wwPDB EM Validation Summary Report

Nov 5, 2026 – 07:44 pm GMT

PDB ID	:	9T3I / pdb_00009t3i
EMDB ID	:	EMD-55496
Title	:	CRYO-EM STRUCTURE OF EKVX HUMAN CANCER CELL LINE RIBOSOME : CLASS 4
Authors	:	Rajan, K.S.; Yonath, A.
Deposited on	:	2025-10-27
Resolution	:	2.06 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:

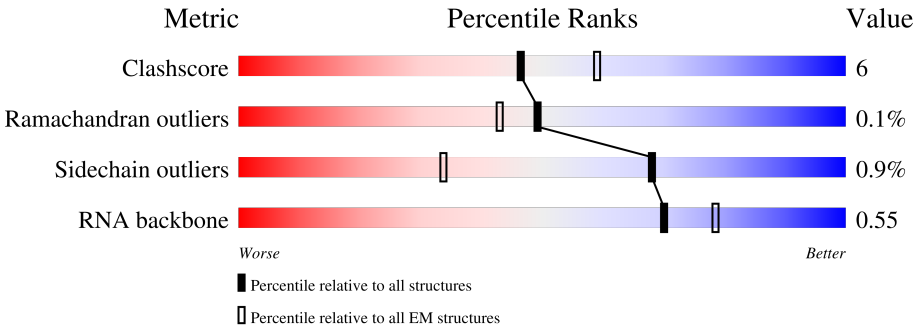
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

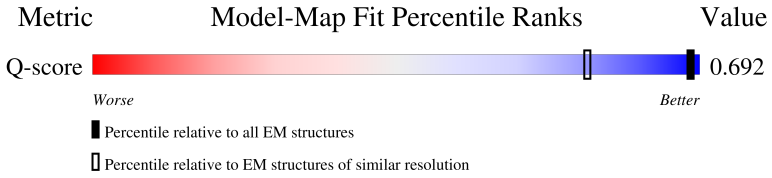
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.06 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1895 (1.56 - 2.56)

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

Mol	Chain	Length	Quality of chain
1	2	76	7% · 5% 84%
2	5	13	54% 31% 15%
3	L5	5069	40% 26% · 30%

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Mol	Chain	Length	Quality of chain
4	L7	120	76% 23%
5	L8	156	57% 39%
6	LA	257	86% 11%
7	LB	403	89% 10%
8	LC	427	79% 7% 15%
9	LD	297	90% 9%
10	LE	288	69% 8% 23%
11	LF	248	80% 11% 9%
12	LG	266	78% 12% 10%
13	LH	192	84% 15%
14	LI	214	88% 7% 5%
15	LJ	178	85% 11%
16	LL	211	90% 8%
17	LM	215	54% 9% 37%
18	LN	204	93% 7%
19	LO	203	88% 11%
20	LP	184	79% 7% 14%
21	LQ	188	91% 8%
22	LR	196	86% 9% 5%
23	LS	176	88% 13%
24	LT	160	89% 9%
25	LU	128	65% 12% 23%
26	LV	140	87% 8% 5%
27	LW	157	64% 10% 26%
28	LX	156	71% 24%

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Mol	Chain	Length	Quality of chain
29	LY	145	85% 7% 8%
30	LZ	136	91% 7%
31	La	148	92% 7%
32	Lb	159	64% 6% 30%
33	Lc	115	75% 11% 14%
34	Ld	125	72% 13% 15%
35	Le	135	86% 9% 5%
36	Lf	110	91% 7%
37	Lg	117	91% 7%
38	Lh	123	93% 7%
39	Li	105	91% 6%
40	Lj	97	87% 11%
41	Lk	70	83% 16%
42	Ll	51	92% 6%
43	Lm	128	38% 59%
44	Ln	25	72% 28%
45	Lo	106	84% 12%
46	Lp	92	92% 5%
47	Lr	137	85% 5% 9%
48	S2	1869	47% 35% 6% 11%
49	SA	295	63% 12% 24%
50	SB	264	73% 12% 16%
51	SC	293	64% 11% 25%
52	SD	243	80% 12% 8%
53	SE	263	86% 13%

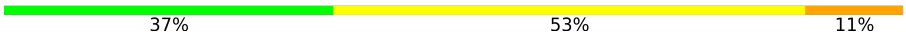
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Mol	Chain	Length	Quality of chain
54	SF	204	78% 11% 10%
55	SG	249	77% 15% 8%
56	SH	194	79% 16%
57	SI	208	80% 19%
58	SJ	194	82% 11% 7%
59	SK	165	49% 9% 42%
60	SL	158	84% 9% 8%
61	SM	132	68% 23% 9%
62	SN	151	90% 9%
63	SO	151	82% 8% 10%
64	SP	145	79% 11% 10%
65	SQ	146	82% 14%
66	SR	135	83% 16%
67	SS	152	84% 13%
68	ST	145	92% 6%
69	SU	119	68% 16% 15%
70	SV	83	84% 16%
71	SW	130	82% 17%
72	SX	143	90% 8%
73	SY	133	73% 22% 5%
74	SZ	125	55% 10% 33%
75	Sa	115	73% 12% 14%
76	Sb	84	86% 13%
77	Sc	69	72% 19% 9%
78	Sd	56	82% 11% 7%

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Mol	Chain	Length	Quality of chain
79	Se	133	
80	Sf	156	
81	Sg	317	
82	3	77	
83	4	19	

2 Entry composition (i)

There are 92 unique types of molecules in this entry. The entry contains 216087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called A-tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	2	12	263	121	47	82	12	1	0	0

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	11	229	103	38	77	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L5	3546	76092	33924	13915	24708	3545	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	L8	156	3316	1482	585	1094	155	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LA	251	1932	1209	397	320	6	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LA	98	VAL	ILE	variant	UNP P62917

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LC	365	Total	C	N	O	S	0	0
			2901	1824	579	484	14		

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LD	294	Total	C	N	O	S	0	0
			2367	1498	431	424	14		

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LE	223	Total	C	N	O	S	0	0
			1782	1147	338	293	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LF	225	Total	C	N	O	S	1	0
			1877	1207	361	300	9		

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LG	240	Total	C	N	O	S	0	0
			1914	1219	369	322	4		

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LH	190	Total	C	N	O	S	0	0
			1514	953	283	272	6		

- Molecule 14 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LI	203	Total	C	N	O	S	0	0
			1641	1043	317	268	13		

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 16 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LL	206	Total	C	N	O	S	0	0
			1652	1033	343	272	4		

- Molecule 17 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LM	136	Total	C	N	O	S	0	0
			1113	714	213	179	7		

- Molecule 18 is a protein called 60S ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LO	202	Total	C	N	O	S	0	0
			1654	1066	322	261	5		

- Molecule 20 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LP	158	Total	C	N	O	S	1	0
			1277	802	249	217	9		

- Molecule 21 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LQ	187	Total	C	N	O	S	0	0
			1509	943	314	247	5		

- Molecule 22 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LR	187	Total	C	N	O	S	0	0
			1558	966	335	248	9		

- Molecule 23 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LS	176	Total	C	N	O	S	0	0
			1456	927	283	235	11		

- Molecule 24 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LT	158	Total	C	N	O	S	2	0
			1284	816	252	211	5		

- Molecule 25 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LU	99	Total	C	N	O	S	0	0
			784	504	137	141	2		

- Molecule 26 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LV	133	Total	C	N	O	S	1	0
			993	627	188	173	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	116	Total	C	N	O	S	0	0
			891	557	180	150	4		

- Molecule 28 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LX	118	Total	C	N	O	S	0	0
			953	609	177	166	1		

- Molecule 29 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LY	133	Total	C	N	O	S	0	0
			1098	690	223	182	3		

- Molecule 30 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LZ	135	Total	C	N	O	S	0	0
			1102	711	205	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LZ	108	CYS	ARG	conflict	UNP P61353

- Molecule 31 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 32 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lb	111	Total	C	N	O	S	0	0
			888	554	191	139	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lc	99	Total	C	N	O	S	0	0
			770	488	136	140	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ld	106	Total	C	N	O	S	0	0
			868	550	170	146	2		

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Le	128	Total	C	N	O	S	1	0
			1061	672	219	165	5		

- Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lf	109	Total	C	N	O	S	0	0
			875	555	174	143	3		

- Molecule 37 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lg	114	Total	C	N	O	S	0	0
			902	563	186	147	6		

- Molecule 38 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lh	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 39 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Li	102	Total	C	N	O	S	0	0
			828	518	176	129	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lk	69	Total	C	N	O	S	0	0
			548	353	100	94	1		

- Molecule 42 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ll	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 43 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lm	52	Total	C	N	O	S	1	0
			432	269	90	67	6		

- Molecule 44 is a protein called 60S ribosomal protein L41.

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

- Molecule 45 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lo	105	Total	C	N	O	S	2	0
			877	552	180	139	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lp	90	Total	C	N	O	S	1	0
			703	444	137	115	7		

- Molecule 47 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lr	124	Total	C	N	O	S	0	0
			986	611	204	167	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lr	2	ACE	-	acetylation	UNP A0A2K6C1I7

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	1664	Total	C	N	O	P	0	0
			35566	15905	6374	11624	1663		

- Molecule 49 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SA	223	Total	C	N	O	S	0	0
			1746	1109	306	323	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	2	ACE	-	acetylation	UNP P08865

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SB	223	Total	C	N	O	S	0	0
			1802	1142	324	322	14		

- Molecule 51 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SC	220	Total	C	N	O	S	0	0
			1707	1104	293	300	10		

- Molecule 52 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SD	223	Total	C	N	O	S	0	0
			1731	1105	313	306	7		

- Molecule 53 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SF	183	Total	C	N	O	S	0	0
			1446	908	269	262	7		

- Molecule 55 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SG	229	Total	C	N	O	S	0	0
			1833	1147	368	311	7		

- Molecule 56 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SH	186	Total	C	N	O	S	0	0
			1474	937	270	266	1		

- Molecule 57 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SI	206	Total	C	N	O	S	0	0
			1671	1046	329	291	5		

- Molecule 58 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SJ	180	Total	C	N	O	S	0	0
			1495	952	299	242	2		

- Molecule 59 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SK	96	Total	C	N	O	S	0	0
			804	527	140	131	6		

- Molecule 60 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SL	146	Total	C	N	O	S	0	0
			1200	766	226	202	6		

- Molecule 61 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SM	120	Total	C	N	O	S	0	0
			920	577	165	171	7		

- Molecule 62 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SN	150	Total	C	N	O	S	0	0
			1207	773	229	204	1		

- Molecule 63 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SO	136	Total	C	N	O	S	0	0
			1008	618	199	185	6		

- Molecule 64 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SP	131	Total	C	N	O	S	0	0
			1072	681	201	183	7		

- Molecule 65 is a protein called 40S ribosomal protein S16.

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

- Molecule 66 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SR	133	Total	C	N	O	S	0	0
			1075	675	200	196	4		

- Molecule 67 is a protein called 40S ribosomal protein S18.

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

- Molecule 68 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	ST	142	Total	C	N	O	S	0	0
			1103	691	212	197	3		

- Molecule 69 is a protein called 40S ribosomal protein S20.

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

- Molecule 70 is a protein called 40S ribosomal protein S21.

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

- Molecule 71 is a protein called 40S ribosomal protein S15a.

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

- Molecule 72 is a protein called 40S ribosomal protein S23.

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

- Molecule 73 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SY	127	Total	C	N	O	S	1	0
			1042	659	203	175	5		

- Molecule 74 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SZ	84	Total	C	N	O	S	0	0
			674	433	126	114	1		

- Molecule 75 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sa	99	Total	C	N	O	S	1	0
			800	497	168	130	5		

- Molecule 76 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sb	83	Total	C	N	O	S	0	0
			647	406	121	113	7		

- Molecule 77 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sc	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 78 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sd	52	Total	C	N	O	S	0	0
			426	268	85	68	5		

- Molecule 79 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Se	50	Total	C	N	O	S	0	0
			394	241	88	64	1		

- Molecule 80 is a protein called Ubiquitin.

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

- Molecule 81 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 82 is a RNA chain called P-site_tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	3	71	Total 1513	C 676	N 277	O 490	P 70	0	0

- Molecule 83 is a RNA chain called E-site_tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	4	19	Total 402	C 180	N 72	O 132	P 18	0	0

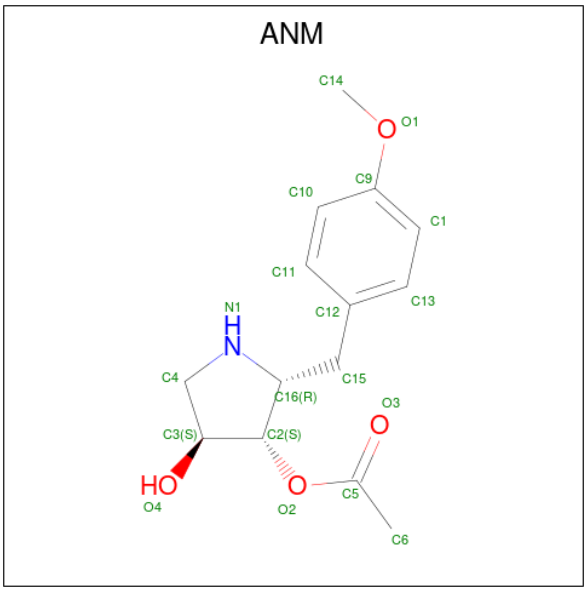
- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	5	1	Total 1	Mg 1	0
84	L5	202	Total 202	Mg 202	0
84	L7	4	Total 4	Mg 4	0
84	L8	3	Total 3	Mg 3	0
84	LI	1	Total 1	Mg 1	0
84	LP	1	Total 1	Mg 1	0
84	LR	1	Total 1	Mg 1	0
84	LV	1	Total 1	Mg 1	0
84	Lj	1	Total 1	Mg 1	0
84	S2	72	Total 72	Mg 72	0
84	SX	1	Total 1	Mg 1	0

- Molecule 85 is POTASSIUM ION (CCD ID: K) (formula: K).

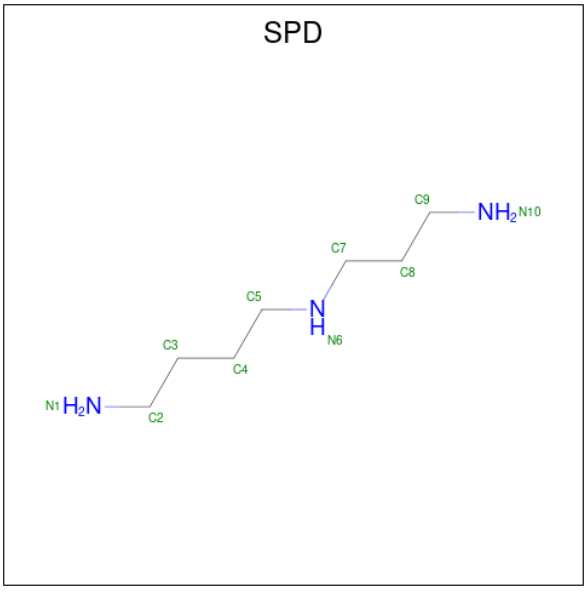
Mol	Chain	Residues	Atoms	AltConf
85	5	1	Total K 1 1	0
85	L5	51	Total K 51 51	0
85	LA	1	Total K 1 1	0
85	LH	1	Total K 1 1	0
85	LI	1	Total K 1 1	0
85	Le	1	Total K 1 1	0
85	Lf	1	Total K 1 1	0
85	Lg	1	Total K 1 1	0
85	Ln	1	Total K 1 1	0
85	S2	25	Total K 25 25	0
85	SL	1	Total K 1 1	0
85	SO	1	Total K 1 1	0
85	Sa	1	Total K 1 1	0
85	Sd	1	Total K 1 1	0

- Molecule 86 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



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

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



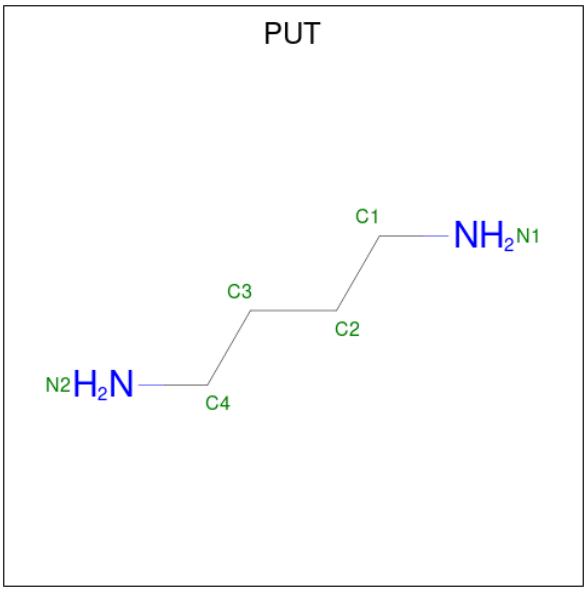
Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms	AltConf
87	L5	1	Total C N 10 7 3	0
87	L5	1	Total C N 10 7 3	0
87	L5	1	Total C N 10 7 3	0
87	L5	1	Total C N 10 7 3	0
87	L5	1	Total C N 10 7 3	0
87	L5	1	Total C N 10 7 3	0
87	L5	1	Total C N 10 7 3	0
87	L5	1	Total C N 10 7 3	0
87	L5	1	Total C N 10 7 3	0
87	LN	1	Total C N 10 7 3	0
87	Ln	1	Total C N 10 7 3	0
87	S2	1	Total C N 10 7 3	0
87	S2	1	Total C N 10 7 3	0
87	S2	1	Total C N 10 7 3	0
87	S2	1	Total C N 10 7 3	0
87	S2	1	Total C N 10 7 3	0
87	S2	1	Total C N 10 7 3	0
87	S2	1	Total C N 10 7 3	0

- Molecule 88 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



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

- Molecule 89 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
89	L5	4	Total Na 4 4	0
89	La	1	Total Na 1 1	0

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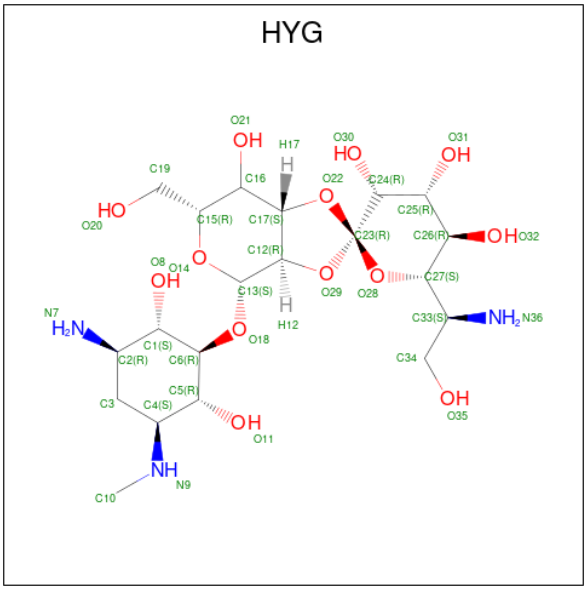
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Mol	Chain	Residues	Atoms	AltConf
89	S2	3	Total Na 3 3	0

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 91 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



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

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	5	6	Total	O	0
			6	6	
92	L5	2336	Total	O	0
			2336	2336	
92	L7	26	Total	O	0
			26	26	
92	L8	37	Total	O	0
			37	37	
92	LA	58	Total	O	0
			58	58	
92	LB	47	Total	O	0
			47	47	
92	LC	41	Total	O	0
			41	41	
92	LD	4	Total	O	0
			4	4	
92	LE	1	Total	O	0
			1	1	
92	LF	16	Total	O	0
			16	16	
92	LG	1	Total	O	0
			1	1	
92	LH	1	Total	O	0
			1	1	
92	LI	5	Total	O	0
			5	5	
92	LL	21	Total	O	0
			21	21	
92	LN	36	Total	O	0
			36	36	
92	LO	7	Total	O	0
			7	7	
92	LP	15	Total	O	0
			15	15	
92	LQ	20	Total	O	0
			20	20	
92	LR	13	Total	O	0
			13	13	

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Mol	Chain	Residues	Atoms	AltConf
92	LS	4	Total O 4 4	0
92	LT	11	Total O 11 11	0
92	LV	9	Total O 9 9	0
92	LX	2	Total O 2 2	0
92	LY	2	Total O 2 2	0
92	LZ	2	Total O 2 2	0
92	La	19	Total O 19 19	0
92	Lb	12	Total O 12 12	0
92	Lc	3	Total O 3 3	0
92	Ld	3	Total O 3 3	0
92	Le	16	Total O 16 16	0
92	Lf	9	Total O 9 9	0
92	Lg	12	Total O 12 12	0
92	Lh	2	Total O 2 2	0
92	Li	1	Total O 1 1	0
92	Lj	13	Total O 13 13	0
92	Ll	2	Total O 2 2	0
92	Lm	1	Total O 1 1	0
92	Ln	11	Total O 11 11	0
92	Lo	13	Total O 13 13	0
92	Lp	17	Total O 17 17	0

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Mol	Chain	Residues	Atoms	AltConf
92	Lr	4	Total O 4 4	0
92	S2	901	Total O 901 901	0
92	SA	2	Total O 2 2	0
92	SB	7	Total O 7 7	0
92	SC	5	Total O 5 5	0
92	SD	3	Total O 3 3	0
92	SE	3	Total O 3 3	0
92	SF	3	Total O 3 3	0
92	SI	6	Total O 6 6	0
92	SL	13	Total O 13 13	0
92	SN	13	Total O 13 13	0
92	SO	13	Total O 13 13	0
92	SQ	5	Total O 5 5	0
92	SR	2	Total O 2 2	0
92	SS	1	Total O 1 1	0
92	SU	5	Total O 5 5	0
92	SW	4	Total O 4 4	0
92	SX	4	Total O 4 4	0
92	Sa	11	Total O 11 11	0
92	Sb	2	Total O 2 2	0
92	Sc	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
92	3	9	Total O 9 9	0
92	4	8	Total O 8 8	0

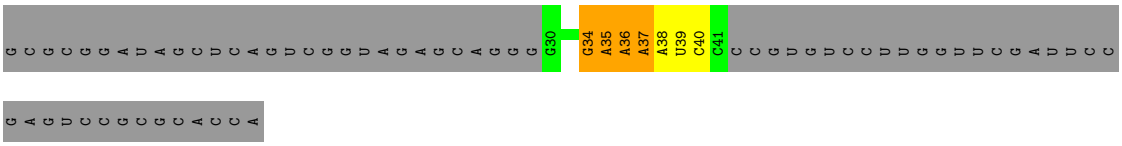
3 Residue-property plots (i)

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

- Molecule 1: A-tRNA-Phe

Chain 2:

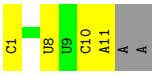




- Molecule 2: mRNA

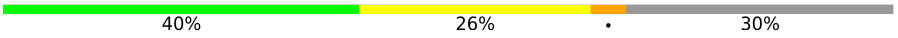
Chain 5:

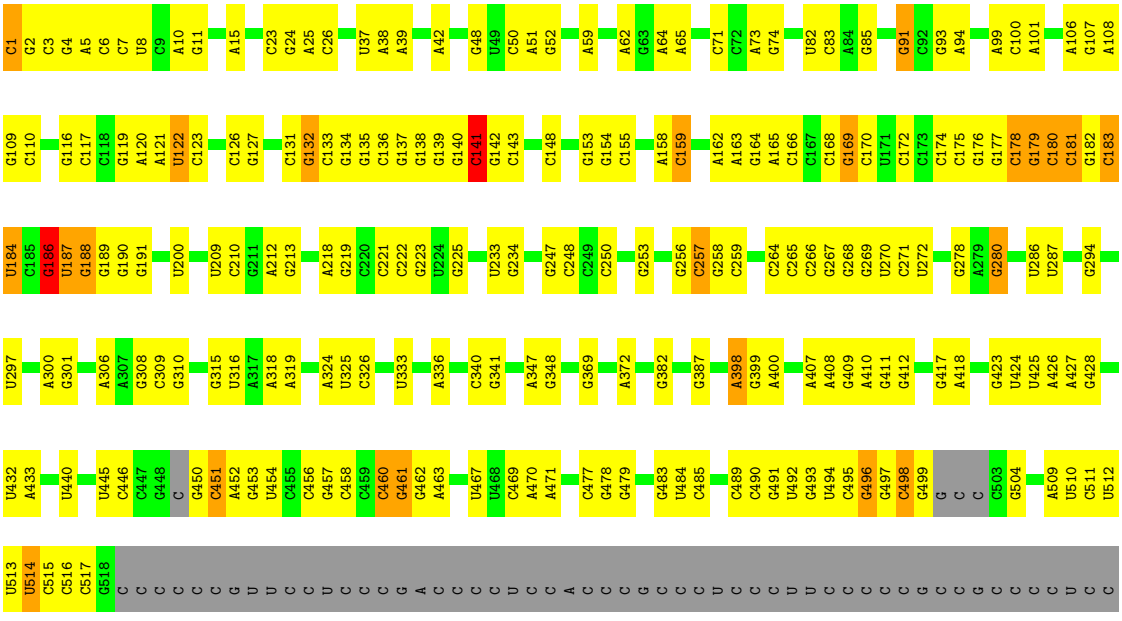


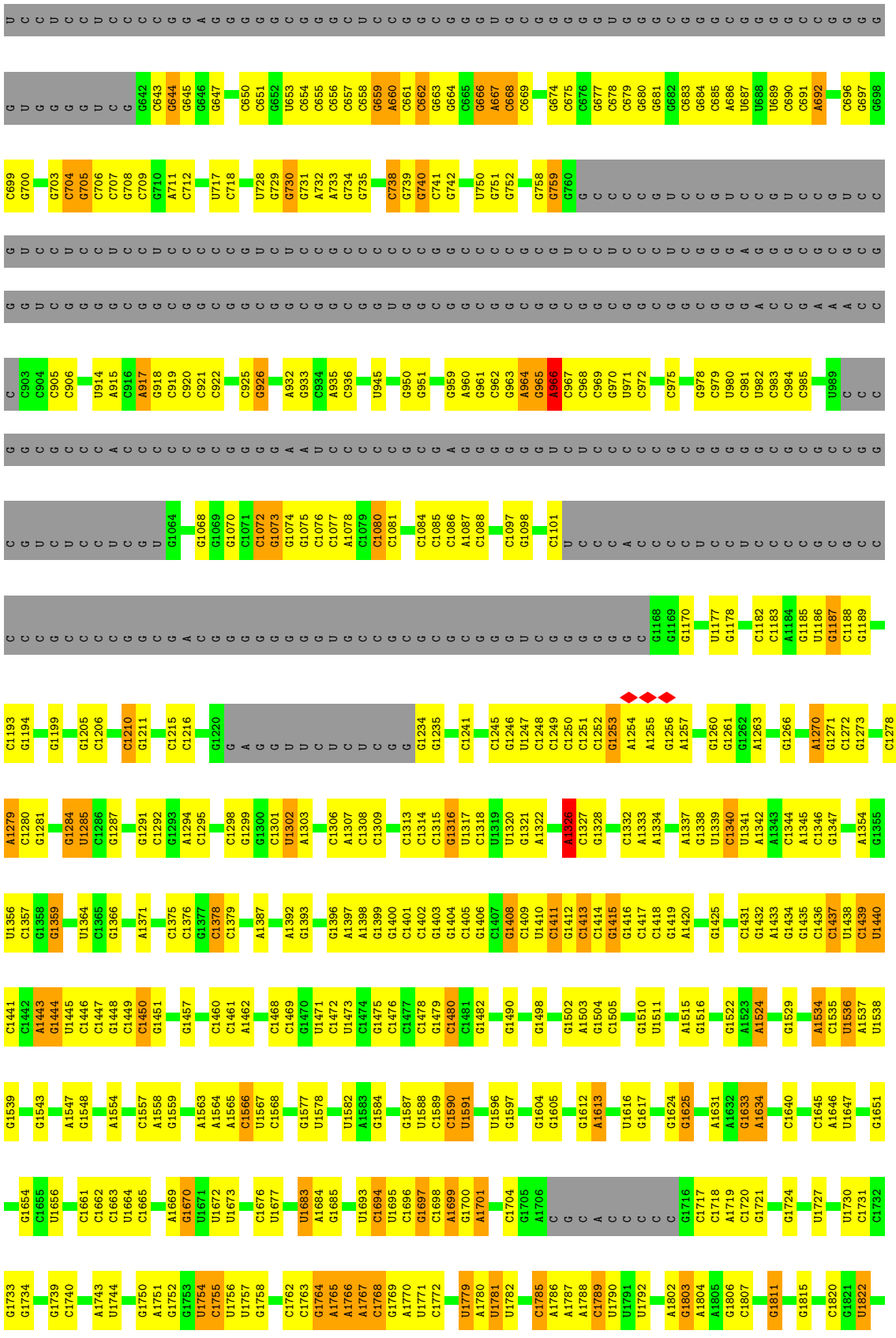


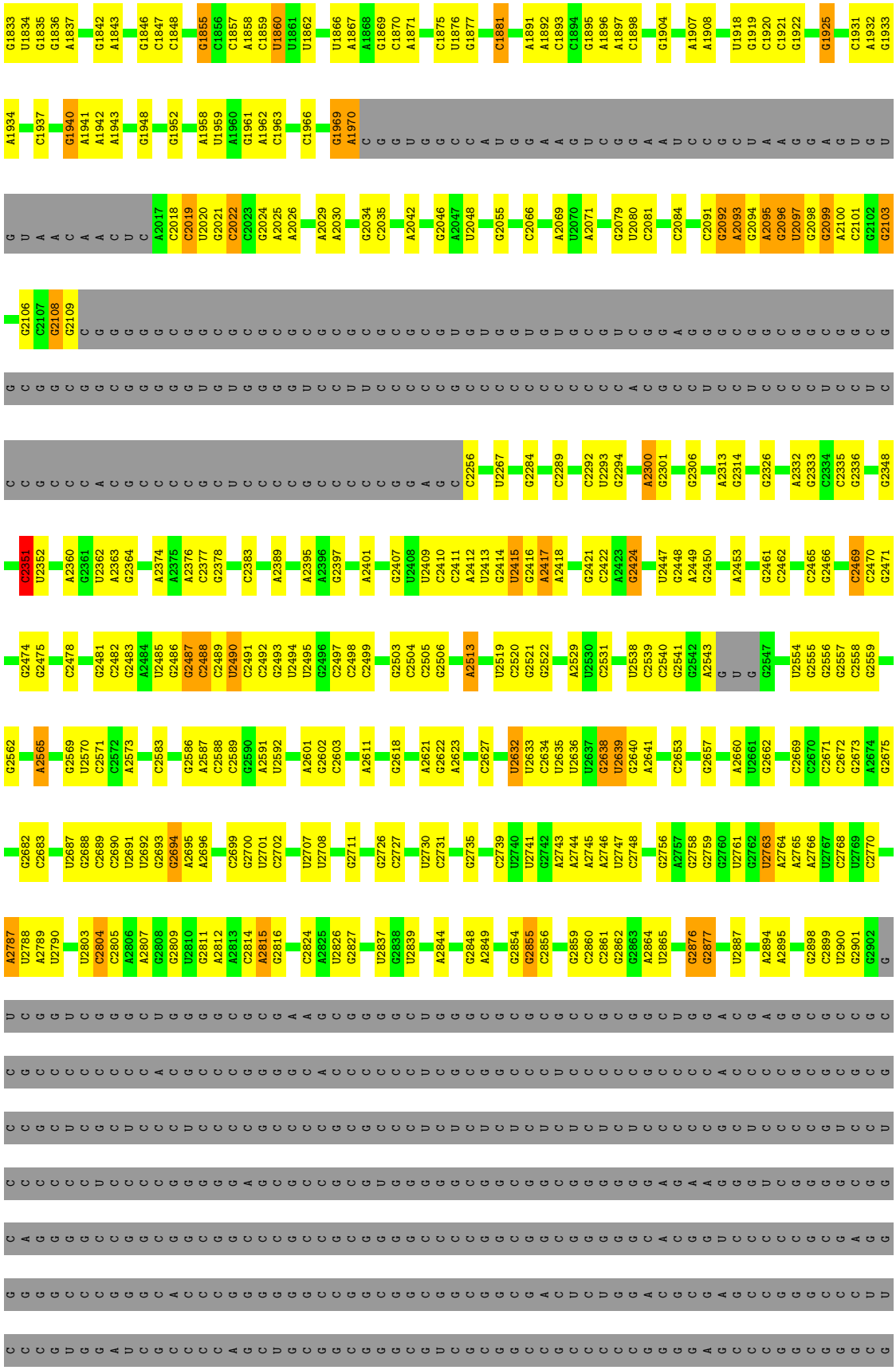
- Molecule 3: 28S rRNA

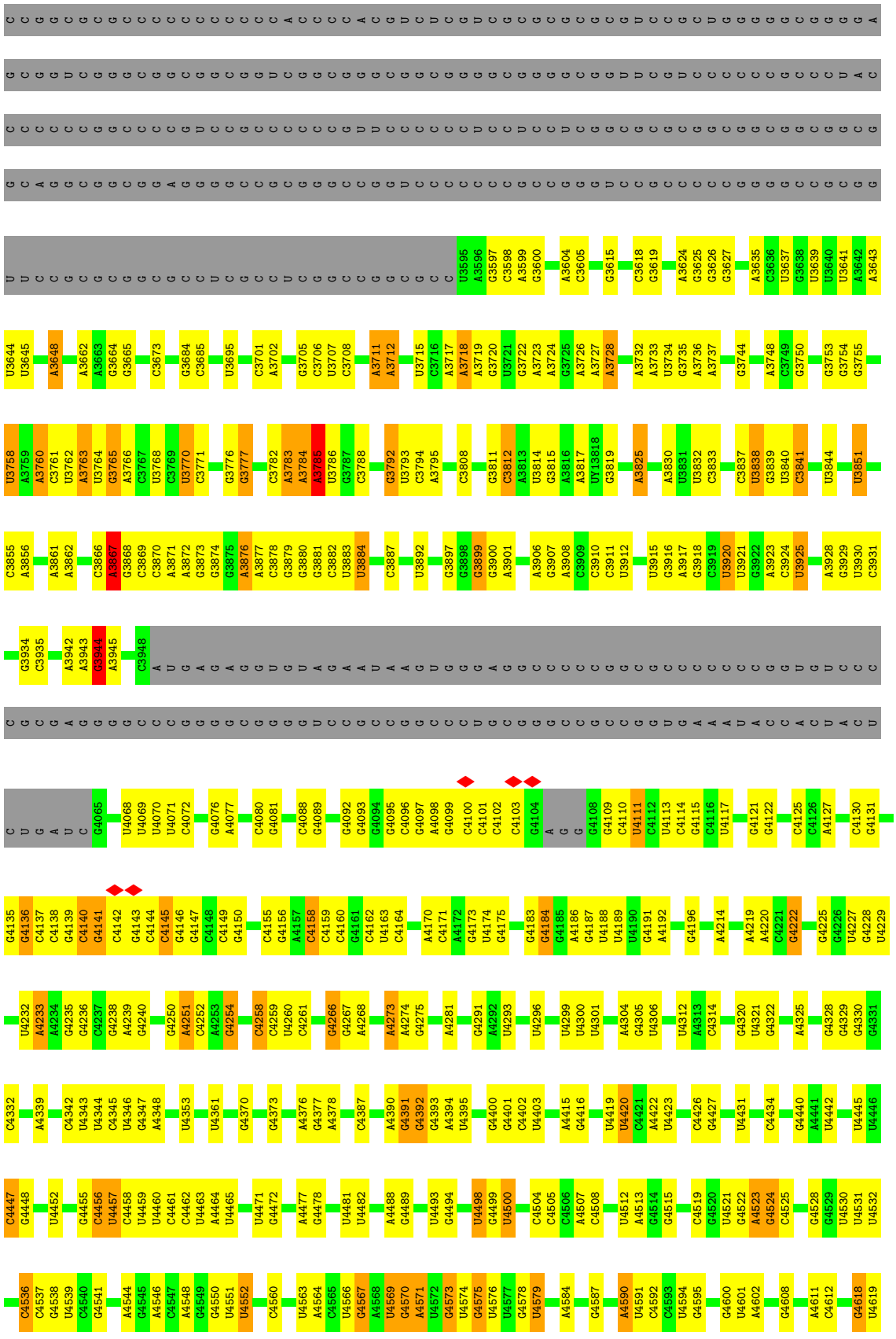
Chain L5:

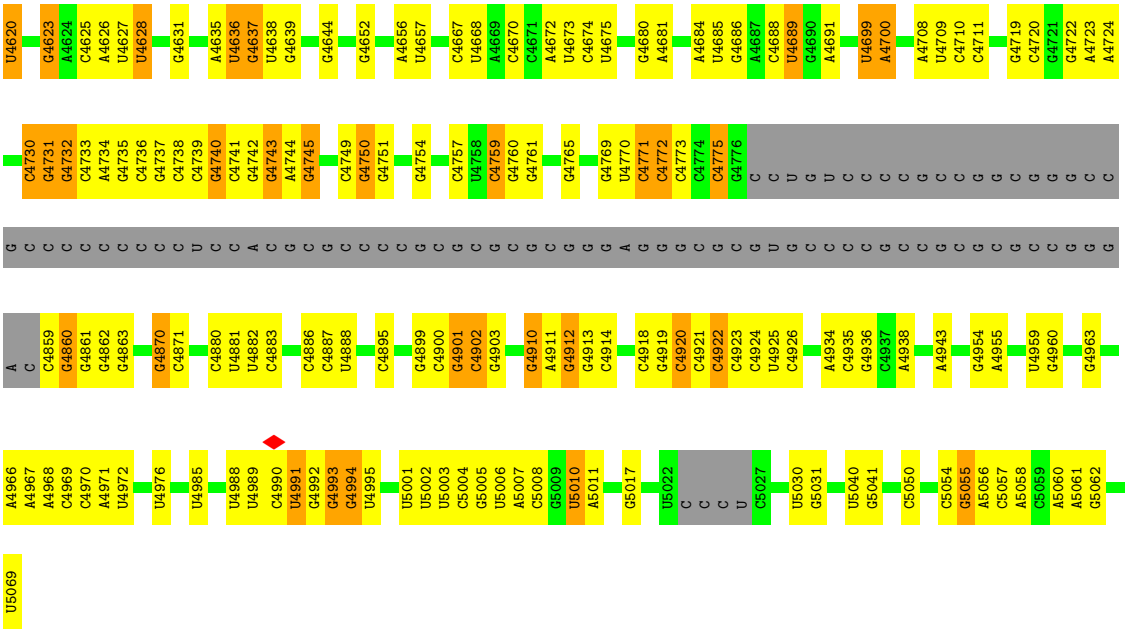








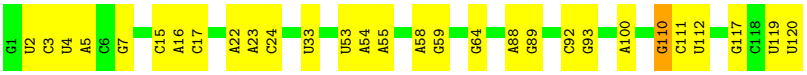




• Molecule 4: 5S rRNA

Chain L7:

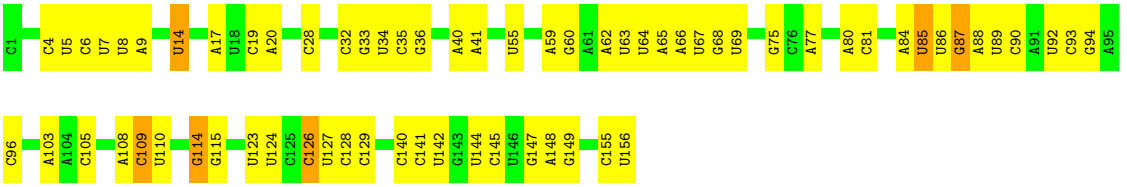




• Molecule 5: 5.8S rRNA

Chain L8:

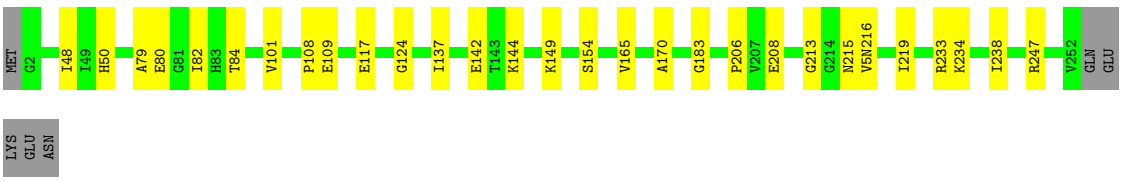




• Molecule 6: Large ribosomal subunit protein uL2

Chain LA:

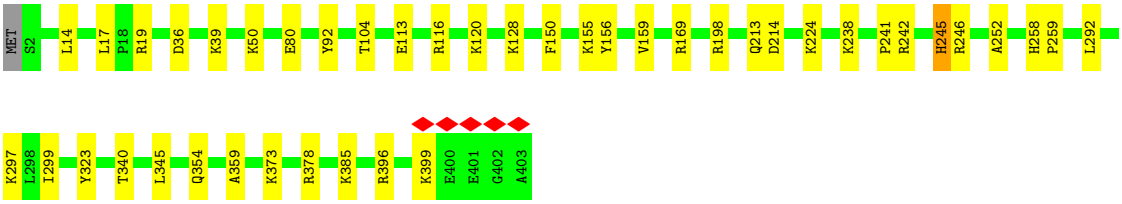




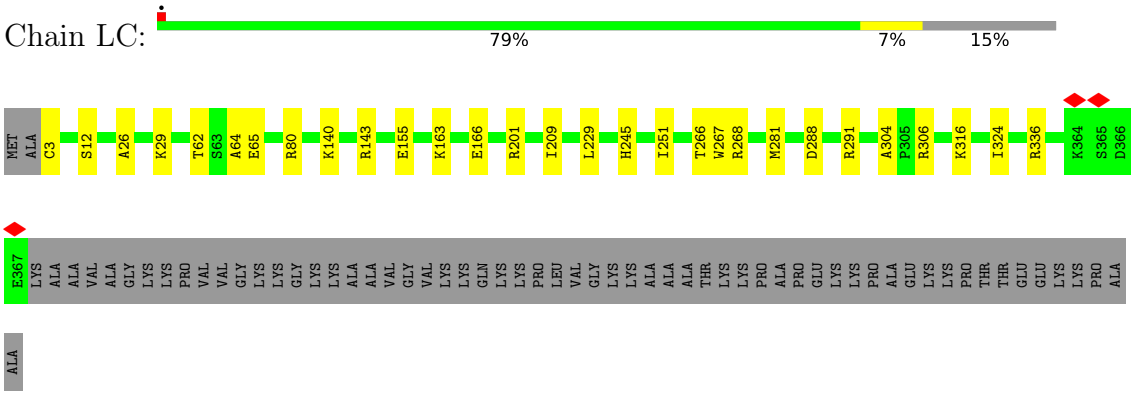
• Molecule 7: Large ribosomal subunit protein uL3

Chain LB:

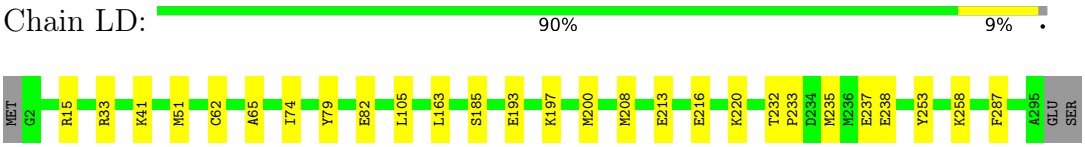




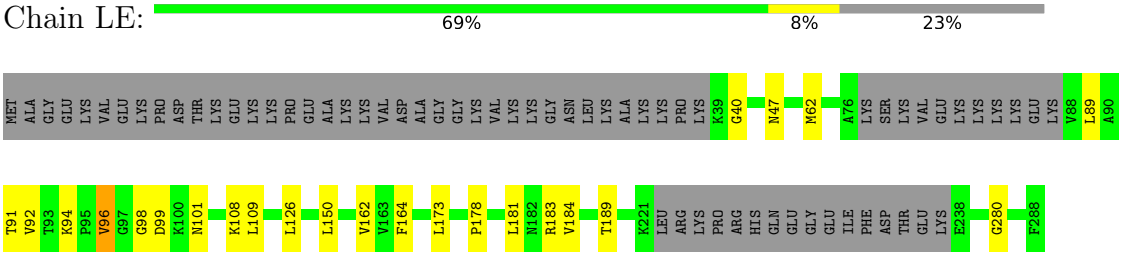
• Molecule 8: 60S ribosomal protein L4



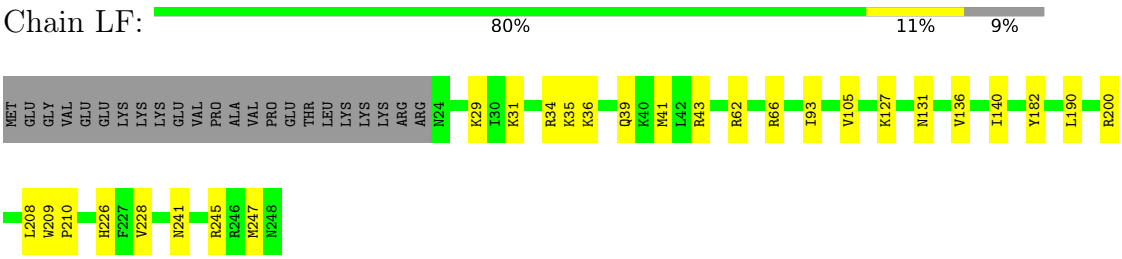
• Molecule 9: 60S ribosomal protein L5



• Molecule 10: Large ribosomal subunit protein eL6

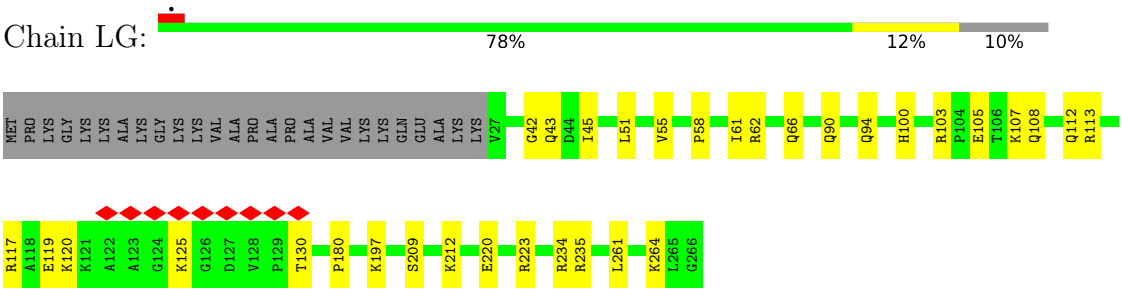


• Molecule 11: Large ribosomal subunit protein uL30



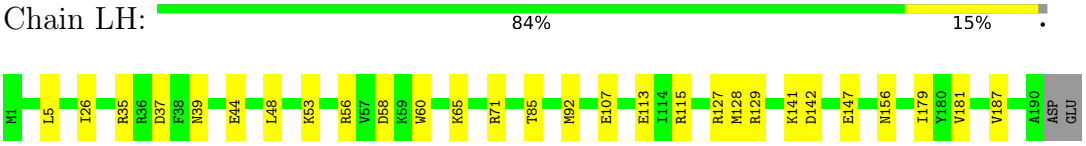
• Molecule 12: 60S ribosomal protein L7a

Chain LG:



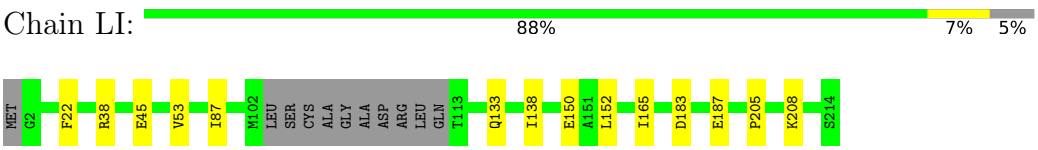
• Molecule 13: 60S ribosomal protein L9

Chain LH:



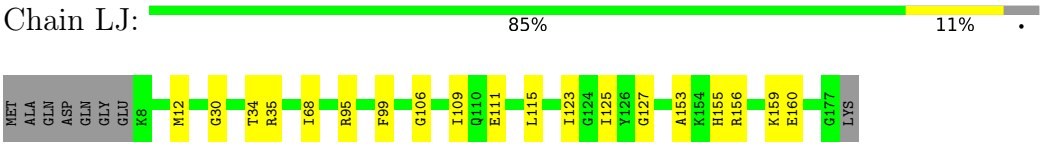
• Molecule 14: 60S ribosomal protein L10

Chain LI:



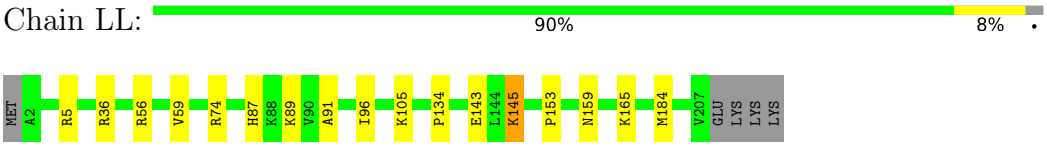
• Molecule 15: 60S ribosomal protein L11

Chain LJ:



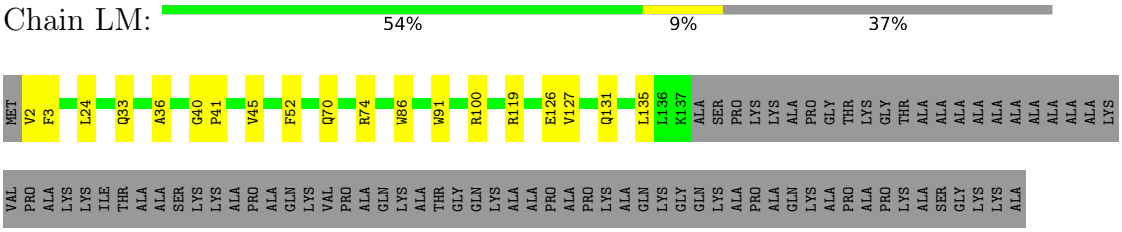
• Molecule 16: Large ribosomal subunit protein eL13

Chain LL:



• Molecule 17: 60S ribosomal protein L14

Chain LM:



• Molecule 18: 60S ribosomal protein L15

Chain LN:





• Molecule 19: 60S ribosomal protein L13a

Chain LO:

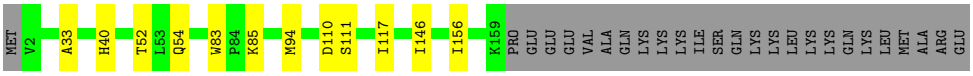




• Molecule 20: 60S ribosomal protein L17

Chain LP:

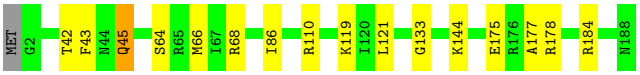




• Molecule 21: 60S ribosomal protein L18

Chain LQ:

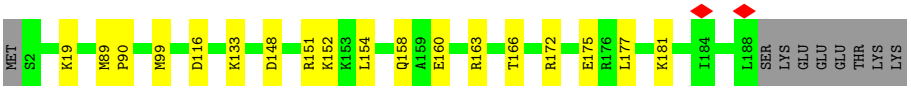




• Molecule 22: 60S ribosomal protein L19

Chain LR:

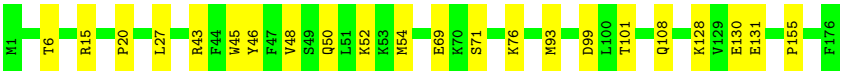




• Molecule 23: 60S ribosomal protein L18a

Chain LS:





• Molecule 24: 60S ribosomal protein L21

Chain LT:

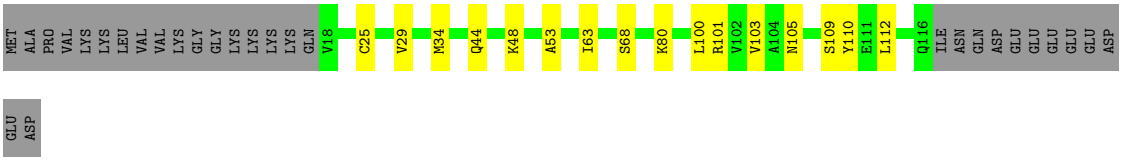




• Molecule 25: 60S ribosomal protein L22

Chain LU:

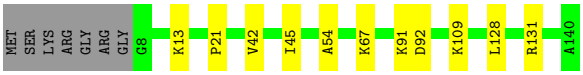




• Molecule 26: 60S ribosomal protein L23

Chain LV:

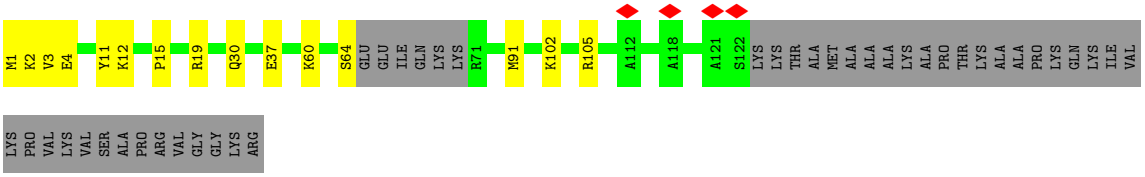




• Molecule 27: 60S ribosomal protein L24

Chain LW:





• Molecule 28: 60S ribosomal protein L23a

Chain LX:

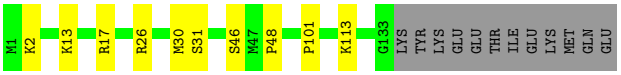




• Molecule 29: 60S ribosomal protein L26

Chain LY:





• Molecule 30: Large ribosomal subunit protein eL27

Chain LZ:

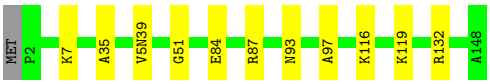




• Molecule 31: Large ribosomal subunit protein uL15

Chain La:

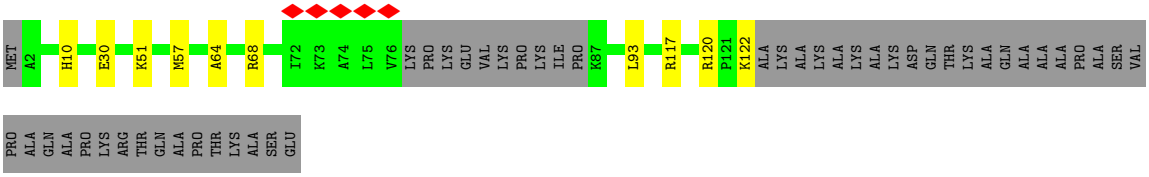




• Molecule 32: Large ribosomal subunit protein eL29

Chain Lb:

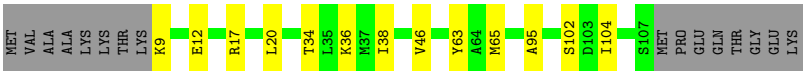




• Molecule 33: 60S ribosomal protein L30

Chain Lc:

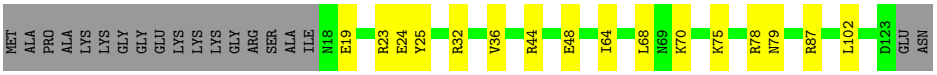




• Molecule 34: 60S ribosomal protein L31

Chain Ld:

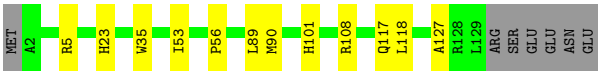




• Molecule 35: 60S ribosomal protein L32

Chain Le:

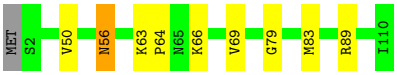




• Molecule 36: 60S ribosomal protein L35a

Chain Lf:





• Molecule 37: 60S ribosomal protein L34

Chain Lg:

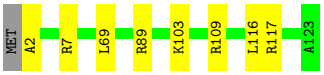




• Molecule 38: 60S ribosomal protein L35

Chain Lh:





• Molecule 39: 60S ribosomal protein L36

Chain Li:

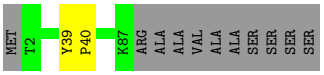




• Molecule 40: Large ribosomal subunit protein eL37

Chain Lj:





• Molecule 41: 60S ribosomal protein L38

Chain Lk:

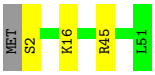




• Molecule 42: 60S ribosomal protein L39

Chain Ll:

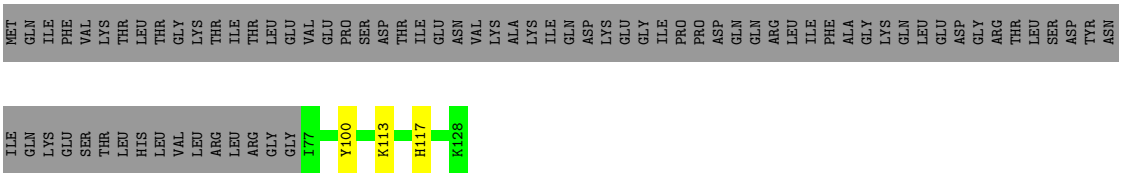




• Molecule 43: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:

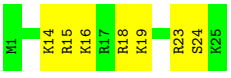




• Molecule 44: 60S ribosomal protein L41

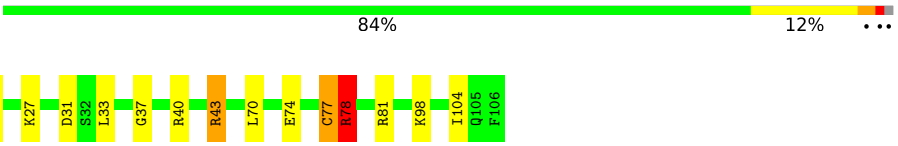
Chain Ln:





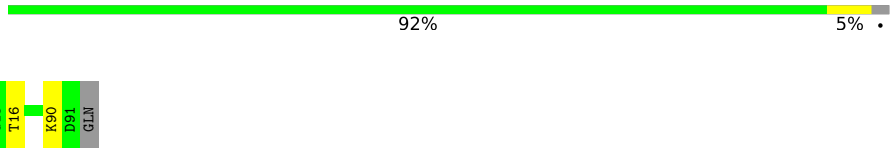
• Molecule 45: Large ribosomal subunit protein eL42

Chain Lo:



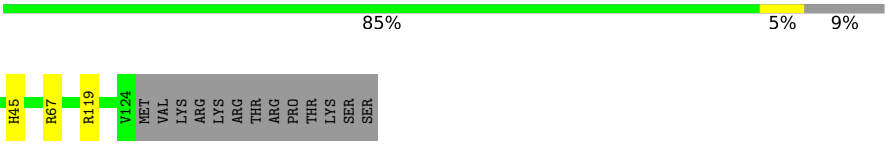
• Molecule 46: 60S ribosomal protein L37a

Chain Lp:



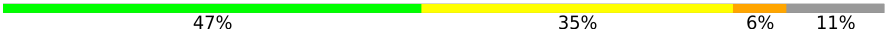
• Molecule 47: Large ribosomal subunit protein eL28

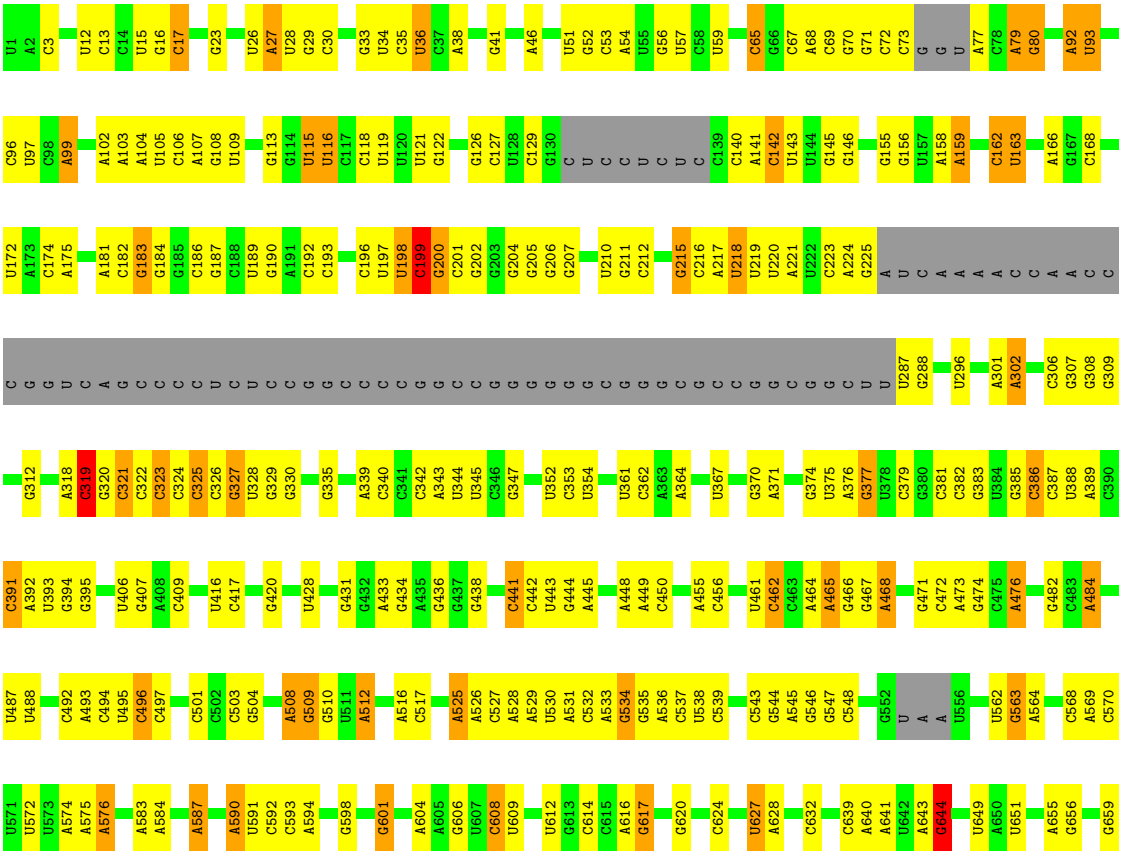
Chain Lr:

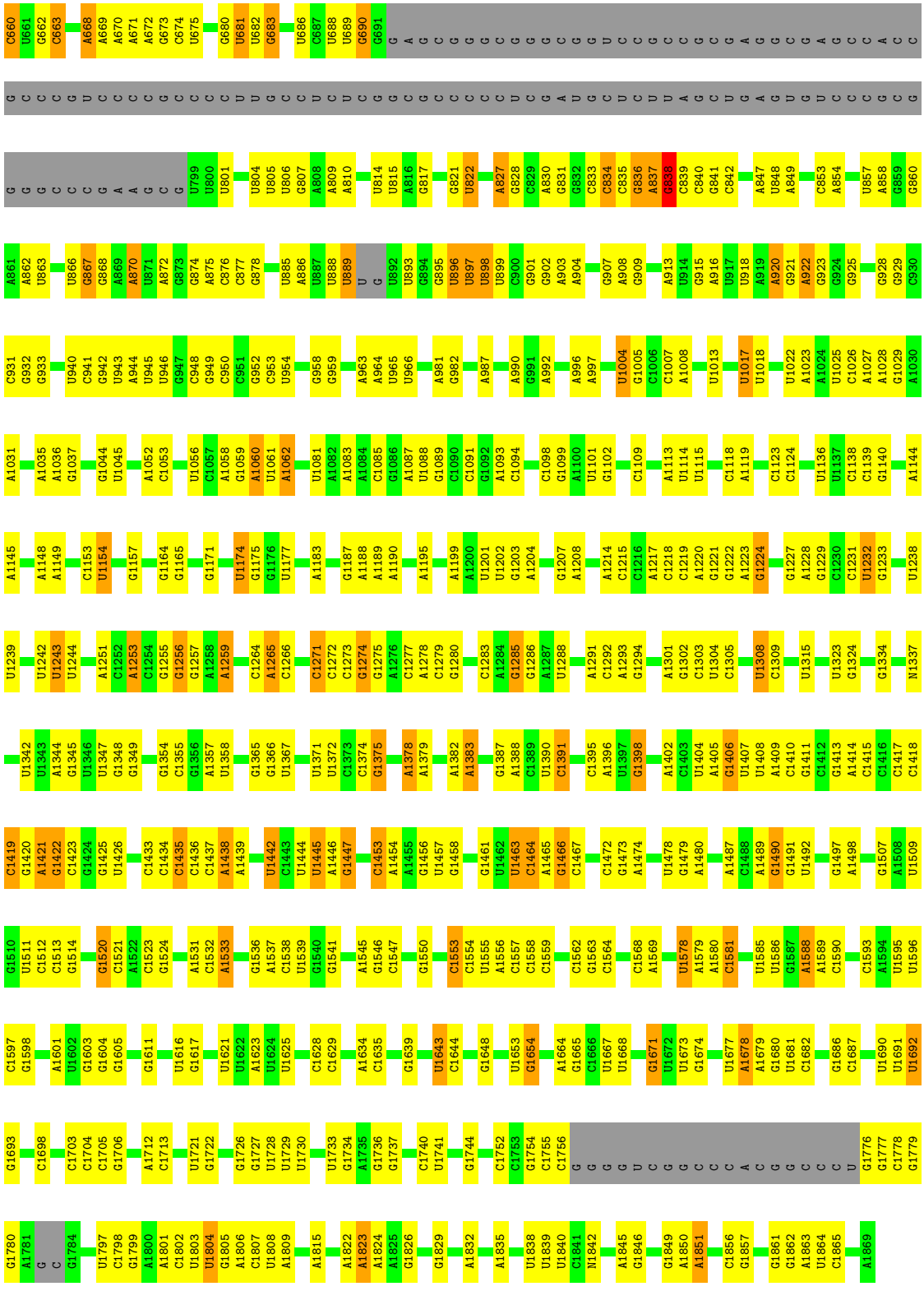


• Molecule 48: 18S rRNA

Chain S2:



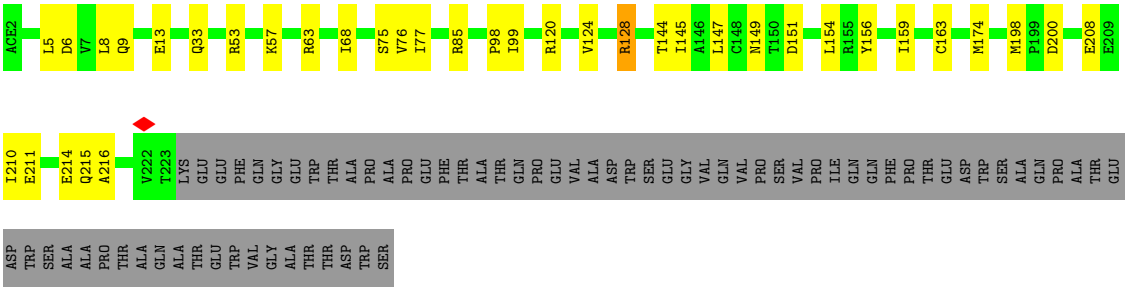




• Molecule 49: Small ribosomal subunit protein uS2

Chain SA:

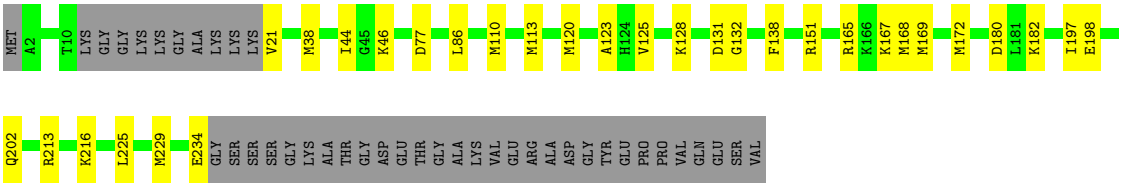




• Molecule 50: 40S ribosomal protein S3a

Chain SB:

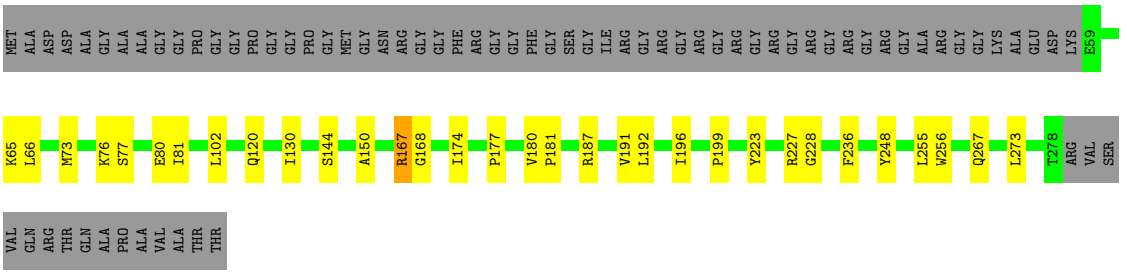




• Molecule 51: 40S ribosomal protein S2

Chain SC:

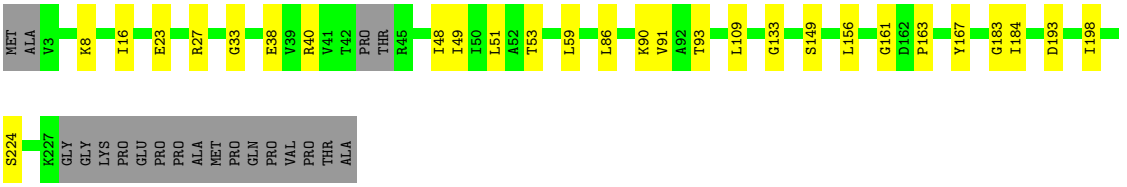




• Molecule 52: 40S ribosomal protein S3

Chain SD:



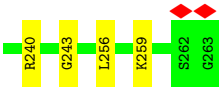


• Molecule 53: Small ribosomal subunit protein eS4, X isoform

Chain SE:







• Molecule 54: 40S ribosomal protein S5

Chain SF:







• Molecule 55: 40S ribosomal protein S6

Chain SG:



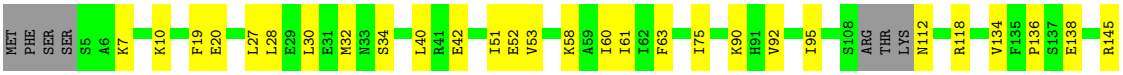




• Molecule 56: 40S ribosomal protein S7

Chain SH:



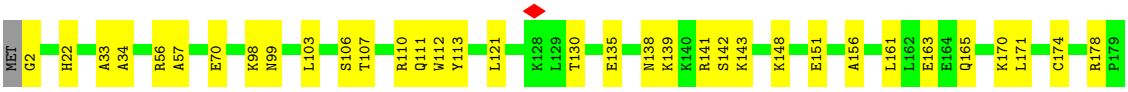




• Molecule 57: 40S ribosomal protein S8

Chain SI:



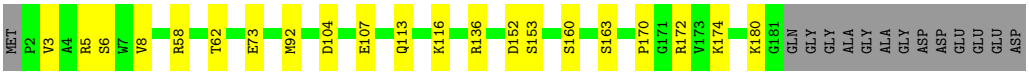




• Molecule 58: 40S ribosomal protein S9

Chain SJ:





• Molecule 59: 40S ribosomal protein S10

Chain SK:





• Molecule 60: 40S ribosomal protein S11

Chain SL:

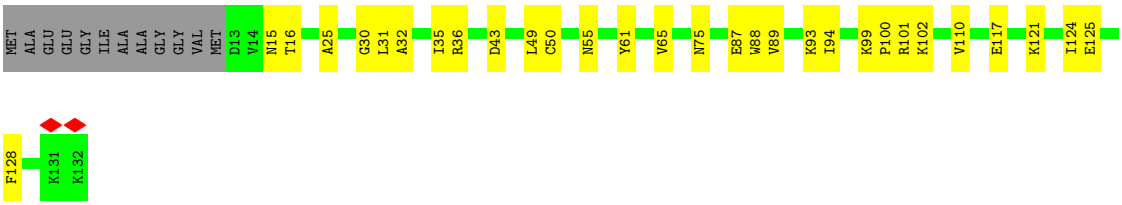




• Molecule 61: 40S ribosomal protein S12

Chain SM:

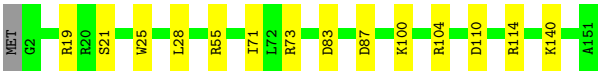




• Molecule 62: 40S ribosomal protein S13

Chain SN:





• Molecule 63: 40S ribosomal protein S14

Chain SO:

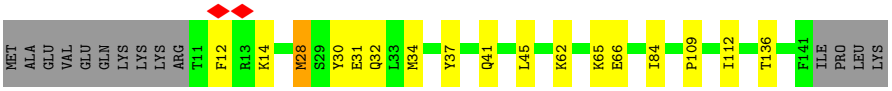




• Molecule 64: 40S ribosomal protein S15

Chain SP:

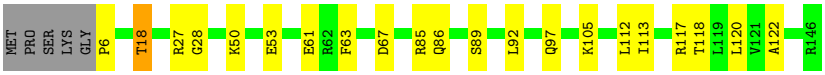




• Molecule 65: 40S ribosomal protein S16

Chain SQ:





• Molecule 66: 40S ribosomal protein S17

Chain SR:





• Molecule 67: 40S ribosomal protein S18

Chain SS:

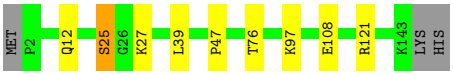




• Molecule 68: 40S ribosomal protein S19

Chain ST:





• Molecule 69: 40S ribosomal protein S20

Chain SU:

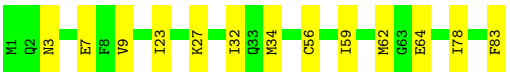




• Molecule 70: 40S ribosomal protein S21

Chain SV:





• Molecule 71: 40S ribosomal protein S15a

Chain SW:





• Molecule 72: 40S ribosomal protein S23

Chain SX:

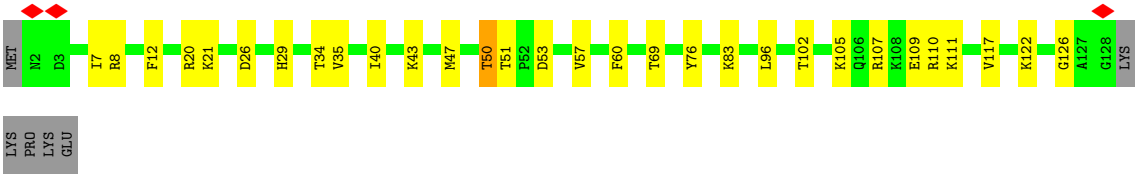




• Molecule 73: 40S ribosomal protein S24

Chain SY:

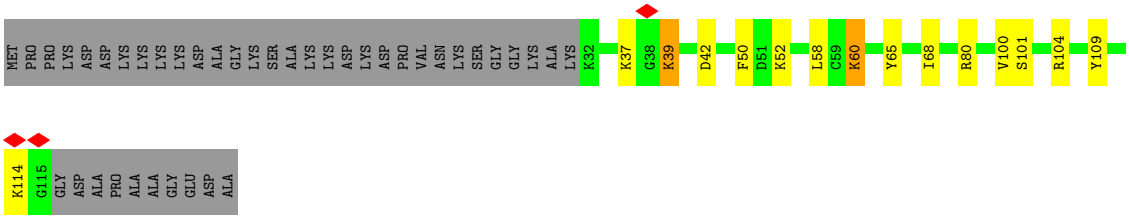




• Molecule 74: 40S ribosomal protein S25

Chain SZ:

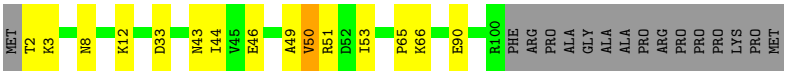




• Molecule 75: 40S ribosomal protein S26

Chain Sa:

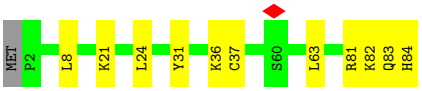




• Molecule 76: 40S ribosomal protein S27

Chain Sb:

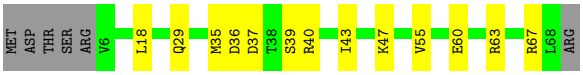




• Molecule 77: 40S ribosomal protein S28

Chain Sc:

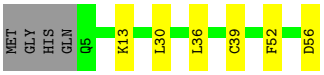




• Molecule 78: 40S ribosomal protein S29

Chain Sd:

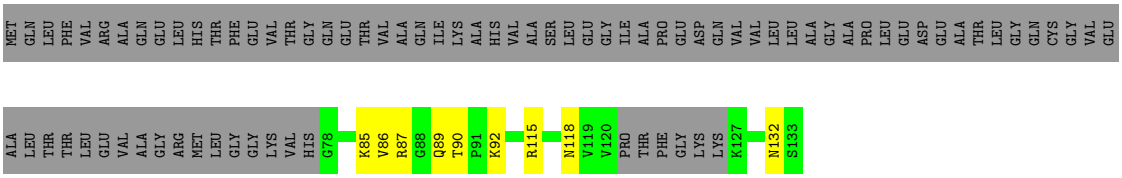




• Molecule 79: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se:

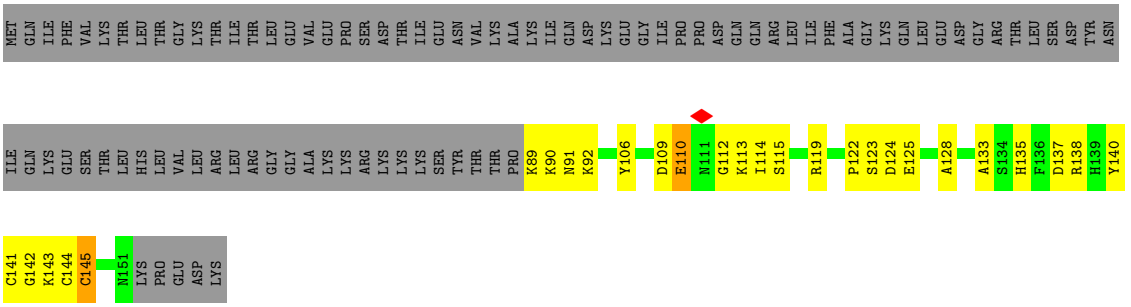




• Molecule 80: Ubiquitin

Chain Sf:

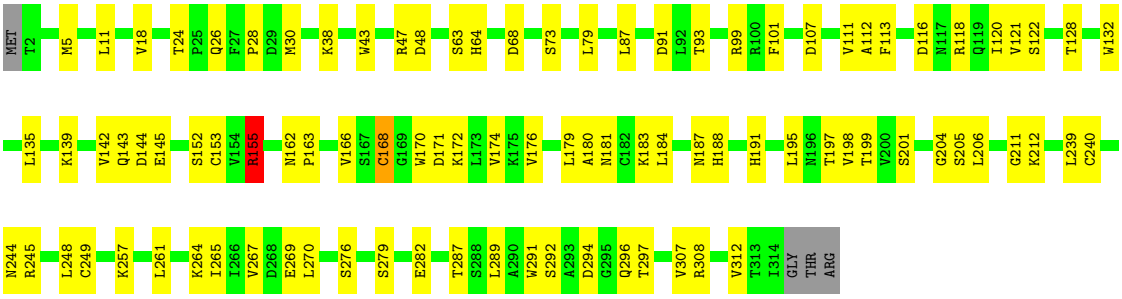




• Molecule 81: Receptor of activated protein C kinase 1

Chain Sg:

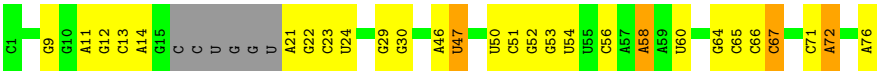




• Molecule 82: P-site_tRNA

Chain 3:

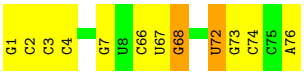




- Molecule 83: E-site_tRNA

Chain 4:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	254167	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	0.917	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, MA6, ACE, HIC, ZN, 4AC, NA, M3L, V5N, OMC, 6MZ, MG, SPD, MIA, OMG, UR3, ANM, 5MC, OMU, HYG, G7M, MLZ, K, PUT, HY3, 1MA, A2M, UY1, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	2	0.22	0/260	0.72	0/400
2	5	0.25	0/254	0.80	0/392
3	L5	0.33	3/82226 (0.0%)	0.78	24/128268 (0.0%)
4	L7	0.25	0/2858	0.69	0/4455
5	L8	0.29	0/3609	0.74	3/5623 (0.1%)
6	LA	0.16	0/1957	0.35	0/2622
7	LB	0.10	0/3294	0.27	0/4406
8	LC	0.10	0/2955	0.27	0/3969
9	LD	0.16	0/2413	0.35	1/3235 (0.0%)
10	LE	0.10	0/1816	0.25	0/2438
11	LF	0.10	0/1915	0.26	0/2553
12	LG	0.11	0/1947	0.29	0/2622
13	LH	0.09	0/1533	0.26	0/2062
14	LI	0.23	0/1679	0.36	0/2242
15	LJ	0.10	0/1385	0.24	0/1852
16	LL	0.42	0/1683	0.62	2/2257 (0.1%)
17	LM	0.09	0/1135	0.22	0/1520
18	LN	0.10	0/1745	0.27	0/2338
19	LO	0.10	0/1686	0.26	0/2257
20	LP	0.10	0/1308	0.28	0/1757
21	LQ	0.10	0/1533	0.28	0/2048
22	LR	0.09	0/1574	0.24	0/2082
23	LS	0.19	0/1496	0.35	2/2009 (0.1%)
24	LT	0.13	0/1317	0.30	0/1762
25	LU	0.10	0/798	0.29	0/1075
26	LV	0.10	0/1010	0.28	0/1355
27	LW	0.12	0/905	0.29	0/1209
28	LX	0.10	0/970	0.25	0/1308
29	LY	0.09	0/1115	0.24	0/1483
30	LZ	0.10	0/1125	0.25	0/1501
31	La	0.10	0/1178	0.27	0/1573

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	Lb	0.15	0/890	0.31	0/1176
33	Lc	0.11	0/780	0.27	0/1046
34	Ld	0.39	0/883	0.57	0/1190
35	Le	0.10	0/1082	0.25	0/1443
36	Lf	0.12	0/894	0.31	0/1198
37	Lg	0.09	0/912	0.25	0/1216
38	Lh	0.25	0/1022	0.40	0/1351
39	Li	0.17	0/839	0.31	0/1111
40	Lj	0.10	0/720	0.27	0/952
41	Lk	0.10	0/554	0.25	0/739
42	Ll	0.09	0/453	0.23	0/599
43	Lm	0.10	0/429	0.30	0/571
44	Ln	0.15	0/240	0.25	0/305
45	Lo	0.33	0/884	0.51	1/1165 (0.1%)
46	Lp	0.11	0/716	0.29	0/951
47	Lr	0.10	0/999	0.24	0/1342
48	S2	0.34	2/37785 (0.0%)	0.78	18/58881 (0.0%)
49	SA	0.36	0/1781	0.56	0/2421
50	SB	0.11	0/1828	0.26	0/2445
51	SC	0.34	0/1744	0.51	0/2357
52	SD	0.10	0/1757	0.25	0/2363
53	SE	0.10	0/2118	0.26	0/2849
54	SF	0.10	0/1467	0.27	0/1973
55	SG	0.09	0/1856	0.25	0/2475
56	SH	0.10	0/1495	0.27	0/2005
57	SI	0.11	0/1700	0.30	0/2271
58	SJ	0.09	0/1520	0.22	0/2031
59	SK	0.09	0/828	0.25	0/1118
60	SL	0.11	0/1221	0.28	0/1632
61	SM	0.15	0/930	0.40	0/1249
62	SN	0.10	0/1231	0.23	0/1656
63	SO	0.13	0/1021	0.32	0/1371
64	SP	0.10	0/1094	0.27	0/1463
65	SQ	0.10	0/1141	0.31	0/1528
66	SR	0.13	0/1090	0.34	0/1464
67	SS	0.24	0/1232	0.40	0/1651
68	ST	0.12	0/1122	0.29	0/1504
69	SU	0.12	0/813	0.31	0/1092
70	SV	0.36	0/643	0.56	1/860 (0.1%)
71	SW	0.13	0/1051	0.31	0/1406
72	SX	0.11	0/1096	0.30	0/1461
73	SY	0.25	0/1060	0.39	0/1409
74	SZ	0.09	0/682	0.25	0/911

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	Sa	0.13	0/816	0.30	0/1093
76	Sb	0.12	0/661	0.32	0/886
77	Sc	0.12	0/497	0.26	0/666
78	Sd	0.09	0/435	0.24	0/578
79	Se	0.07	0/396	0.23	0/519
80	Sf	0.26	0/525	0.75	2/695 (0.3%)
81	Sg	0.33	0/2493	0.58	1/3394 (0.0%)
82	3	0.23	0/1690	0.70	0/2631
83	4	0.77	0/447	0.94	0/693
All	All	0.27	5/222242 (0.0%)	0.64	55/326029 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
45	Lo	0	1
49	SA	0	1
67	SS	0	2
81	Sg	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3760	A2M	O3'-P	5.52	1.61	1.56
3	L5	3785	A2M	O3'-P	5.22	1.61	1.56
3	L5	4523	A2M	O3'-P	5.12	1.61	1.56
48	S2	1383	A2M	O3'-P	5.07	1.61	1.56
48	S2	1031	A2M	O3'-P	5.04	1.61	1.56

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	S2	199	C	N1-C2-O2	8.71	124.13	118.90
3	L5	2022	C	N3-C2-O2	-8.22	116.15	121.90
23	LS	20	PRO	N-CD-CG	-7.80	91.50	103.20
48	S2	199	C	C2-N1-C1'	7.57	127.13	118.80
3	L5	2469	C	C2-N1-C1'	7.48	127.02	118.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
45	Lo	78	ARG	Sidechain
49	SA	128	ARG	Sidechain
67	SS	38	ARG	Sidechain
67	SS	39	ARG	Sidechain
81	Sg	155	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	263	0	141	5	0
2	5	229	0	119	2	0
3	L5	76092	0	38524	926	0
4	L7	2558	0	1295	22	0
5	L8	3316	0	1687	42	0
6	LA	1932	0	2025	18	0
7	LB	3239	0	3377	34	0
8	LC	2901	0	3070	22	0
9	LD	2367	0	2378	16	0
10	LE	1782	0	1934	16	0
11	LF	1877	0	2009	19	0
12	LG	1914	0	2052	23	0
13	LH	1514	0	1589	21	0
14	LI	1641	0	1690	9	0
15	LJ	1362	0	1399	14	0
16	LL	1652	0	1747	11	0
17	LM	1113	0	1167	16	0
18	LN	1700	0	1749	10	0
19	LO	1654	0	1799	18	0
20	LP	1277	0	1310	8	0
21	LQ	1509	0	1626	10	0
22	LR	1558	0	1714	13	0
23	LS	1456	0	1491	12	0
24	LT	1284	0	1340	10	0
25	LU	784	0	789	10	0
26	LV	993	0	1056	9	0
27	LW	891	0	891	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	LX	953	0	1009	5	0
29	LY	1098	0	1182	6	0
30	LZ	1102	0	1174	8	0
31	La	1162	0	1206	9	0
32	Lb	888	0	961	9	0
33	Lc	770	0	809	8	0
34	Ld	868	0	914	10	0
35	Le	1061	0	1160	9	0
36	Lf	875	0	912	9	0
37	Lg	902	0	987	5	0
38	Lh	1014	0	1148	10	0
39	Li	828	0	906	5	0
40	Lj	705	0	737	1	0
41	Lk	548	0	596	6	0
42	Ll	443	0	483	3	0
43	Lm	432	0	466	2	0
44	Ln	239	0	289	5	0
45	Lo	877	0	942	12	0
46	Lp	703	0	759	4	0
47	Lr	986	0	1043	6	0
48	S2	35566	0	18005	456	0
49	SA	1746	0	1751	24	0
50	SB	1802	0	1877	20	0
51	SC	1707	0	1791	19	0
52	SD	1731	0	1827	15	0
53	SE	2076	0	2177	20	0
54	SF	1446	0	1492	17	0
55	SG	1833	0	1978	27	0
56	SH	1474	0	1540	22	0
57	SI	1671	0	1730	23	0
58	SJ	1495	0	1607	16	0
59	SK	804	0	825	10	0
60	SL	1200	0	1271	10	0
61	SM	920	0	943	19	0
62	SN	1207	0	1293	12	0
63	SO	1008	0	1033	10	0
64	SP	1072	0	1110	10	0
65	SQ	1123	0	1193	11	0
66	SR	1075	0	1128	18	0
67	SS	1214	0	1275	15	0
68	ST	1103	0	1133	8	0
69	SU	803	0	873	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	SV	636	0	637	8	0
71	SW	1034	0	1080	21	0
72	SX	1088	0	1149	9	0
73	SY	1042	0	1104	18	0
74	SZ	674	0	748	11	0
75	Sa	800	0	853	10	0
76	Sb	647	0	668	11	0
77	Sc	495	0	523	10	0
78	Sd	426	0	419	6	0
79	Se	394	0	434	9	0
80	Sf	515	0	521	24	0
81	Sg	2436	0	2391	65	0
82	3	1513	0	774	19	0
83	4	402	0	209	5	0
84	5	1	0	0	0	0
84	L5	202	0	0	0	0
84	L7	4	0	0	0	0
84	L8	3	0	0	0	0
84	LI	1	0	0	0	0
84	LP	1	0	0	0	0
84	LR	1	0	0	0	0
84	LV	1	0	0	0	0
84	Lj	1	0	0	0	0
84	S2	72	0	0	1	0
84	SX	1	0	0	0	0
85	5	1	0	0	0	0
85	L5	51	0	0	0	0
85	LA	1	0	0	0	0
85	LH	1	0	0	0	0
85	LI	1	0	0	0	0
85	Le	1	0	0	0	0
85	Lf	1	0	0	0	0
85	Lg	1	0	0	0	0
85	Ln	1	0	0	0	0
85	S2	25	0	0	0	0
85	SL	1	0	0	0	0
85	SO	1	0	0	0	0
85	Sa	1	0	0	0	0
85	Sd	1	0	0	0	0
86	L5	19	0	19	1	0
87	L5	120	0	228	13	0
87	LN	10	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	Ln	10	0	19	3	0
87	S2	70	0	133	4	0
88	L5	48	0	96	7	0
88	S2	12	0	24	1	0
89	L5	4	0	0	0	0
89	La	1	0	0	0	0
89	S2	3	0	0	0	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
90	Sd	1	0	0	0	0
90	Sf	1	0	0	0	0
91	S2	36	0	36	1	0
92	3	9	0	0	0	0
92	4	8	0	0	0	0
92	5	6	0	0	0	0
92	L5	2336	0	0	5	0
92	L7	26	0	0	0	0
92	L8	37	0	0	0	0
92	LA	58	0	0	0	0
92	LB	47	0	0	0	0
92	LC	41	0	0	0	0
92	LD	4	0	0	0	0
92	LE	1	0	0	0	0
92	LF	16	0	0	0	0
92	LG	1	0	0	0	0
92	LH	1	0	0	0	0
92	LI	5	0	0	0	0
92	LL	21	0	0	1	0
92	LN	36	0	0	0	0
92	LO	7	0	0	0	0
92	LP	15	0	0	0	0
92	LQ	20	0	0	0	0
92	LR	13	0	0	0	0
92	LS	4	0	0	0	0
92	LT	11	0	0	0	0
92	LV	9	0	0	0	0
92	LX	2	0	0	0	0
92	LY	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	LZ	2	0	0	0	0
92	La	19	0	0	0	0
92	Lb	12	0	0	0	0
92	Lc	3	0	0	0	0
92	Ld	3	0	0	0	0
92	Le	16	0	0	0	0
92	Lf	9	0	0	0	0
92	Lg	12	0	0	0	0
92	Lh	2	0	0	0	0
92	Li	1	0	0	0	0
92	Lj	13	0	0	0	0
92	Ll	2	0	0	0	0
92	Lm	1	0	0	0	0
92	Ln	11	0	0	0	0
92	Lo	13	0	0	0	0
92	Lp	17	0	0	0	0
92	Lr	4	0	0	0	0
92	S2	901	0	0	3	0
92	SA	2	0	0	0	0
92	SB	7	0	0	0	0
92	SC	5	0	0	0	0
92	SD	3	0	0	0	0
92	SE	3	0	0	0	0
92	SF	3	0	0	0	0
92	SI	6	0	0	0	0
92	SL	13	0	0	0	0
92	SN	13	0	0	0	0
92	SO	13	0	0	0	0
92	SQ	5	0	0	0	0
92	SR	2	0	0	0	0
92	SS	1	0	0	0	0
92	SU	5	0	0	0	0
92	SW	4	0	0	0	0
92	SX	4	0	0	0	0
92	Sa	11	0	0	0	0
92	Sb	2	0	0	0	0
92	Sc	1	0	0	0	0
All	All	216087	0	157587	2232	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 2232 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:3:50:U:H3	82:3:64:G:H1	0.98	0.97
81:Sg:87:LEU:HB2	81:Sg:101:PHE:HB2	1.51	0.93
3:L5:181:C:H2'	3:L5:182:G:H8	1.36	0.90
48:S2:394:G:H5"	60:SL:81:LYS:HB3	1.53	0.89
3:L5:181:C:H2'	3:L5:182:G:C8	2.08	0.88

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	LA	249/257 (97%)	242 (97%)	7 (3%)	0	100	100
7	LB	399/403 (99%)	394 (99%)	5 (1%)	0	100	100
8	LC	363/427 (85%)	360 (99%)	3 (1%)	0	100	100
9	LD	292/297 (98%)	288 (99%)	4 (1%)	0	100	100
10	LE	217/288 (75%)	212 (98%)	4 (2%)	1 (0%)	24	17
11	LF	224/248 (90%)	218 (97%)	6 (3%)	0	100	100
12	LG	238/266 (90%)	233 (98%)	5 (2%)	0	100	100
13	LH	188/192 (98%)	188 (100%)	0	0	100	100
14	LI	199/214 (93%)	198 (100%)	1 (0%)	0	100	100
15	LJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
16	LL	204/211 (97%)	200 (98%)	3 (2%)	1 (0%)	24	17
17	LM	134/215 (62%)	133 (99%)	1 (1%)	0	100	100
18	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
19	LO	200/203 (98%)	199 (100%)	1 (0%)	0	100	100
20	LP	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
21	LQ	185/188 (98%)	179 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	LR	185/196 (94%)	185 (100%)	0	0	100	100
23	LS	174/176 (99%)	174 (100%)	0	0	100	100
24	LT	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
25	LU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
26	LV	132/140 (94%)	131 (99%)	1 (1%)	0	100	100
27	LW	112/157 (71%)	109 (97%)	3 (3%)	0	100	100
28	LX	116/156 (74%)	116 (100%)	0	0	100	100
29	LY	131/145 (90%)	131 (100%)	0	0	100	100
30	LZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
31	La	144/148 (97%)	139 (96%)	5 (4%)	0	100	100
32	Lb	106/159 (67%)	104 (98%)	2 (2%)	0	100	100
33	Lc	97/115 (84%)	97 (100%)	0	0	100	100
34	Ld	104/125 (83%)	104 (100%)	0	0	100	100
35	Le	127/135 (94%)	126 (99%)	1 (1%)	0	100	100
36	Lf	107/110 (97%)	107 (100%)	0	0	100	100
37	Lg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
38	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
39	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
40	Lj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
41	Lk	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
42	Ll	48/51 (94%)	48 (100%)	0	0	100	100
43	Lm	50/128 (39%)	50 (100%)	0	0	100	100
44	Ln	23/25 (92%)	23 (100%)	0	0	100	100
45	Lo	104/106 (98%)	102 (98%)	1 (1%)	1 (1%)	12	5
46	Lp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
47	Lr	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
49	SA	221/295 (75%)	214 (97%)	7 (3%)	0	100	100
50	SB	219/264 (83%)	216 (99%)	3 (1%)	0	100	100
51	SC	218/293 (74%)	212 (97%)	5 (2%)	1 (0%)	24	17
52	SD	219/243 (90%)	213 (97%)	6 (3%)	0	100	100
53	SE	260/263 (99%)	256 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	SF	179/204 (88%)	174 (97%)	5 (3%)	0	100	100
55	SG	227/249 (91%)	223 (98%)	4 (2%)	0	100	100
56	SH	182/194 (94%)	178 (98%)	4 (2%)	0	100	100
57	SI	204/208 (98%)	199 (98%)	5 (2%)	0	100	100
58	SJ	178/194 (92%)	175 (98%)	3 (2%)	0	100	100
59	SK	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
60	SL	142/158 (90%)	139 (98%)	3 (2%)	0	100	100
61	SM	118/132 (89%)	106 (90%)	12 (10%)	0	100	100
62	SN	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
63	SO	134/151 (89%)	130 (97%)	4 (3%)	0	100	100
64	SP	129/145 (89%)	127 (98%)	2 (2%)	0	100	100
65	SQ	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
66	SR	131/135 (97%)	128 (98%)	3 (2%)	0	100	100
67	SS	146/152 (96%)	143 (98%)	3 (2%)	0	100	100
68	ST	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
69	SU	99/119 (83%)	96 (97%)	3 (3%)	0	100	100
70	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
71	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
72	SX	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
73	SY	126/133 (95%)	126 (100%)	0	0	100	100
74	SZ	82/125 (66%)	80 (98%)	1 (1%)	1 (1%)	10	4
75	Sa	98/115 (85%)	98 (100%)	0	0	100	100
76	Sb	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
77	Sc	61/69 (88%)	57 (93%)	4 (7%)	0	100	100
78	Sd	50/56 (89%)	50 (100%)	0	0	100	100
79	Se	46/133 (35%)	46 (100%)	0	0	100	100
80	Sf	61/156 (39%)	44 (72%)	16 (26%)	1 (2%)	7	2
81	Sg	311/317 (98%)	298 (96%)	11 (4%)	2 (1%)	21	13
All	All	11246/12762 (88%)	11028 (98%)	210 (2%)	8 (0%)	49	44

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	LE	96	VAL
45	Lo	78	ARG
81	Sg	171	ASP
81	Sg	205	SER
51	SC	256	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	LA	193/198 (98%)	188 (97%)	5 (3%)	40 37
7	LB	347/348 (100%)	347 (100%)	0	100 100
8	LC	303/348 (87%)	302 (100%)	1 (0%)	86 89
9	LD	241/250 (96%)	238 (99%)	3 (1%)	63 65
10	LE	195/252 (77%)	193 (99%)	2 (1%)	68 71
11	LF	195/215 (91%)	195 (100%)	0	100 100
12	LG	201/223 (90%)	197 (98%)	4 (2%)	48 47
13	LH	168/171 (98%)	167 (99%)	1 (1%)	78 82
14	LI	172/181 (95%)	172 (100%)	0	100 100
15	LJ	143/149 (96%)	143 (100%)	0	100 100
16	LL	169/177 (96%)	168 (99%)	1 (1%)	78 82
17	LM	114/161 (71%)	114 (100%)	0	100 100
18	LN	171/172 (99%)	171 (100%)	0	100 100
19	LO	173/174 (99%)	171 (99%)	2 (1%)	63 65
20	LP	137/163 (84%)	137 (100%)	0	100 100
21	LQ	163/165 (99%)	162 (99%)	1 (1%)	78 82
22	LR	164/175 (94%)	162 (99%)	2 (1%)	63 65
23	LS	156/157 (99%)	155 (99%)	1 (1%)	78 82
24	LT	135/140 (96%)	132 (98%)	3 (2%)	45 43
25	LU	83/115 (72%)	83 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	LV	102/107 (95%)	102 (100%)	0	100 100
27	LW	83/126 (66%)	82 (99%)	1 (1%)	63 65
28	LX	103/133 (77%)	103 (100%)	0	100 100
29	LY	121/135 (90%)	120 (99%)	1 (1%)	73 77
30	LZ	117/118 (99%)	116 (99%)	1 (1%)	70 74
31	La	119/120 (99%)	119 (100%)	0	100 100
32	Lb	88/125 (70%)	88 (100%)	0	100 100
33	Lc	84/97 (87%)	84 (100%)	0	100 100
34	Ld	94/110 (86%)	93 (99%)	1 (1%)	65 68
35	Le	115/121 (95%)	115 (100%)	0	100 100
36	Lf	88/89 (99%)	87 (99%)	1 (1%)	65 68
37	Lg	97/100 (97%)	95 (98%)	2 (2%)	47 45
38	Lh	109/110 (99%)	109 (100%)	0	100 100
39	Li	85/89 (96%)	85 (100%)	0	100 100
40	Lj	73/80 (91%)	73 (100%)	0	100 100
41	Lk	59/65 (91%)	58 (98%)	1 (2%)	53 53
42	Ll	47/48 (98%)	47 (100%)	0	100 100
43	Lm	47/115 (41%)	47 (100%)	0	100 100
44	Ln	24/24 (100%)	22 (92%)	2 (8%)	10 4
45	Lo	93/93 (100%)	88 (95%)	5 (5%)	20 12
46	Lp	73/75 (97%)	73 (100%)	0	100 100
47	Lr	106/120 (88%)	106 (100%)	0	100 100
49	SA	183/242 (76%)	179 (98%)	4 (2%)	45 43
50	SB	201/231 (87%)	200 (100%)	1 (0%)	81 85
51	SC	186/225 (83%)	181 (97%)	5 (3%)	39 35
52	SD	185/202 (92%)	181 (98%)	4 (2%)	45 43
53	SE	224/225 (100%)	221 (99%)	3 (1%)	61 62
54	SF	155/170 (91%)	154 (99%)	1 (1%)	78 82
55	SG	194/218 (89%)	194 (100%)	0	100 100
56	SH	161/174 (92%)	158 (98%)	3 (2%)	50 49
57	SI	174/180 (97%)	172 (99%)	2 (1%)	65 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
58	SJ	159/168 (95%)	157 (99%)	2 (1%)	61 62
59	SK	86/136 (63%)	86 (100%)	0	100 100
60	SL	132/142 (93%)	132 (100%)	0	100 100
61	SM	98/108 (91%)	96 (98%)	2 (2%)	48 47
62	SN	130/131 (99%)	129 (99%)	1 (1%)	73 77
63	SO	104/119 (87%)	104 (100%)	0	100 100
64	SP	116/130 (89%)	114 (98%)	2 (2%)	53 53
65	SQ	117/121 (97%)	114 (97%)	3 (3%)	40 37
66	SR	120/122 (98%)	120 (100%)	0	100 100
67	SS	128/132 (97%)	127 (99%)	1 (1%)	73 77
68	ST	112/115 (97%)	111 (99%)	1 (1%)	70 74
69	SU	93/107 (87%)	92 (99%)	1 (1%)	65 68
70	SV	67/67 (100%)	66 (98%)	1 (2%)	57 58
71	SW	112/113 (99%)	112 (100%)	0	100 100
72	SX	111/114 (97%)	110 (99%)	1 (1%)	70 74
73	SY	110/115 (96%)	109 (99%)	1 (1%)	70 74
74	SZ	74/103 (72%)	71 (96%)	3 (4%)	27 21
75	Sa	87/98 (89%)	86 (99%)	1 (1%)	65 68
76	Sb	74/76 (97%)	74 (100%)	0	100 100
77	Sc	56/62 (90%)	55 (98%)	1 (2%)	51 51
78	Sd	44/49 (90%)	44 (100%)	0	100 100
79	Se	40/104 (38%)	40 (100%)	0	100 100
80	Sf	56/140 (40%)	55 (98%)	1 (2%)	51 51
81	Sg	272/275 (99%)	266 (98%)	6 (2%)	45 43
All	All	9711/10848 (90%)	9619 (99%)	92 (1%)	68 74

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	SE	240	ARG
65	SQ	18	THR
56	SH	75	ILE
58	SJ	163	SER
68	ST	25	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
57	SI	64	ASN
72	SX	26	GLN
59	SK	7	ASN
62	SN	58	HIS
77	Sc	7	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	11/76 (14%)	4 (36%)	1 (9%)
2	5	10/13 (76%)	1 (10%)	0
3	L5	3529/5069 (69%)	548 (15%)	10 (0%)
4	L7	119/120 (99%)	7 (5%)	0
48	S2	1655/1869 (88%)	258 (15%)	2 (0%)
5	L8	155/156 (99%)	18 (11%)	0
82	3	69/77 (89%)	8 (11%)	0
83	4	17/19 (89%)	4 (23%)	0
All	All	5565/7399 (75%)	848 (15%)	13 (0%)

5 of 848 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	34	G
1	2	35	A
1	2	36	A
1	2	38	A
2	5	8	U

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	1754	U
3	L5	3765	G
48	S2	1520	G
3	L5	4699	U
48	S2	1344	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	1MA	L5	1322	84,3	21,25,26	2.89	6 (28%)	31,37,40	2.87	8 (25%)
48	PSU	S2	1238	48	18,21,22	4.46	7 (38%)	22,30,33	1.72	5 (22%)
3	OMG	L5	2424	3	23,26,27	2.37	8 (34%)	33,38,41	1.83	9 (27%)
48	OMC	S2	1703	48	19,22,23	3.00	8 (42%)	26,31,34	0.67	0
3	OMG	L5	3744	3	23,26,27	2.39	8 (34%)	33,38,41	1.90	10 (30%)
48	PSU	S2	1081	48	18,21,22	4.51	9 (50%)	22,30,33	1.61	4 (18%)
5	OMU	L8	14	5,3	19,22,23	2.97	8 (42%)	26,31,34	1.66	4 (15%)
3	OMG	L5	4392	3	23,26,27	2.36	8 (34%)	33,38,41	1.94	10 (30%)
3	PSU	L5	4353	3	18,21,22	4.45	7 (38%)	22,30,33	1.86	5 (22%)
3	PSU	L5	4457	3	18,21,22	4.46	7 (38%)	22,30,33	1.61	5 (22%)
7	HIC	LB	245	7	10,11,12	1.52	1 (10%)	8,14,16	1.41	2 (25%)
48	PSU	S2	814	48	18,21,22	4.43	7 (38%)	22,30,33	1.66	4 (18%)
48	OMG	S2	1328	85,48	23,26,27	0.29	0	33,38,41	0.37	0
48	A2M	S2	1678	48	22,25,26	3.47	9 (40%)	31,36,39	2.36	11 (35%)
3	OMU	L5	2415	3	19,22,23	3.02	8 (42%)	26,31,34	1.69	5 (19%)
48	PSU	S2	36	48	18,21,22	4.46	7 (38%)	22,30,33	1.74	5 (22%)
48	A2M	S2	576	48	22,25,26	0.18	0	31,36,39	0.46	0
48	PSU	S2	966	48	18,21,22	4.47	7 (38%)	22,30,33	1.68	5 (22%)
48	OMG	S2	1490	84,48	23,26,27	0.33	0	33,38,41	0.38	0
48	PSU	S2	801	48	18,21,22	4.46	7 (38%)	22,30,33	1.71	5 (22%)
3	PSU	L5	4293	3	18,21,22	4.41	7 (38%)	22,30,33	1.61	4 (18%)
48	PSU	S2	1445	48	18,21,22	4.44	7 (38%)	22,30,33	1.75	6 (27%)
3	PSU	L5	1792	85,3	18,21,22	4.42	7 (38%)	22,30,33	1.67	4 (18%)
3	A2M	L5	400	3	22,25,26	3.40	9 (40%)	31,36,39	2.32	10 (32%)
3	PSU	L5	1536	3	18,21,22	4.45	7 (38%)	22,30,33	1.81	5 (22%)
3	5MC	L5	3782	84,3	18,22,23	3.53	7 (38%)	26,32,35	1.06	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	6MZ	S2	1832	85,84,48	22,25,26	2.57	4 (18%)	30,36,39	2.15	9 (30%)
3	PSU	L5	1781	3	18,21,22	4.47	7 (38%)	22,30,33	1.67	5 (22%)
3	OMU	L5	4227	3	19,22,23	3.03	8 (42%)	26,31,34	1.72	4 (15%)
72	HY3	SX	62	72	6,8,9	0.88	0	5,10,12	1.15	1 (20%)
3	OMG	L5	4228	3	23,26,27	2.37	9 (39%)	33,38,41	1.96	10 (30%)
3	PSU	L5	4628	3	18,21,22	4.41	7 (38%)	22,30,33	1.71	5 (22%)
3	OMG	L5	4623	3	23,26,27	2.36	8 (34%)	33,38,41	1.93	10 (30%)
3	5MC	L5	4447	85,3	18,22,23	3.56	7 (38%)	26,32,35	1.11	1 (3%)
3	OMU	L5	4620	3	19,22,23	2.98	8 (42%)	26,31,34	1.56	4 (15%)
48	PSU	S2	1643	84,48	18,21,22	4.46	7 (38%)	22,30,33	1.73	6 (27%)
48	OMG	S2	509	84,48	23,26,27	2.38	8 (34%)	33,38,41	1.94	9 (27%)
3	PSU	L5	4423	3	18,21,22	4.47	7 (38%)	22,30,33	1.73	5 (22%)
3	PSU	L5	4689	3	18,21,22	4.48	7 (38%)	22,30,33	1.76	5 (22%)
48	PSU	S2	686	48	18,21,22	4.45	7 (38%)	22,30,33	1.69	5 (22%)
3	PSU	L5	4403	85,3	18,21,22	4.43	7 (38%)	22,30,33	1.79	6 (27%)
3	A2M	L5	2363	84,3	22,25,26	0.16	0	31,36,39	0.37	0
5	OMG	L8	75	5	23,26,27	2.38	8 (34%)	33,38,41	1.91	9 (27%)
48	PSU	S2	815	48	18,21,22	4.46	7 (38%)	22,30,33	1.72	5 (22%)
48	PSU	S2	866	48	18,21,22	4.46	7 (38%)	22,30,33	1.73	5 (22%)
48	PSU	S2	1056	48	18,21,22	4.48	7 (38%)	22,30,33	1.81	5 (22%)
3	PSU	L5	2839	3	18,21,22	4.48	7 (38%)	22,30,33	1.71	5 (22%)
48	PSU	S2	863	48	18,21,22	4.47	7 (38%)	22,30,33	1.62	4 (18%)
3	PSU	L5	1744	85,3	18,21,22	4.47	7 (38%)	22,30,33	1.66	5 (22%)
3	PSU	L5	5001	3	18,21,22	4.43	7 (38%)	22,30,33	1.71	5 (22%)
48	A2M	S2	1383	48	22,25,26	3.38	9 (40%)	31,36,39	2.37	12 (38%)
48	A2M	S2	484	48	22,25,26	3.37	9 (40%)	31,36,39	2.36	11 (35%)
3	A2M	L5	1534	84,3	22,25,26	3.39	9 (40%)	31,36,39	2.36	10 (32%)
3	OMG	L5	3944	3	23,26,27	2.39	8 (34%)	33,38,41	1.89	10 (30%)
48	A2M	S2	99	84,48	22,25,26	3.40	9 (40%)	31,36,39	2.33	11 (35%)
3	OMG	L5	4370	3	23,26,27	2.36	7 (30%)	33,38,41	1.87	9 (27%)
3	OMC	L5	2422	84,3	19,22,23	2.97	8 (42%)	26,31,34	0.70	0
3	OMG	L5	1522	3	23,26,27	2.38	8 (34%)	33,38,41	1.88	10 (30%)
3	OMC	L5	2824	3	19,22,23	2.98	8 (42%)	26,31,34	0.68	0
3	OMG	L5	1316	3	23,26,27	2.40	7 (30%)	33,38,41	1.91	10 (30%)
3	PSU	L5	4552	3	18,21,22	4.44	7 (38%)	22,30,33	1.73	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OMC	L5	2351	84,3	19,22,23	2.99	8 (42%)	26,31,34	0.98	1 (3%)
3	PSU	L5	5010	3	18,21,22	4.47	7 (38%)	22,30,33	1.70	5 (22%)
48	OMU	S2	1804	48	19,22,23	3.00	8 (42%)	26,31,34	1.71	4 (15%)
48	OMU	S2	354	48	19,22,23	3.00	8 (42%)	26,31,34	1.73	4 (15%)
48	PSU	S2	1177	48	18,21,22	4.42	7 (38%)	22,30,33	1.70	5 (22%)
3	PSU	L5	4493	85,3	18,21,22	4.46	7 (38%)	22,30,33	1.74	5 (22%)
3	A2M	L5	1871	84,3	22,25,26	0.18	0	31,36,39	0.59	0
3	OMC	L5	1340	3	19,22,23	2.97	8 (42%)	26,31,34	0.64	0
3	A2M	L5	2787	3	22,25,26	3.38	9 (40%)	31,36,39	2.26	11 (35%)
3	OMC	L5	3887	3	19,22,23	2.94	8 (42%)	26,31,34	0.72	0
3	A2M	L5	3724	3	22,25,26	0.18	0	31,36,39	0.42	0
48	OMU	S2	172	48	19,22,23	2.98	8 (42%)	26,31,34	1.74	4 (15%)
3	A2M	L5	2815	84,3	22,25,26	3.38	8 (36%)	31,36,39	2.33	10 (32%)
3	A2M	L5	1326	3	22,25,26	3.40	9 (40%)	31,36,39	2.30	10 (32%)
48	OMU	S2	116	48	19,22,23	3.03	8 (42%)	26,31,34	1.66	4 (15%)
48	A2M	S2	590	48	22,25,26	3.42	9 (40%)	31,36,39	2.46	10 (32%)
48	PSU	S2	651	48	18,21,22	4.45	7 (38%)	22,30,33	1.74	5 (22%)
3	OMC	L5	4536	3	19,22,23	2.97	8 (42%)	26,31,34	0.74	0
48	OMC	S2	517	48	19,22,23	2.97	8 (42%)	26,31,34	0.76	0
48	OMC	S2	1391	48	19,22,23	2.99	8 (42%)	26,31,34	0.72	0
3	PSU	L5	3920	84,3	18,21,22	4.50	7 (38%)	22,30,33	1.75	6 (27%)
3	PSU	L5	3884	3	18,21,22	4.46	7 (38%)	22,30,33	1.73	5 (22%)
48	PSU	S2	296	48	18,21,22	4.47	7 (38%)	22,30,33	1.71	5 (22%)
3	PSU	L5	1683	85,3	18,21,22	4.45	7 (38%)	22,30,33	1.66	4 (18%)
48	PSU	S2	1232	48	18,21,22	4.47	7 (38%)	22,30,33	1.73	5 (22%)
3	OMC	L5	1881	84,3	19,22,23	2.97	8 (42%)	26,31,34	0.79	0
3	PSU	L5	3639	3	18,21,22	4.52	7 (38%)	22,30,33	1.65	5 (22%)
3	PSU	L5	4500	3	18,21,22	4.46	7 (38%)	22,30,33	1.73	5 (22%)
3	PSU	L5	4673	3	18,21,22	4.45	7 (38%)	22,30,33	1.75	5 (22%)
3	PSU	L5	4972	3	18,21,22	4.45	7 (38%)	22,30,33	1.71	5 (22%)
3	A2M	L5	4590	3	22,25,26	3.42	9 (40%)	31,36,39	2.35	10 (32%)
3	OMC	L5	3808	3	19,22,23	2.98	8 (42%)	26,31,34	0.76	0
48	4AC	S2	1337	48	21,24,25	3.34	9 (42%)	29,34,37	0.98	2 (6%)
3	PSU	L5	1782	3	18,21,22	4.47	7 (38%)	22,30,33	1.69	5 (22%)
31	V5N	La	39	31	9,11,12	2.60	2 (22%)	9,14,16	1.19	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PSU	L5	4299	3	18,21,22	4.48	7 (38%)	22,30,33	1.68	5 (22%)
3	OMG	L5	2364	84,3	23,26,27	0.28	0	33,38,41	0.36	0
3	OMU	L5	3925	3	19,22,23	3.02	8 (42%)	26,31,34	1.72	4 (15%)
3	PSU	L5	3758	3	18,21,22	0.86	1 (5%)	22,30,33	0.74	1 (4%)
3	A2M	L5	3830	3	22,25,26	3.40	9 (40%)	31,36,39	2.32	10 (32%)
48	OMG	S2	1447	48	23,26,27	2.37	8 (34%)	33,38,41	1.88	10 (30%)
48	MA6	S2	1850	48	23,26,27	1.37	3 (13%)	34,38,41	2.95	12 (35%)
3	PSU	L5	3734	3	18,21,22	4.44	7 (38%)	22,30,33	1.73	5 (22%)
3	PSU	L5	4296	3	18,21,22	4.43	7 (38%)	22,30,33	1.68	5 (22%)
3	A2M	L5	3867	3	22,25,26	3.41	9 (40%)	31,36,39	2.30	11 (35%)
48	PSU	S2	681	48	18,21,22	4.48	7 (38%)	22,30,33	1.74	5 (22%)
3	PSU	L5	3851	3	18,21,22	0.88	1 (5%)	22,30,33	0.59	0
3	OMG	L5	4618	3	23,26,27	2.38	8 (34%)	33,38,41	1.95	9 (27%)
3	PSU	L5	4521	85,84,3	18,21,22	4.43	7 (38%)	22,30,33	1.70	6 (27%)
3	6MZ	L5	4220	3	22,25,26	0.14	0	30,36,39	0.30	0
48	OMG	S2	436	48	23,26,27	2.38	7 (30%)	33,38,41	1.89	10 (30%)
3	PSU	L5	4420	3	18,21,22	4.44	8 (44%)	22,30,33	1.69	5 (22%)
48	PSU	S2	1239	48	18,21,22	4.46	7 (38%)	22,30,33	1.69	5 (22%)
3	UY1	L5	3818	85,84,3	19,22,23	0.18	0	22,31,34	0.32	0
3	OMG	L5	4499	3	23,26,27	2.36	7 (30%)	33,38,41	1.89	9 (27%)
48	OMG	S2	683	48	23,26,27	2.39	8 (34%)	33,38,41	1.88	10 (30%)
3	PSU	L5	4579	3	18,21,22	4.45	7 (38%)	22,30,33	1.71	5 (22%)
3	PSU	L5	2632	3	18,21,22	4.46	7 (38%)	22,30,33	1.62	4 (18%)
3	A2M	L5	3718	3	22,25,26	3.41	9 (40%)	31,36,39	2.24	11 (35%)
3	PSU	L5	4312	3	18,21,22	4.47	7 (38%)	22,30,33	1.73	5 (22%)
48	PSU	S2	1004	48	18,21,22	4.50	7 (38%)	22,30,33	1.68	5 (22%)
48	PSU	S2	1174	48	18,21,22	4.46	7 (38%)	22,30,33	1.66	4 (18%)
43	M3L	Lm	98	43	10,11,12	0.51	0	9,14,16	0.46	0
3	OMU	L5	4498	3	19,22,23	2.99	8 (42%)	26,31,34	1.65	4 (15%)
3	OMG	L5	4637	3	23,26,27	0.29	0	33,38,41	0.45	0
3	PSU	L5	4361	3	18,21,22	4.44	7 (38%)	22,30,33	1.74	5 (22%)
48	OMG	S2	601	48	23,26,27	2.37	7 (30%)	33,38,41	1.87	9 (27%)
48	OMU	S2	627	48	19,22,23	2.96	8 (42%)	26,31,34	1.65	4 (15%)
48	PSU	S2	918	48	18,21,22	4.44	8 (44%)	22,30,33	1.82	6 (27%)
48	PSU	S2	1367	48	18,21,22	4.47	7 (38%)	22,30,33	1.73	5 (22%)
3	OMG	L5	3627	3	23,26,27	2.38	8 (34%)	33,38,41	1.97	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	PSU	S2	218	48	18,21,22	4.46	7 (38%)	22,30,33	1.71	5 (22%)
3	PSU	L5	3844	84,3	18,21,22	0.88	1 (5%)	22,30,33	0.64	0
48	4AC	S2	1842	48	21,24,25	3.34	9 (42%)	29,34,37	1.08	2 (6%)
3	A2M	L5	3785	3	22,25,26	3.34	10 (45%)	31,36,39	2.51	12 (38%)
48	A2M	S2	166	48	22,25,26	3.41	9 (40%)	31,36,39	2.35	12 (38%)
48	PSU	S2	649	48	18,21,22	4.47	7 (38%)	22,30,33	1.73	5 (22%)
3	OMG	L5	1625	85,3	23,26,27	2.37	7 (30%)	33,38,41	1.83	9 (27%)
48	A2M	S2	668	84,48	22,25,26	3.40	10 (45%)	31,36,39	2.32	10 (32%)
6	V5N	LA	216	6	9,11,12	0.52	0	9,14,16	1.01	1 (11%)
5	PSU	L8	55	5	18,21,22	4.46	7 (38%)	22,30,33	1.73	5 (22%)
48	PSU	S2	1244	48	18,21,22	0.87	1 (5%)	22,30,33	0.64	0
48	PSU	S2	93	48	18,21,22	4.48	7 (38%)	22,30,33	1.64	4 (18%)
3	PSU	L5	1860	3	18,21,22	4.45	7 (38%)	22,30,33	1.76	5 (22%)
3	OMC	L5	3701	85,3	19,22,23	2.92	8 (42%)	26,31,34	0.66	0
3	PSU	L5	1582	3	18,21,22	4.39	8 (44%)	22,30,33	1.66	3 (13%)
3	A2M	L5	4571	3	22,25,26	3.44	9 (40%)	31,36,39	2.34	11 (35%)
48	PSU	S2	406	48	18,21,22	4.45	7 (38%)	22,30,33	1.73	5 (22%)
3	OMC	L5	4456	3	19,22,23	2.99	8 (42%)	26,31,34	0.70	0
3	PSU	L5	4576	3	18,21,22	4.45	7 (38%)	22,30,33	1.73	5 (22%)
3	A2M	L5	398	3	22,25,26	3.41	9 (40%)	31,36,39	2.34	11 (35%)
3	A2M	L5	1524	3	22,25,26	3.41	10 (45%)	31,36,39	2.38	11 (35%)
48	A2M	S2	468	48	22,25,26	3.42	9 (40%)	31,36,39	2.31	10 (32%)
3	OMG	L5	3899	84,3	23,26,27	2.37	9 (39%)	33,38,41	1.95	10 (30%)
48	OMG	S2	644	48	23,26,27	2.37	8 (34%)	33,38,41	1.93	9 (27%)
48	OMG	S2	867	48	23,26,27	2.38	8 (34%)	33,38,41	1.92	10 (30%)
48	PSU	S2	1692	48	18,21,22	4.49	7 (38%)	22,30,33	1.71	5 (22%)
48	OMU	S2	1442	84,48	19,22,23	3.03	8 (42%)	26,31,34	1.65	4 (15%)
3	PSU	L5	1862	3	18,21,22	0.85	1 (5%)	22,30,33	0.66	0
48	PSU	S2	1347	48	18,21,22	4.45	7 (38%)	22,30,33	1.77	5 (22%)
3	PSU	L5	3715	3	18,21,22	0.89	1 (5%)	22,30,33	0.61	0
3	PSU	L5	4431	3	18,21,22	4.45	7 (38%)	22,30,33	1.75	5 (22%)
48	OMC	S2	462	48	19,22,23	2.98	8 (42%)	26,31,34	0.72	0
48	A2M	S2	27	84,48	22,25,26	3.38	9 (40%)	31,36,39	2.34	11 (35%)
48	PSU	S2	1136	48	18,21,22	4.46	7 (38%)	22,30,33	1.73	5 (22%)
48	PSU	S2	1243	48	18,21,22	0.86	1 (5%)	22,30,33	0.89	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MIA	2	37	1	28,31,32	2.60	5 (17%)	40,44,47	4.79	19 (47%)
48	PSU	S2	109	48	18,21,22	4.44	7 (38%)	22,30,33	1.74	5 (22%)
3	OMC	L5	2861	3	19,22,23	3.00	8 (42%)	26,31,34	0.71	0
3	OMG	L5	3792	3	23,26,27	2.39	7 (30%)	33,38,41	1.87	9 (27%)
3	OMG	L5	4196	82,3	23,26,27	0.29	0	33,38,41	0.40	0
3	A2M	L5	4523	84,3	22,25,26	3.39	9 (40%)	31,36,39	2.35	12 (38%)
3	PSU	L5	4442	3	18,21,22	4.44	7 (38%)	22,30,33	1.75	6 (27%)
3	OMC	L5	3841	3	19,22,23	2.97	8 (42%)	26,31,34	0.69	0
3	A2M	L5	3760	3	22,25,26	0.16	0	31,36,39	0.66	0
3	PSU	L5	3768	3	18,21,22	4.44	7 (38%)	22,30,33	1.66	4 (18%)
48	UY1	S2	1326	84,48	19,22,23	0.19	0	22,31,34	0.34	0
48	MA6	S2	1851	48	23,26,27	1.37	3 (13%)	34,38,41	3.03	12 (35%)
48	OMU	S2	121	48	19,22,23	3.01	8 (42%)	26,31,34	1.67	4 (15%)
45	MLZ	Lo	53	45	8,9,10	0.73	0	4,9,11	0.60	0
48	A2M	S2	159	48	22,25,26	3.40	9 (40%)	31,36,39	2.35	11 (35%)
3	PSU	L5	4569	3	18,21,22	4.53	7 (38%)	22,30,33	1.74	5 (22%)
3	OMU	L5	2837	3	19,22,23	3.00	8 (42%)	26,31,34	1.76	4 (15%)
48	PSU	S2	1625	48	18,21,22	4.48	7 (38%)	22,30,33	1.66	4 (18%)
48	PSU	S2	34	48	18,21,22	4.48	7 (38%)	22,30,33	1.71	5 (22%)
3	PSU	L5	3695	85,3	18,21,22	0.84	1 (5%)	22,30,33	0.61	0
3	OMG	L5	2876	3	23,26,27	2.41	8 (34%)	33,38,41	1.89	9 (27%)
3	A2M	L5	2401	3	22,25,26	3.39	10 (45%)	31,36,39	2.34	11 (35%)
3	OMC	L5	2365	3	19,22,23	0.26	0	26,31,34	0.46	0
3	PSU	L5	1779	3	18,21,22	4.47	7 (38%)	22,30,33	1.77	5 (22%)
3	PSU	L5	3637	85,3	18,21,22	4.46	7 (38%)	22,30,33	1.80	4 (18%)
3	A2M	L5	3723	3	22,25,26	0.17	0	31,36,39	0.37	0
3	OMG	L5	4494	3	23,26,27	2.37	7 (30%)	33,38,41	1.88	10 (30%)
3	PSU	L5	4531	3	18,21,22	4.39	7 (38%)	22,30,33	1.81	5 (22%)
48	PSU	S2	572	48	18,21,22	0.85	1 (5%)	22,30,33	0.62	0
5	PSU	L8	69	5	18,21,22	4.42	7 (38%)	22,30,33	1.66	6 (27%)
48	G7M	S2	1639	82,48	23,26,27	2.64	8 (34%)	35,39,42	2.50	11 (31%)
48	OMC	S2	174	48	19,22,23	2.98	8 (42%)	26,31,34	0.71	0
3	A2M	L5	3825	3	22,25,26	3.37	9 (40%)	31,36,39	2.31	10 (32%)
48	A2M	S2	1031	85,48	22,25,26	3.39	9 (40%)	31,36,39	2.32	10 (32%)
48	OMU	S2	1288	48	19,22,23	3.00	8 (42%)	26,31,34	1.64	4 (15%)
48	A2M	S2	512	48	22,25,26	3.40	8 (36%)	31,36,39	2.33	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	MLZ	Lb	5	32	8,9,10	0.39	0	4,9,11	0.21	0
48	PSU	S2	119	48	18,21,22	4.45	8 (44%)	22,30,33	1.63	4 (18%)
48	PSU	S2	105	48	18,21,22	4.48	7 (38%)	22,30,33	1.67	4 (18%)
3	OMC	L5	3869	3	19,22,23	3.00	8 (42%)	26,31,34	0.69	0
3	UR3	L5	4530	3	19,22,23	2.77	7 (36%)	26,32,35	1.27	3 (11%)
3	PSU	L5	4532	3	18,21,22	4.52	7 (38%)	22,30,33	1.62	4 (18%)
48	PSU	S2	822	48	18,21,22	4.45	8 (44%)	22,30,33	1.71	6 (27%)
48	OMU	S2	428	48	19,22,23	2.97	8 (42%)	26,31,34	1.68	4 (15%)
3	PSU	L5	3770	3	18,21,22	4.48	7 (38%)	22,30,33	1.74	5 (22%)
48	B8N	S2	1248	48	24,29,30	0.41	0	29,42,45	0.52	0
3	OMC	L5	2804	3	19,22,23	2.95	8 (42%)	26,31,34	0.73	0
3	OMU	L5	4306	3	19,22,23	3.00	8 (42%)	26,31,34	1.68	4 (15%)
3	PSU	L5	4471	3	18,21,22	4.50	7 (38%)	22,30,33	1.66	5 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1MA	L5	1322	84,3	-	2/7/25/26	0/3/3/3
48	PSU	S2	1238	48	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
48	OMC	S2	1703	48	-	0/9/27/28	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
48	PSU	S2	1081	48	-	1/7/25/26	0/2/2/2
5	OMU	L8	14	5,3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
7	HIC	LB	245	7	-	1/5/6/8	0/1/1/1
48	PSU	S2	814	48	-	0/7/25/26	0/2/2/2
48	OMG	S2	1328	85,48	-	1/9/27/28	0/3/3/3
48	A2M	S2	1678	48	-	1/9/27/28	0/3/3/3
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
48	PSU	S2	36	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	576	48	-	2/9/27/28	0/3/3/3
48	PSU	S2	966	48	-	0/7/25/26	0/2/2/2
48	OMG	S2	1490	84,48	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	S2	801	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	1445	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	1792	85,3	-	2/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	84,3	-	0/7/25/26	0/2/2/2
48	6MZ	S2	1832	85,84,48	-	2/9/27/28	0/3/3/3
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
72	HY3	SX	62	72	-	0/1/12/14	0/1/1/1
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	4447	85,3	-	4/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
48	PSU	S2	1643	84,48	-	0/7/25/26	0/2/2/2
48	OMG	S2	509	84,48	-	0/9/27/28	0/3/3/3
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	686	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	85,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2363	84,3	-	0/9/27/28	0/3/3/3
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
48	PSU	S2	815	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	866	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1056	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	863	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	85,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
48	A2M	S2	1383	48	-	1/9/27/28	0/3/3/3
48	A2M	S2	484	48	-	1/9/27/28	0/3/3/3
3	A2M	L5	1534	84,3	-	3/9/27/28	0/3/3/3
3	OMG	L5	3944	3	-	2/9/27/28	0/3/3/3
48	A2M	S2	99	84,48	-	3/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	2422	84,3	-	3/9/27/28	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	1316	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	84,3	-	3/9/27/28	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
48	OMU	S2	1804	48	-	0/9/27/28	0/2/2/2
48	OMU	S2	354	48	-	0/9/27/28	0/2/2/2
48	PSU	S2	1177	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	85,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	84,3	-	0/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2787	3	-	3/9/27/28	0/3/3/3
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
48	OMU	S2	172	48	-	0/9/27/28	0/2/2/2
3	A2M	L5	2815	84,3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	1/9/27/28	0/3/3/3
48	OMU	S2	116	48	-	0/9/27/28	0/2/2/2
48	A2M	S2	590	48	-	3/9/27/28	0/3/3/3
48	PSU	S2	651	48	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
48	OMC	S2	517	48	-	0/9/27/28	0/2/2/2
48	OMC	S2	1391	48	-	0/9/27/28	0/2/2/2
3	PSU	L5	3920	84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	296	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	85,3	-	0/7/25/26	0/2/2/2
48	PSU	S2	1232	48	-	0/7/25/26	0/2/2/2
3	OMC	L5	1881	84,3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
48	4AC	S2	1337	48	-	0/11/29/30	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
31	V5N	La	39	31	-	1/9/10/12	0/1/1/1
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2364	84,3	-	2/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
48	OMG	S2	1447	48	-	3/9/27/28	0/3/3/3
48	MA6	S2	1850	48	-	0/11/29/30	0/3/3/3
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	2/9/27/28	0/3/3/3
48	PSU	S2	681	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4521	85,84,3	-	0/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
48	OMG	S2	436	48	-	0/9/27/28	0/3/3/3
3	PSU	L5	4420	3	-	2/7/25/26	0/2/2/2
48	PSU	S2	1239	48	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	85,84,3	-	2/9/27/28	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
48	OMG	S2	683	48	-	2/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	1004	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1174	48	-	0/7/25/26	0/2/2/2
43	M3L	Lm	98	43	-	0/9/10/12	-
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
48	OMG	S2	601	48	-	1/9/27/28	0/3/3/3
48	OMU	S2	627	48	-	2/9/27/28	0/2/2/2
48	PSU	S2	918	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1367	48	-	0/7/25/26	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
48	PSU	S2	218	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	84,3	-	1/7/25/26	0/2/2/2
48	4AC	S2	1842	48	-	0/11/29/30	0/2/2/2
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
48	A2M	S2	166	48	-	1/9/27/28	0/3/3/3
48	PSU	S2	649	48	-	0/7/25/26	0/2/2/2
3	OMG	L5	1625	85,3	-	1/9/27/28	0/3/3/3
48	A2M	S2	668	84,48	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	V5N	LA	216	6	-	1/9/10/12	0/1/1/1
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
48	PSU	S2	1244	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	93	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3701	85,3	-	4/9/27/28	0/2/2/2
3	PSU	L5	1582	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
48	PSU	S2	406	48	-	0/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	2/9/27/28	0/3/3/3
48	A2M	S2	468	48	-	0/9/27/28	0/3/3/3
3	OMG	L5	3899	84,3	-	0/9/27/28	0/3/3/3
48	OMG	S2	644	48	-	4/9/27/28	0/3/3/3
48	OMG	S2	867	48	-	1/9/27/28	0/3/3/3
48	PSU	S2	1692	48	-	0/7/25/26	0/2/2/2
48	OMU	S2	1442	84,48	-	0/9/27/28	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	1347	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
48	OMC	S2	462	48	-	0/9/27/28	0/2/2/2
48	A2M	S2	27	84,48	-	0/9/27/28	0/3/3/3
48	PSU	S2	1136	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1243	48	-	3/7/25/26	0/2/2/2
1	MIA	2	37	1	-	2/15/33/34	0/3/3/3
48	PSU	S2	109	48	-	0/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3792	3	-	3/9/27/28	0/3/3/3
3	OMG	L5	4196	82,3	-	3/9/27/28	0/3/3/3
3	A2M	L5	4523	84,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3760	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
48	UY1	S2	1326	84,48	-	1/9/27/28	0/2/2/2
48	MA6	S2	1851	48	-	3/11/29/30	0/3/3/3
48	OMU	S2	121	48	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	MLZ	Lo	53	45	-	0/7/8/10	-
48	A2M	S2	159	48	-	1/9/27/28	0/3/3/3
3	PSU	L5	4569	3	-	2/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
48	PSU	S2	1625	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	34	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	85,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2401	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	85,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	572	48	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
48	G7M	S2	1639	82,48	-	0/7/25/26	0/3/3/3
48	OMC	S2	174	48	-	0/9/27/28	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
48	A2M	S2	1031	85,48	-	0/9/27/28	0/3/3/3
48	OMU	S2	1288	48	-	1/9/27/28	0/2/2/2
48	A2M	S2	512	48	-	2/9/27/28	0/3/3/3
32	MLZ	Lb	5	32	-	2/7/8/10	-
48	PSU	S2	119	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	105	48	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	822	48	-	2/7/25/26	0/2/2/2
48	OMU	S2	428	48	-	6/9/27/28	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
48	B8N	S2	1248	48	-	3/16/34/35	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4471	3	-	2/7/25/26	0/2/2/2

The worst 5 of 1411 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4532	PSU	C6-C5	11.84	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4569	PSU	C6-C5	11.82	1.49	1.35
3	L5	3639	PSU	C6-C5	11.78	1.49	1.35
48	S2	1081	PSU	C6-C5	11.76	1.49	1.35
3	L5	4471	PSU	C6-C5	11.76	1.49	1.35

The worst 5 of 1108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	37	MIA	C1'-N9-C8	-14.56	94.25	127.14
1	2	37	MIA	C4-N9-C1'	12.80	157.09	126.59
48	S2	1851	MA6	N1-C6-N6	-11.26	104.77	117.08
48	S2	1850	MA6	N1-C6-N6	-10.87	105.20	117.08
1	2	37	MIA	C11-S10-C2	10.16	109.85	102.27

There are no chirality outliers.

5 of 146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	LA	216	V5N	O-C-CA-CB
7	LB	245	HIC	O-C-CA-CB
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	1316	OMG	C1'-C2'-O2'-CM2
3	L5	1781	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

86 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2424	OMG	1	0
5	L8	14	OMU	1	0
3	L5	4392	OMG	2	0
3	L5	4457	PSU	1	0
7	LB	245	HIC	1	0
48	S2	1678	A2M	2	0
3	L5	2415	OMU	3	0
48	S2	36	PSU	1	0
48	S2	576	A2M	1	0
48	S2	1490	OMG	2	0
48	S2	1445	PSU	2	0
3	L5	1536	PSU	1	0
3	L5	4628	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4623	OMG	1	0
3	L5	4447	5MC	1	0
3	L5	4620	OMU	2	0
48	S2	1643	PSU	1	0
48	S2	509	OMG	4	0
3	L5	4689	PSU	1	0
3	L5	2363	A2M	2	0
48	S2	1383	A2M	1	0
48	S2	484	A2M	1	0
3	L5	3944	OMG	1	0
3	L5	1316	OMG	1	0
3	L5	4552	PSU	1	0
3	L5	2351	OMC	1	0
3	L5	5010	PSU	2	0
48	S2	1804	OMU	1	0
3	L5	1871	A2M	1	0
3	L5	1340	OMC	1	0
3	L5	2787	A2M	1	0
3	L5	3724	A2M	2	0
3	L5	2815	A2M	1	0
3	L5	1326	A2M	1	0
48	S2	116	OMU	2	0
3	L5	4536	OMC	1	0
48	S2	1391	OMC	2	0
3	L5	3920	PSU	1	0
3	L5	3884	PSU	1	0
3	L5	1683	PSU	2	0
48	S2	1232	PSU	2	0
3	L5	1881	OMC	1	0
3	L5	2364	OMG	1	0
3	L5	3925	OMU	1	0
3	L5	3758	PSU	1	0
48	S2	1447	OMG	3	0
3	L5	3867	A2M	4	0
48	S2	681	PSU	2	0
3	L5	4618	OMG	1	0
3	L5	4220	6MZ	3	0
3	L5	4579	PSU	3	0
3	L5	2632	PSU	1	0
3	L5	3718	A2M	3	0
48	S2	1004	PSU	2	0
48	S2	1174	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4498	OMU	1	0
3	L5	4637	OMG	1	0
48	S2	601	OMG	1	0
48	S2	218	PSU	1	0
3	L5	3785	A2M	1	0
48	S2	93	PSU	1	0
3	L5	1860	PSU	1	0
3	L5	4571	A2M	2	0
3	L5	4456	OMC	2	0
3	L5	398	A2M	2	0
3	L5	1524	A2M	1	0
48	S2	468	A2M	1	0
3	L5	3899	OMG	1	0
48	S2	644	OMG	1	0
48	S2	867	OMG	1	0
48	S2	1692	PSU	1	0
48	S2	1442	OMU	1	0
48	S2	462	OMC	2	0
48	S2	27	A2M	3	0
1	2	37	MIA	2	0
3	L5	3792	OMG	3	0
3	L5	4196	OMG	1	0
3	L5	4523	A2M	1	0
3	L5	3841	OMC	1	0
48	S2	159	A2M	3	0
3	L5	2876	OMG	2	0
3	L5	1779	PSU	1	0
3	L5	3723	A2M	2	0
3	L5	3825	A2M	1	0
3	L5	3770	PSU	1	0
3	L5	2804	OMC	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 425 ligands modelled in this entry, 392 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
87	SPD	Ln	101	-	9,9,9	0.45	0	8,8,8	0.31	0
87	SPD	LN	301	-	9,9,9	0.44	0	8,8,8	0.44	0
88	PUT	L5	5117	-	5,5,5	0.23	0	4,4,4	0.16	0
87	SPD	S2	1905	-	9,9,9	0.44	0	8,8,8	0.22	0
88	PUT	L5	5110	-	5,5,5	0.21	0	4,4,4	0.22	0
88	PUT	S2	1907	-	5,5,5	0.22	0	4,4,4	0.17	0
87	SPD	L5	5102	-	9,9,9	0.42	0	8,8,8	0.35	0
87	SPD	L5	5107	-	9,9,9	0.43	0	8,8,8	0.33	0
88	PUT	L5	5119	-	5,5,5	0.21	0	4,4,4	0.16	0
87	SPD	S2	1909	-	9,9,9	0.44	0	8,8,8	0.41	0
87	SPD	S2	1903	-	9,9,9	0.45	0	8,8,8	0.33	0
87	SPD	S2	1908	-	9,9,9	0.44	0	8,8,8	0.22	0
87	SPD	L5	5112	-	9,9,9	0.46	0	8,8,8	0.27	0
88	PUT	L5	5118	-	5,5,5	0.24	0	4,4,4	0.23	0
87	SPD	S2	1910	-	9,9,9	0.43	0	8,8,8	0.31	0
88	PUT	L5	5111	-	5,5,5	0.24	0	4,4,4	0.08	0
88	PUT	L5	5113	-	5,5,5	0.22	0	4,4,4	0.17	0
87	SPD	L5	5108	-	9,9,9	0.42	0	8,8,8	0.30	0
87	SPD	L5	5120	-	9,9,9	0.44	0	8,8,8	0.29	0
88	PUT	L5	5109	-	5,5,5	0.22	0	4,4,4	0.18	0
87	SPD	L5	5121	-	9,9,9	0.41	0	8,8,8	0.28	0
87	SPD	S2	1906	-	9,9,9	0.45	0	8,8,8	0.31	0
91	HYG	S2	1904	85	35,39,39	0.61	1 (2%)	43,60,60	1.16	5 (11%)
86	ANM	L5	5101	85	20,20,20	0.46	0	22,27,27	0.45	0
87	SPD	L5	5105	-	9,9,9	0.43	0	8,8,8	0.25	0
87	SPD	L5	5104	-	9,9,9	0.43	0	8,8,8	0.22	0
88	PUT	L5	5114	-	5,5,5	0.21	0	4,4,4	0.21	0
87	SPD	L5	5115	-	9,9,9	0.43	0	8,8,8	0.34	0
87	SPD	L5	5106	-	9,9,9	0.45	0	8,8,8	0.33	0
87	SPD	S2	1901	-	9,9,9	0.44	0	8,8,8	0.36	0
87	SPD	L5	5116	-	9,9,9	0.43	0	8,8,8	0.31	0
88	PUT	S2	1902	-	5,5,5	0.21	0	4,4,4	0.22	0
87	SPD	L5	5103	-	9,9,9	0.43	0	8,8,8	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	Ln	101	-	-	0/7/7/7	-
87	SPD	LN	301	-	-	3/7/7/7	-
88	PUT	L5	5117	-	-	0/3/3/3	-
87	SPD	S2	1905	-	-	1/7/7/7	-
88	PUT	L5	5110	-	-	0/3/3/3	-
88	PUT	S2	1907	-	-	0/3/3/3	-
87	SPD	L5	5102	-	-	1/7/7/7	-
87	SPD	L5	5107	-	-	1/7/7/7	-
88	PUT	L5	5119	-	-	1/3/3/3	-
87	SPD	S2	1909	-	-	2/7/7/7	-
87	SPD	S2	1903	-	-	0/7/7/7	-
87	SPD	S2	1908	-	-	3/7/7/7	-
87	SPD	L5	5112	-	-	0/7/7/7	-
88	PUT	L5	5118	-	-	2/3/3/3	-
87	SPD	S2	1910	-	-	2/7/7/7	-
88	PUT	L5	5111	-	-	0/3/3/3	-
88	PUT	L5	5113	-	-	0/3/3/3	-
87	SPD	L5	5108	-	-	2/7/7/7	-
87	SPD	L5	5120	-	-	1/7/7/7	-
88	PUT	L5	5109	-	-	0/3/3/3	-
87	SPD	L5	5121	-	-	1/7/7/7	-
87	SPD	S2	1906	-	-	2/7/7/7	-
91	HYG	S2	1904	85	-	2/12/87/87	0/4/4/4
86	ANM	L5	5101	85	-	0/10/23/23	0/2/2/2
87	SPD	L5	5105	-	-	3/7/7/7	-
87	SPD	L5	5104	-	-	0/7/7/7	-
88	PUT	L5	5114	-	-	0/3/3/3	-
87	SPD	L5	5115	-	-	1/7/7/7	-
87	SPD	L5	5106	-	-	3/7/7/7	-
87	SPD	S2	1901	-	-	0/7/7/7	-
87	SPD	L5	5116	-	-	1/7/7/7	-
88	PUT	S2	1902	-	-	1/3/3/3	-
87	SPD	L5	5103	-	-	0/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	S2	1904	HYG	C3-C4	-2.31	1.49	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	S2	1904	HYG	O29-C12-C13	3.58	120.27	110.86
91	S2	1904	HYG	O22-C17-C16	2.90	118.29	111.22
91	S2	1904	HYG	C16-C17-C12	-2.77	106.77	113.50
91	S2	1904	HYG	O14-C13-C12	-2.43	104.69	109.51
91	S2	1904	HYG	O11-C5-C4	-2.42	104.47	109.47

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	S2	1909	SPD	C4-C5-N6-C7
87	L5	5106	SPD	C3-C4-C5-N6
87	L5	5105	SPD	C3-C4-C5-N6
87	L5	5107	SPD	N6-C7-C8-C9
87	S2	1910	SPD	N6-C7-C8-C9

There are no ring outliers.

23 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	Ln	101	SPD	3	0
87	LN	301	SPD	2	0
88	L5	5117	PUT	2	0
87	S2	1905	SPD	1	0
88	L5	5110	PUT	1	0
88	S2	1907	PUT	1	0
87	L5	5102	SPD	1	0
87	L5	5107	SPD	2	0
88	L5	5119	PUT	2	0
87	S2	1903	SPD	1	0
87	L5	5112	SPD	1	0
88	L5	5111	PUT	1	0
87	L5	5108	SPD	2	0
87	L5	5121	SPD	1	0
87	S2	1906	SPD	1	0
91	S2	1904	HYG	1	0
86	L5	5101	ANM	1	0
87	L5	5105	SPD	1	0
87	L5	5104	SPD	2	0
88	L5	5114	PUT	1	0
87	L5	5115	SPD	1	0

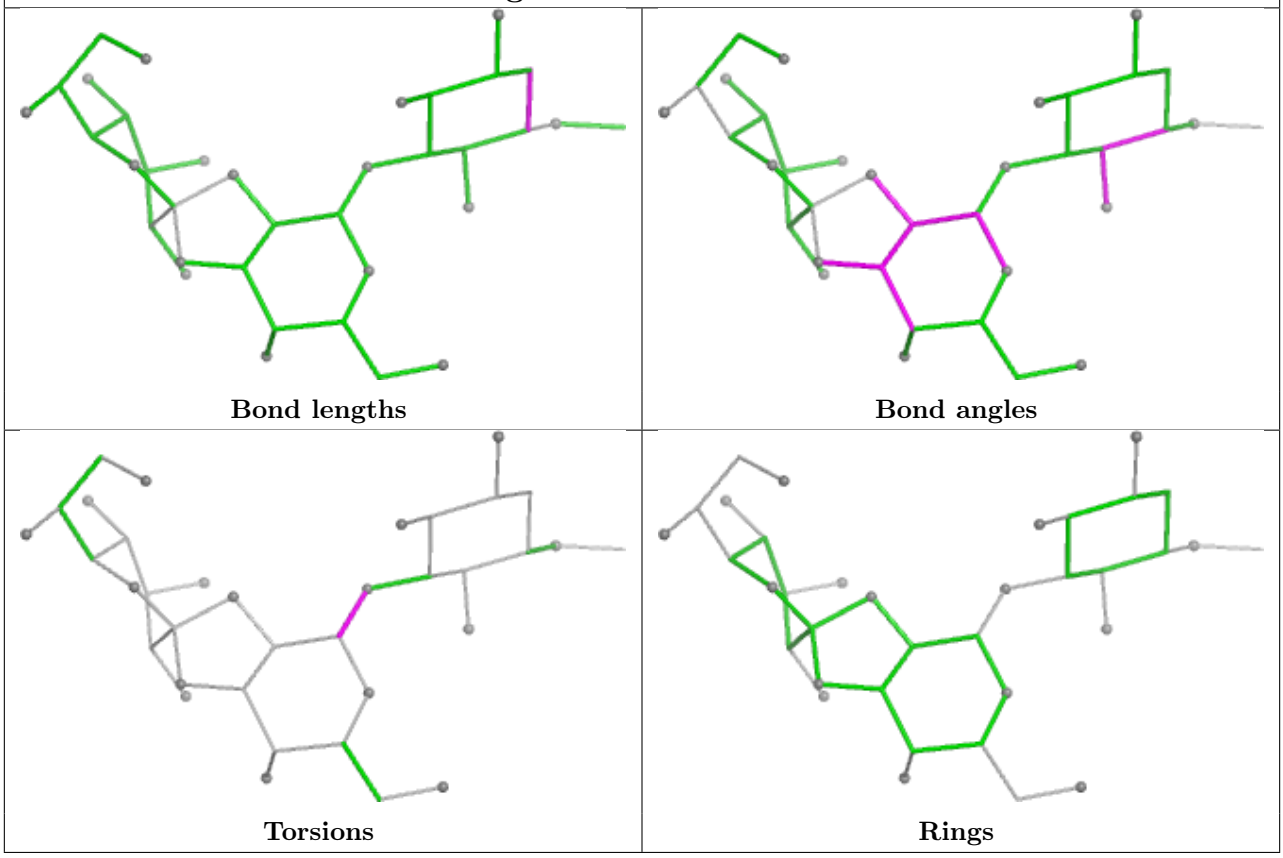
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	S2	1901	SPD	1	0
87	L5	5116	SPD	2	0

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

Ligand HYG S2 1904



5.7 Other polymers

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
83	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	8:U	O3'	66:C	P	13.80

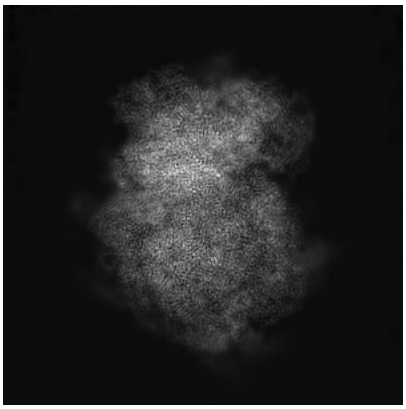
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55496. These allow visual inspection of the internal detail of the map and identification of artifacts.

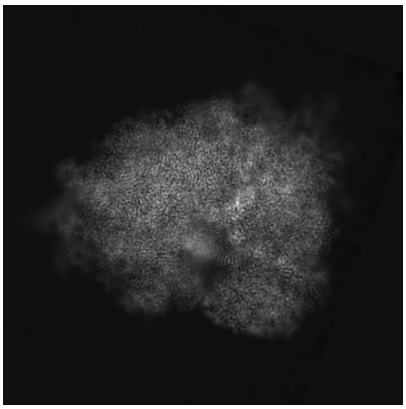
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

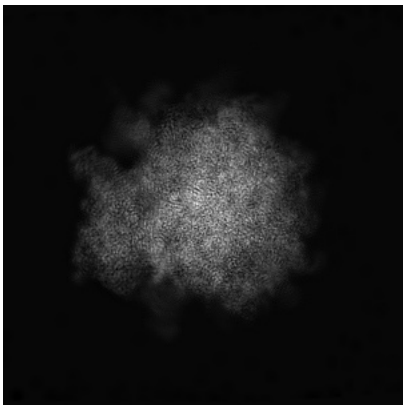
6.1.1 Primary map



X

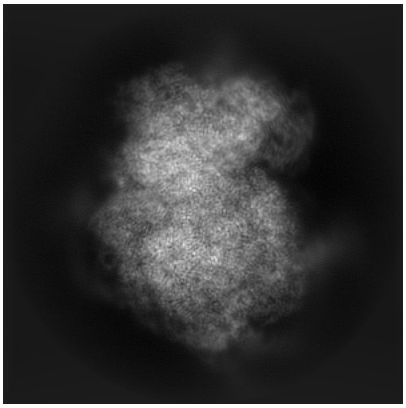


Y

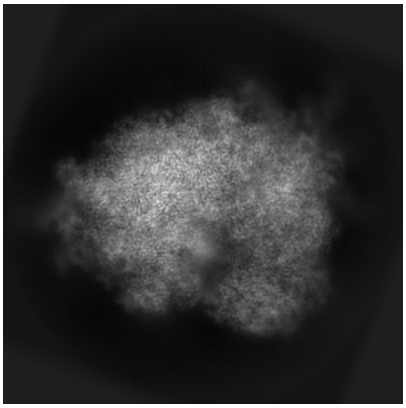


Z

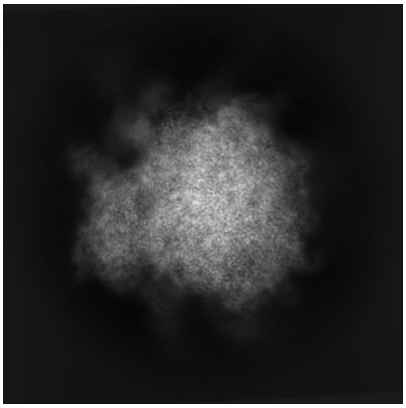
6.1.2 Raw map



X



Y

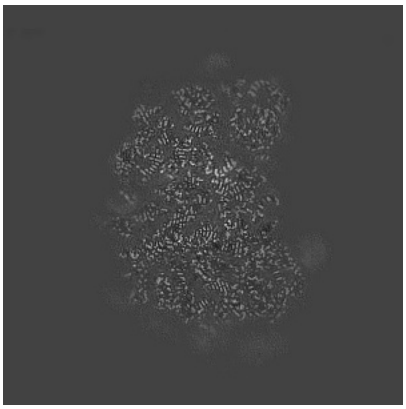


Z

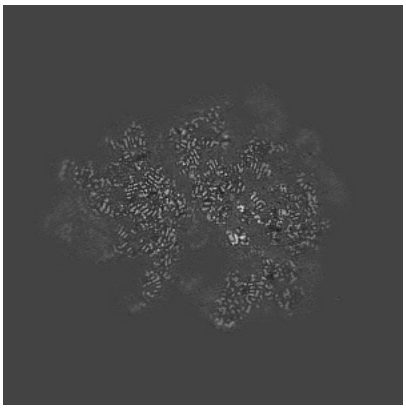
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

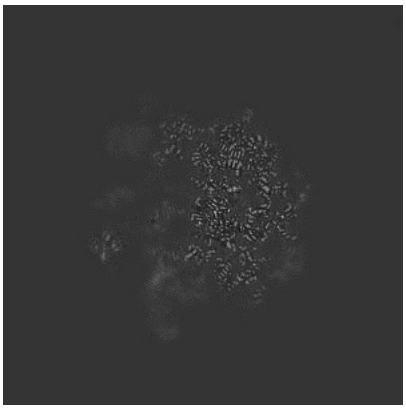
6.2.1 Primary map



X Index: 240

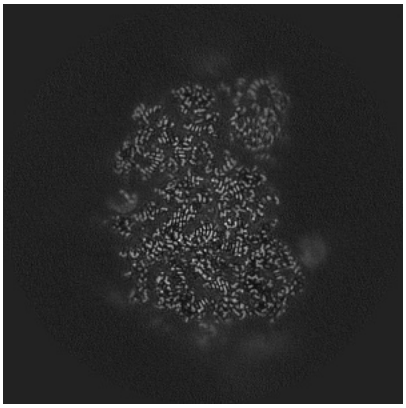


Y Index: 240

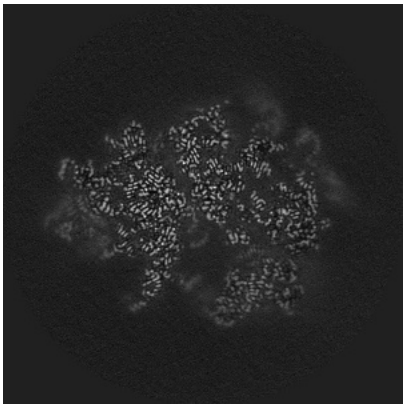


Z Index: 240

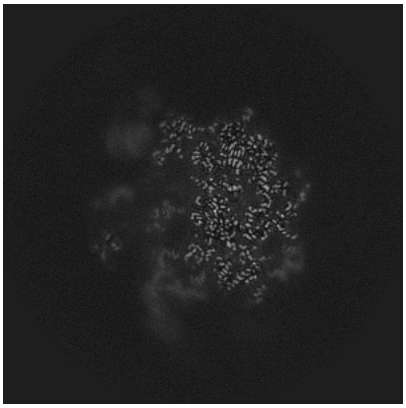
6.2.2 Raw map



X Index: 240



Y Index: 240

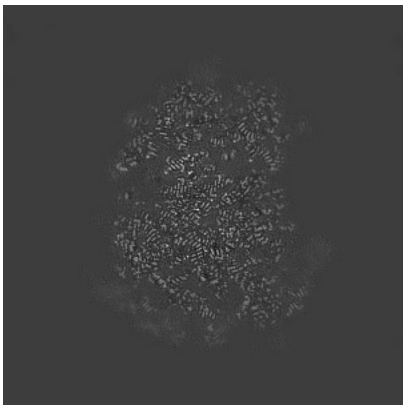


Z Index: 240

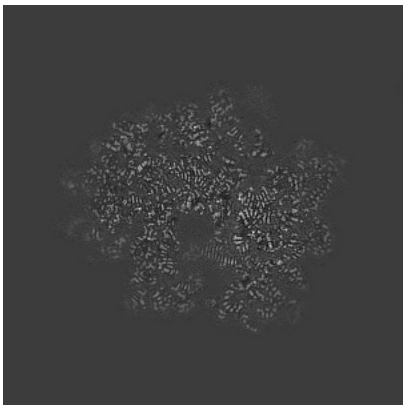
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 253

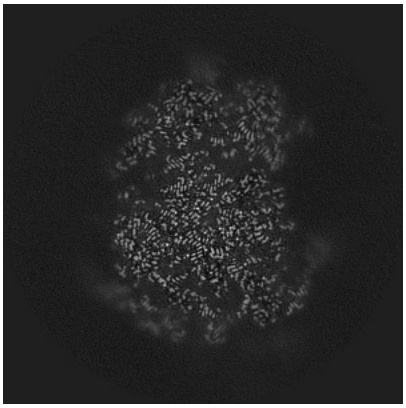


Y Index: 217

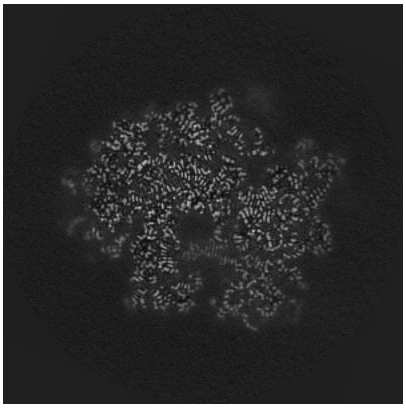


Z Index: 281

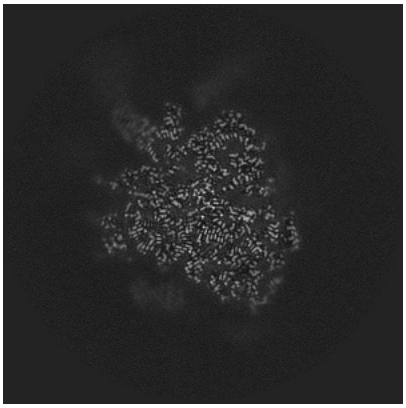
6.3.2 Raw map



X Index: 253



Y Index: 217

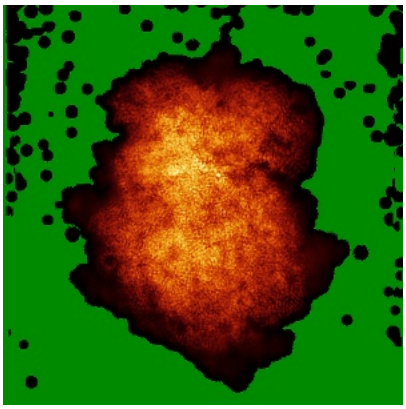


Z Index: 197

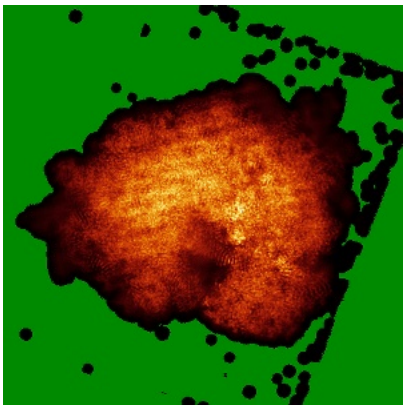
The images above show the largest variance slices of the map in three orthogonal directions.

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

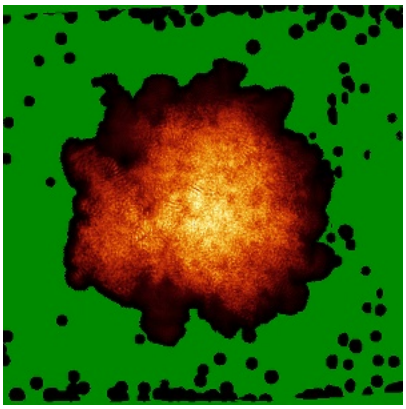
6.4.1 Primary map



X

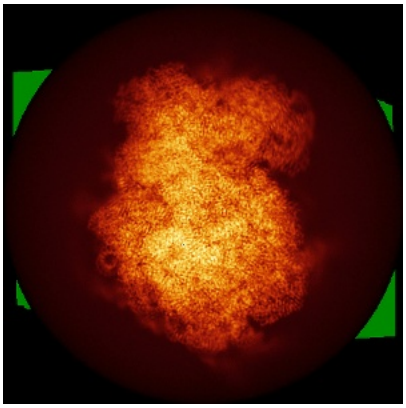


Y

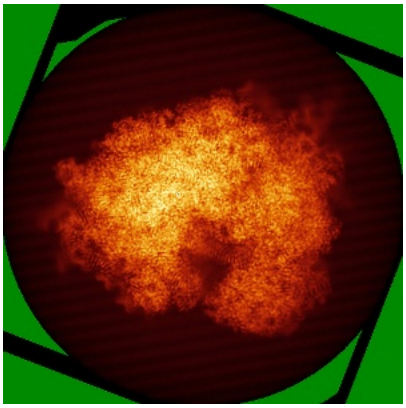


Z

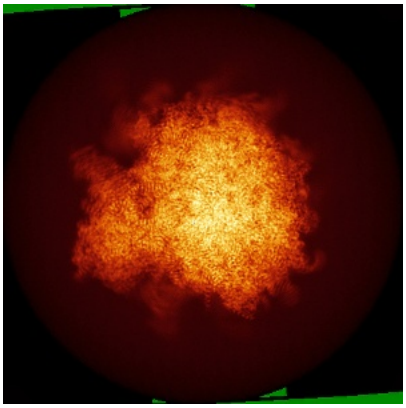
6.4.2 Raw map



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)

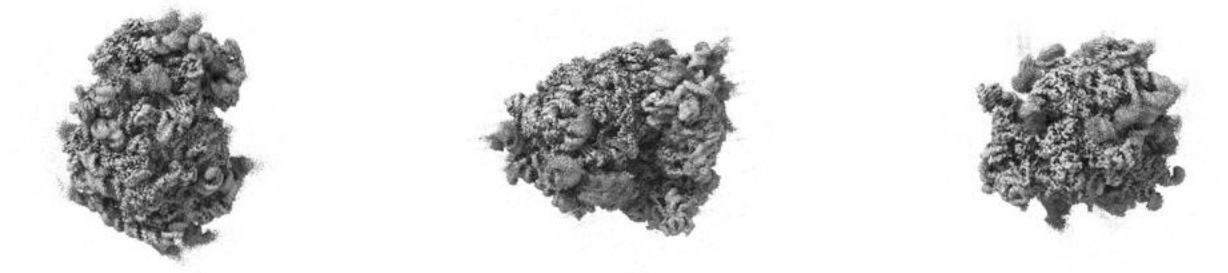
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

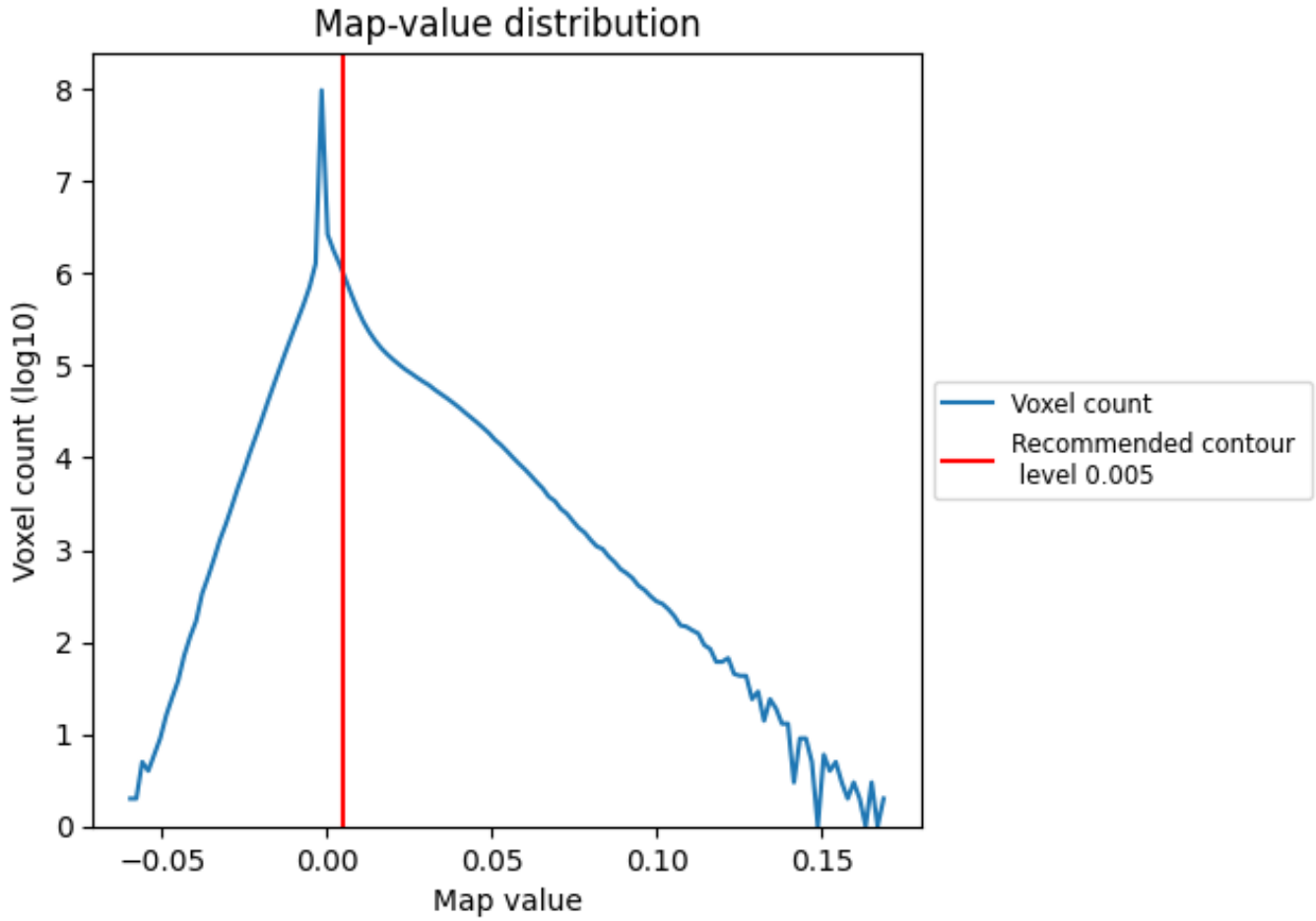
6.6 Mask visualisation (i)

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

7 Map analysis

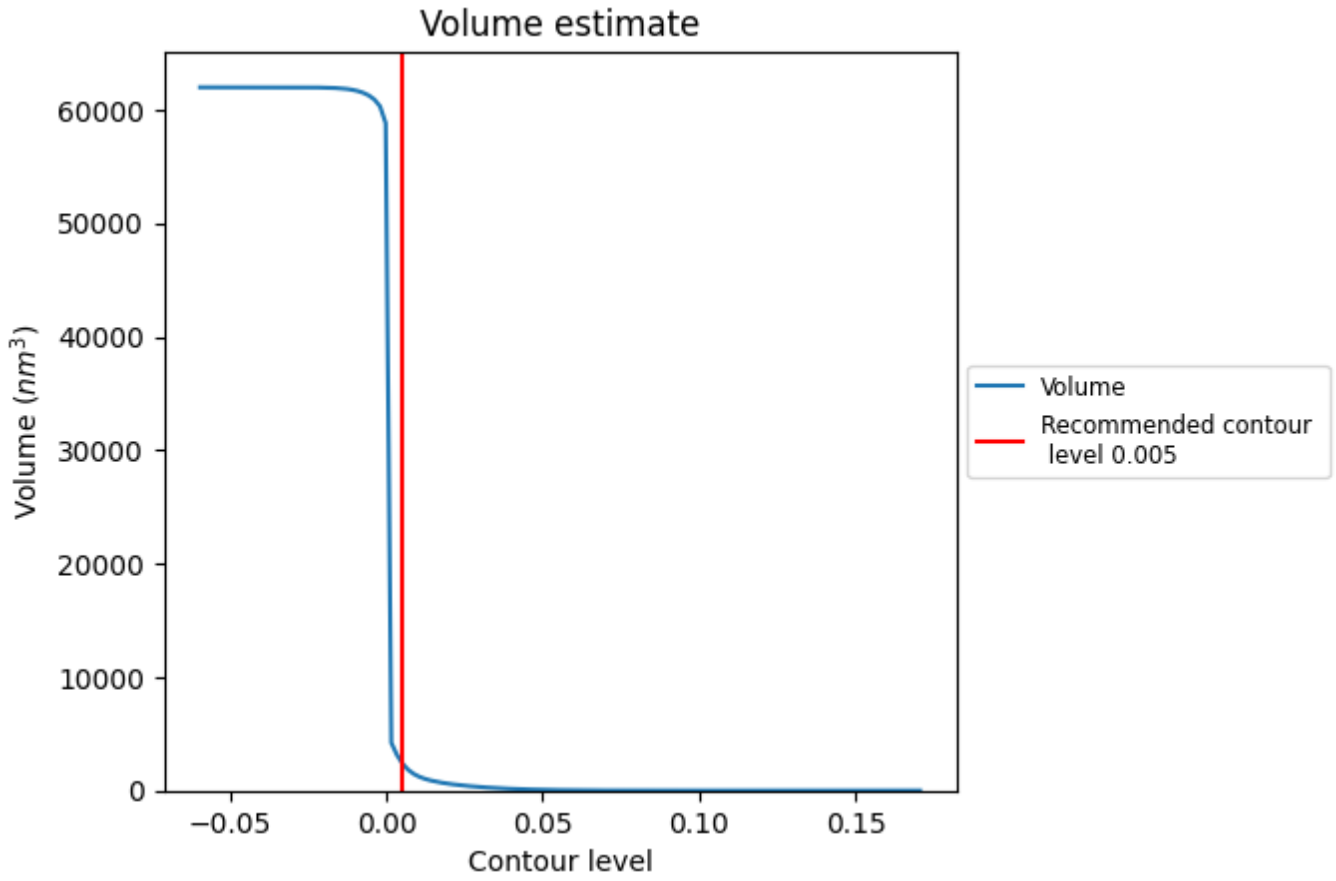
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

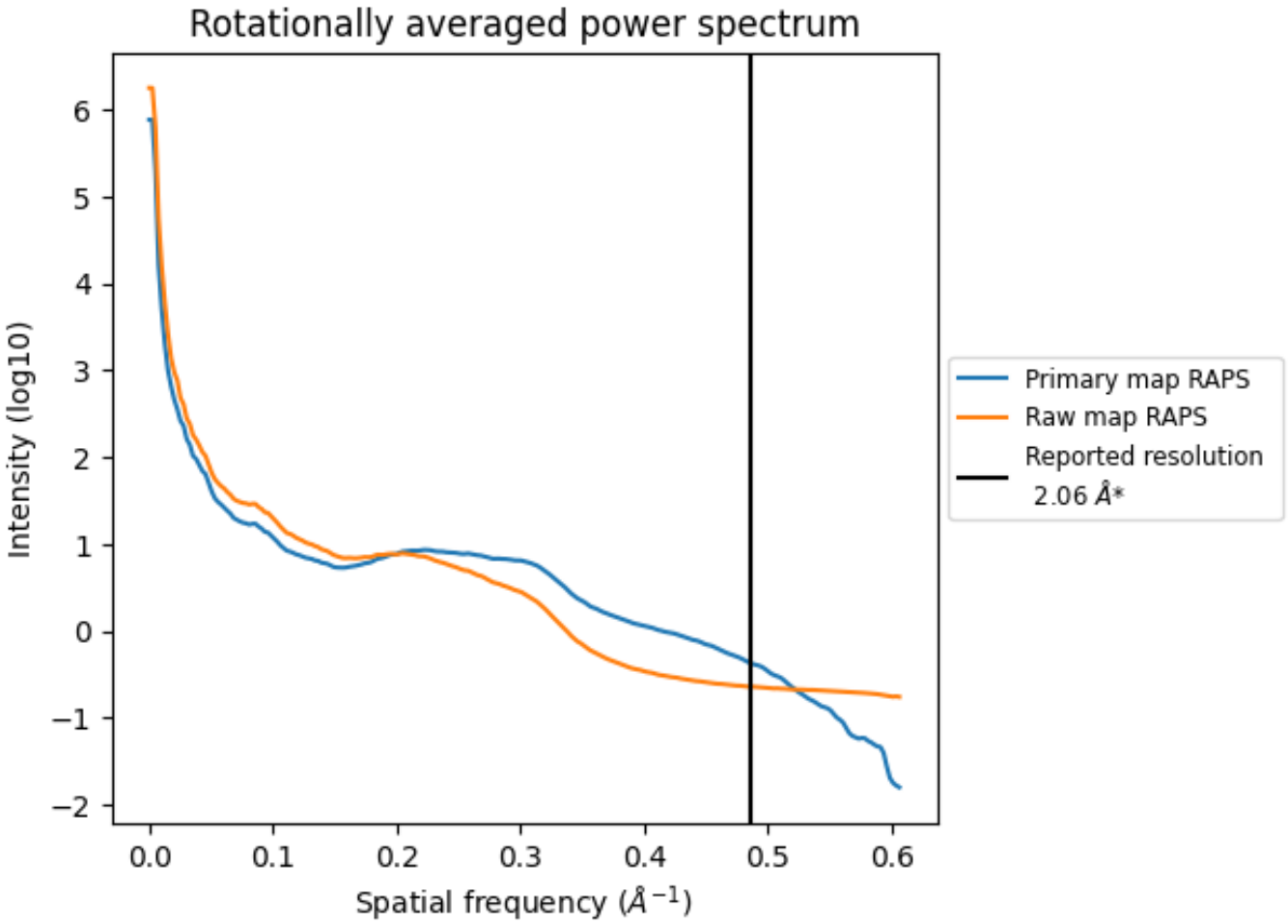
7.2 Volume estimate



The volume at the recommended contour level is 2443 nm^3; this corresponds to an approximate mass of 2206 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

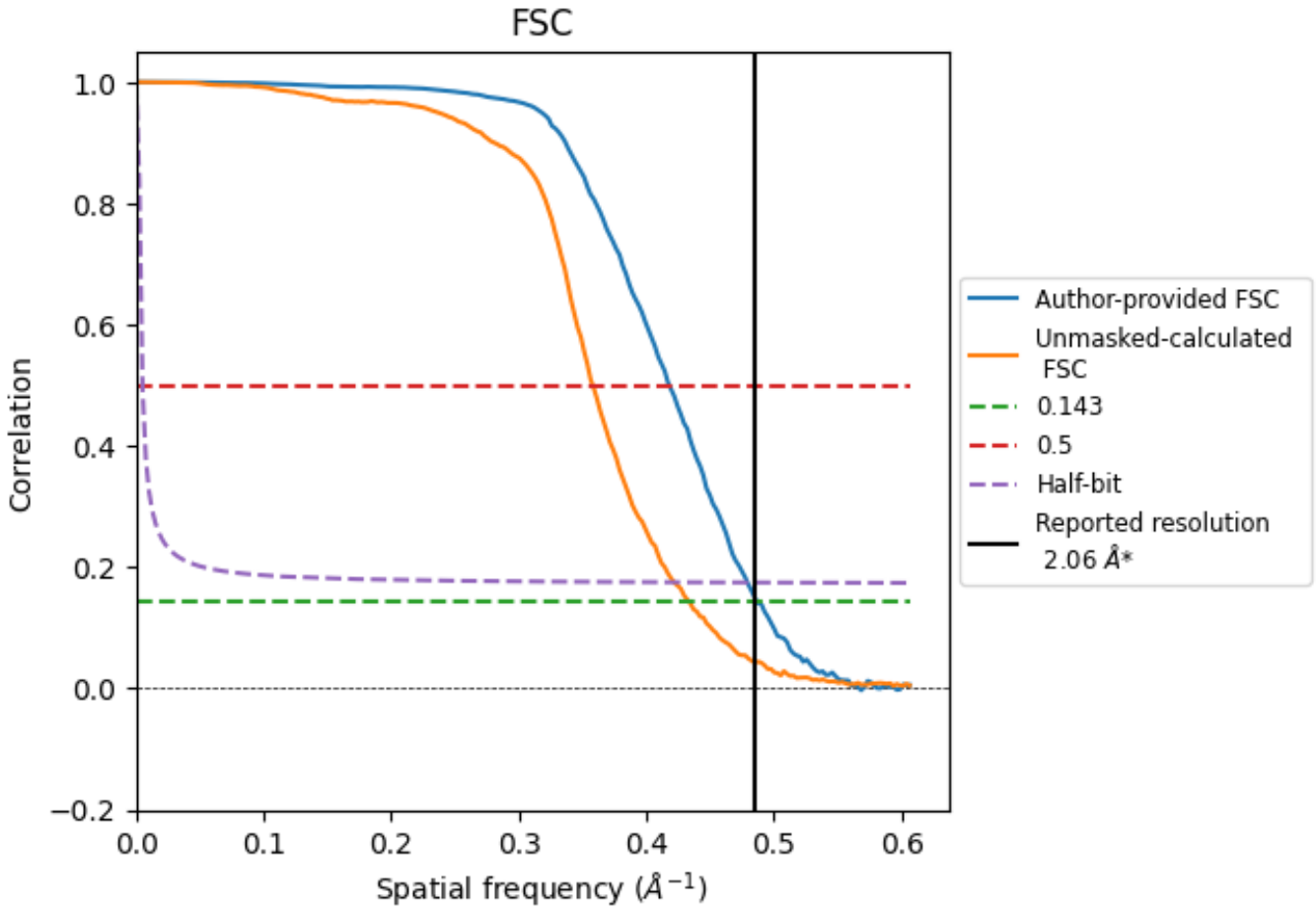


*Reported resolution corresponds to spatial frequency of 0.485 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.485 Å^{-1}

8.2 Resolution estimates (i)

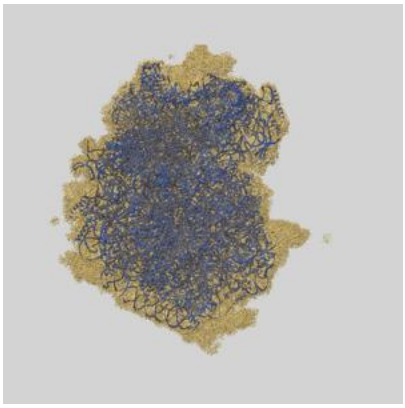
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.05	2.39	2.09
Unmasked-calculated*	2.31	2.79	2.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.31 differs from the reported value 2.06 by more than 10 %

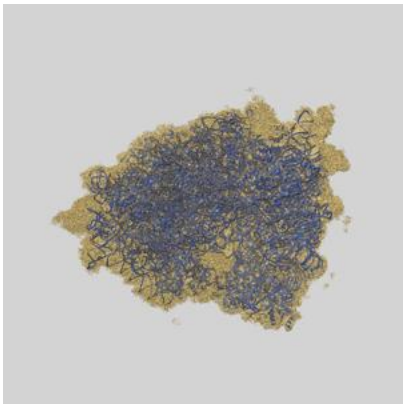
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55496 and PDB model 9T3I. Per-residue inclusion information can be found in section 3 on page 29.

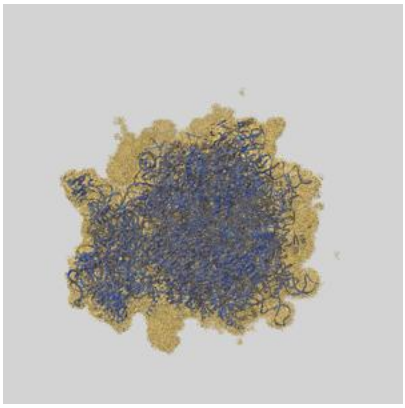
9.1 Map-model overlay



X



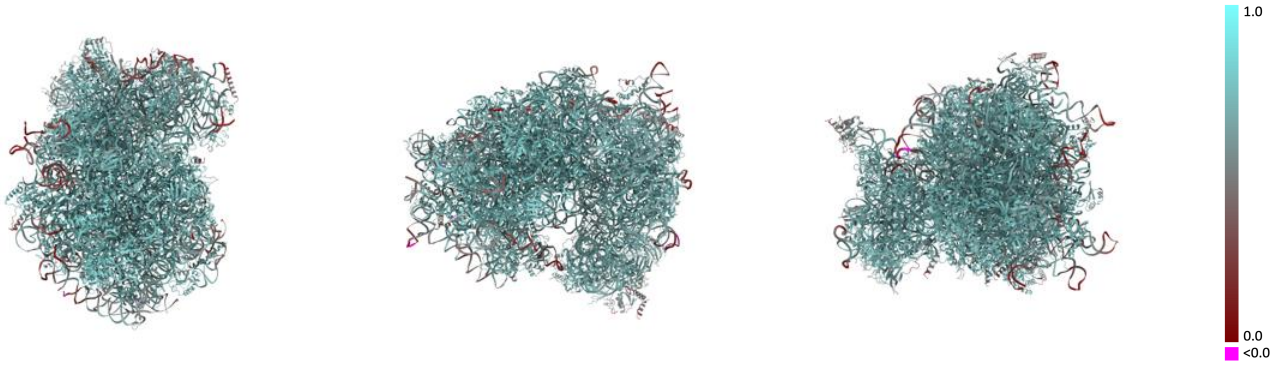
Y



Z

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

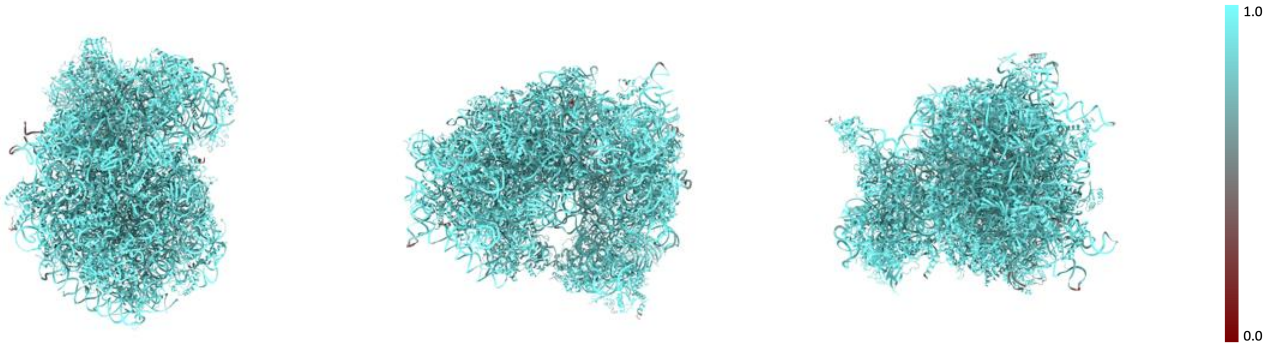
9.2 Q-score mapped to coordinate model



X Y Z

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

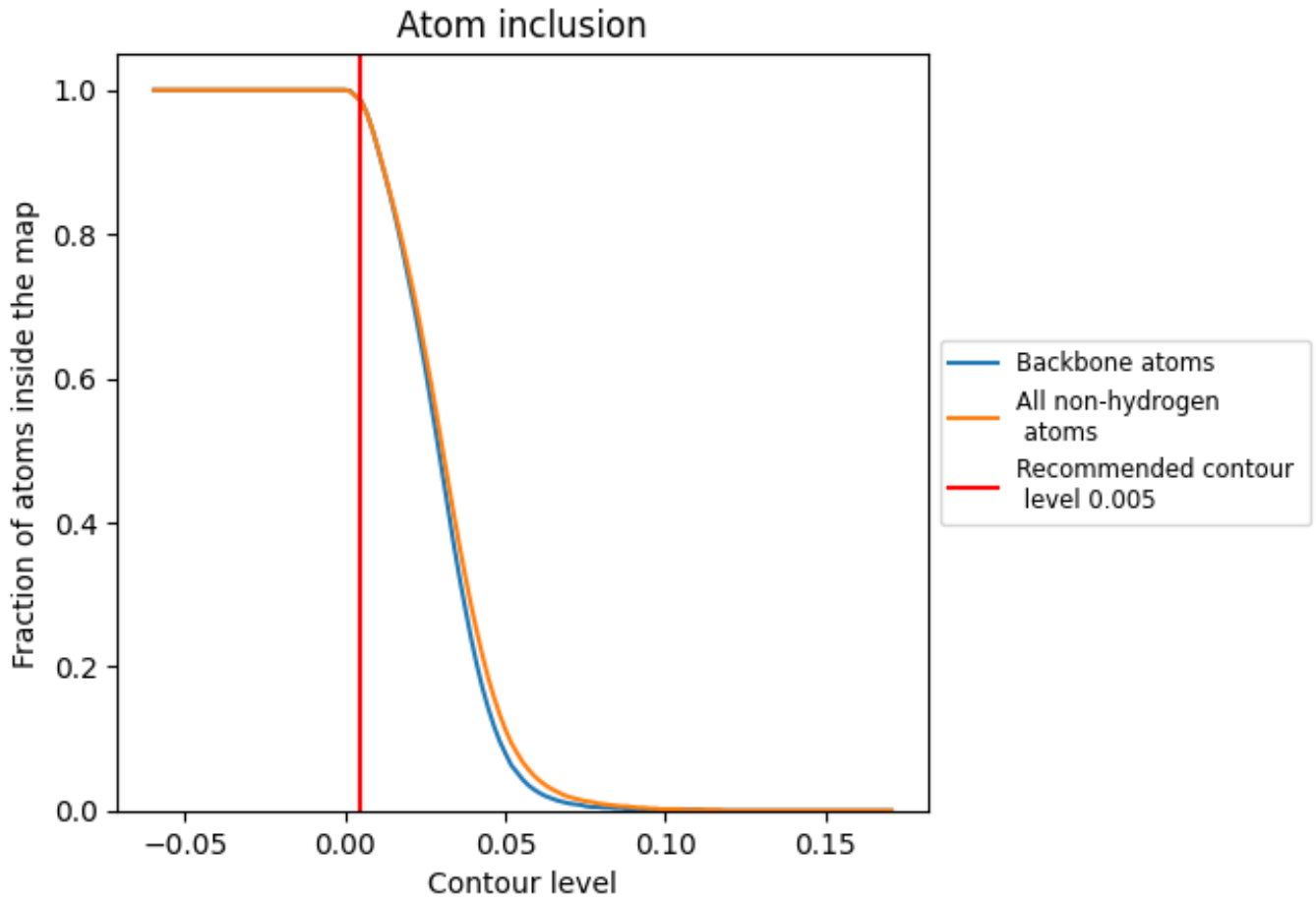
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.9850	0.6920
2	0.9200	0.5590
3	0.9750	0.6020
4	0.9950	0.6290
5	0.9830	0.6390
L5	0.9820	0.6760
L7	0.9970	0.7220
L8	0.9890	0.7000
LA	0.9980	0.7790
LB	0.9860	0.7500
LC	0.9890	0.7570
LD	0.9850	0.7070
LE	0.9900	0.7110
LF	0.9950	0.7590
LG	0.9590	0.6830
LH	0.9930	0.7320
LI	0.9930	0.7450
LJ	0.9910	0.6860
LL	0.9860	0.7380
LM	0.9970	0.7390
LN	0.9990	0.7820
LO	0.9920	0.7560
LP	0.9920	0.7620
LQ	1.0000	0.7780
LR	0.9650	0.6990
LS	0.9990	0.7580
LT	0.9860	0.7280
LU	0.9880	0.6390
LV	0.9990	0.7660
LW	0.9320	0.6270
LX	0.9930	0.7480
LY	0.9890	0.7420
LZ	0.9940	0.7190
La	0.9920	0.7710
Lb	0.9520	0.6640



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Chain	Atom inclusion	Q-score
Lc	0.9870	0.7400
Ld	0.9940	0.7320
Le	0.9970	0.7740
Lf	0.9960	0.7770
Lg	0.9830	0.7410
Lh	0.9970	0.7410
Li	0.9910	0.7210
Lj	1.0000	0.7810
Lk	0.9850	0.6710
Ll	1.0000	0.7600
Lm	0.9900	0.7450
Ln	1.0000	0.7370
Lo	0.9870	0.7350
Lp	0.9940	0.7720
Lr	0.9990	0.7590
S2	0.9900	0.6750
SA	0.9810	0.6970
SB	0.9970	0.7110
SC	0.9920	0.7230
SD	0.9790	0.6740
SE	0.9850	0.6910
SF	0.9940	0.7220
SG	0.9720	0.6510
SH	0.9480	0.6340
SI	0.9800	0.6840
SJ	0.9850	0.6860
SK	0.9900	0.6830
SL	0.9880	0.7050
SM	0.9370	0.4750
SN	0.9940	0.7370
SO	0.9960	0.7300
SP	0.9730	0.6720
SQ	0.9920	0.7210
SR	0.9680	0.6610
SS	0.9930	0.7020
ST	0.9870	0.7090
SU	0.9450	0.6400
SV	0.9860	0.7050
SW	0.9980	0.7390
SX	0.9930	0.7180
SY	0.9680	0.6570
SZ	0.9570	0.6730

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Chain	Atom inclusion	Q-score
Sa	0.9910	0.7340
Sb	0.9470	0.6630
Sc	0.9980	0.6850
Sd	0.9760	0.6930
Se	0.9790	0.6610
Sf	0.8980	0.5260
Sg	0.9790	0.6370