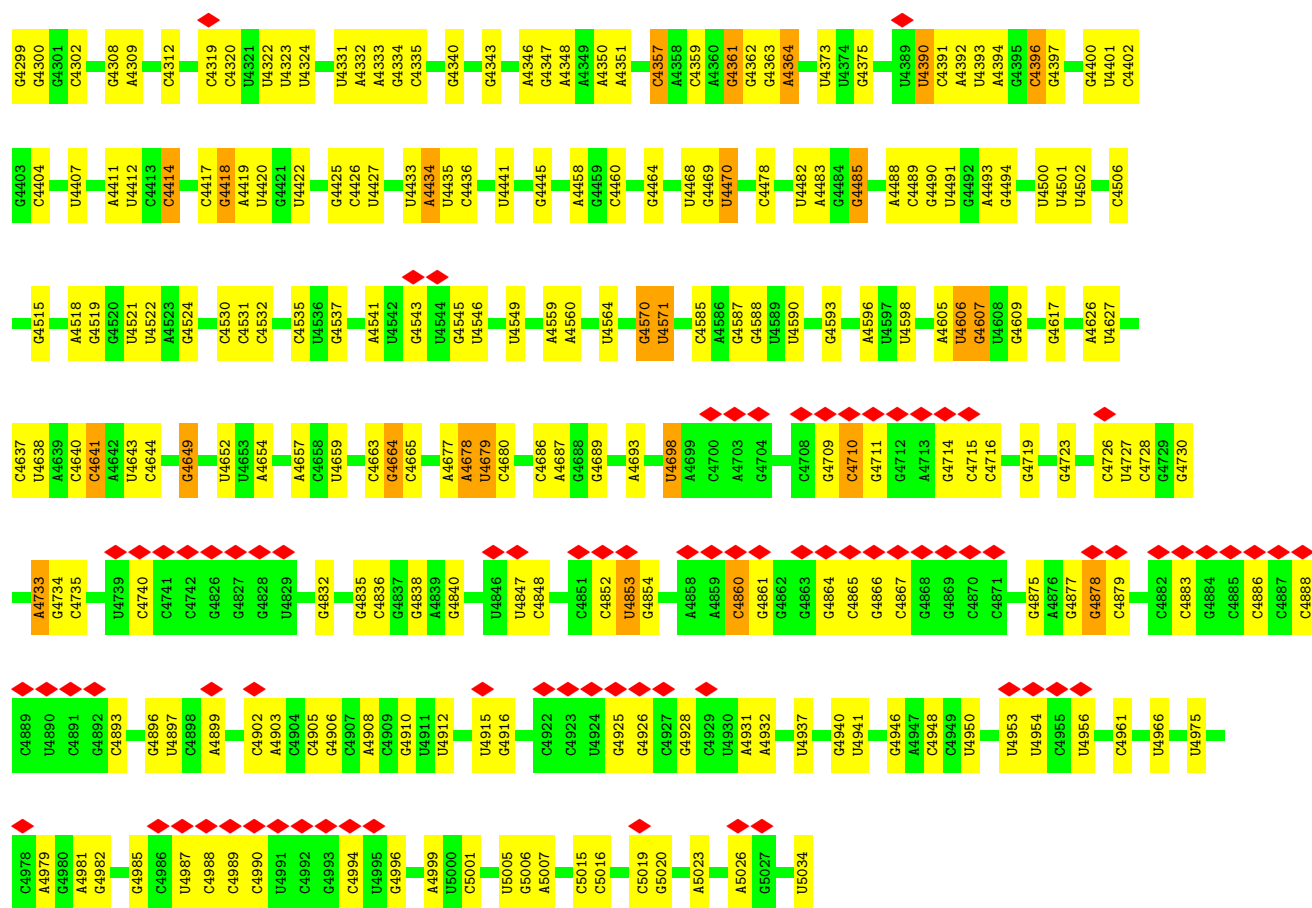
Mol	Chain	Residues	Atoms		AltConf
86	Lg	1	Total	Zn	0
			1	1	
86	Lj	1	Total	Zn	0
			1	1	
86	Lm	1	Total	Zn	0
			1	1	
86	Lo	1	Total	Zn	0
			1	1	
86	Lp	1	Total	Zn	0
			1	1	
86	Sa	1	Total	Zn	0
			1	1	
86	Sd	1	Total	Zn	0
			1	1	
86	Sf	1	Total	Zn	0
			1	1	

- Molecule 87 is POTASSIUM ION (CCD ID: K) (formula: K).

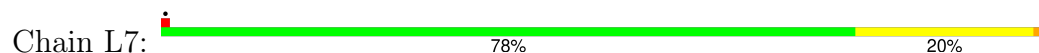
Mol	Chain	Residues	Atoms		AltConf
87	Bv	2	Total	K	0
			2	2	



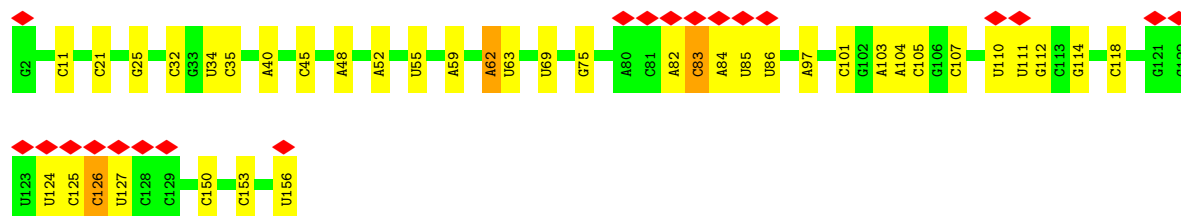
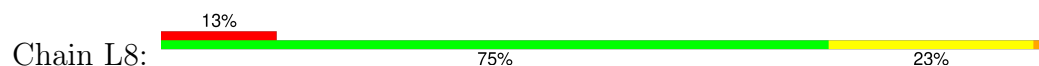




• Molecule 4: 5S rRNA

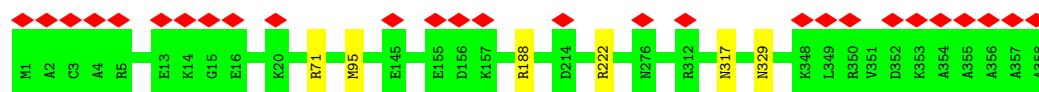


• Molecule 5: 5.8S rRNA

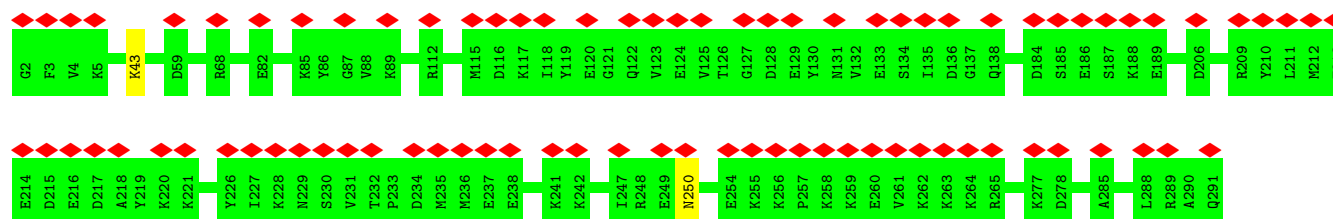


• Molecule 6: 60S ribosomal protein L4





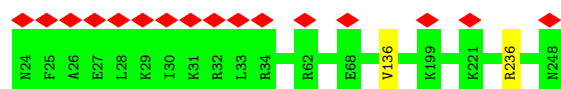
• Molecule 7: 60S ribosomal protein L5



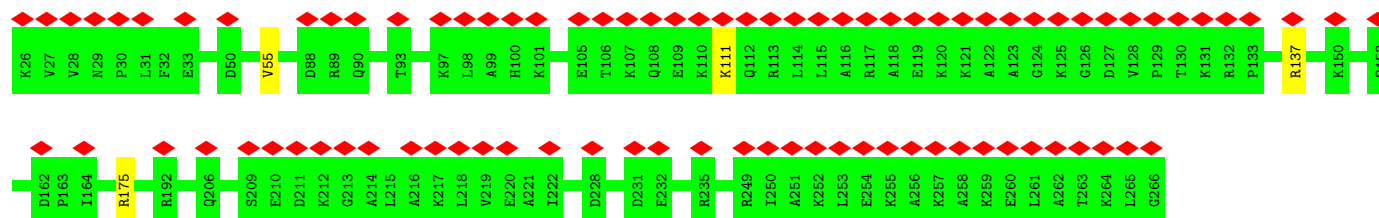
• Molecule 8: 60S ribosomal protein L6



• Molecule 9: 60S ribosomal protein L7

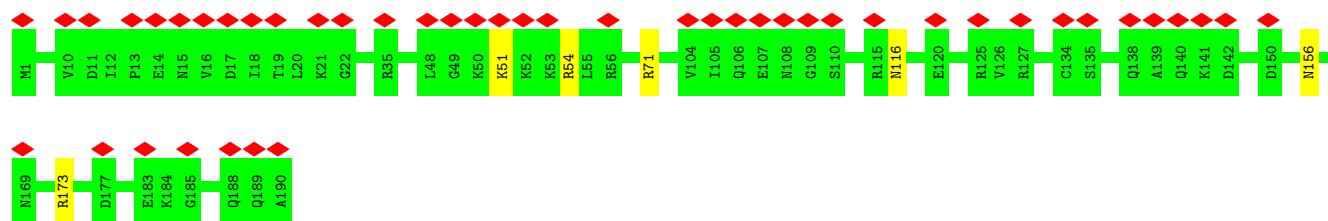


• Molecule 10: 60S ribosomal protein L7a



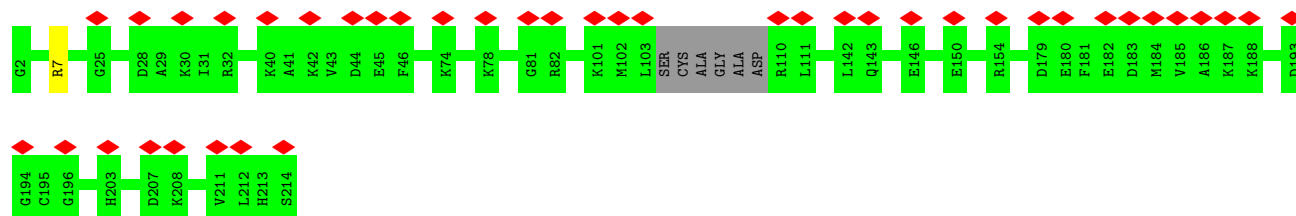
• Molecule 11: 60S ribosomal protein L9





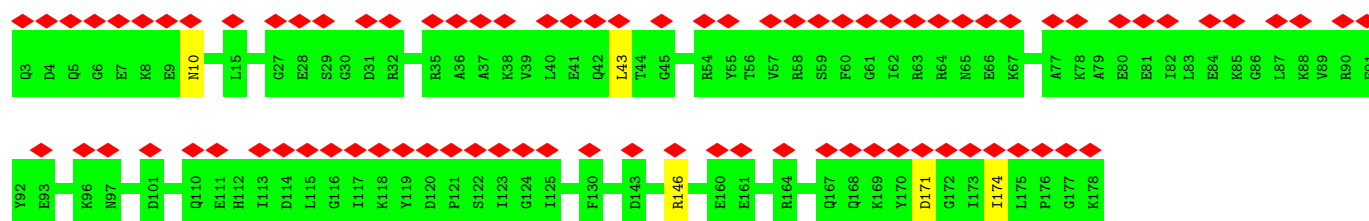
- Molecule 12: 60S ribosomal protein L10-like

Chain LI: 19% 97%



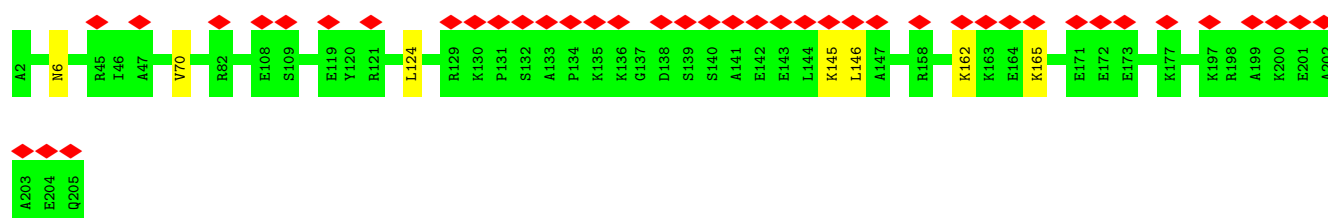
- Molecule 13: 60S ribosomal protein L11

Chain LJ: 48% 97%



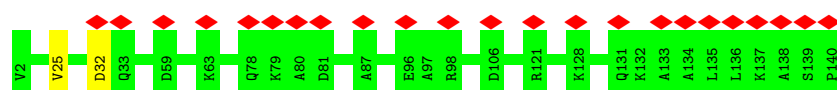
- Molecule 14: 60S ribosomal protein L13

Chain LL: 21% 97%



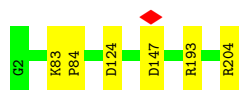
- Molecule 15: 60S ribosomal protein L14

Chain LM: 17% 99%



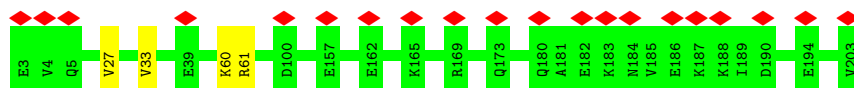
- Molecule 16: 60S ribosomal protein L15

Chain LN:  97%



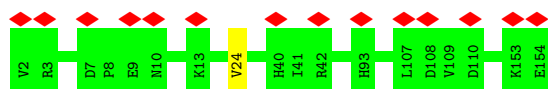
- Molecule 17: 60S ribosomal protein L13a

Chain LO:  98%



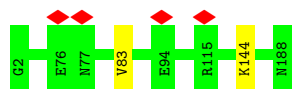
- Molecule 18: 60S ribosomal protein L17

Chain LP:  99%



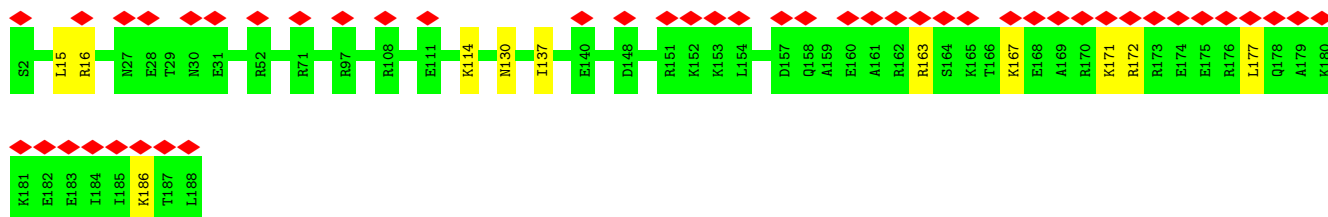
- Molecule 19: 60S ribosomal protein L18

Chain LQ:  99%



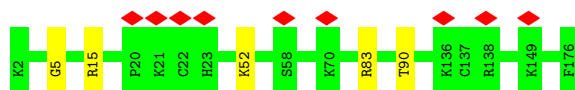
- Molecule 20: 60S ribosomal protein L19

Chain LR:  94% 6%



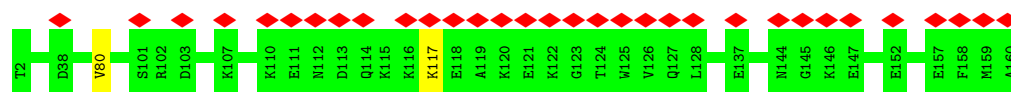
- Molecule 21: 60S ribosomal protein L18a

Chain LS:  97%



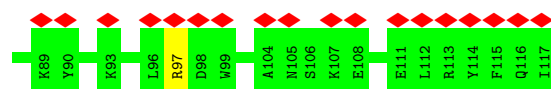
- Molecule 22: 60S ribosomal protein L21

Chain LT:  99%



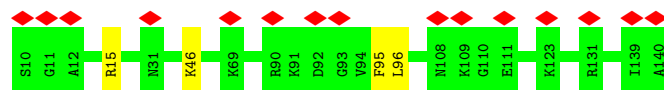
- Molecule 23: Heparin-binding protein HBp15

Chain LU: 72% 99%



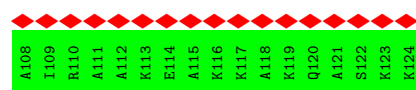
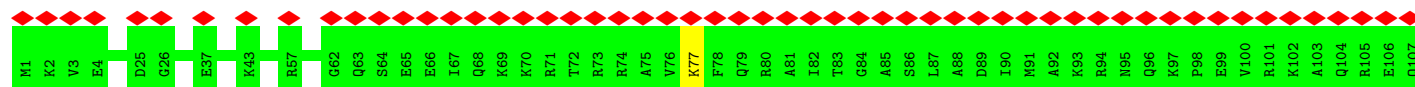
- Molecule 24: 60S ribosomal protein L23

Chain LV: 11% 97%



- Molecule 25: 60S ribosomal protein L24

Chain LW: 58% 99%



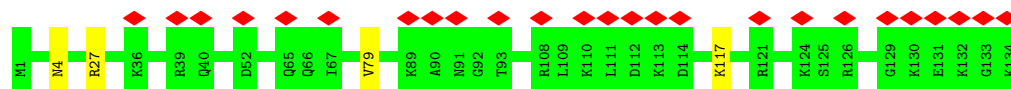
- Molecule 26: 60S ribosomal protein L23a

Chain LX: 23% 99%

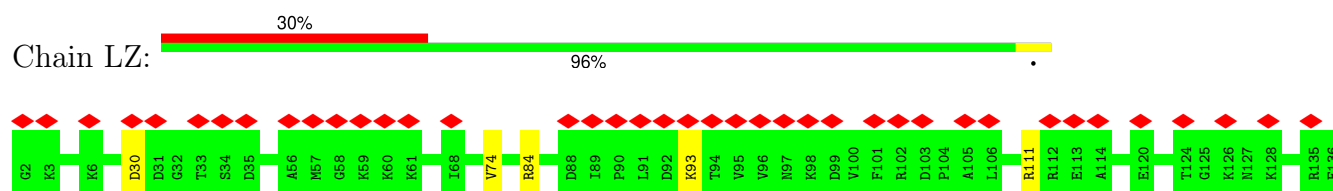


- Molecule 27: 60S ribosomal protein L26

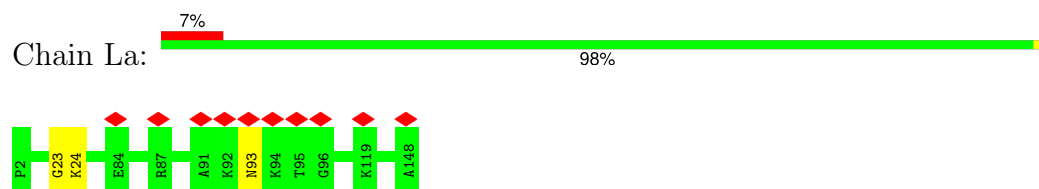
Chain LY: 19% 97%



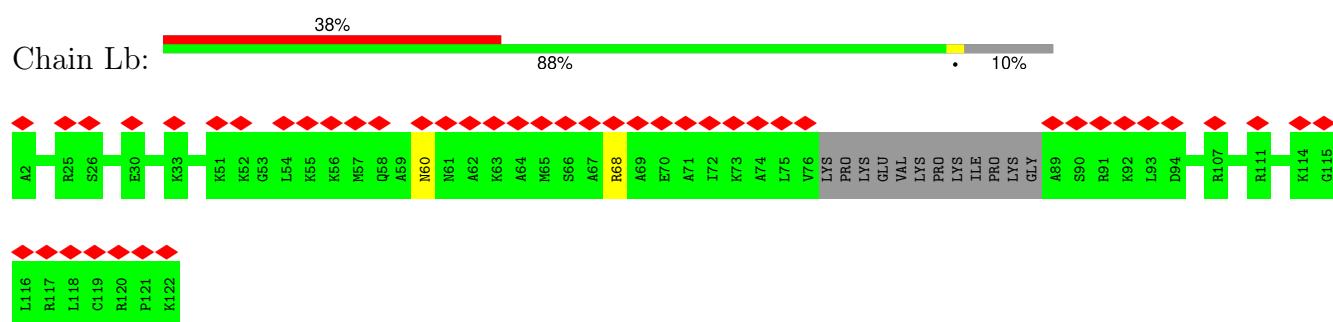
- Molecule 28: 60S ribosomal protein L27



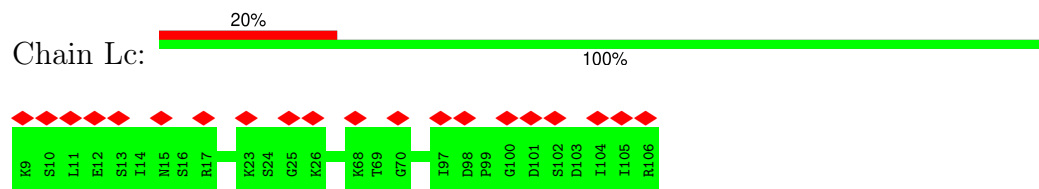
- Molecule 29: 60S ribosomal protein L27a



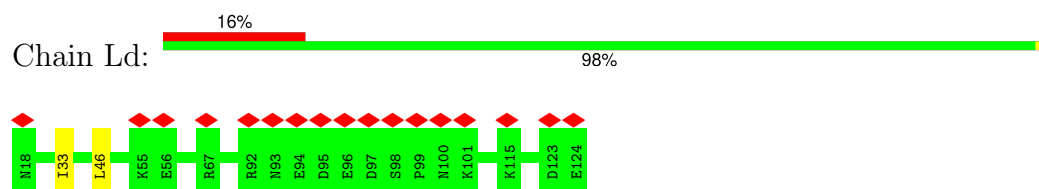
- Molecule 30: 60S ribosomal protein L29



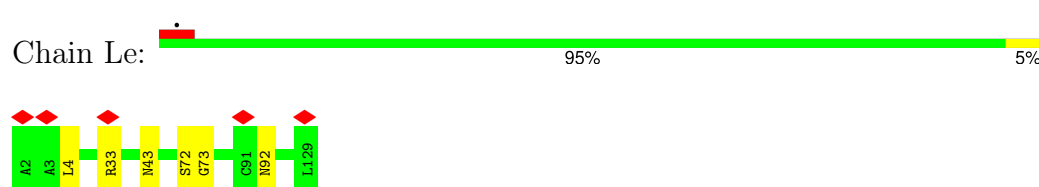
- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31

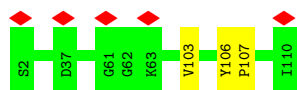


- Molecule 33: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L35a

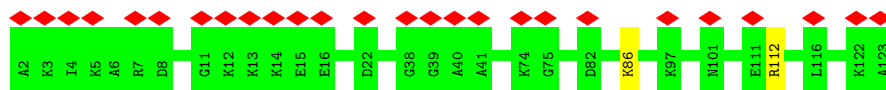




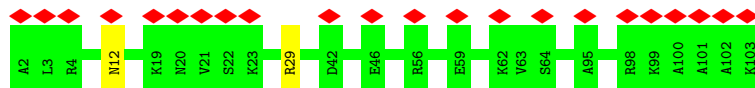
- Molecule 35: 60S ribosomal protein L34



- Molecule 36: 60S ribosomal protein L35



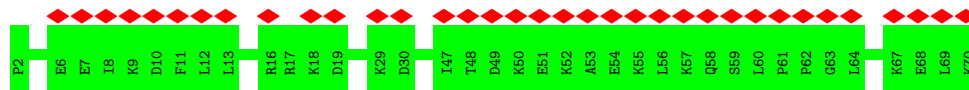
- Molecule 37: 60S ribosomal protein L36



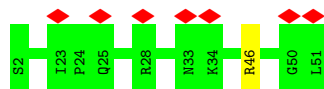
- Molecule 38: 60S ribosomal protein L37



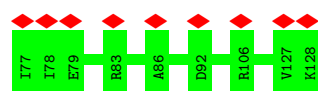
- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39



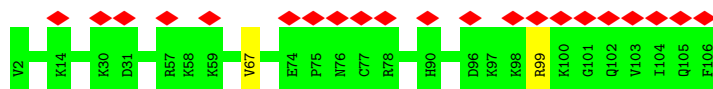
- Molecule 41: 60S ribosomal protein L40



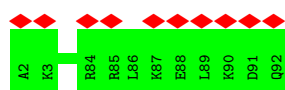
- Molecule 42: 60S ribosomal protein L41



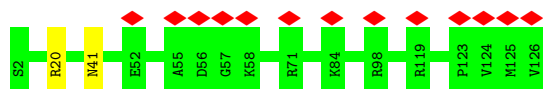
- Molecule 43: 60S ribosomal protein L36a



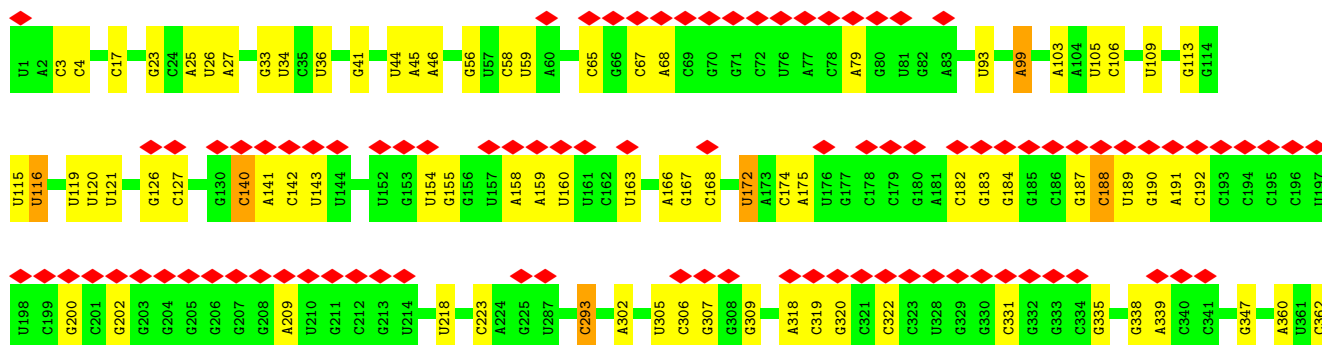
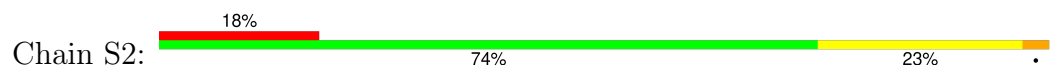
- Molecule 44: 60S ribosomal protein L37a

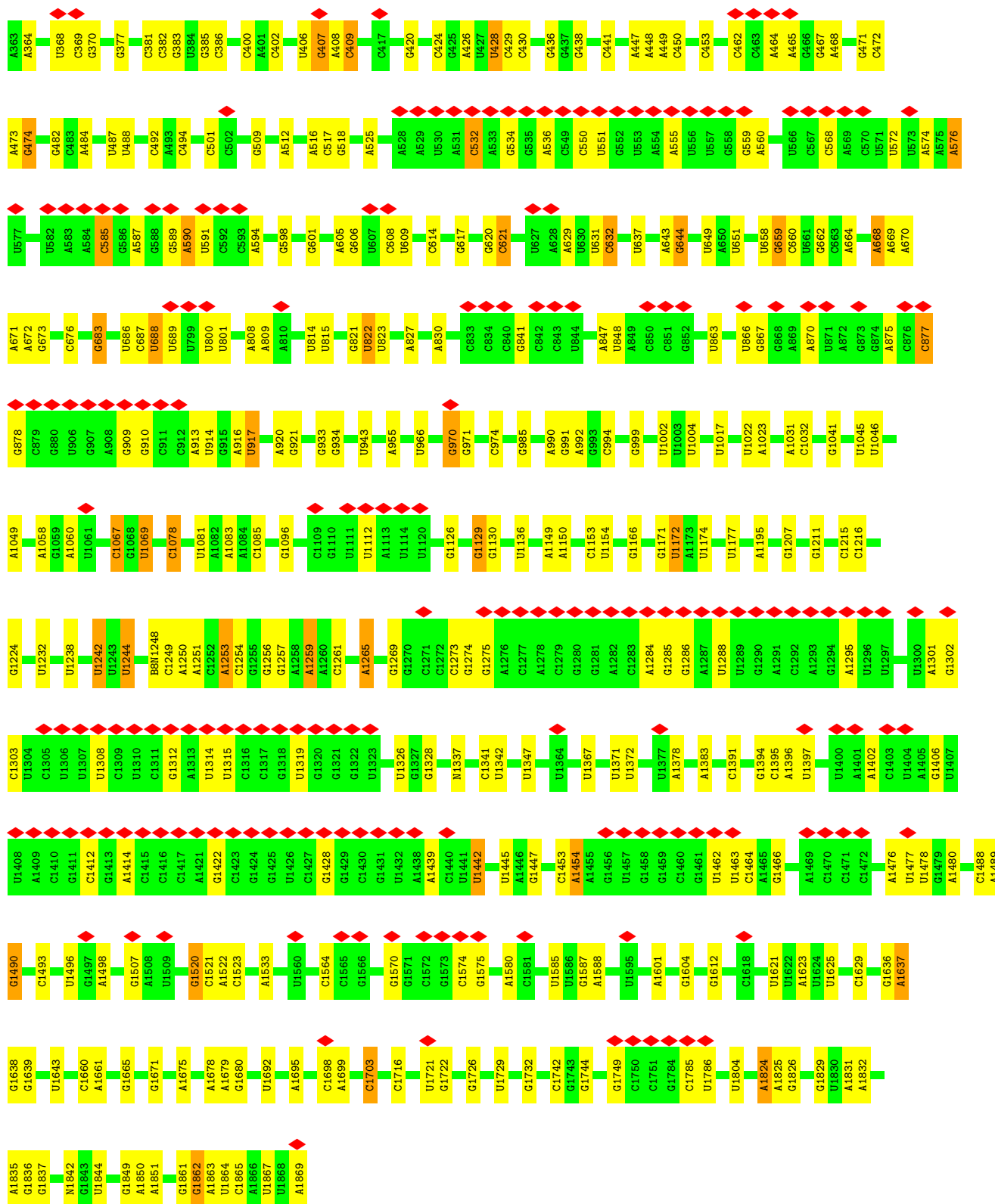


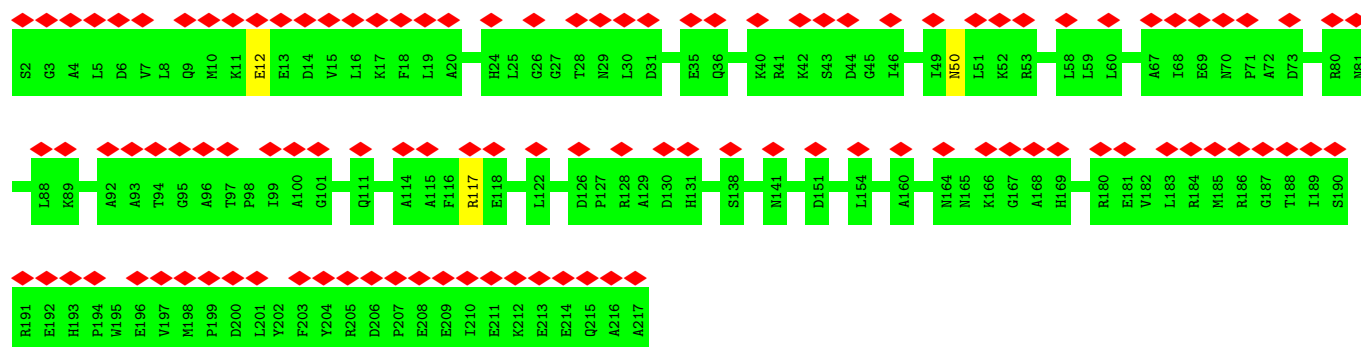
- Molecule 45: 60S ribosomal protein L28



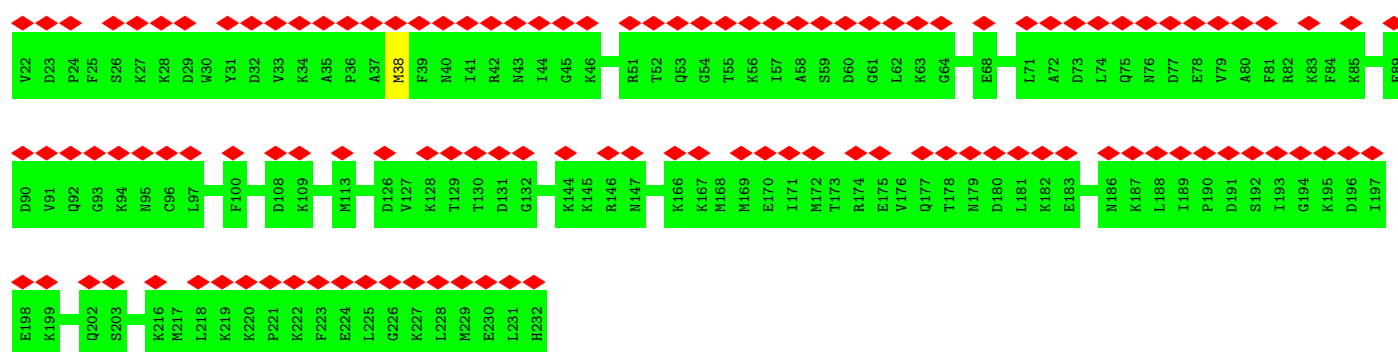
- Molecule 46: 18S rRNA



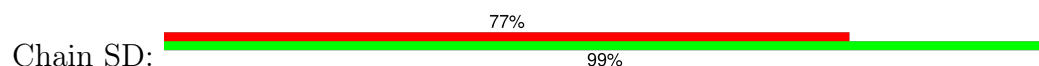




• Molecule 48: 40S ribosomal protein S3a

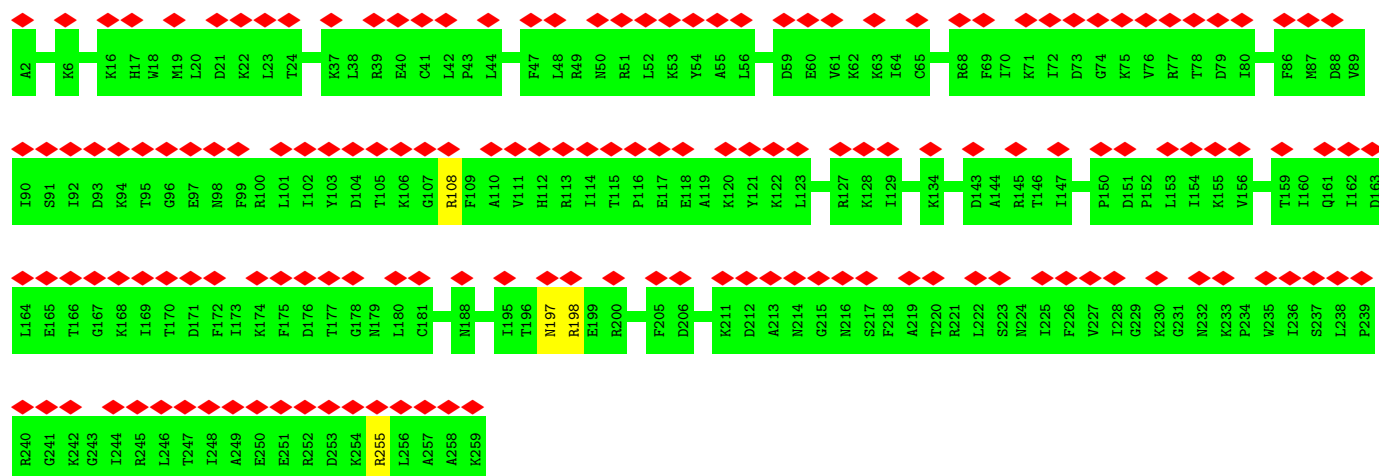


• Molecule 49: 40S ribosomal protein S3

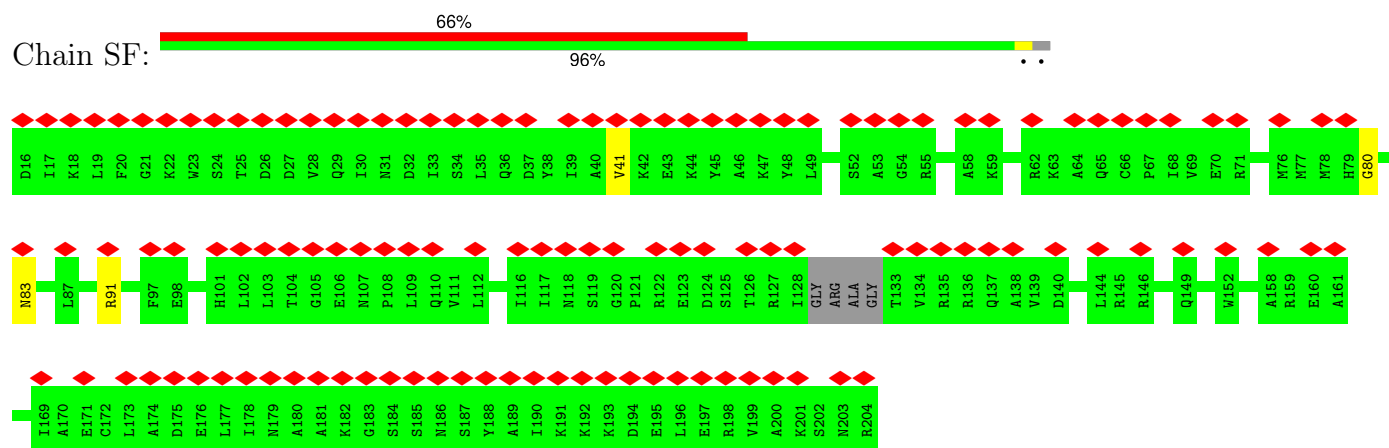


• Molecule 50: 40S ribosomal protein S4, X isoform

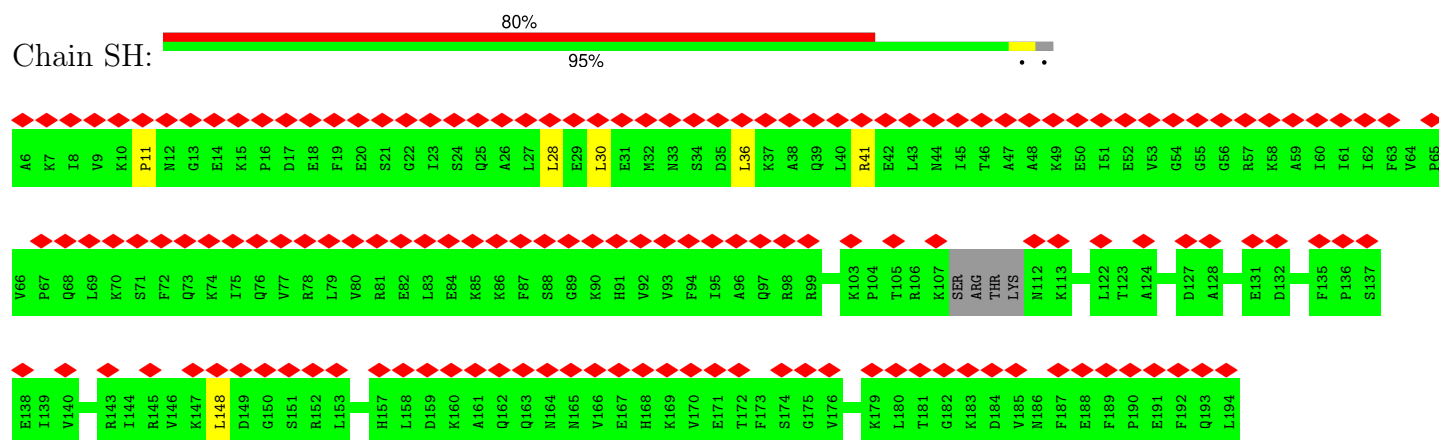




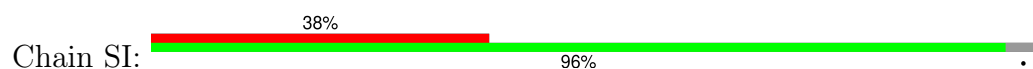
- Molecule 51: 40S ribosomal protein S5

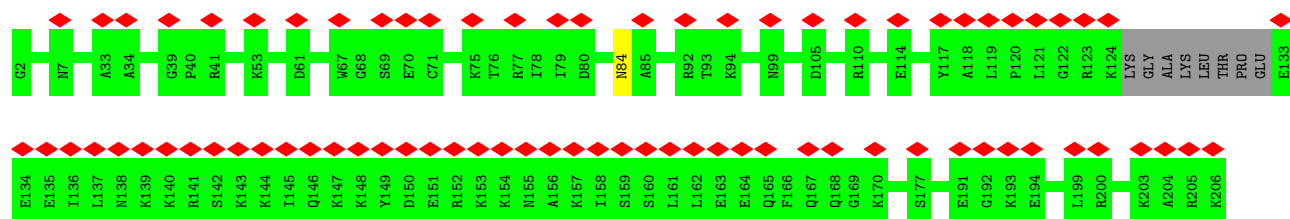


- Molecule 52: 40S ribosomal protein S7



- Molecule 53: 40S ribosomal protein S8

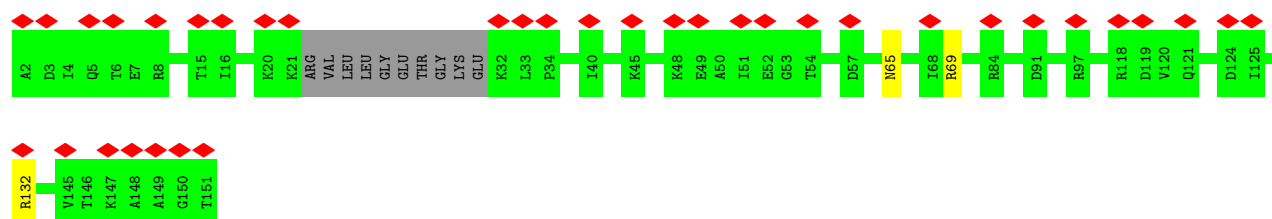
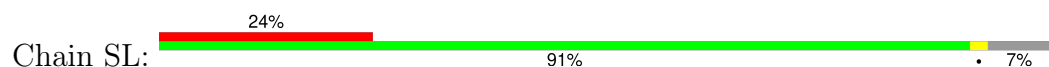




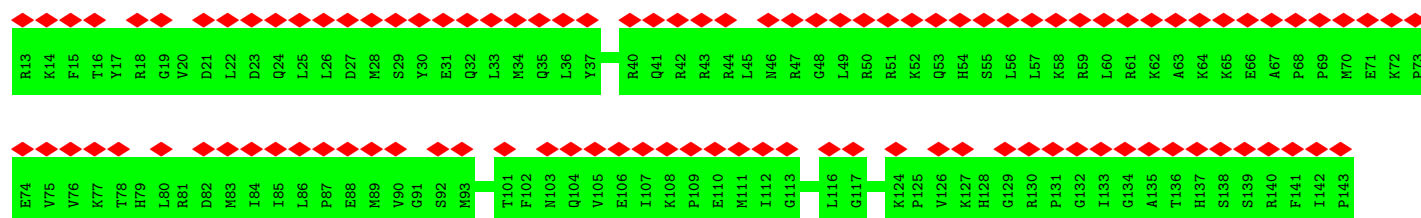
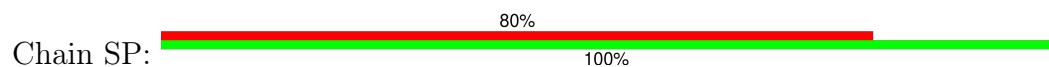
• Molecule 54: 40S ribosomal protein S10



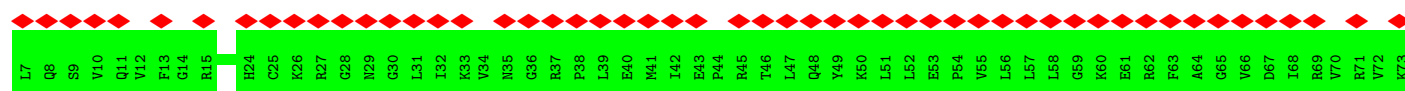
• Molecule 55: 40S ribosomal protein S11

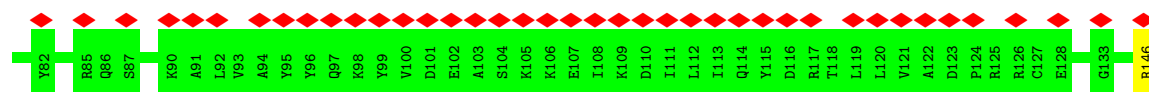


• Molecule 56: 40S ribosomal protein S15



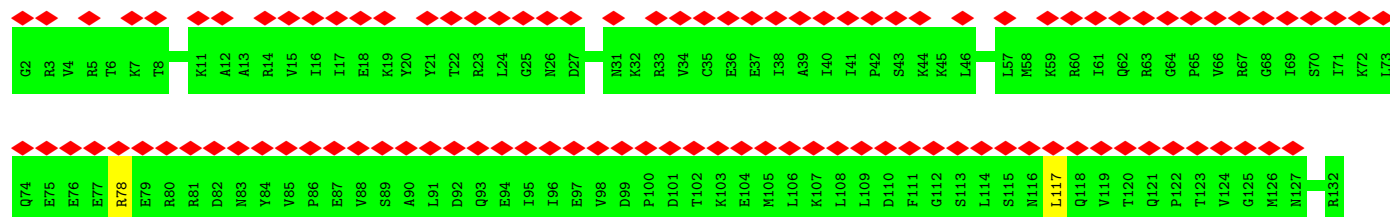
• Molecule 57: 40S ribosomal protein S16





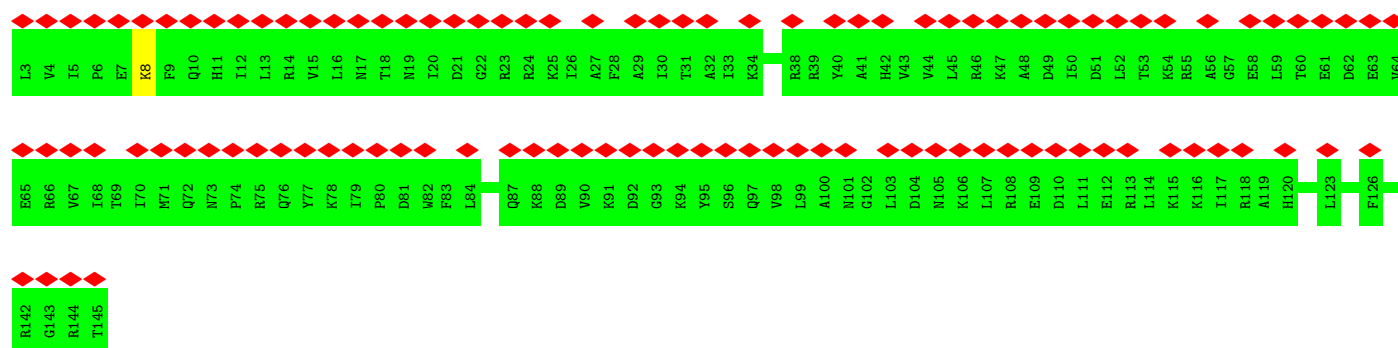
- Molecule 58: 40S ribosomal protein S17

Chain SR: 79% 98%



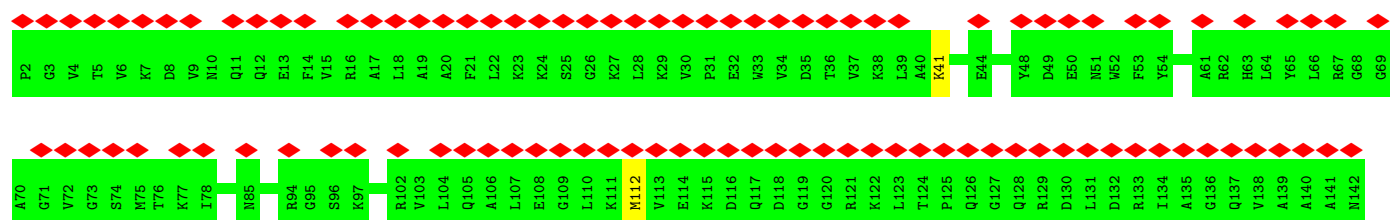
- Molecule 59: 40S ribosomal protein S18

Chain SS: 75% 99%



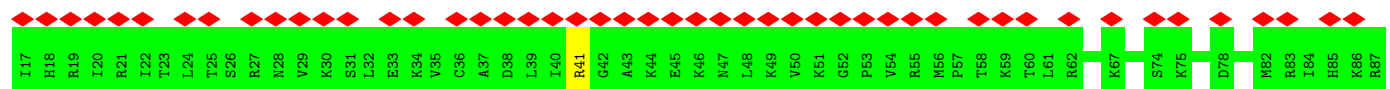
- Molecule 60: 40S ribosomal protein S19

Chain ST: 71% 99%



- Molecule 61: 40S ribosomal protein S20

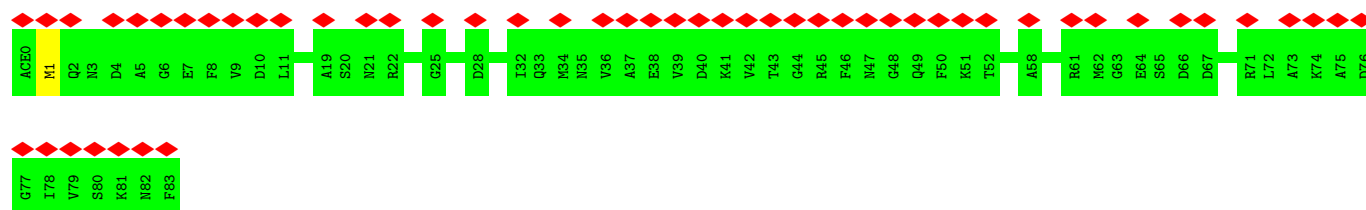
Chain SU: 77% 99%





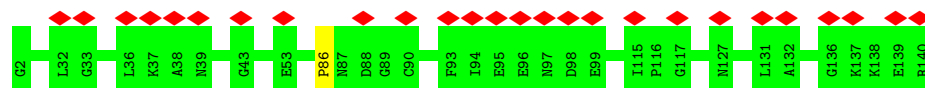
- Molecule 62: 40S ribosomal protein S21

Chain SV: 63% 99%



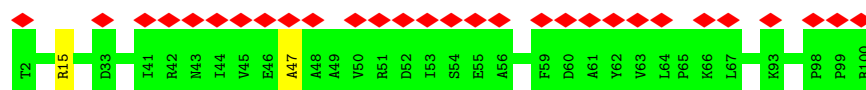
- Molecule 63: 40S ribosomal protein S23

Chain SX: 19% 99%



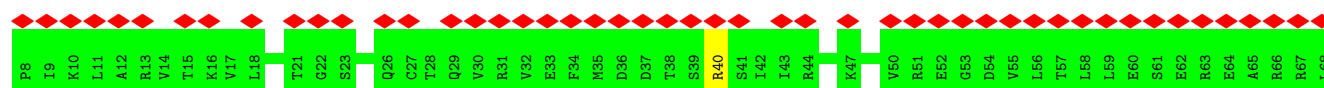
- Molecule 64: 40S ribosomal protein S26

Chain Sa: 29% 98%



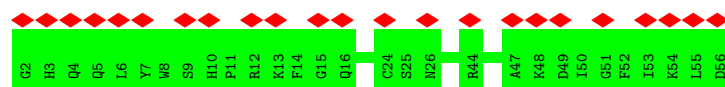
- Molecule 65: 40S ribosomal protein S28

Chain Sc: 80% 98%



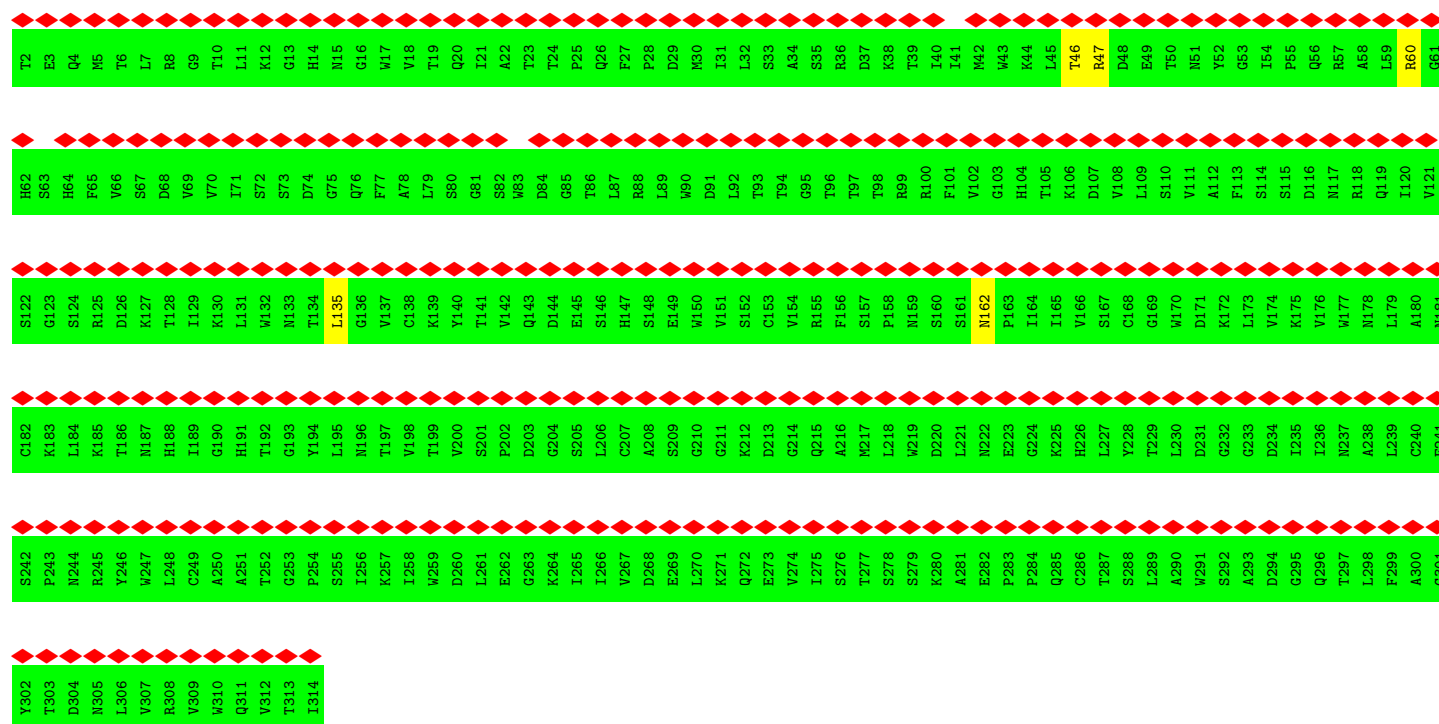
- Molecule 66: 40S ribosomal protein S29

Chain Sd: 42% 100%

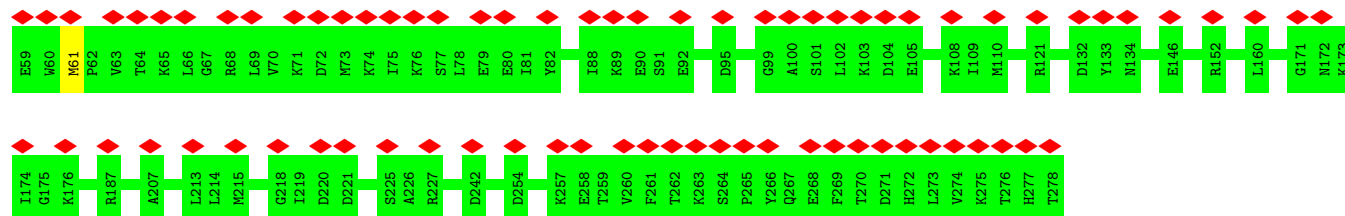


- Molecule 67: Receptor of activated protein C kinase 1

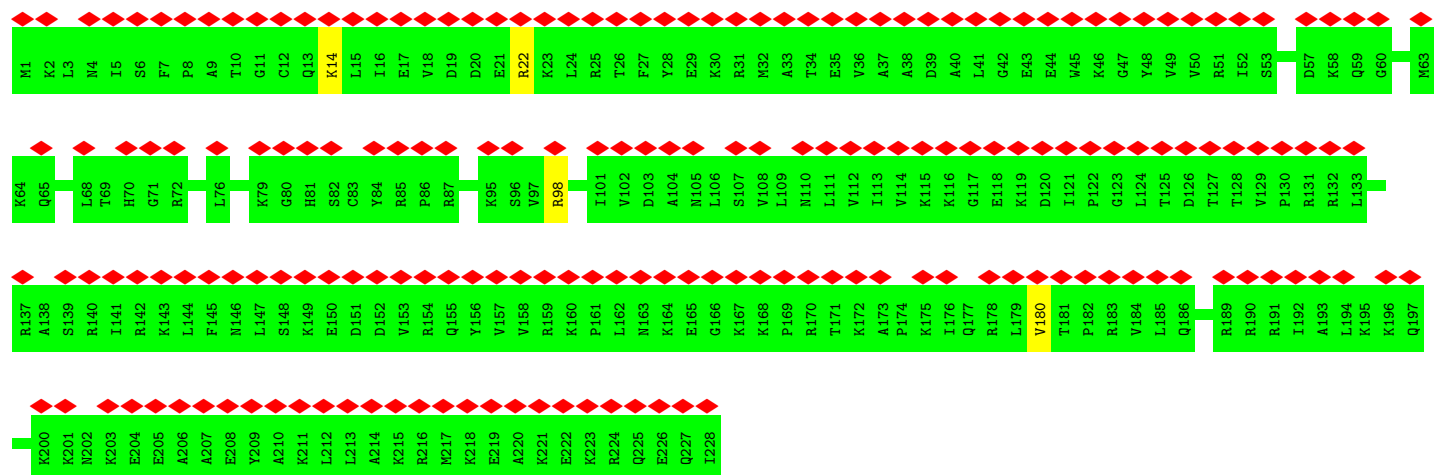
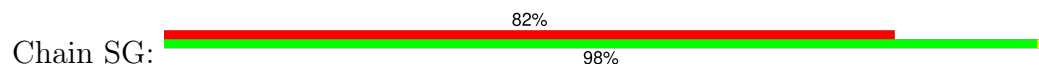
Chain Sg: 99% 98%



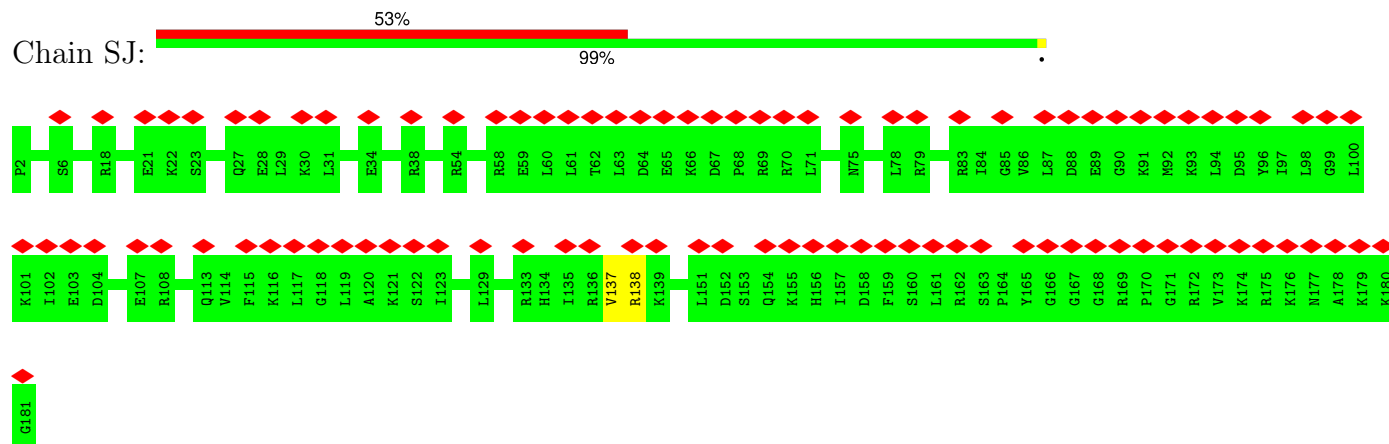
• Molecule 68: 40S ribosomal protein S2



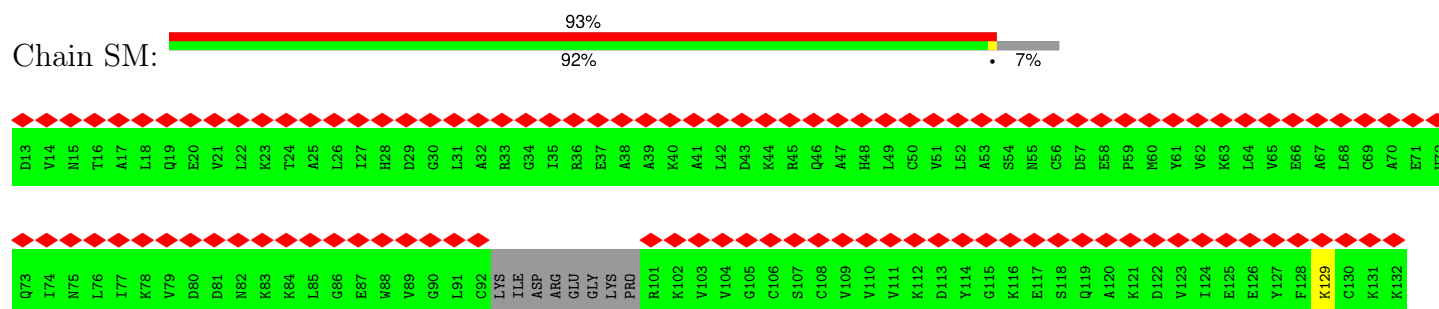
• Molecule 69: 40S ribosomal protein S6



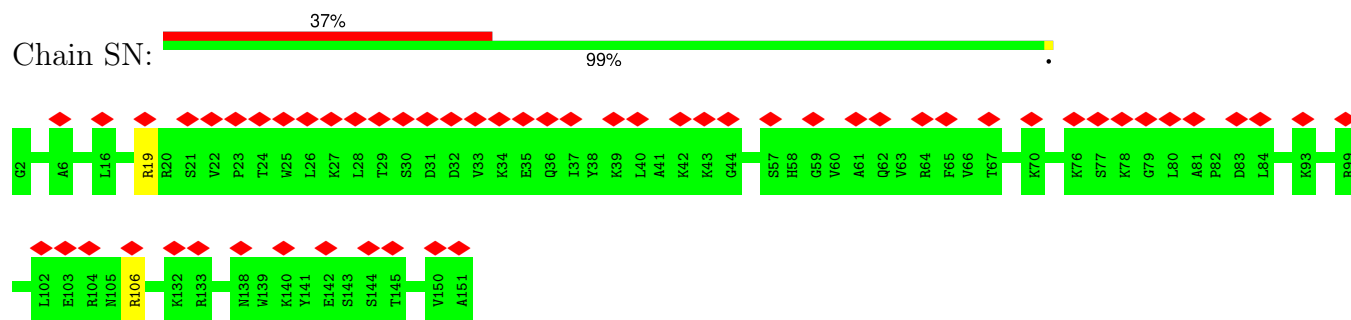
- Molecule 70: 40S ribosomal protein S9



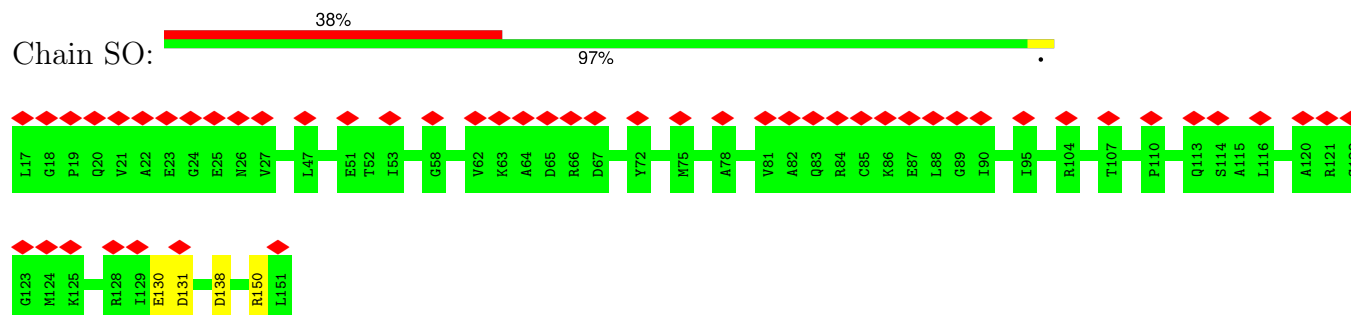
- Molecule 71: 40S ribosomal protein S12



- Molecule 72: 40S ribosomal protein S13

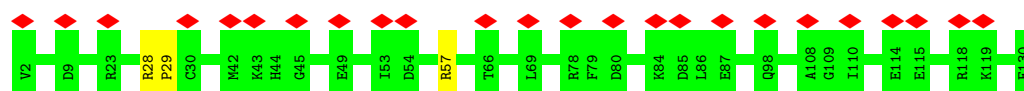


- Molecule 73: 40S ribosomal protein S14

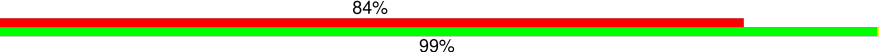


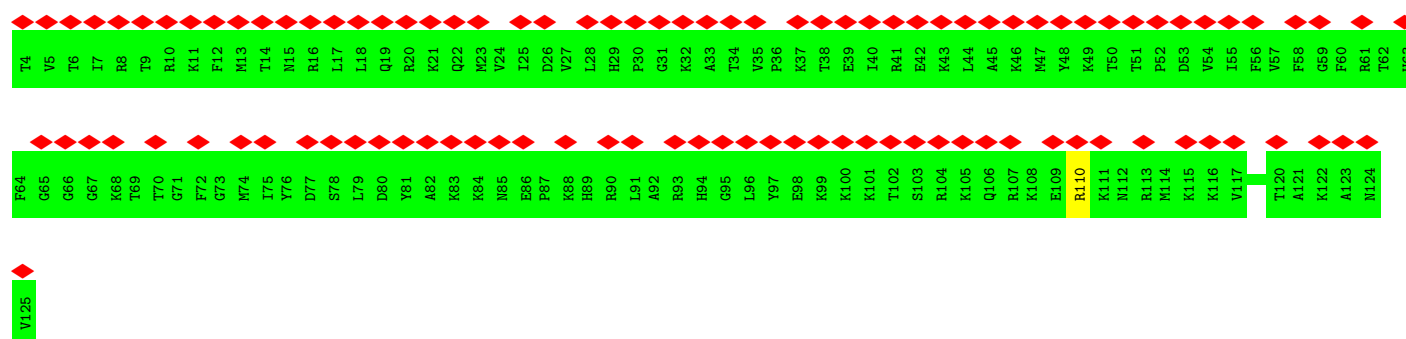
- Molecule 74: 40S ribosomal protein S15a

Chain SW: 



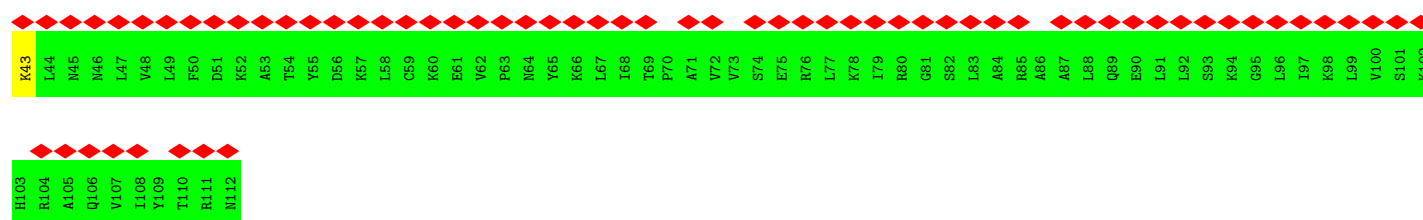
- Molecule 75: 40S ribosomal protein S24

Chain SY: 



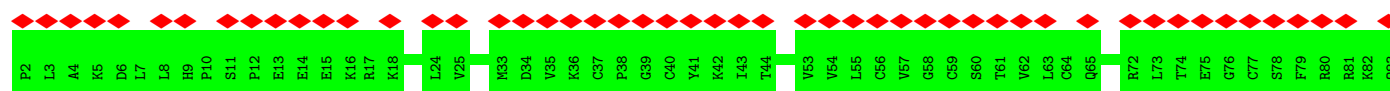
- Molecule 76: 40S ribosomal protein S25

Chain SZ: 



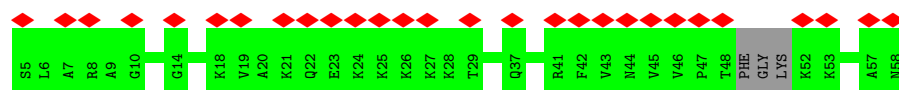
- Molecule 77: 40S ribosomal protein S27

Chain Sb: 



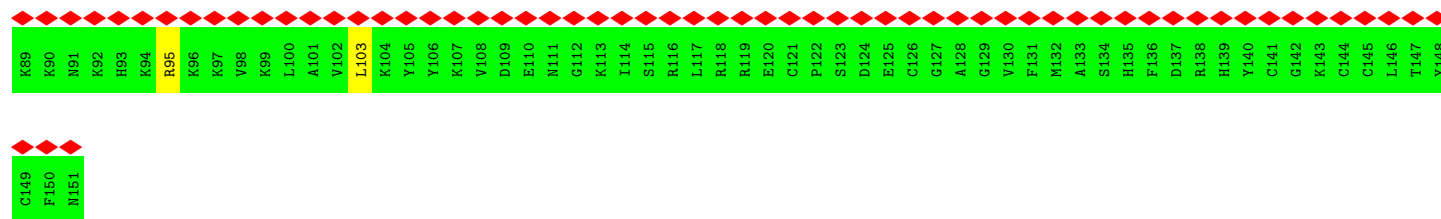
- Molecule 78: 40S ribosomal protein S30

Chain Se: 

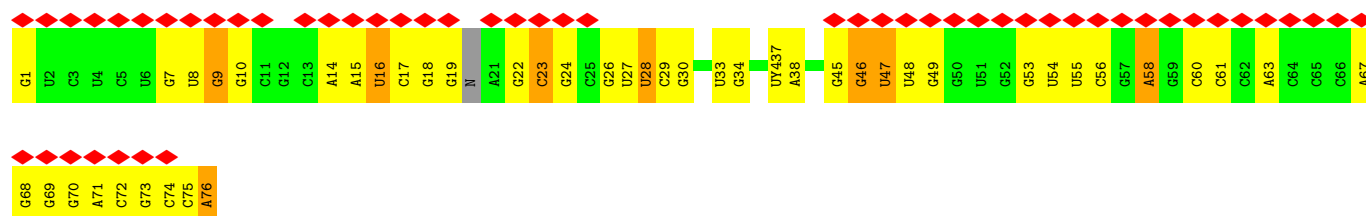


- Molecule 79: 40S ribosomal protein S27a

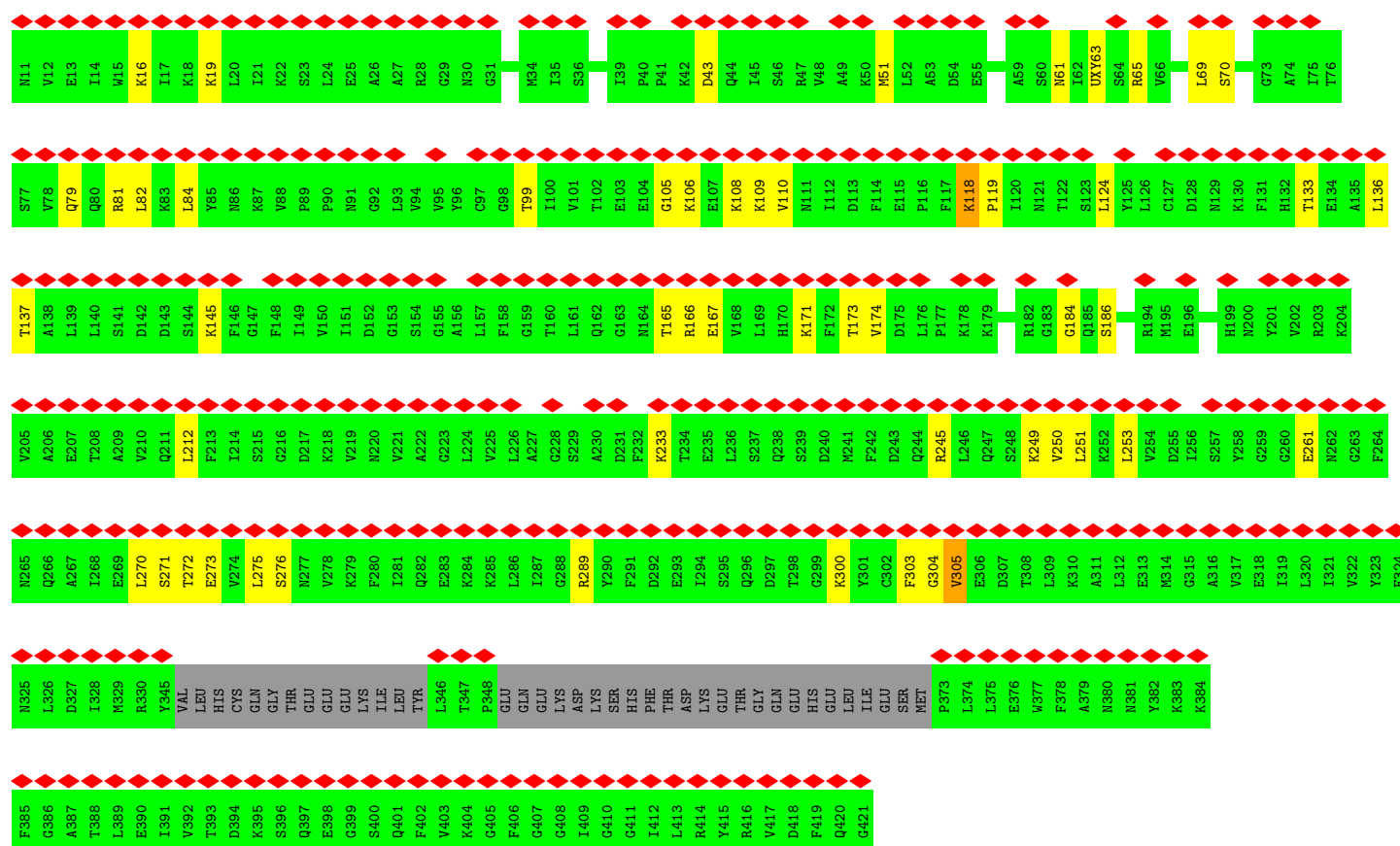
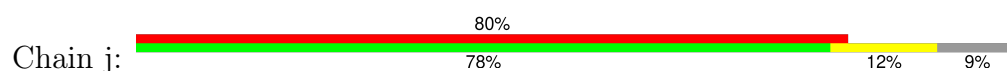
Chain Sf: 



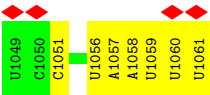
• Molecule 80: P-tRNA



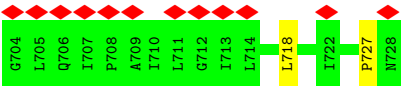
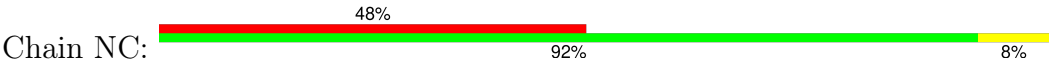
• Molecule 81: Eukaryotic peptide chain release factor subunit 1



• Molecule 82: mRNA



● Molecule 83: Stalled Nascent chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57324	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.260	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	494.5, 494.5, 494.5	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.15, 1.15, 1.15	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, A2M, 1MG, PSU, M2G, OMC, H2U, UXY, IAS, MEQ, OMU, UY1, 4AC, ACE, UY4, UR3, 5MC, MG, 1MA, 6MZ, ZN, MVM, 2MG, K, G7M, MA6, B8N, MLZ

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	LA	0.80	1/1936 (0.1%)	0.75	0/2596
2	LB	0.74	0/3265	0.70	1/4370 (0.0%)
3	L5	1.67	159/81383 (0.2%)	1.48	579/126935 (0.5%)
4	L7	1.57	2/2862 (0.1%)	1.17	14/4459 (0.3%)
5	L8	1.55	1/3612 (0.0%)	1.18	17/5627 (0.3%)
6	LC	0.72	0/2898	0.66	0/3891
7	LD	0.67	0/2403	0.61	0/3219
8	LE	0.61	0/1942	0.68	1/2606 (0.0%)
9	LF	0.77	0/1916	0.72	1/2553 (0.0%)
10	LG	0.66	1/1971 (0.1%)	0.70	0/2651
11	LH	0.67	0/1537	0.67	0/2066
12	LI	0.65	0/1716	0.63	0/2291
13	LJ	0.62	0/1433	0.76	2/1915 (0.1%)
14	LL	0.67	0/1680	0.72	1/2249 (0.0%)
15	LM	0.67	0/1161	0.66	0/1554
16	LN	0.86	0/1746	0.78	1/2338 (0.0%)
17	LO	0.80	2/1682 (0.1%)	0.71	0/2250
18	LP	0.75	0/1268	0.68	0/1701
19	LQ	0.77	0/1537	0.71	0/2052
20	LR	0.64	0/1582	0.68	2/2091 (0.1%)
21	LS	0.75	0/1493	0.63	0/2003
22	LT	0.76	0/1326	0.64	0/1770
23	LU	0.54	0/839	0.71	0/1126
24	LV	0.70	0/993	0.75	1/1332 (0.1%)
25	LW	0.61	0/1030	0.65	0/1364
26	LX	0.63	0/1002	0.63	1/1345 (0.1%)
27	LY	0.70	0/1132	0.71	0/1504
28	LZ	0.70	0/1130	0.69	1/1507 (0.1%)
29	La	0.79	0/1191	0.68	0/1591
30	Lb	0.60	0/895	0.64	0/1182
31	Lc	0.71	0/774	0.71	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.71	0/903	0.69	2/1216 (0.2%)
33	Le	0.83	2/1071 (0.2%)	0.68	0/1429
34	Lf	0.82	0/895	0.75	0/1198
35	Lg	0.72	0/916	0.70	0/1220
36	Lh	0.60	0/1023	0.63	0/1351
37	Li	0.57	0/843	0.60	0/1115
38	Lj	0.78	0/731	0.75	1/966 (0.1%)
39	Lk	0.58	0/575	0.66	0/761
40	Ll	0.69	0/454	0.67	0/599
41	Lm	0.65	0/425	0.61	0/561
42	Ln	0.69	0/231	0.92	2/294 (0.7%)
43	Lo	0.72	1/887 (0.1%)	0.71	0/1170
44	Lp	0.75	0/718	0.65	0/953
45	Lr	0.71	0/1017	0.74	0/1364
46	S2	1.97	10/36169 (0.0%)	1.10	107/56356 (0.2%)
47	SA	0.43	0/1742	0.56	0/2367
48	SB	0.49	0/1745	0.58	0/2335
49	SD	0.39	0/1773	0.55	0/2387
50	SE	0.44	0/2092	0.57	0/2816
51	SF	0.41	0/1491	0.55	0/2003
52	SH	0.41	0/1512	0.65	4/2025 (0.2%)
53	SI	0.52	0/1651	0.59	0/2200
54	SK	0.39	0/823	0.59	1/1111 (0.1%)
55	SL	0.59	0/1164	0.61	0/1558
56	SP	0.40	0/1097	0.55	0/1467
57	SQ	0.40	0/1134	0.57	0/1517
58	SR	0.37	0/1078	0.61	1/1447 (0.1%)
59	SS	0.39	0/1202	0.58	0/1610
60	ST	0.41	0/1113	0.56	0/1493
61	SU	0.36	0/808	0.56	0/1085
62	SV	0.45	0/644	0.57	0/862
63	SX	0.51	0/1097	0.61	0/1464
64	Sa	0.52	0/805	0.60	0/1079
65	Sc	0.37	0/481	0.56	0/643
66	Sd	0.49	0/470	0.56	0/623
67	Sg	0.34	0/2493	0.63	1/3394 (0.0%)
68	SC	0.49	0/1755	0.61	0/2371
69	SG	0.38	0/1871	0.58	1/2492 (0.0%)
70	SJ	0.40	0/1524	0.53	0/2035
71	SM	0.29	0/868	0.56	0/1165
72	SN	0.50	0/1232	0.55	0/1656
73	SO	0.51	0/1014	0.60	0/1358
74	SW	0.52	0/1051	0.58	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SY	0.40	0/1019	0.53	0/1354
76	SZ	0.39	0/565	0.59	0/759
77	Sb	0.45	0/653	0.55	0/876
78	Se	0.36	0/410	0.55	0/539
79	Sf	0.38	0/525	0.63	1/695 (0.1%)
80	Bv	0.56	2/1527 (0.1%)	0.76	1/2373 (0.0%)
81	j	0.35	0/2954	0.70	5/3968 (0.1%)
82	k	0.29	0/300	0.67	0/463
83	NC	0.21	0/178	0.47	0/243
All	All	1.37	181/222054 (0.1%)	1.13	749/324968 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	LA	0	1
7	LD	0	1
8	LE	0	1
11	LH	0	1
13	LJ	0	1
21	LS	0	1
22	LT	0	1
23	LU	0	1
29	La	0	1
34	Lf	0	2
36	Lh	0	1
38	Lj	0	1
45	Lr	0	1
46	S2	1	0
52	SH	0	1
63	SX	0	1
70	SJ	0	1
74	SW	0	1
All	All	1	18

The worst 5 of 181 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	970	G	C6-N1	171.12	2.59	1.39
46	S2	970	G	N1-C2	140.33	2.50	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	970	G	N3-C4	134.05	2.29	1.35
46	S2	970	G	C2-N3	117.01	2.26	1.32
46	S2	970	G	C5-C4	116.58	2.19	1.38

The worst 5 of 749 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3690	A	N1-C2-N3	-237.89	10.36	129.30
3	L5	3690	A	C2-N3-C4	85.13	153.17	110.60
3	L5	3690	A	C6-N1-C2	73.75	162.85	118.60
3	L5	3690	A	C4-C5-C6	-44.98	94.51	117.00
46	S2	970	G	C4-C5-N7	-37.55	95.78	110.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
46	S2	1248	B8N	C33

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	LA	246	LEU	Peptide
7	LD	43	LYS	Peptide
8	LE	176	THR	Peptide
11	LH	173	ARG	Peptide
13	LJ	10	ASN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LA	246/248 (99%)	229 (93%)	17 (7%)	0	100	100
2	LB	394/396 (100%)	379 (96%)	15 (4%)	0	100	100
6	LC	355/358 (99%)	340 (96%)	14 (4%)	1 (0%)	37	67
7	LD	288/290 (99%)	275 (96%)	13 (4%)	0	100	100
8	LE	232/247 (94%)	206 (89%)	26 (11%)	0	100	100
9	LF	224/225 (100%)	212 (95%)	12 (5%)	0	100	100
10	LG	240/241 (100%)	223 (93%)	17 (7%)	0	100	100
11	LH	188/190 (99%)	171 (91%)	17 (9%)	0	100	100
12	LI	203/213 (95%)	191 (94%)	12 (6%)	0	100	100
13	LJ	174/176 (99%)	154 (88%)	20 (12%)	0	100	100
14	LL	202/204 (99%)	182 (90%)	20 (10%)	0	100	100
15	LM	137/139 (99%)	127 (93%)	9 (7%)	1 (1%)	19	48
16	LN	201/203 (99%)	193 (96%)	5 (2%)	3 (2%)	8	29
17	LO	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
18	LP	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
19	LQ	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
20	LR	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
21	LS	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
22	LT	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
23	LU	99/101 (98%)	85 (86%)	14 (14%)	0	100	100
24	LV	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
25	LW	122/124 (98%)	108 (88%)	14 (12%)	0	100	100
26	LX	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
27	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
28	LZ	133/135 (98%)	120 (90%)	13 (10%)	0	100	100
29	La	145/147 (99%)	136 (94%)	8 (6%)	1 (1%)	19	48
30	Lb	105/121 (87%)	95 (90%)	10 (10%)	0	100	100
31	Lc	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
32	Ld	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
33	Le	126/128 (98%)	118 (94%)	7 (6%)	1 (1%)	16	44
34	Lf	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	14	42
35	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
38	Lj	85/86 (99%)	78 (92%)	6 (7%)	1 (1%)	11	34
39	Lk	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
40	Ll	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
41	Lm	49/52 (94%)	47 (96%)	2 (4%)	0	100	100
42	Ln	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
43	Lo	104/105 (99%)	99 (95%)	5 (5%)	0	100	100
44	Lp	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
45	Lr	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
47	SA	214/216 (99%)	199 (93%)	14 (6%)	1 (0%)	25	56
48	SB	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
49	SD	222/224 (99%)	210 (95%)	12 (5%)	0	100	100
50	SE	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
51	SF	181/189 (96%)	168 (93%)	12 (7%)	1 (1%)	22	51
52	SH	181/189 (96%)	167 (92%)	14 (8%)	0	100	100
53	SI	193/205 (94%)	185 (96%)	8 (4%)	0	100	100
54	SK	93/95 (98%)	83 (89%)	10 (11%)	0	100	100
55	SL	136/150 (91%)	130 (96%)	6 (4%)	0	100	100
56	SP	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
57	SQ	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
58	SR	129/131 (98%)	119 (92%)	10 (8%)	0	100	100
59	SS	141/143 (99%)	133 (94%)	8 (6%)	0	100	100
60	ST	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
61	SU	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
62	SV	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
63	SX	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
64	Sa	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	13	39
65	Sc	59/61 (97%)	54 (92%)	5 (8%)	0	100	100
66	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
67	Sg	311/313 (99%)	271 (87%)	40 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	SC	219/220 (100%)	212 (97%)	7 (3%)	0	100	100
69	SG	226/228 (99%)	212 (94%)	14 (6%)	0	100	100
70	SJ	178/180 (99%)	174 (98%)	3 (2%)	1 (1%)	22	51
71	SM	108/120 (90%)	102 (94%)	6 (6%)	0	100	100
72	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
73	SO	131/135 (97%)	121 (92%)	10 (8%)	0	100	100
74	SW	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	44
75	SY	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
76	SZ	68/70 (97%)	68 (100%)	0	0	100	100
77	Sb	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
78	Se	47/54 (87%)	44 (94%)	3 (6%)	0	100	100
79	Sf	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
81	j	365/411 (89%)	325 (89%)	34 (9%)	6 (2%)	8	27
83	NC	23/25 (92%)	22 (96%)	0	1 (4%)	2	7
All	All	11569/11850 (98%)	10840 (94%)	708 (6%)	21 (0%)	45	73

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	LC	222	ARG
16	LN	124	ASP
29	La	24	LYS
81	j	305	VAL
33	Le	73	GLY

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	LA	190/190 (100%)	183 (96%)	7 (4%)	29	63
2	LB	345/345 (100%)	341 (99%)	4 (1%)	67	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	LC	298/298 (100%)	293 (98%)	5 (2%)	56	84
7	LD	244/245 (100%)	243 (100%)	1 (0%)	89	96
8	LE	209/220 (95%)	204 (98%)	5 (2%)	44	77
9	LF	195/194 (100%)	194 (100%)	1 (0%)	86	95
10	LG	204/205 (100%)	200 (98%)	4 (2%)	50	81
11	LH	169/169 (100%)	164 (97%)	5 (3%)	36	70
12	LI	177/180 (98%)	176 (99%)	1 (1%)	84	95
13	LJ	148/148 (100%)	146 (99%)	2 (1%)	62	87
14	LL	170/170 (100%)	164 (96%)	6 (4%)	31	65
15	LM	118/118 (100%)	117 (99%)	1 (1%)	79	93
16	LN	171/171 (100%)	169 (99%)	2 (1%)	67	89
17	LO	173/173 (100%)	171 (99%)	2 (1%)	67	89
18	LP	134/134 (100%)	133 (99%)	1 (1%)	81	94
19	LQ	164/164 (100%)	162 (99%)	2 (1%)	67	89
20	LR	166/166 (100%)	157 (95%)	9 (5%)	18	48
21	LS	156/156 (100%)	152 (97%)	4 (3%)	41	75
22	LT	139/139 (100%)	138 (99%)	1 (1%)	81	94
23	LU	91/91 (100%)	91 (100%)	0	100	100
24	LV	101/101 (100%)	98 (97%)	3 (3%)	36	70
25	LW	103/103 (100%)	102 (99%)	1 (1%)	73	91
26	LX	108/108 (100%)	108 (100%)	0	100	100
27	LY	124/124 (100%)	120 (97%)	4 (3%)	34	68
28	LZ	117/117 (100%)	113 (97%)	4 (3%)	32	66
29	La	120/120 (100%)	119 (99%)	1 (1%)	79	93
30	Lb	89/100 (89%)	87 (98%)	2 (2%)	47	79
31	Lc	83/83 (100%)	83 (100%)	0	100	100
32	Ld	98/98 (100%)	98 (100%)	0	100	100
33	Le	114/114 (100%)	111 (97%)	3 (3%)	41	75
34	Lf	88/88 (100%)	88 (100%)	0	100	100
35	Lg	98/98 (100%)	97 (99%)	1 (1%)	73	91
36	Lh	109/109 (100%)	108 (99%)	1 (1%)	75	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	Li	86/86 (100%)	84 (98%)	2 (2%)	45	78
38	Lj	74/73 (101%)	74 (100%)	0	100	100
39	Lk	64/64 (100%)	64 (100%)	0	100	100
40	Ll	47/47 (100%)	46 (98%)	1 (2%)	48	80
41	Lm	47/47 (100%)	47 (100%)	0	100	100
42	Ln	23/23 (100%)	23 (100%)	0	100	100
43	Lo	94/93 (101%)	93 (99%)	1 (1%)	70	90
44	Lp	74/74 (100%)	74 (100%)	0	100	100
45	Lr	109/109 (100%)	108 (99%)	1 (1%)	75	92
47	SA	180/180 (100%)	178 (99%)	2 (1%)	70	90
48	SB	193/193 (100%)	192 (100%)	1 (0%)	86	95
49	SD	188/188 (100%)	186 (99%)	2 (1%)	70	90
50	SE	221/221 (100%)	217 (98%)	4 (2%)	54	83
51	SF	158/159 (99%)	155 (98%)	3 (2%)	52	82
52	SH	165/169 (98%)	164 (99%)	1 (1%)	84	95
53	SI	172/178 (97%)	171 (99%)	1 (1%)	84	95
54	SK	86/86 (100%)	85 (99%)	1 (1%)	67	89
55	SL	126/134 (94%)	123 (98%)	3 (2%)	44	77
56	SP	117/117 (100%)	117 (100%)	0	100	100
57	SQ	116/116 (100%)	115 (99%)	1 (1%)	75	92
58	SR	119/119 (100%)	118 (99%)	1 (1%)	79	93
59	SS	124/124 (100%)	123 (99%)	1 (1%)	79	93
60	ST	111/111 (100%)	109 (98%)	2 (2%)	54	83
61	SU	93/93 (100%)	92 (99%)	1 (1%)	70	90
62	SV	67/67 (100%)	66 (98%)	1 (2%)	60	86
63	SX	111/111 (100%)	111 (100%)	0	100	100
64	Sa	86/86 (100%)	85 (99%)	1 (1%)	67	89
65	Sc	54/54 (100%)	53 (98%)	1 (2%)	52	82
66	Sd	48/48 (100%)	48 (100%)	0	100	100
67	Sg	272/272 (100%)	268 (98%)	4 (2%)	60	86
68	SC	187/186 (100%)	186 (100%)	1 (0%)	86	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	SG	199/199 (100%)	196 (98%)	3 (2%)	60	86
70	SJ	160/160 (100%)	160 (100%)	0	100	100
71	SM	93/102 (91%)	92 (99%)	1 (1%)	70	90
72	SN	130/130 (100%)	128 (98%)	2 (2%)	60	86
73	SO	104/104 (100%)	101 (97%)	3 (3%)	37	71
74	SW	112/112 (100%)	111 (99%)	1 (1%)	75	92
75	SY	107/107 (100%)	106 (99%)	1 (1%)	75	92
76	SZ	62/62 (100%)	61 (98%)	1 (2%)	58	85
77	Sb	74/74 (100%)	74 (100%)	0	100	100
78	Se	42/44 (96%)	42 (100%)	0	100	100
79	Sf	56/56 (100%)	55 (98%)	1 (2%)	54	83
81	j	317/353 (90%)	272 (86%)	45 (14%)	2	9
83	NC	19/19 (100%)	18 (95%)	1 (5%)	19	49
All	All	10100/10189 (99%)	9921 (98%)	179 (2%)	54	83

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
67	Sg	46	THR
81	j	82	LEU
68	SC	61	MET
75	SY	110	ARG
81	j	118	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
47	SA	50	ASN
54	SK	7	ASN
48	SB	179	ASN
50	SE	188	ASN
56	SP	41	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3484/3510 (99%)	797 (22%)	14 (0%)
4	L7	119/120 (99%)	19 (15%)	0
46	S2	1571/1590 (98%)	324 (20%)	10 (0%)
5	L8	154/155 (99%)	27 (17%)	1 (0%)
80	Bv	72/76 (94%)	40 (55%)	0
82	k	12/13 (92%)	7 (58%)	0
All	All	5412/5464 (99%)	1214 (22%)	25 (0%)

5 of 1214 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	8	U
3	L5	12	A
3	L5	13	U
3	L5	17	A
3	L5	21	G

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L8	83	C
46	S2	688	U
46	S2	1824	A
46	S2	407	G
46	S2	1129	G

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

217 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	S2	649	46	18,21,22	1.60	4 (22%)	21,30,33	2.16	4 (19%)
46	PSU	S2	1004	46	18,21,22	1.56	5 (27%)	21,30,33	2.24	3 (14%)
3	PSU	L5	1769	3	18,21,22	1.65	5 (27%)	21,30,33	2.39	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	A2M	S2	1678	46	18,25,26	0.65	0	20,36,39	0.79	1 (5%)
3	5MC	L5	4417	3	19,22,23	1.22	1 (5%)	26,32,35	2.09	7 (26%)
46	OMU	S2	1804	46	19,22,23	1.35	4 (21%)	25,31,34	1.93	6 (24%)
3	PSU	L5	1569	3	18,21,22	1.71	5 (27%)	21,30,33	2.19	4 (19%)
3	PSU	L5	4282	3	18,21,22	1.69	4 (22%)	21,30,33	2.34	5 (23%)
3	PSU	L5	4502	3	18,21,22	1.78	6 (33%)	21,30,33	2.01	5 (23%)
3	OMG	L5	1612	84,3	19,26,27	1.16	1 (5%)	21,38,41	1.23	3 (14%)
3	PSU	L5	3713	3	18,21,22	1.46	5 (27%)	21,30,33	2.25	5 (23%)
3	5MC	L5	3761	3	19,22,23	1.24	2 (10%)	26,32,35	1.71	6 (23%)
80	UY4	Bv	37	80	26,34,35	1.77	3 (11%)	28,49,52	2.06	8 (28%)
46	A2M	S2	1383	46	18,25,26	0.68	0	20,36,39	0.98	1 (5%)
46	A2M	S2	590	46	18,25,26	0.62	0	20,36,39	1.06	2 (10%)
3	PSU	L5	3741	3	18,21,22	1.55	5 (27%)	21,30,33	2.36	5 (23%)
3	A2M	L5	3846	3	18,25,26	0.68	0	20,36,39	1.10	2 (10%)
46	A2M	S2	99	46	18,25,26	0.68	0	20,36,39	0.90	1 (5%)
46	PSU	S2	1136	46	18,21,22	1.50	3 (16%)	21,30,33	2.16	5 (23%)
3	OMG	L5	4166	80,3	19,26,27	1.18	2 (10%)	21,38,41	1.31	5 (23%)
46	OMC	S2	462	46	19,22,23	0.83	0	25,31,34	1.06	2 (8%)
3	OMG	L5	3878	3	19,26,27	1.25	1 (5%)	21,38,41	1.30	4 (19%)
80	2MG	Bv	10	80	18,26,27	0.96	1 (5%)	16,38,41	1.47	3 (18%)
3	PSU	L5	4401	3	18,21,22	1.72	5 (27%)	21,30,33	2.25	4 (19%)
3	OMG	L5	1303	3	19,26,27	1.43	2 (10%)	21,38,41	1.04	1 (4%)
46	PSU	S2	1692	46	18,21,22	1.67	5 (27%)	21,30,33	2.25	5 (23%)
3	OMG	L5	2411	3	19,26,27	1.10	1 (5%)	21,38,41	1.15	2 (9%)
3	PSU	L5	1779	3	18,21,22	1.65	4 (22%)	21,30,33	1.97	4 (19%)
3	PSU	L5	3743	3	18,21,22	1.60	4 (22%)	21,30,33	2.13	4 (19%)
81	MEQ	j	185	81	8,9,10	0.47	0	5,10,12	0.48	0
3	PSU	L5	4659	3	18,21,22	1.82	5 (27%)	21,30,33	2.34	6 (28%)
3	PSU	L5	1664	3	18,21,22	1.74	5 (27%)	21,30,33	2.44	6 (28%)
3	PSU	L5	1523	3	18,21,22	1.94	5 (27%)	21,30,33	2.26	4 (19%)
3	A2M	L5	3739	3	18,25,26	0.70	0	20,36,39	0.92	1 (5%)
3	A2M	L5	1313	3	18,25,26	1.06	1 (5%)	20,36,39	1.63	3 (15%)
3	PSU	L5	4975	3	18,21,22	1.65	4 (22%)	21,30,33	2.30	3 (14%)
3	PSU	L5	3737	3	18,21,22	1.63	4 (22%)	21,30,33	2.06	4 (19%)
3	PSU	L5	3616	3	18,21,22	2.02	5 (27%)	21,30,33	2.38	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	S2	1177	46	18,21,22	1.61	4 (22%)	21,30,33	1.95	4 (19%)
46	OMU	S2	428	46	19,22,23	1.24	3 (15%)	25,31,34	1.82	5 (20%)
46	OMU	S2	1442	46	19,22,23	1.36	4 (21%)	25,31,34	1.87	4 (16%)
3	A2M	L5	2350	84,3	18,25,26	0.76	0	20,36,39	0.90	1 (5%)
3	PSU	L5	4522	3	18,21,22	1.86	5 (27%)	21,30,33	2.47	5 (23%)
80	PSU	Bv	55	80	18,21,22	1.34	2 (11%)	21,30,33	2.14	5 (23%)
46	OMU	S2	121	46	19,22,23	1.35	3 (15%)	25,31,34	1.92	4 (16%)
3	PSU	L5	4373	3	18,21,22	1.67	5 (27%)	21,30,33	2.09	4 (19%)
3	PSU	L5	4491	84,3	18,21,22	1.85	5 (27%)	21,30,33	2.40	6 (28%)
80	H2U	Bv	47	80	18,21,22	1.02	2 (11%)	19,30,33	1.35	3 (15%)
3	OMC	L5	3866	3	19,22,23	0.93	1 (5%)	25,31,34	0.94	1 (4%)
3	PSU	L5	4937	3	18,21,22	1.60	5 (27%)	21,30,33	2.03	5 (23%)
46	OMG	S2	509	46,84	19,26,27	0.97	1 (5%)	21,38,41	1.07	1 (4%)
3	OMG	L5	4593	3	19,26,27	1.17	1 (5%)	21,38,41	1.23	2 (9%)
3	PSU	L5	2619	3	18,21,22	1.67	5 (27%)	21,30,33	2.27	5 (23%)
5	PSU	L8	69	5	18,21,22	1.60	5 (27%)	21,30,33	2.39	4 (19%)
3	A2M	L5	389	3	18,25,26	0.73	0	20,36,39	1.01	2 (10%)
46	OMG	S2	1328	46	19,26,27	0.98	1 (5%)	21,38,41	1.09	2 (9%)
3	OMG	L5	4464	3	19,26,27	1.32	2 (10%)	21,38,41	1.11	3 (14%)
3	OMG	L5	4362	3	19,26,27	1.30	2 (10%)	21,38,41	1.15	2 (9%)
3	OMG	L5	4607	3	19,26,27	1.29	2 (10%)	21,38,41	1.23	4 (19%)
46	PSU	S2	801	46	18,21,22	1.52	4 (22%)	21,30,33	2.08	4 (19%)
3	OMG	L5	2351	3	19,26,27	1.14	1 (5%)	21,38,41	1.36	4 (19%)
5	OMG	L8	75	5	19,26,27	1.06	1 (5%)	21,38,41	1.09	2 (9%)
46	A2M	S2	159	46	18,25,26	0.63	0	20,36,39	0.76	1 (5%)
46	OMU	S2	172	46	19,22,23	1.31	4 (21%)	25,31,34	1.96	5 (20%)
46	A2M	S2	468	46	18,25,26	0.65	0	20,36,39	0.89	1 (5%)
46	A2M	S2	484	46	18,25,26	0.66	0	20,36,39	0.91	1 (5%)
46	PSU	S2	1174	46	18,21,22	1.60	5 (27%)	21,30,33	2.32	4 (19%)
3	PSU	L5	4412	3	18,21,22	1.66	5 (27%)	21,30,33	2.28	4 (19%)
3	PSU	L5	4266	3	18,21,22	1.57	4 (22%)	21,30,33	2.19	4 (19%)
3	OMC	L5	2791	3	19,22,23	1.03	2 (10%)	25,31,34	0.91	1 (4%)
5	PSU	L8	55	5	18,21,22	1.55	5 (27%)	21,30,33	2.26	4 (19%)
80	PSU	Bv	27	80	18,21,22	1.36	2 (11%)	21,30,33	2.09	4 (19%)
3	OMU	L5	4276	3	19,22,23	1.58	4 (21%)	25,31,34	1.92	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	OMC	S2	621	46	19,22,23	0.96	2 (10%)	25,31,34	1.62	5 (20%)
46	A2M	S2	576	46	18,25,26	0.64	0	20,36,39	0.85	1 (5%)
3	OMC	L5	3787	3	19,22,23	0.99	2 (10%)	25,31,34	1.08	2 (8%)
46	PSU	S2	1045	46	18,21,22	1.51	3 (16%)	21,30,33	2.26	4 (19%)
3	A2M	L5	1521	3	18,25,26	0.79	0	20,36,39	0.91	1 (5%)
3	A2M	L5	3703	3	18,25,26	0.67	0	20,36,39	0.83	1 (5%)
3	A2M	L5	2388	84,3	18,25,26	0.73	1 (5%)	20,36,39	0.80	1 (5%)
3	PSU	L5	1768	3	18,21,22	1.59	5 (27%)	21,30,33	2.22	3 (14%)
3	OMU	L5	3904	3	19,22,23	1.81	4 (21%)	25,31,34	2.12	8 (32%)
3	OMC	L5	1327	3	19,22,23	0.95	2 (10%)	25,31,34	0.88	1 (4%)
3	PSU	L5	3749	3	18,21,22	1.64	4 (22%)	21,30,33	2.13	3 (14%)
3	PSU	L5	4427	3	18,21,22	1.71	5 (27%)	21,30,33	2.44	5 (23%)
46	PSU	S2	218	46	18,21,22	1.47	4 (22%)	21,30,33	2.14	5 (23%)
46	PSU	S2	36	46	18,21,22	1.52	4 (22%)	21,30,33	2.24	3 (14%)
46	PSU	S2	572	46	18,21,22	1.44	4 (22%)	21,30,33	2.21	5 (23%)
46	PSU	S2	822	46	18,21,22	1.52	5 (27%)	21,30,33	2.16	4 (19%)
46	PSU	S2	814	46	18,21,22	1.54	4 (22%)	21,30,33	2.12	4 (19%)
46	OMG	S2	1490	46	19,26,27	1.08	2 (10%)	21,38,41	1.32	4 (19%)
3	OMC	L5	3820	3	19,22,23	1.16	2 (10%)	25,31,34	1.45	4 (16%)
46	OMU	S2	116	46	19,22,23	1.29	3 (15%)	25,31,34	1.84	6 (24%)
46	OMC	S2	1391	46	19,22,23	0.84	0	25,31,34	1.03	1 (4%)
46	PSU	S2	406	46	18,21,22	1.64	5 (27%)	21,30,33	2.23	5 (23%)
46	OMG	S2	436	46	19,26,27	1.00	1 (5%)	21,38,41	1.24	3 (14%)
3	PSU	L5	4470	3	18,21,22	1.60	6 (33%)	21,30,33	2.33	3 (14%)
3	PSU	L5	4263	3	18,21,22	1.77	6 (33%)	21,30,33	2.21	4 (19%)
46	PSU	S2	93	46	18,21,22	1.47	4 (22%)	21,30,33	2.07	4 (19%)
46	PSU	S2	1232	46	18,21,22	1.62	4 (22%)	21,30,33	2.16	3 (14%)
3	OMC	L5	2848	3	19,22,23	0.97	2 (10%)	25,31,34	0.61	0
46	4AC	S2	1337	46	21,24,25	1.21	2 (9%)	28,34,37	2.60	9 (32%)
3	PSU	L5	3618	3	18,21,22	2.02	5 (27%)	21,30,33	2.32	5 (23%)
3	PSU	L5	1849	3	18,21,22	1.75	4 (22%)	21,30,33	2.14	5 (23%)
3	A2M	L5	391	3	18,25,26	0.73	0	20,36,39	0.96	1 (5%)
46	PSU	S2	1367	46	18,21,22	1.51	4 (22%)	21,30,33	2.14	3 (14%)
3	OMU	L5	4197	3	19,22,23	1.48	4 (21%)	25,31,34	2.00	6 (24%)
3	PSU	L5	2495	3	18,21,22	1.61	4 (22%)	21,30,33	2.10	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3709	3	18,21,22	1.47	4 (22%)	21,30,33	2.17	4 (19%)
3	OMC	L5	3680	3	19,22,23	1.03	2 (10%)	25,31,34	0.80	0
6	MLZ	LC	333	6	8,9,10	0.94	0	4,9,11	0.68	0
3	6MZ	L5	4190	3	17,25,26	0.88	1 (5%)	15,36,39	2.40	4 (26%)
46	PSU	S2	686	46	18,21,22	1.56	5 (27%)	21,30,33	2.27	5 (23%)
3	UR3	L5	4500	3	19,22,23	1.07	1 (5%)	26,32,35	2.00	6 (23%)
46	OMC	S2	1703	46	19,22,23	0.88	2 (10%)	25,31,34	1.21	2 (8%)
3	PSU	L5	4441	3	18,21,22	1.71	5 (27%)	21,30,33	2.35	4 (19%)
46	PSU	S2	105	46	18,21,22	1.57	4 (22%)	21,30,33	2.13	4 (19%)
3	OMG	L5	2863	3	19,26,27	1.13	2 (10%)	21,38,41	1.24	4 (19%)
3	PSU	L5	3899	84,3	18,21,22	1.88	5 (27%)	21,30,33	2.48	5 (23%)
80	H2U	Bv	16	80	18,21,22	1.01	2 (11%)	19,30,33	1.26	3 (15%)
3	A2M	L5	4541	3	18,25,26	0.72	0	20,36,39	0.81	1 (5%)
46	PSU	S2	1046	46	18,21,22	1.59	5 (27%)	21,30,33	2.03	4 (19%)
46	MA6	S2	1851	46	19,26,27	0.96	1 (5%)	18,38,41	2.12	3 (16%)
3	A2M	L5	4493	84,3	18,25,26	0.68	0	20,36,39	0.97	2 (10%)
46	OMC	S2	174	46	19,22,23	0.87	1 (5%)	25,31,34	0.96	1 (4%)
3	OMG	L5	1509	3	19,26,27	1.27	2 (10%)	21,38,41	1.43	4 (19%)
46	A2M	S2	668	46,84	18,25,26	0.76	0	20,36,39	1.16	2 (10%)
46	MA6	S2	1850	46	19,26,27	0.85	0	18,38,41	2.08	4 (22%)
46	OMG	S2	601	46	19,26,27	1.10	1 (5%)	21,38,41	0.91	1 (4%)
3	A2M	L5	3697	3	18,25,26	0.65	0	20,36,39	0.87	1 (5%)
3	PSU	L5	3832	84,3	18,21,22	1.82	4 (22%)	21,30,33	2.09	4 (19%)
3	OMU	L5	4468	3	19,22,23	1.53	4 (21%)	25,31,34	1.96	5 (20%)
46	PSU	S2	866	46	18,21,22	1.47	4 (22%)	21,30,33	2.08	4 (19%)
46	PSU	S2	119	46	18,21,22	1.49	5 (27%)	21,30,33	2.04	5 (23%)
3	OMG	L5	4469	3	19,26,27	1.08	1 (5%)	21,38,41	1.06	2 (9%)
3	OMG	L5	3771	3	19,26,27	1.08	1 (5%)	21,38,41	1.51	5 (23%)
80	1MA	Bv	58	80	17,25,26	1.61	2 (11%)	17,37,40	1.30	3 (17%)
46	PSU	S2	34	46	18,21,22	1.49	4 (22%)	21,30,33	2.15	5 (23%)
3	PSU	L5	2402	3	18,21,22	1.62	4 (22%)	21,30,33	2.45	5 (23%)
3	PSU	L5	4269	3	18,21,22	1.75	4 (22%)	21,30,33	1.97	4 (19%)
3	PSU	L5	1670	3	18,21,22	1.97	4 (22%)	21,30,33	2.15	3 (14%)
46	PSU	S2	1081	46	18,21,22	1.62	5 (27%)	21,30,33	2.26	5 (23%)
46	PSU	S2	651	46	18,21,22	1.51	4 (22%)	21,30,33	2.16	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	G7M	S2	1639	46,80	20,26,27	1.15	2 (10%)	16,39,42	0.56	0
46	PSU	S2	109	46	18,21,22	1.52	4 (22%)	21,30,33	2.17	4 (19%)
46	OMG	S2	867	46	19,26,27	0.95	1 (5%)	21,38,41	1.08	2 (9%)
3	OMC	L5	4506	3	19,22,23	1.00	2 (10%)	25,31,34	1.03	1 (4%)
3	PSU	L5	4643	3	18,21,22	1.82	5 (27%)	21,30,33	2.11	3 (14%)
46	A2M	S2	512	46	18,25,26	0.67	0	20,36,39	0.95	1 (5%)
3	OMG	L5	4340	3	19,26,27	1.16	2 (10%)	21,38,41	1.25	3 (14%)
41	MLZ	Lm	98	41	8,9,10	0.89	0	4,9,11	0.75	0
3	PSU	L5	3694	3	18,21,22	1.52	4 (22%)	21,30,33	2.07	4 (19%)
46	PSU	S2	1244	46	18,21,22	1.43	4 (22%)	21,30,33	2.08	4 (19%)
3	PSU	L5	3830	3	18,21,22	1.77	5 (27%)	21,30,33	2.17	6 (28%)
3	A2M	L5	2802	3	18,25,26	0.66	0	20,36,39	1.11	2 (10%)
3	PSU	L5	3747	3	18,21,22	1.65	5 (27%)	21,30,33	2.19	4 (19%)
46	PSU	S2	863	46	18,21,22	1.58	5 (27%)	21,30,33	2.13	4 (19%)
3	PSU	L5	4323	3	18,21,22	1.78	5 (27%)	21,30,33	2.43	5 (23%)
3	PSU	L5	4393	3	18,21,22	1.62	4 (22%)	21,30,33	2.06	4 (19%)
46	OMU	S2	1326	46	19,22,23	1.31	4 (21%)	25,31,34	2.03	7 (28%)
80	1MG	Bv	9	80	19,26,27	1.06	1 (5%)	18,39,42	1.45	4 (22%)
3	PSU	L5	1847	3	18,21,22	1.70	5 (27%)	21,30,33	2.30	5 (23%)
3	PSU	L5	4598	3	18,21,22	1.78	5 (27%)	21,30,33	2.38	4 (19%)
46	OMG	S2	683	46	19,26,27	1.04	1 (5%)	21,38,41	1.13	3 (14%)
46	A2M	S2	1031	46	18,25,26	0.71	0	20,36,39	0.87	1 (5%)
46	PSU	S2	609	46	18,21,22	1.45	4 (22%)	21,30,33	2.14	3 (14%)
46	B8N	S2	1248	46	25,29,30	1.44	4 (16%)	28,42,45	1.64	6 (21%)
3	2MG	L5	1504	3	18,26,27	1.25	2 (11%)	16,38,41	1.66	5 (31%)
3	A2M	L5	3804	3	18,25,26	0.71	0	20,36,39	0.86	1 (5%)
46	PSU	S2	966	46	18,21,22	1.51	4 (22%)	21,30,33	2.19	5 (23%)
3	PSU	L5	3823	3	18,21,22	1.74	5 (27%)	21,30,33	2.48	4 (19%)
3	OMC	L5	2352	3	19,22,23	0.88	2 (10%)	25,31,34	0.73	0
3	A2M	L5	2774	84,3	18,25,26	0.68	0	20,36,39	1.12	2 (10%)
3	A2M	L5	1511	3	18,25,26	0.70	0	20,36,39	1.11	1 (5%)
3	A2M	L5	3809	3	18,25,26	0.72	0	20,36,39	0.88	1 (5%)
46	PSU	S2	1625	46	18,21,22	1.44	4 (22%)	21,30,33	2.01	4 (19%)
46	PSU	S2	1643	46	18,21,22	1.51	5 (27%)	21,30,33	2.07	4 (19%)
46	4AC	S2	1842	46	21,24,25	1.12	3 (14%)	28,34,37	2.93	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1731	3	18,21,22	1.70	4 (22%)	21,30,33	2.31	3 (14%)
3	OMC	L5	2338	3	19,22,23	1.07	2 (10%)	25,31,34	1.47	3 (12%)
3	A2M	L5	3764	3	18,25,26	0.79	0	20,36,39	1.26	4 (20%)
46	PSU	S2	815	46	18,21,22	1.50	4 (22%)	21,30,33	2.11	3 (14%)
3	OMC	L5	4426	3	19,22,23	1.01	2 (10%)	25,31,34	0.96	1 (4%)
81	UXY	j	63	81	7,9,10	0.75	0	7,10,12	1.36	1 (14%)
3	OMG	L5	4588	3	19,26,27	1.11	1 (5%)	21,38,41	1.25	4 (19%)
46	PSU	S2	1445	46	18,21,22	1.44	4 (22%)	21,30,33	2.00	4 (19%)
3	OMC	L5	2409	84,3	19,22,23	1.00	2 (10%)	25,31,34	1.15	2 (8%)
3	OMC	L5	2811	3	19,22,23	0.93	2 (10%)	25,31,34	0.88	1 (4%)
3	PSU	L5	4390	3	18,21,22	1.35	3 (16%)	21,30,33	2.02	4 (19%)
3	1MA	L5	1309	84,3	17,25,26	1.36	4 (23%)	17,37,40	1.29	3 (17%)
80	M2G	Bv	26	80	20,27,28	1.40	4 (20%)	19,40,43	1.22	3 (15%)
46	OMC	S2	517	46	19,22,23	0.84	1 (5%)	25,31,34	0.80	1 (4%)
46	PSU	S2	1238	46	18,21,22	1.55	4 (22%)	21,30,33	2.09	3 (14%)
3	OMG	L5	3723	3	19,26,27	1.14	1 (5%)	21,38,41	1.20	3 (14%)
3	A2M	L5	1858	84,3	18,25,26	0.84	0	20,36,39	0.97	1 (5%)
3	OMG	L5	4198	3	19,26,27	1.00	1 (5%)	21,38,41	1.20	2 (9%)
46	OMU	S2	1288	46	19,22,23	1.31	4 (21%)	25,31,34	1.79	4 (16%)
3	PSU	L5	3674	3	18,21,22	1.84	5 (27%)	21,30,33	2.24	5 (23%)
46	A2M	S2	27	46,84	18,25,26	0.68	0	20,36,39	0.82	1 (5%)
3	OMG	L5	3606	3	19,26,27	1.27	2 (10%)	21,38,41	1.14	2 (9%)
46	6MZ	S2	1832	46	17,25,26	0.87	1 (5%)	15,36,39	2.85	4 (26%)
46	A2M	S2	166	46	18,25,26	0.71	0	20,36,39	0.93	1 (5%)
73	IAS	SO	138	73	6,7,8	1.30	1 (16%)	3,8,10	1.21	0
3	PSU	L5	4606	3	18,21,22	1.59	4 (22%)	21,30,33	1.98	4 (19%)
3	OMU	L5	2824	3	19,22,23	1.47	4 (21%)	25,31,34	2.14	4 (16%)
80	G7M	Bv	46	80	20,26,27	1.27	3 (15%)	16,39,42	1.42	1 (6%)
46	OMG	S2	644	46	19,26,27	1.00	1 (5%)	21,38,41	1.11	2 (9%)
3	PSU	L5	4549	3	18,21,22	1.70	5 (27%)	21,30,33	2.39	6 (28%)
3	PSU	L5	4546	3	18,21,22	1.59	5 (27%)	21,30,33	2.27	3 (14%)
3	PSU	L5	4331	3	18,21,22	1.80	5 (27%)	21,30,33	2.14	5 (23%)
3	OMG	L5	364	3	19,26,27	1.34	2 (10%)	21,38,41	1.37	4 (19%)
3	OMC	L5	3848	3	19,22,23	0.96	1 (5%)	25,31,34	0.95	1 (4%)
46	PSU	S2	1347	46	18,21,22	1.44	4 (22%)	21,30,33	2.05	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4966	3	18,21,22	1.80	5 (27%)	21,30,33	2.16	4 (19%)
80	PSU	Bv	28	80	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
3	OMU	L5	4590	3	19,22,23	1.64	3 (15%)	25,31,34	1.80	6 (24%)
3	UY1	L5	3797	84,3	19,22,23	1.58	5 (26%)	21,31,34	2.01	4 (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
46	PSU	S2	649	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1004	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	1769	3	-	0/7/25/26	0/2/2/2
46	A2M	S2	1678	46	-	0/5/27/28	0/3/3/3
3	5MC	L5	4417	3	-	3/7/25/26	0/2/2/2
46	OMU	S2	1804	46	-	2/9/27/28	0/2/2/2
3	PSU	L5	1569	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4282	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4502	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1612	84,3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3713	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	3761	3	-	0/7/25/26	0/2/2/2
80	UY4	Bv	37	80	-	3/19/50/51	0/3/3/3
46	A2M	S2	1383	46	-	0/5/27/28	0/3/3/3
46	A2M	S2	590	46	-	3/5/27/28	0/3/3/3
3	PSU	L5	3741	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	3846	3	-	2/5/27/28	0/3/3/3
46	A2M	S2	99	46	-	2/5/27/28	0/3/3/3
46	PSU	S2	1136	46	-	2/7/25/26	0/2/2/2
3	OMG	L5	4166	80,3	-	0/5/27/28	0/3/3/3
46	OMC	S2	462	46	-	0/9/27/28	0/2/2/2
3	OMG	L5	3878	3	-	1/5/27/28	0/3/3/3
80	2MG	Bv	10	80	-	0/5/27/28	0/3/3/3
3	PSU	L5	4401	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1303	3	-	2/5/27/28	0/3/3/3
46	PSU	S2	1692	46	-	0/7/25/26	0/2/2/2
3	OMG	L5	2411	3	-	2/5/27/28	0/3/3/3
3	PSU	L5	1779	3	-	2/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3743	3	-	2/7/25/26	0/2/2/2
81	MEQ	j	185	81	-	0/8/9/11	-
3	PSU	L5	4659	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1664	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	1523	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3739	3	-	2/5/27/28	0/3/3/3
3	A2M	L5	1313	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4975	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3737	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3616	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	1177	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	428	46	-	6/9/27/28	0/2/2/2
46	OMU	S2	1442	46	-	2/9/27/28	0/2/2/2
3	A2M	L5	2350	84,3	-	1/5/27/28	0/3/3/3
3	PSU	L5	4522	3	-	0/7/25/26	0/2/2/2
80	PSU	Bv	55	80	-	1/7/25/26	0/2/2/2
46	OMU	S2	121	46	-	0/9/27/28	0/2/2/2
3	PSU	L5	4373	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4491	84,3	-	0/7/25/26	0/2/2/2
80	H2U	Bv	47	80	-	1/7/38/39	0/2/2/2
3	OMC	L5	3866	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4937	3	-	0/7/25/26	0/2/2/2
46	OMG	S2	509	46,84	-	0/5/27/28	0/3/3/3
3	OMG	L5	4593	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	2619	3	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	5	-	1/7/25/26	0/2/2/2
3	A2M	L5	389	3	-	0/5/27/28	0/3/3/3
46	OMG	S2	1328	46	-	0/5/27/28	0/3/3/3
3	OMG	L5	4464	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	4362	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	4607	3	-	0/5/27/28	0/3/3/3
46	PSU	S2	801	46	-	1/7/25/26	0/2/2/2
3	OMG	L5	2351	3	-	2/5/27/28	0/3/3/3
5	OMG	L8	75	5	-	0/5/27/28	0/3/3/3
46	A2M	S2	159	46	-	0/5/27/28	0/3/3/3
46	OMU	S2	172	46	-	2/9/27/28	0/2/2/2
46	A2M	S2	468	46	-	1/5/27/28	0/3/3/3
46	A2M	S2	484	46	-	0/5/27/28	0/3/3/3
46	PSU	S2	1174	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	4412	3	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4266	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	2791	3	-	0/9/27/28	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
80	PSU	Bv	27	80	-	0/7/25/26	0/2/2/2
3	OMU	L5	4276	3	-	0/9/27/28	0/2/2/2
46	OMC	S2	621	46	-	4/9/27/28	0/2/2/2
46	A2M	S2	576	46	-	3/5/27/28	0/3/3/3
3	OMC	L5	3787	3	-	0/9/27/28	0/2/2/2
46	PSU	S2	1045	46	-	2/7/25/26	0/2/2/2
3	A2M	L5	1521	3	-	1/5/27/28	0/3/3/3
3	A2M	L5	3703	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	2388	84,3	-	1/5/27/28	0/3/3/3
3	PSU	L5	1768	3	-	2/7/25/26	0/2/2/2
3	OMU	L5	3904	3	-	2/9/27/28	0/2/2/2
3	OMC	L5	1327	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3749	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4427	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	218	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	36	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	572	46	-	1/7/25/26	0/2/2/2
46	PSU	S2	822	46	-	2/7/25/26	0/2/2/2
46	PSU	S2	814	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	1490	46	-	3/5/27/28	0/3/3/3
3	OMC	L5	3820	3	-	2/9/27/28	0/2/2/2
46	OMU	S2	116	46	-	3/9/27/28	0/2/2/2
46	OMC	S2	1391	46	-	2/9/27/28	0/2/2/2
46	PSU	S2	406	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	436	46	-	2/5/27/28	0/3/3/3
3	PSU	L5	4470	3	-	3/7/25/26	0/2/2/2
3	PSU	L5	4263	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	93	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1232	46	-	0/7/25/26	0/2/2/2
3	OMC	L5	2848	3	-	0/9/27/28	0/2/2/2
46	4AC	S2	1337	46	-	1/11/29/30	0/2/2/2
3	PSU	L5	3618	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1849	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	391	3	-	1/5/27/28	0/3/3/3
46	PSU	S2	1367	46	-	0/7/25/26	0/2/2/2
3	OMU	L5	4197	3	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	2495	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3709	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3680	3	-	4/9/27/28	0/2/2/2
6	MLZ	LC	333	6	-	4/7/8/10	-
3	6MZ	L5	4190	3	-	0/5/27/28	0/3/3/3
46	PSU	S2	686	46	-	0/7/25/26	0/2/2/2
3	UR3	L5	4500	3	-	0/7/25/26	0/2/2/2
46	OMC	S2	1703	46	-	2/9/27/28	0/2/2/2
3	PSU	L5	4441	3	-	1/7/25/26	0/2/2/2
46	PSU	S2	105	46	-	0/7/25/26	0/2/2/2
3	OMG	L5	2863	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3899	84,3	-	2/7/25/26	0/2/2/2
80	H2U	Bv	16	80	-	2/7/38/39	0/2/2/2
3	A2M	L5	4541	3	-	0/5/27/28	0/3/3/3
46	PSU	S2	1046	46	-	0/7/25/26	0/2/2/2
46	MA6	S2	1851	46	-	2/7/29/30	0/3/3/3
3	A2M	L5	4493	84,3	-	0/5/27/28	0/3/3/3
46	OMC	S2	174	46	-	1/9/27/28	0/2/2/2
3	OMG	L5	1509	3	-	0/5/27/28	0/3/3/3
46	A2M	S2	668	46,84	-	3/5/27/28	0/3/3/3
46	MA6	S2	1850	46	-	2/7/29/30	0/3/3/3
46	OMG	S2	601	46	-	0/5/27/28	0/3/3/3
3	A2M	L5	3697	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3832	84,3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4468	3	-	0/9/27/28	0/2/2/2
46	PSU	S2	866	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	119	46	-	0/7/25/26	0/2/2/2
3	OMG	L5	4469	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	3771	3	-	0/5/27/28	0/3/3/3
80	1MA	Bv	58	80	-	2/3/25/26	0/3/3/3
46	PSU	S2	34	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	2402	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4269	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1670	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	1081	46	-	2/7/25/26	0/2/2/2
46	PSU	S2	651	46	-	0/7/25/26	0/2/2/2
46	G7M	S2	1639	46,80	-	0/3/25/26	0/3/3/3
46	PSU	S2	109	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	867	46	-	0/5/27/28	0/3/3/3
3	OMC	L5	4506	3	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4643	3	-	0/7/25/26	0/2/2/2
46	A2M	S2	512	46	-	2/5/27/28	0/3/3/3
3	OMG	L5	4340	3	-	0/5/27/28	0/3/3/3
41	MLZ	Lm	98	41	-	1/7/8/10	-
3	PSU	L5	3694	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	1244	46	-	2/7/25/26	0/2/2/2
3	PSU	L5	3830	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	2802	3	-	4/5/27/28	0/3/3/3
3	PSU	L5	3747	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	863	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	4323	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4393	3	-	0/7/25/26	0/2/2/2
46	OMU	S2	1326	46	-	0/9/27/28	0/2/2/2
80	1MG	Bv	9	80	-	1/3/25/26	0/3/3/3
3	PSU	L5	1847	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	4598	3	-	0/7/25/26	0/2/2/2
46	OMG	S2	683	46	-	2/5/27/28	0/3/3/3
46	A2M	S2	1031	46	-	0/5/27/28	0/3/3/3
46	PSU	S2	609	46	-	0/7/25/26	0/2/2/2
46	B8N	S2	1248	46	1/1/7/7	1/16/34/35	0/2/2/2
3	2MG	L5	1504	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	3804	3	-	0/5/27/28	0/3/3/3
46	PSU	S2	966	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	3823	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	2352	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2774	84,3	-	1/5/27/28	0/3/3/3
3	A2M	L5	1511	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	3809	3	-	0/5/27/28	0/3/3/3
46	PSU	S2	1625	46	-	2/7/25/26	0/2/2/2
46	PSU	S2	1643	46	-	0/7/25/26	0/2/2/2
46	4AC	S2	1842	46	-	2/11/29/30	0/2/2/2
3	PSU	L5	1731	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2338	3	-	2/9/27/28	0/2/2/2
3	A2M	L5	3764	3	-	2/5/27/28	0/3/3/3
46	PSU	S2	815	46	-	0/7/25/26	0/2/2/2
3	OMC	L5	4426	3	-	0/9/27/28	0/2/2/2
81	UXY	j	63	81	-	3/8/9/11	-
3	OMG	L5	4588	3	-	1/5/27/28	0/3/3/3
46	PSU	S2	1445	46	-	0/7/25/26	0/2/2/2
3	OMC	L5	2409	84,3	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	2811	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4390	3	-	2/7/25/26	0/2/2/2
3	1MA	L5	1309	84,3	-	0/3/25/26	0/3/3/3
80	M2G	Bv	26	80	-	0/7/29/30	0/3/3/3
46	OMC	S2	517	46	-	1/9/27/28	0/2/2/2
46	PSU	S2	1238	46	-	0/7/25/26	0/2/2/2
3	OMG	L5	3723	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	1858	84,3	-	0/5/27/28	0/3/3/3
3	OMG	L5	4198	3	-	0/5/27/28	0/3/3/3
46	OMU	S2	1288	46	-	0/9/27/28	0/2/2/2
3	PSU	L5	3674	3	-	0/7/25/26	0/2/2/2
46	A2M	S2	27	46,84	-	0/5/27/28	0/3/3/3
3	OMG	L5	3606	3	-	1/5/27/28	0/3/3/3
46	6MZ	S2	1832	46	-	0/5/27/28	0/3/3/3
46	A2M	S2	166	46	-	0/5/27/28	0/3/3/3
73	IAS	SO	138	73	-	3/7/7/8	-
3	PSU	L5	4606	3	-	3/7/25/26	0/2/2/2
3	OMU	L5	2824	3	-	0/9/27/28	0/2/2/2
80	G7M	Bv	46	80	-	3/3/25/26	0/3/3/3
46	OMG	S2	644	46	-	3/5/27/28	0/3/3/3
3	PSU	L5	4549	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4546	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4331	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	364	3	-	1/5/27/28	0/3/3/3
3	OMC	L5	3848	3	-	0/9/27/28	0/2/2/2
46	PSU	S2	1347	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	4966	3	-	0/7/25/26	0/2/2/2
80	PSU	Bv	28	80	-	2/7/25/26	0/2/2/2
3	OMU	L5	4590	3	-	0/9/27/28	0/2/2/2
3	UY1	L5	3797	84,3	-	7/9/27/28	0/2/2/2

The worst 5 of 597 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	Bv	37	UY4	C04-C02	5.17	1.60	1.52
80	Bv	58	1MA	C2-N3	5.03	1.34	1.28
80	Bv	37	UY4	C6-N1	5.00	1.40	1.34
3	L5	3904	OMU	C4-N3	-4.73	1.30	1.38
3	L5	1303	OMG	C6-N1	-4.67	1.30	1.37

The worst 5 of 733 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1842	4AC	CM7-C7-N4	11.26	133.45	115.27
46	S2	1337	4AC	N4-C4-N3	9.21	128.82	113.87
46	S2	1832	6MZ	C2-N1-C6	8.42	123.13	116.60
3	L5	3899	PSU	N1-C2-N3	7.90	123.50	115.17
3	L5	4522	PSU	N1-C2-N3	7.89	123.49	115.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
46	S2	1248	B8N	C33

5 of 173 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	LC	333	MLZ	N-CA-CB-CG
6	LC	333	MLZ	C-CA-CB-CG
6	LC	333	MLZ	O-C-CA-CB
6	LC	333	MLZ	CD-CE-NZ-CM
3	L5	2351	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 201 ligands modelled in this entry, 200 are monoatomic - leaving 1 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	MVM	L5	5246	-	32,35,35	1.09	1 (3%)	39,49,49	1.41	6 (15%)

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	MVM	L5	5246	-	-	0/20/28/28	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	L5	5246	MVM	N6-N5	-3.30	1.28	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	L5	5246	MVM	C1-C9-N1	-3.54	107.27	116.16
85	L5	5246	MVM	C6-N1-C9	3.30	123.30	118.40
85	L5	5246	MVM	C20-C19-C18	-3.11	115.84	120.09
85	L5	5246	MVM	N6-N5-N4	2.90	109.59	106.37
85	L5	5246	MVM	C21-N7-C22	-2.83	113.42	116.81

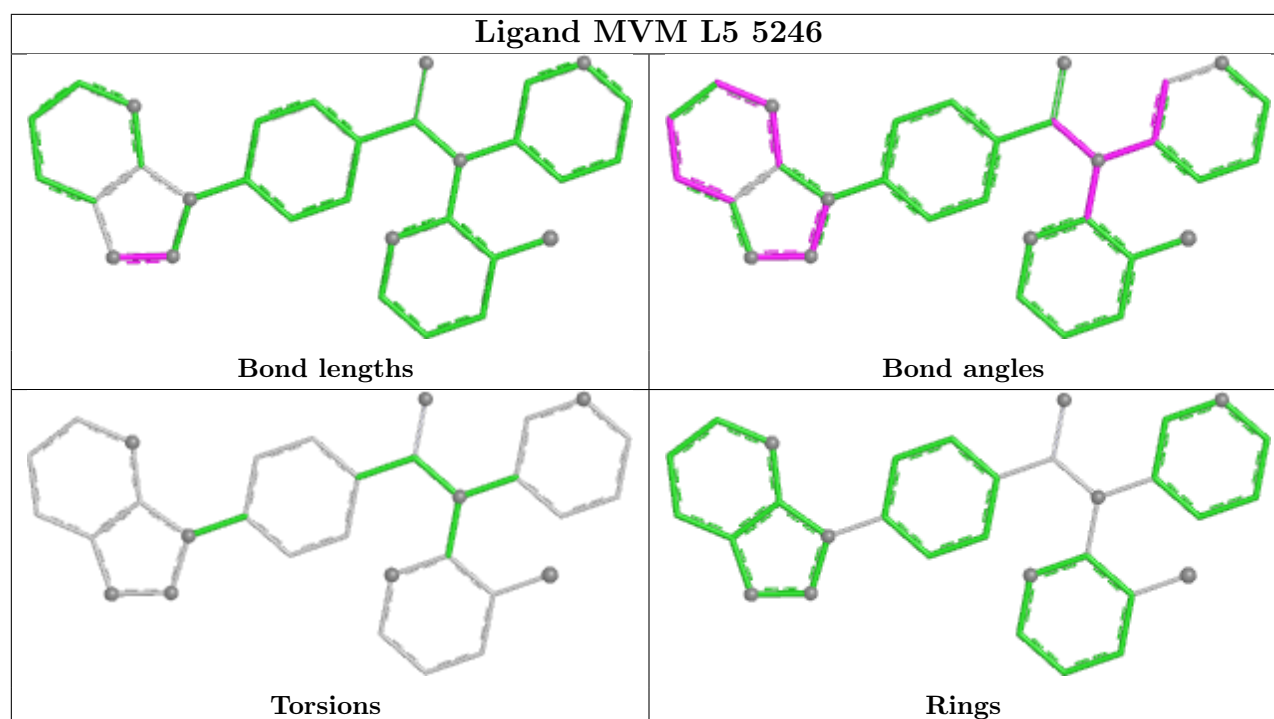
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



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
3	L5	22
46	S2	13
81	j	2

The worst 5 of 37 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	482:G	O3'	495:G	P	26.99
1	L5	173:G	O3'	186:G	P	24.85
1	S2	689:U	O3'	799:U	P	24.17
1	L5	250:G	O3'	253:G	P	24.06
1	L5	646:C	O3'	659:C	P	21.79

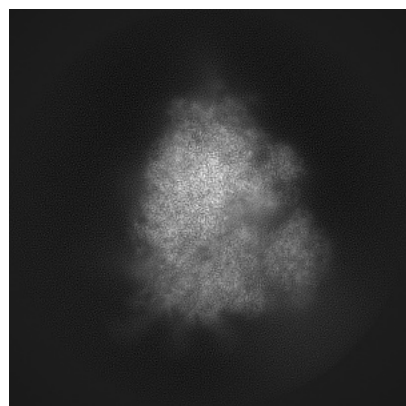
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22085. These allow visual inspection of the internal detail of the map and identification of artifacts.

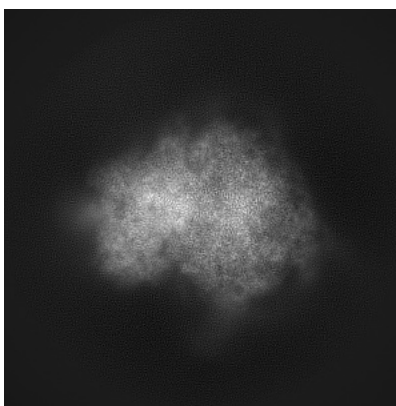
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

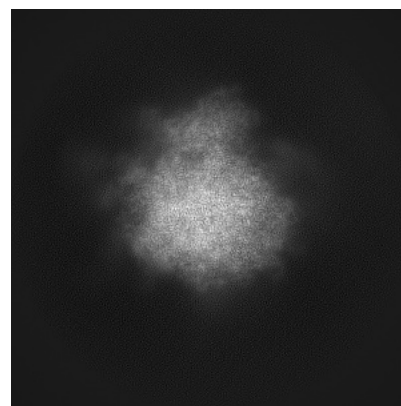
6.1.1 Primary map



X

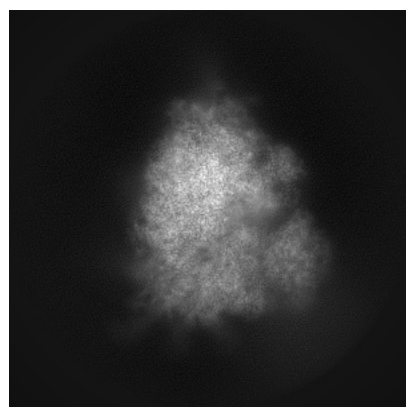


Y

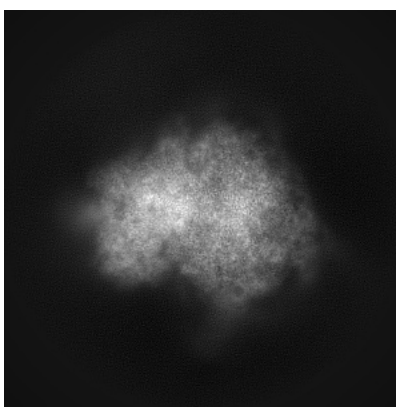


Z

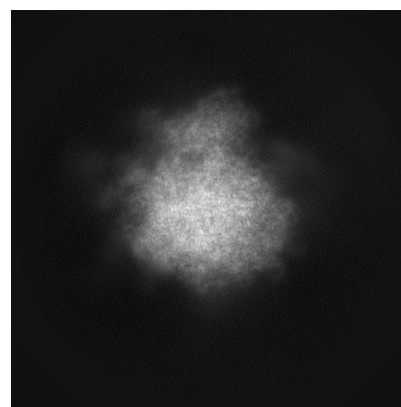
6.1.2 Raw map



X



Y

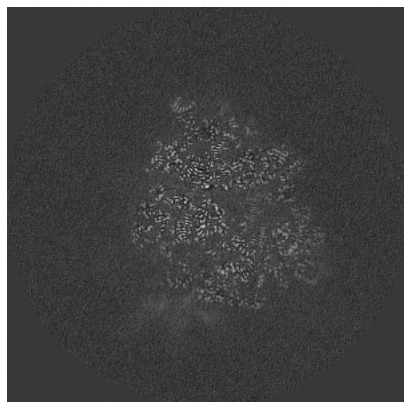


Z

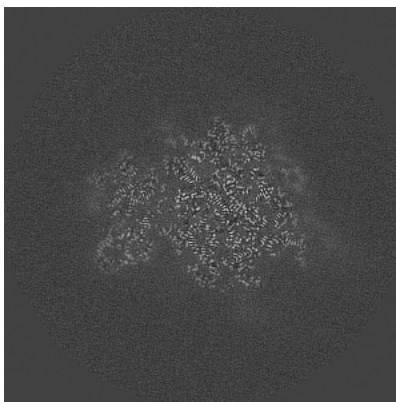
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

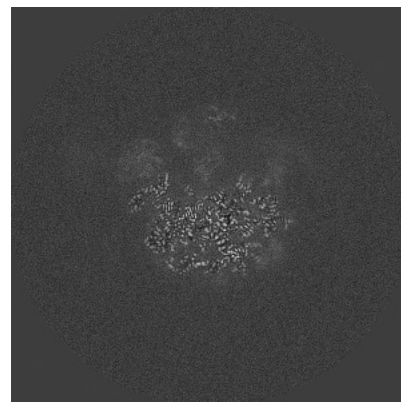
6.2.1 Primary map



X Index: 215

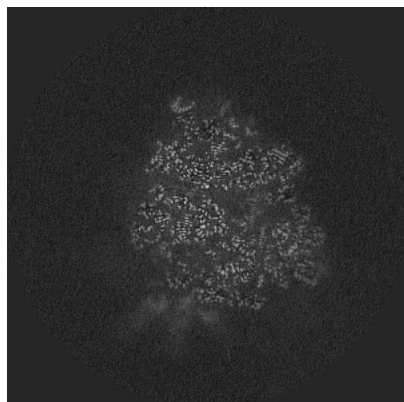


Y Index: 215

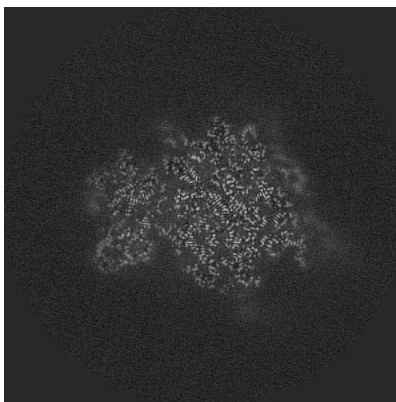


Z Index: 215

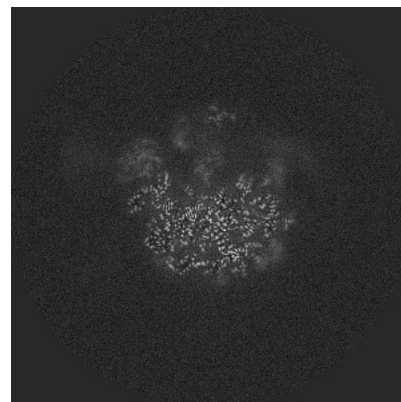
6.2.2 Raw map



X Index: 215



Y Index: 215

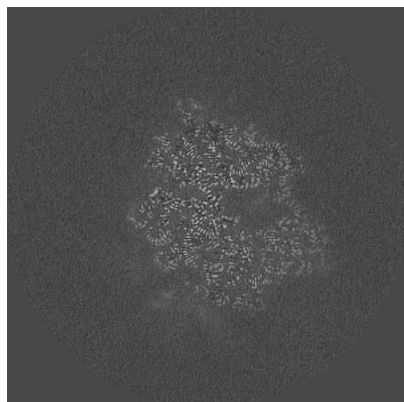


Z Index: 215

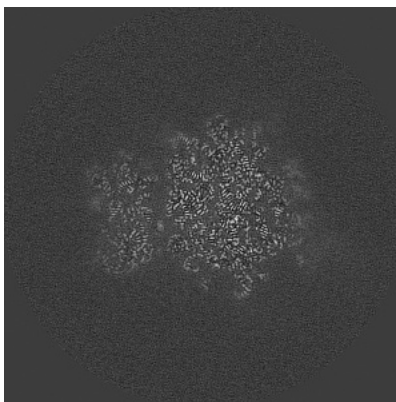
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

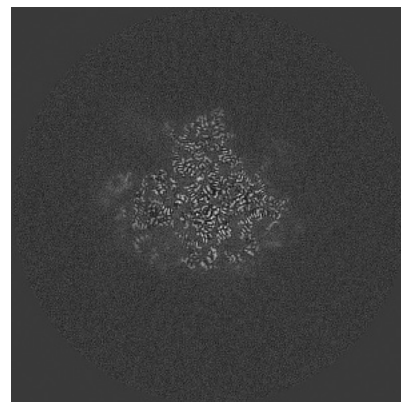
6.3.1 Primary map



X Index: 222

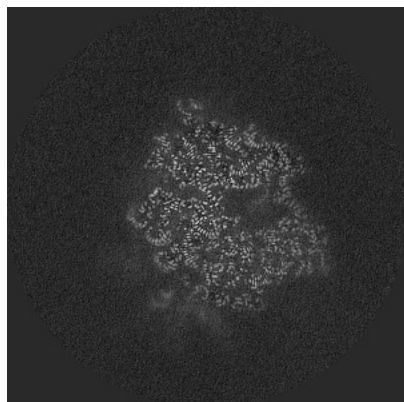


Y Index: 210

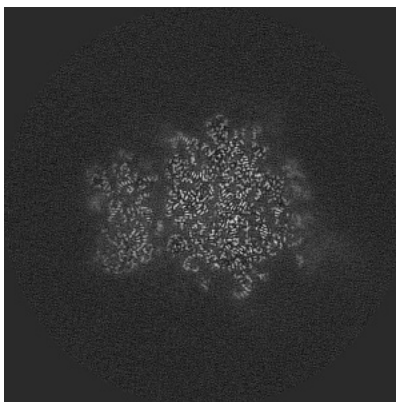


Z Index: 255

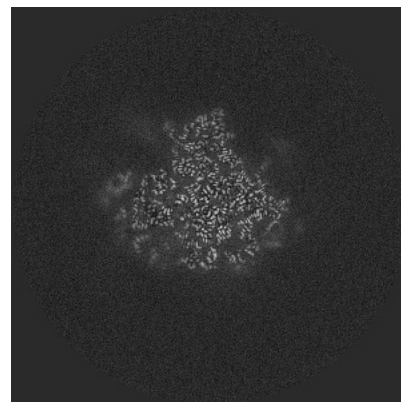
6.3.2 Raw map



X Index: 222



Y Index: 210

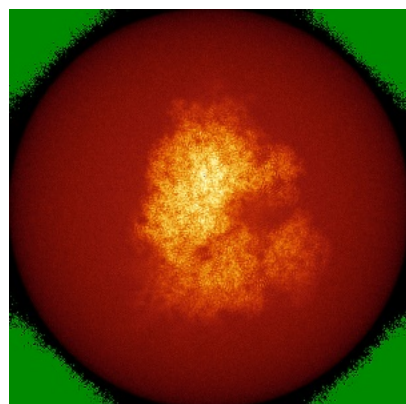


Z Index: 255

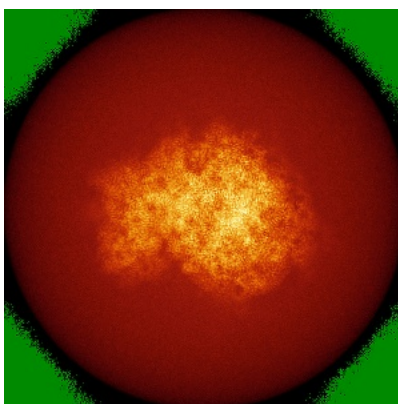
The images above show the largest variance slices of the map in three orthogonal directions.

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

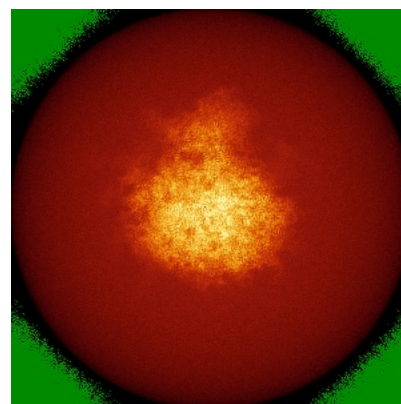
6.4.1 Primary map



X

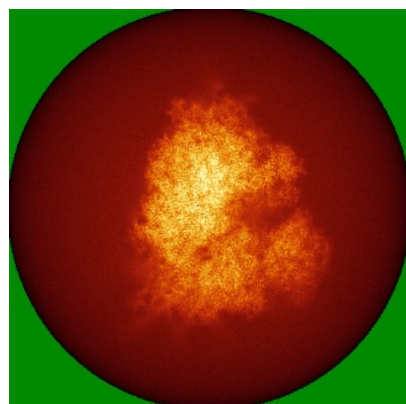


Y

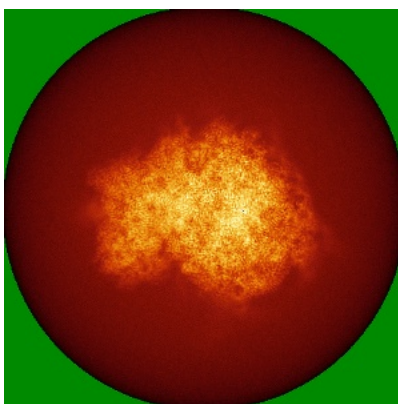


Z

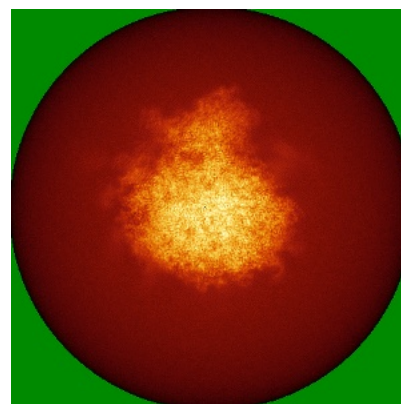
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



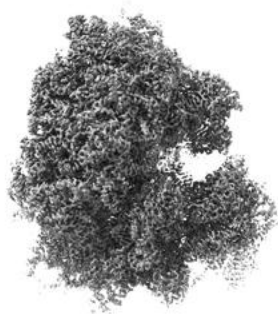
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

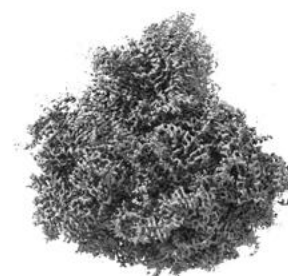
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

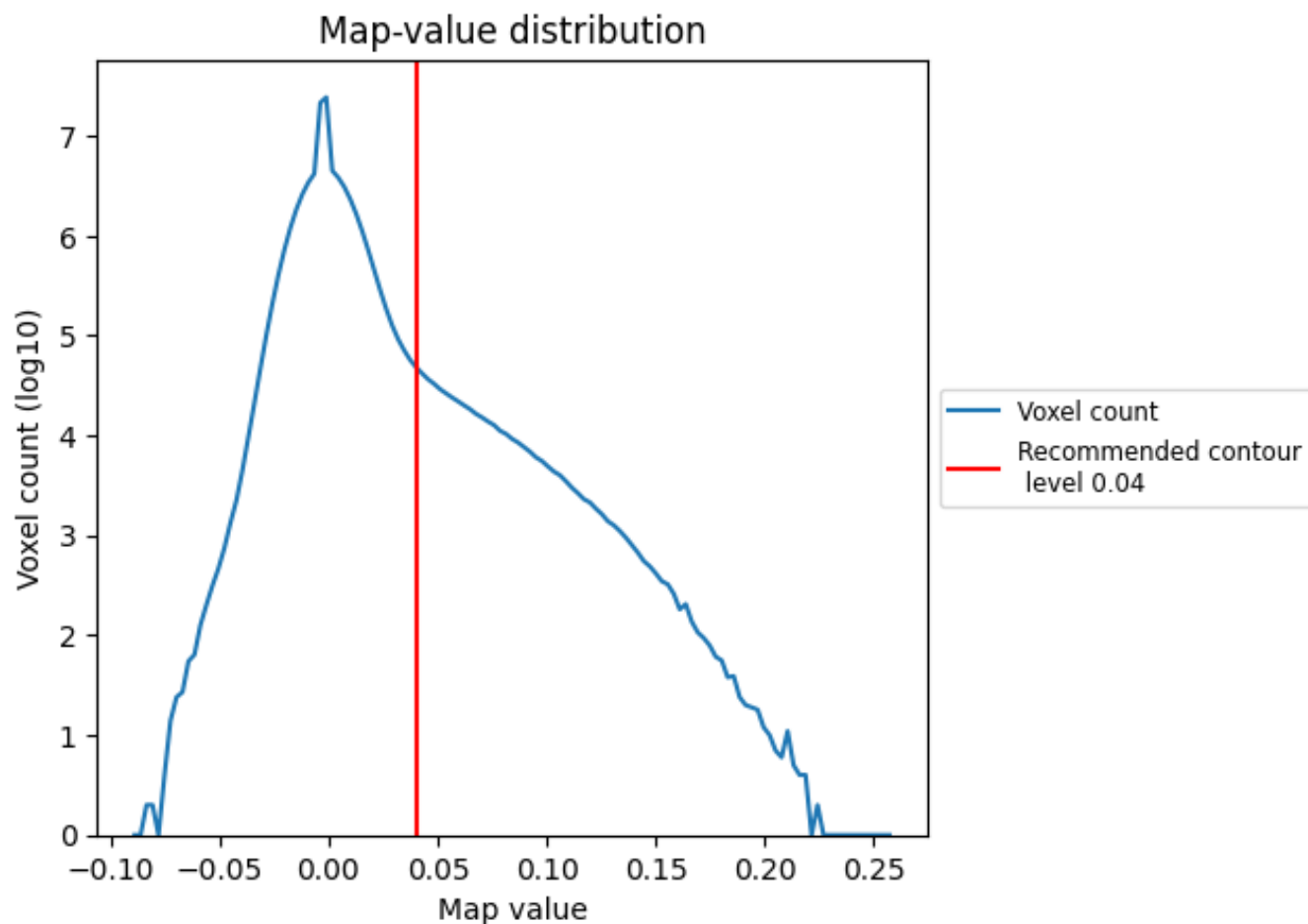
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

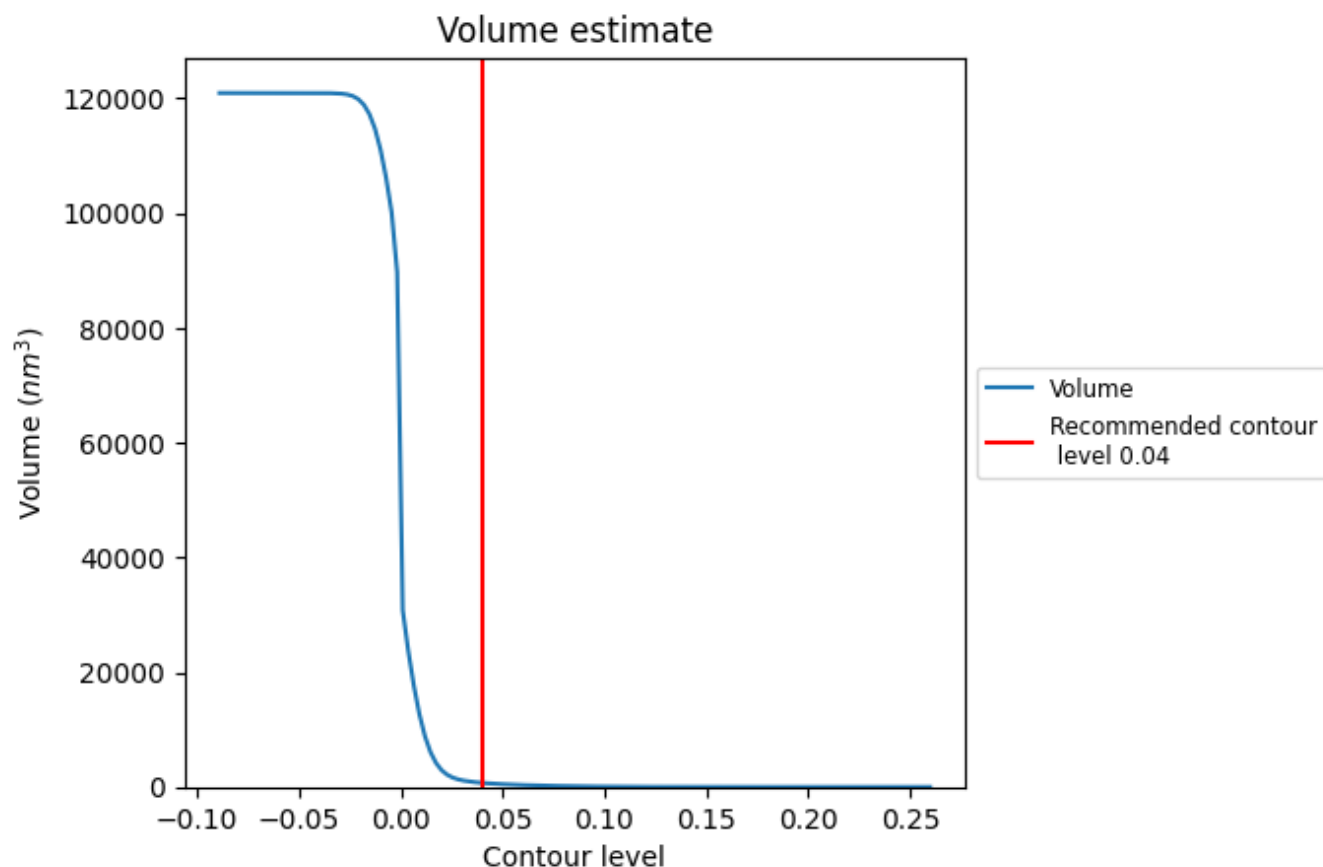
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

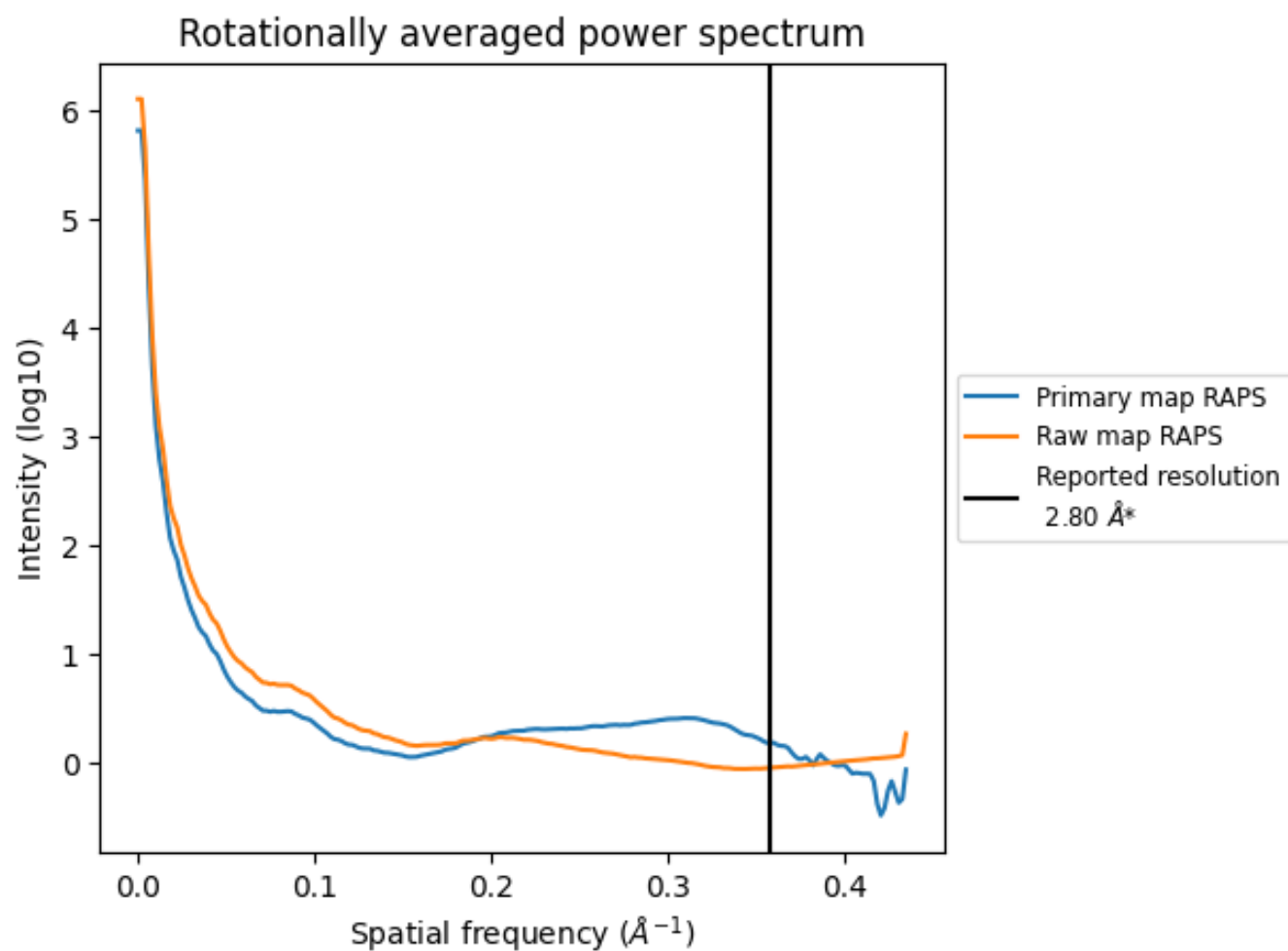
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 709 nm^3 ; this corresponds to an approximate mass of 641 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 ⓘ

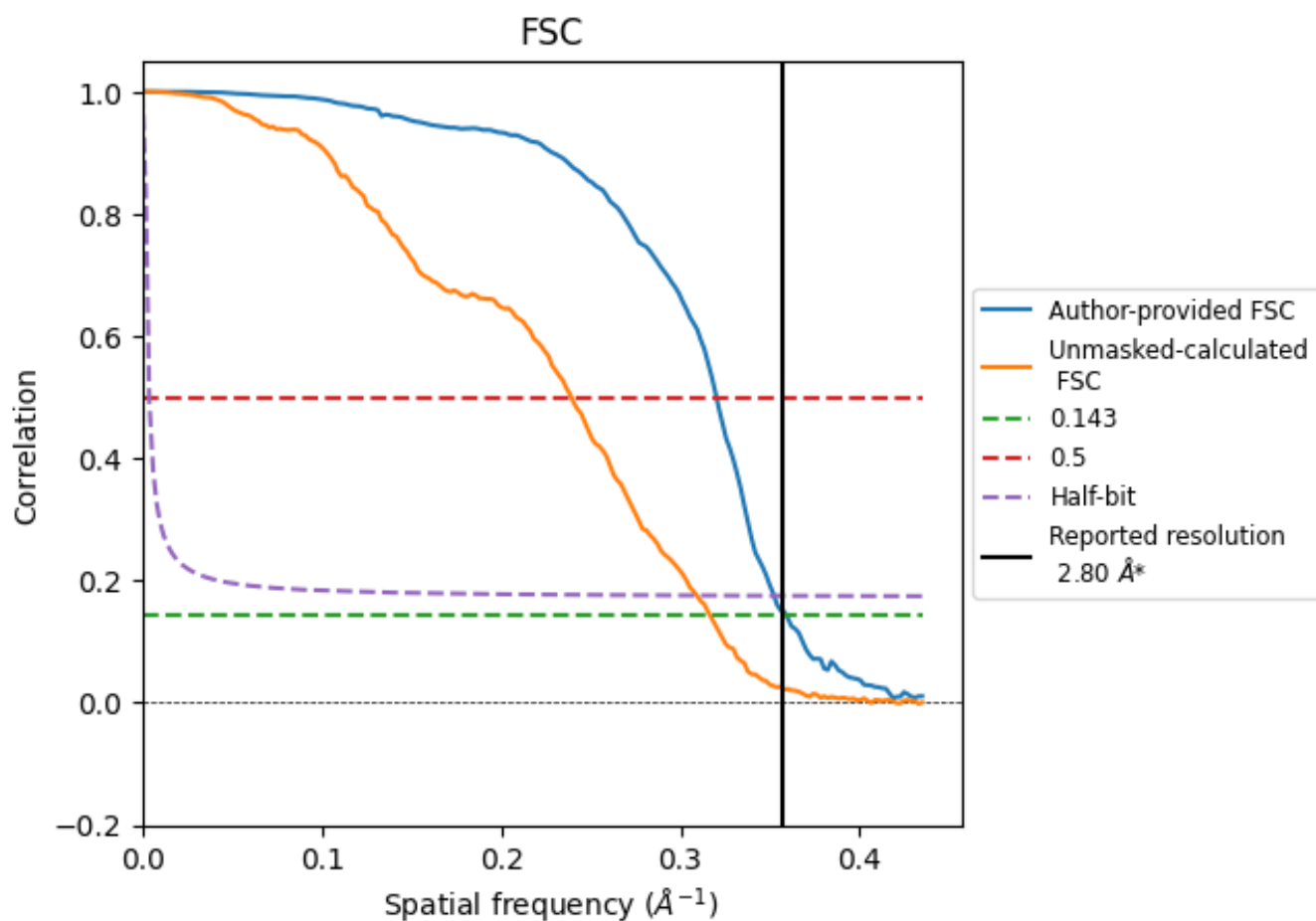


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

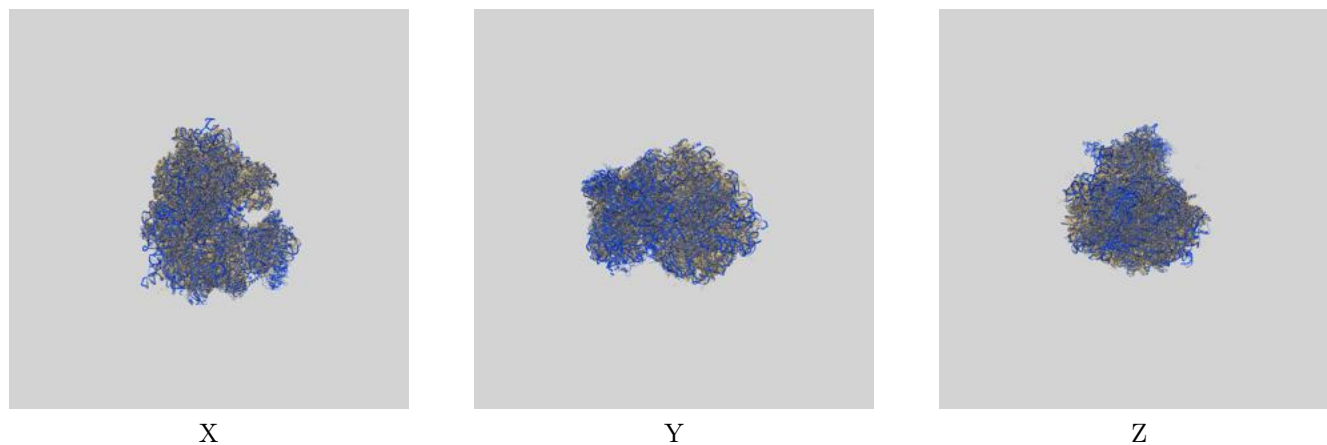
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.79	3.12	2.84
Unmasked-calculated*	3.16	4.18	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

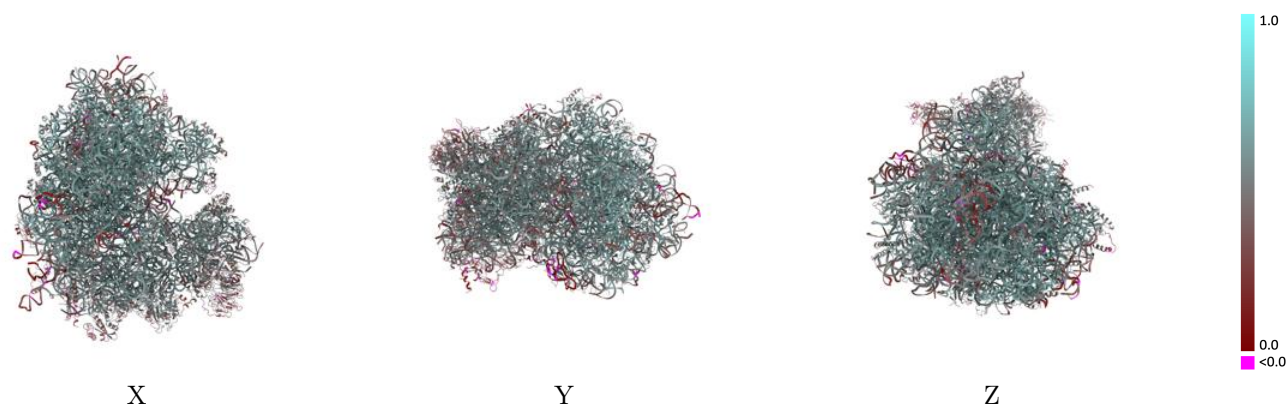
This section contains information regarding the fit between EMDB map EMD-22085 and PDB model 6XA1. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



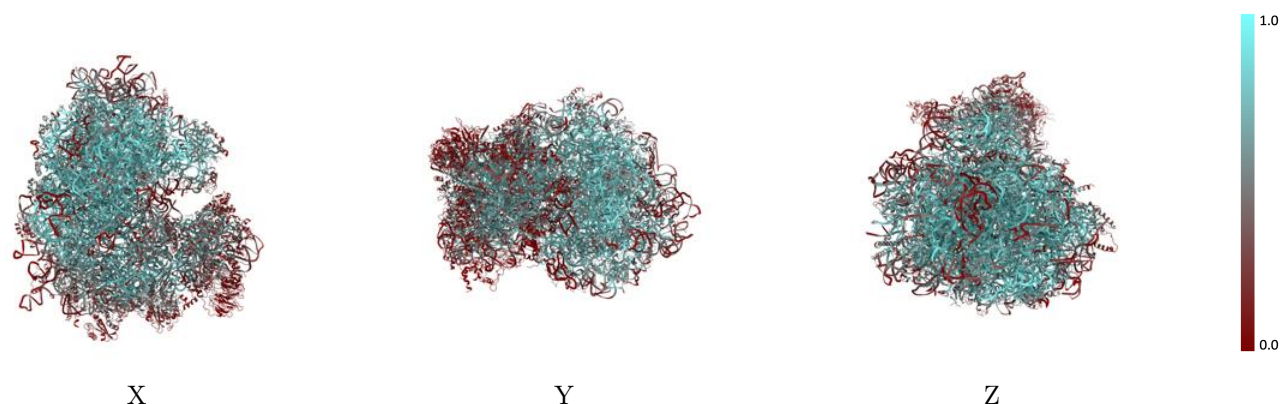
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



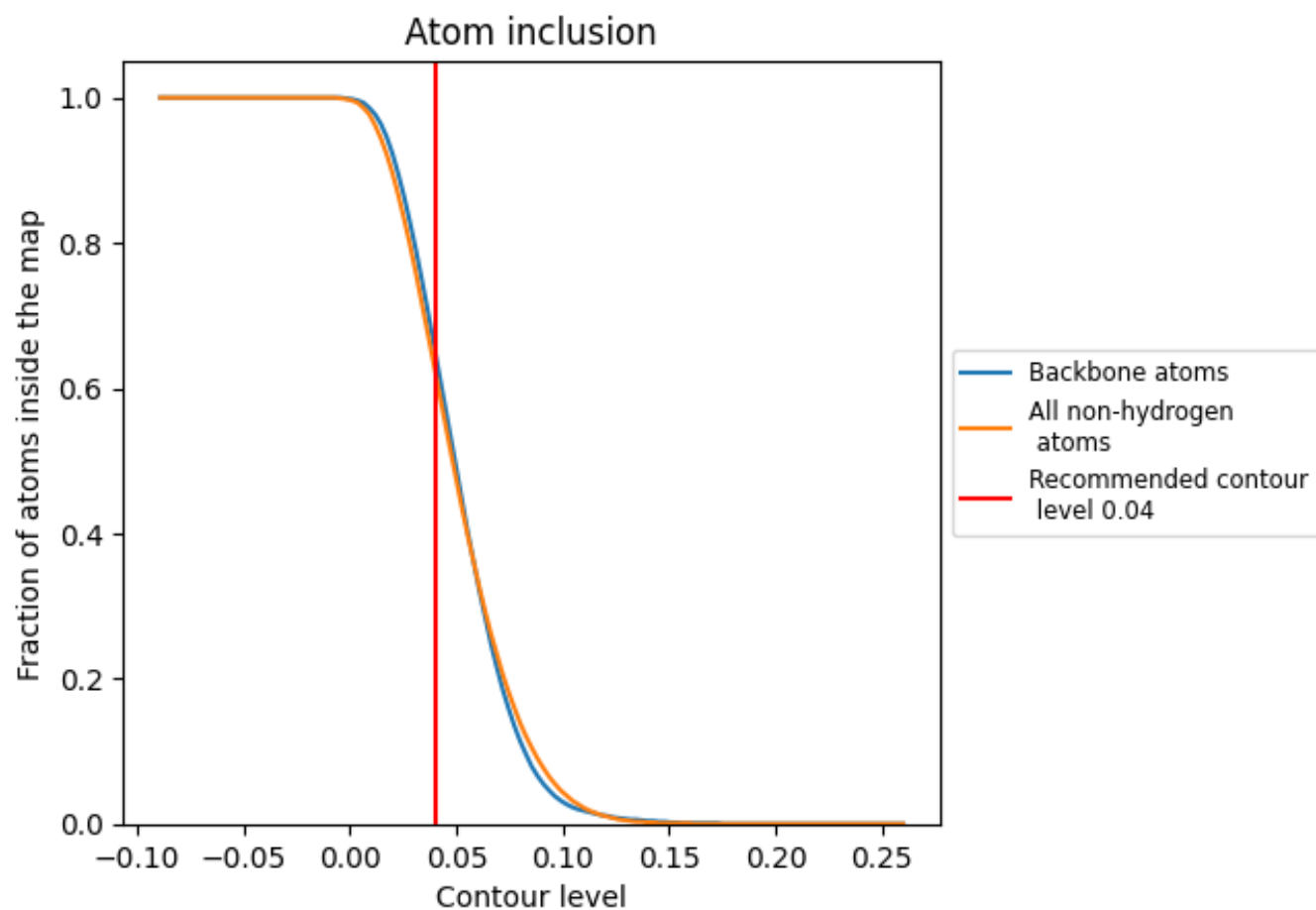
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 62% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6240	 0.5350
Bv	 0.2910	 0.4180
L5	 0.7530	 0.5620
L7	 0.8360	 0.6110
L8	 0.7940	 0.5730
LA	 0.8070	 0.6000
LB	 0.6830	 0.5690
LC	 0.7420	 0.6000
LD	 0.5550	 0.5440
LE	 0.4890	 0.4950
LF	 0.7550	 0.5880
LG	 0.5150	 0.4920
LH	 0.5370	 0.5200
LI	 0.6450	 0.5490
LJ	 0.4100	 0.4390
LL	 0.6300	 0.5520
LM	 0.6120	 0.5480
LN	 0.8590	 0.6190
LO	 0.7330	 0.5730
LP	 0.7380	 0.5870
LQ	 0.7760	 0.6090
LR	 0.5960	 0.4970
LS	 0.7360	 0.5900
LT	 0.6650	 0.5430
LU	 0.2970	 0.4320
LV	 0.7030	 0.5660
LW	 0.3300	 0.3420
LX	 0.6140	 0.5400
LY	 0.6460	 0.5600
LZ	 0.5640	 0.5300
La	 0.8010	 0.6140
Lb	 0.5350	 0.5060
Lc	 0.5860	 0.5160
Ld	 0.6310	 0.5330
Le	 0.7680	 0.6030

















Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lf	 0.7920	 0.5980
Lg	 0.6950	 0.5600
Lh	 0.6000	 0.5500
Li	 0.5830	 0.5370
Lj	 0.8380	 0.6010
Lk	 0.4090	 0.4600
Ll	 0.7520	 0.5630
Lm	 0.6550	 0.5470
Ln	 0.7750	 0.5660
Lo	 0.6370	 0.5440
Lp	 0.6910	 0.5640
Lr	 0.6990	 0.5760
NC	 0.4180	 0.5180
S2	 0.6580	 0.5500
SA	 0.3770	 0.4910
SB	 0.3680	 0.5050
SC	 0.4780	 0.5110
SD	 0.2190	 0.4090
SE	 0.3620	 0.4870
SF	 0.3380	 0.4960
SG	 0.1820	 0.3930
SH	 0.1890	 0.3800
SI	 0.4680	 0.5040
SJ	 0.3930	 0.4920
SK	 0.1590	 0.4240
SL	 0.5810	 0.5350
SM	 0.0010	 0.1650
SN	 0.5010	 0.5230
SO	 0.4830	 0.5300
SP	 0.2320	 0.4310
SQ	 0.3280	 0.4820
SR	 0.2120	 0.4120
SS	 0.2500	 0.4570
ST	 0.2730	 0.4870
SU	 0.2330	 0.3680
SV	 0.3480	 0.4750
SW	 0.5670	 0.5380
SX	 0.5870	 0.5430
SY	 0.2360	 0.4300
SZ	 0.1560	 0.4540
Sa	 0.5560	 0.5290
Sb	 0.3190	 0.4510

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Sc	 0.2130	 0.4180
Sd	 0.4590	 0.5040
Se	 0.3370	 0.4500
Sf	 0.0120	 0.2590
Sg	 0.0600	 0.3550
j	 0.1570	 0.4010
k	 0.4940	 0.5190