



wwPDB EM Validation Summary Report ⓘ

Jun 17, 2026 – 04:51 pm BST

PDB ID : 9I14 / pdb_00009i14
EMDB ID : EMD-52565
Title : CRYO-EM STRUCTURE OF HCT15 POLYSOMES IN HYBRID-PRE STATE
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2025-01-15
Resolution : 3.34 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

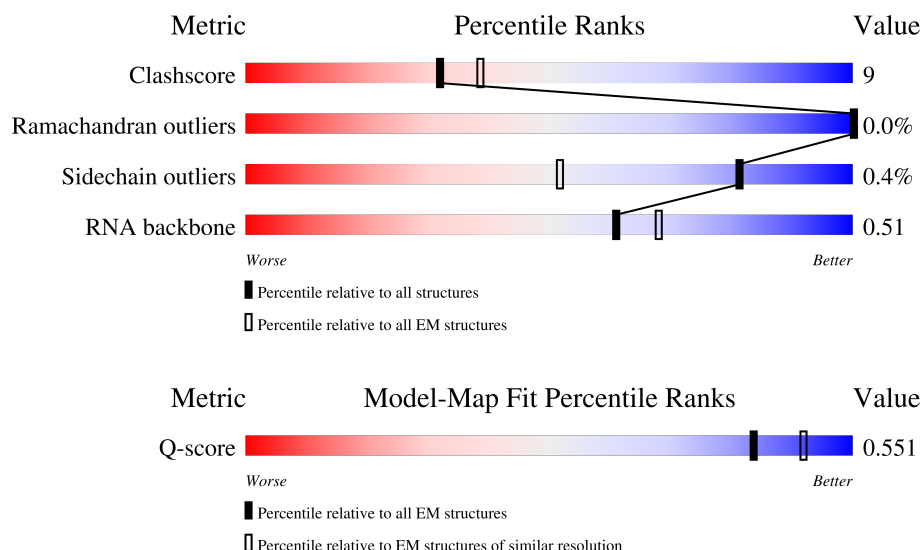
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.34 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	14446 (2.84 - 3.84)

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

Mol	Chain	Length	Quality of chain
1	LA	257	
2	SA	295	
3	LB	403	

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Mol	Chain	Length	Quality of chain
4	SB	264	
5	A4	13	
6	B4	75	
7	D4	76	
8	L5	5070	
9	L7	120	
10	L8	156	
11	LC	427	
12	LD	297	
13	LE	288	
14	LF	248	
15	LG	266	
16	LH	192	
17	LJ	178	
18	LL	211	
19	LM	215	
20	LN	204	
21	LO	203	
22	LP	184	
23	LQ	188	
24	LR	196	
25	LS	176	
26	LT	160	
27	LU	128	
28	LV	140	

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Mol	Chain	Length	Quality of chain
29	LW	157	
30	LX	156	
31	LY	145	
32	LZ	136	
33	La	148	
34	Lb	159	
35	Lc	115	
36	Ld	125	
37	Lf	110	
38	Lg	117	
39	Lh	123	
40	Li	105	
41	Lj	97	
42	Lk	70	
43	Ll	51	
44	Lm	128	
45	Ln	25	
46	Lo	106	
47	Lp	92	
48	Lr	137	
49	S2	1869	
50	SC	293	
51	SD	243	
52	SE	263	
53	SF	204	

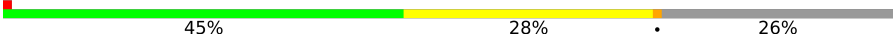
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Mol	Chain	Length	Quality of chain
54	SG	249	
55	SH	194	
56	SI	208	
57	SJ	194	
58	SK	165	
59	SL	158	
60	SN	151	
61	SO	151	
62	SP	145	
63	SQ	146	
64	SR	135	
65	SS	152	
66	ST	145	
67	SU	119	
68	SV	83	
69	SW	130	
70	SX	143	
71	SY	133	
72	SZ	125	
73	Sa	115	
74	Sb	84	
75	Sc	69	
76	Sd	56	
77	Se	59	
78	Sf	156	

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Mol	Chain	Length	Quality of chain
79	Sg	317	 74% 23%
80	SM	132	 45% 28% 26%
81	Le	135	 73% 21% 6%
82	LI	214	 74% 19% 5%

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 206575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LA	248	Total	C	N	O	S	0	0
			1886	1183	386	311	6		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SA	217	Total	C	N	O	S	0	0
			1705	1084	300	313	8		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LB	398	Total	C	N	O	S	0	0
			3147	2008	591	534	14		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SB	213	Total	C	N	O	S	0	0
			1727	1096	309	308	14		

- Molecule 5 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A4	11	Total	C	N	O	P	0	0
			231	104	37	79	11		

- Molecule 6 is a RNA chain called P/E tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B4	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 7 is a RNA chain called A/P tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D4	63	Total	C	N	O	P	0	0
			1349	601	243	442	63		

- Molecule 8 is a RNA chain called LSU 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L5	3465	Total	C	N	O	P	0	0
			74335	33126	13606	24139	3464		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 10 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L8	147	Total	C	N	O	P	0	0
			3132	1399	557	1030	146		

- Molecule 11 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC	362	Total	C	N	O	S	0	0
			2874	1808	574	477	15		

- Molecule 12 is a protein called 60S ribosomal protein L5.

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

- Molecule 13 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	209	Total	C	N	O	S	0	0
			1648	1061	313	270	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LF	222	Total	C	N	O	S	0	0
			1846	1186	354	297	9		

- Molecule 15 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	224	Total	C	N	O	S	0	0
			1793	1143	343	303	4		

- Molecule 16 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	191	Total	C	N	O	S	0	0
			1526	960	285	275	6		

- Molecule 17 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LJ	167	Total	C	N	O	S	0	0
			1330	841	249	234	6		

- Molecule 18 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LL	198	Total	C	N	O	S	0	0
			1588	994	333	257	4		

- Molecule 19 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LM	137	Total	C	N	O	S	0	0
			1121	719	215	180	7		

- Molecule 20 is a protein called 60S ribosomal protein L15.

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

- Molecule 21 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LO	201	Total	C	N	O	S	0	0
			1646	1061	321	259	5		

- Molecule 22 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LP	157	Total	C	N	O	S	0	0
			1267	794	243	221	9		

- Molecule 23 is a protein called 60S ribosomal protein L18.

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

- Molecule 24 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LR	175	Total	C	N	O	S	0	0
			1458	902	317	230	9		

- Molecule 25 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LS	173	Total	C	N	O	S	0	0
			1431	912	278	232	9		

- Molecule 26 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LT	155	Total	C	N	O	S	0	0
			1247	789	244	208	6		

- Molecule 27 is a protein called 60S ribosomal protein L22.

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

- Molecule 28 is a protein called 60S ribosomal protein L23.

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

- Molecule 29 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LW	89	Total	C	N	O	S	0	0
			663	420	129	112	2		

- Molecule 30 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LX	118	Total	C	N	O	S	0	0
			962	615	180	166	1		

- Molecule 31 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LY	134	Total	C	N	O	S	0	0
			1103	692	223	185	3		

- Molecule 32 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LZ	135	Total	C	N	O	S	1	0
			1115	719	211	182	3		

- Molecule 33 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	La	147	Total	C	N	O	S	0	0
			1159	735	236	185	3		

- Molecule 34 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lb	92	Total	C	N	O	S	0	0
			747	465	163	117	2		

- Molecule 35 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lc	93	Total	C	N	O	S	0	0
			725	462	128	128	7		

- Molecule 36 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ld	106	Total	C	N	O	S	0	0
			871	552	170	147	2		

- Molecule 37 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lf	109	Total	C	N	O	S	0	0
			867	550	173	141	3		

- Molecule 38 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lg	110	Total	C	N	O	S	0	0
			861	539	177	139	6		

- Molecule 39 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lh	122	Total	C	N	O	S	0	0
			1011	638	204	168	1		

- Molecule 40 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Li	100	Total	C	N	O	S	0	0
			818	512	174	127	5		

- Molecule 41 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lj	87	Total	C	N	O	S	0	0
			715	440	158	112	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lj	57	THR	ASN	conflict	UNP P61927

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lk	69	Total	C	N	O	S	0	0
			553	356	100	96	1		

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ll	49	Total	C	N	O	S	0	0
			435	275	97	62	1		

- Molecule 44 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lm	51	Total	C	N	O	S	0	0
			411	255	87	63	6		

- Molecule 45 is a protein called 60S ribosomal protein L41.

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

- Molecule 46 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lo	103	Total	C	N	O	S	0	0
			839	525	172	136	6		

- Molecule 47 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lp	91	Total	C	N	O	S	0	0
			707	445	136	119	7		

- Molecule 48 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lr	125	Total	C	N	O	S	0	0
			992	615	207	166	4		

- Molecule 49 is a RNA chain called SSU 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S2	1577	Total	C	N	O	P	0	0
			33711	15068	6064	11003	1576		

- Molecule 50 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SC	220	Total	C	N	O	S	0	0
			1704	1102	293	300	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SD	223	Total	C	N	O	S	0	0
			1689	1077	304	301	7		

- Molecule 52 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	187	Total	C	N	O	S	0	0
			1486	929	282	268	7		

- Molecule 54 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SG	221	Total	C	N	O	S	0	0
			1749	1097	349	296	7		

- Molecule 55 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	SH	177	Total	C	N	O		
			1360	876	251	233	0	0

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SI	197	Total	C	N	O	S		
			1582	991	311	275	5	0	0

- Molecule 57 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SJ	178	Total	C	N	O	S		
			1482	944	296	240	2	0	0

- Molecule 58 is a protein called 40S ribosomal protein S10.

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

- Molecule 59 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SL	140	Total	C	N	O	S		
			1147	731	216	194	6	0	0

- Molecule 60 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SN	150	Total	C	N	O	S		
			1205	772	229	203	1	0	0

- Molecule 61 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SO	129	Total	C	N	O	S		
			959	586	190	177	6	0	0

- Molecule 62 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SP	129	Total	C	N	O	S	0	0
			1060	672	202	179	7		

- Molecule 63 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SQ	141	Total	C	N	O	S	0	0
			1120	713	212	192	3		

- Molecule 64 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SR	130	Total	C	N	O	S	0	0
			1053	663	197	189	4		

- Molecule 65 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SS	142	Total	C	N	O	S	0	0
			1171	735	239	196	1		

- Molecule 66 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	ST	141	Total	C	N	O	S	0	0
			1098	689	210	196	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ST	4	PHE	VAL	conflict	UNP P39019

- Molecule 67 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SU	101	Total	C	N	O	S	0	0
			790	495	152	139	4		

- Molecule 68 is a protein called 40S ribosomal protein S21.

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

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

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

- Molecule 70 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SX	141	Total	C	N	O	S	0	0
			1082	685	213	181	3		

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SY	123	Total	C	N	O	S	0	0
			988	625	191	167	5		

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SZ	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sa	99	Total	C	N	O	S	0	0
			788	490	165	128	5		

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sb	83	Total	C	N	O	S	0	0
			633	398	117	112	6		

- Molecule 75 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sc	63	Total	C	N	O	S	0	0
			489	299	97	91	2		

- Molecule 76 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sd	52	Total	C	N	O	S	0	0
			436	273	88	70	5		

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Se	50	Total	C	N	O	S	0	0
			400	245	91	63	1		

- Molecule 78 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sf	61	Total	C	N	O	S	0	0
			489	308	91	83	7		

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sg	306	Total	C	N	O	S	0	0
			2389	1507	417	453	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SM	98	Total	C	N	O	S	0	0
			722	451	134	130	7		

- Molecule 81 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Le	127	Total	C	N	O	S	0	0
			1044	662	214	163	5		

- Molecule 82 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	LI	203	Total	C	N	O	S	0	0
			1641	1042	316	270	13		

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
83	LA	1	Total	K	0
			1	1	
83	B4	3	Total	K	0
			3	3	
83	L5	17	Total	K	0
			17	17	
83	L8	1	Total	K	0
			1	1	
83	La	1	Total	K	0
			1	1	
83	S2	15	Total	K	0
			15	15	
83	SN	1	Total	K	0
			1	1	
83	Le	1	Total	K	0
			1	1	

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
84	A4	2	Total	Mg	0
			2	2	
84	B4	4	Total	Mg	0
			4	4	
84	D4	1	Total	Mg	0
			1	1	
84	L5	157	Total	Mg	0
			157	157	
84	L7	2	Total	Mg	0
			2	2	
84	L8	3	Total	Mg	0
			3	3	
84	LN	1	Total	Mg	0
			1	1	
84	LP	1	Total	Mg	0
			1	1	

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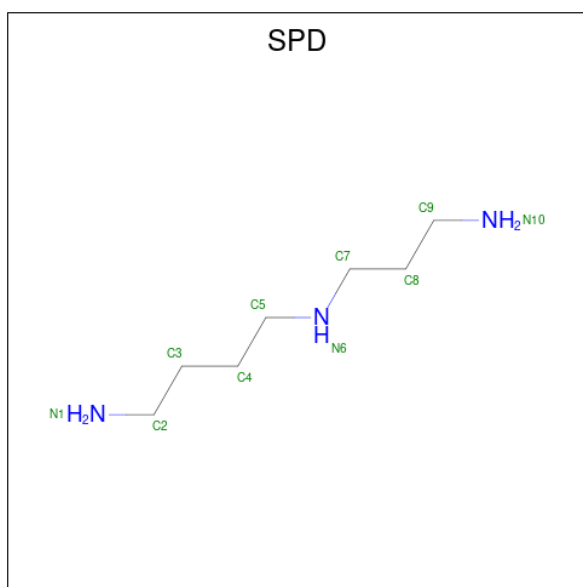
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
84	LT	1	Total 1	Mg 1	0
84	Lp	1	Total 1	Mg 1	0
84	S2	93	Total 93	Mg 93	0
84	LI	1	Total 1	Mg 1	0

- Molecule 85 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

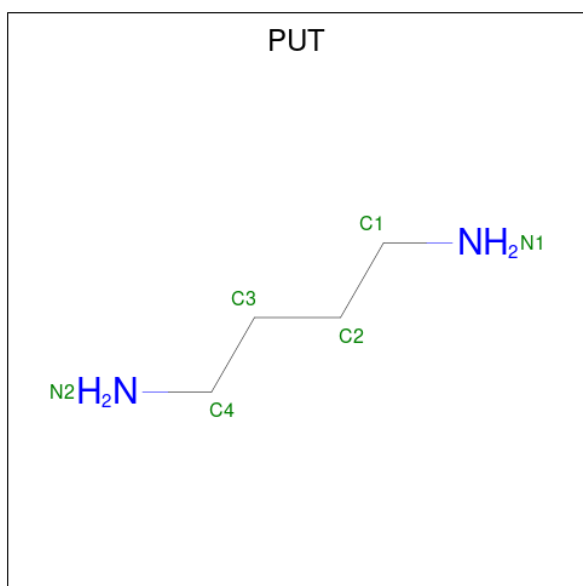
Mol	Chain	Residues	Atoms		AltConf
85	L5	12	Total 12	Na 12	0
85	L7	1	Total 1	Na 1	0
85	L8	1	Total 1	Na 1	0
85	LP	1	Total 1	Na 1	0
85	L1	1	Total 1	Na 1	0
85	S2	7	Total 7	Na 7	0

- Molecule 86 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 87 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).

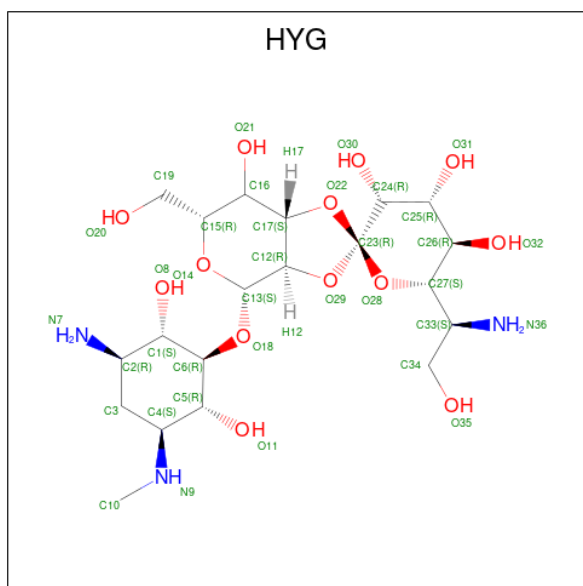


Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			6	4	2	

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
88	Lg	1	Total	Zn	0
			1	1	
88	Lj	1	Total	Zn	0
			1	1	
88	Lo	1	Total	Zn	0
			1	1	
88	Lp	1	Total	Zn	0
			1	1	
88	Sd	1	Total	Zn	0
			1	1	
88	Sf	1	Total	Zn	0
			1	1	
88	SM	1	Total	Zn	0
			1	1	

- Molecule 89 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 90 is water.

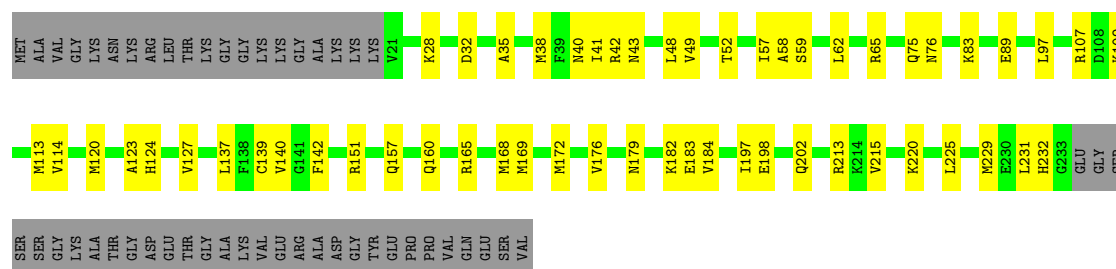
Mol	Chain	Residues	Atoms		AltConf
90	L5	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
90	L8	1	Total 1	O 1	0
90	LH	1	Total 1	O 1	0
90	LV	1	Total 1	O 1	0
90	S2	1	Total 1	O 1	0
90	SX	1	Total 1	O 1	0
90	LI	1	Total 1	O 1	0

Chain SB:  60% 21% 19%

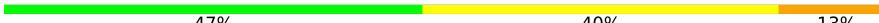


- Molecule 5: mRNA

Chain A4:  38% 46% 15%



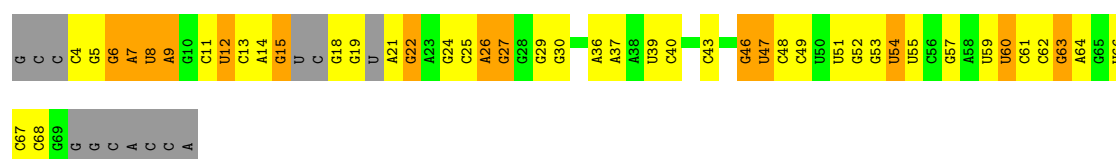
- Molecule 6: P/E tRNA

Chain B4:  47% 40% 13%

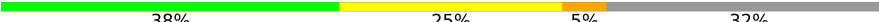


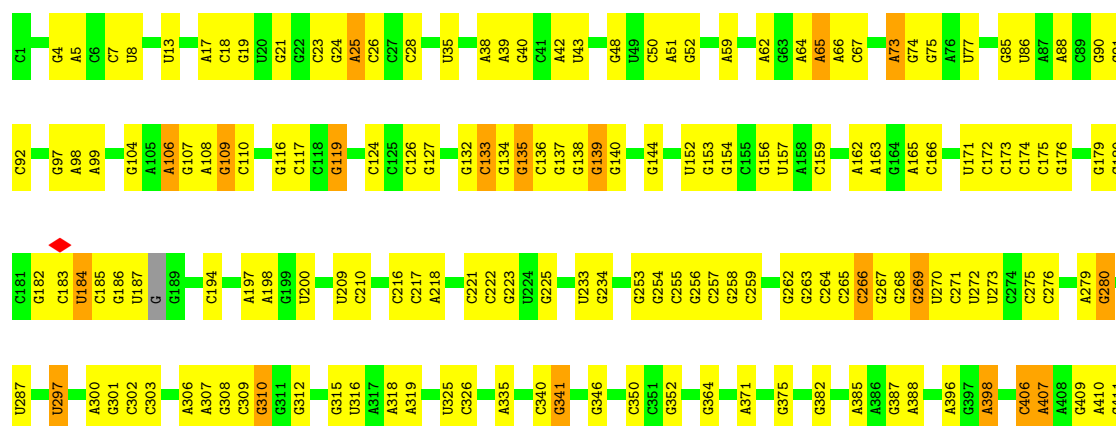
- Molecule 7: A/P tRNA

Chain D4:  24% 41% 18% 17%



- Molecule 8: LSU 28S rRNA

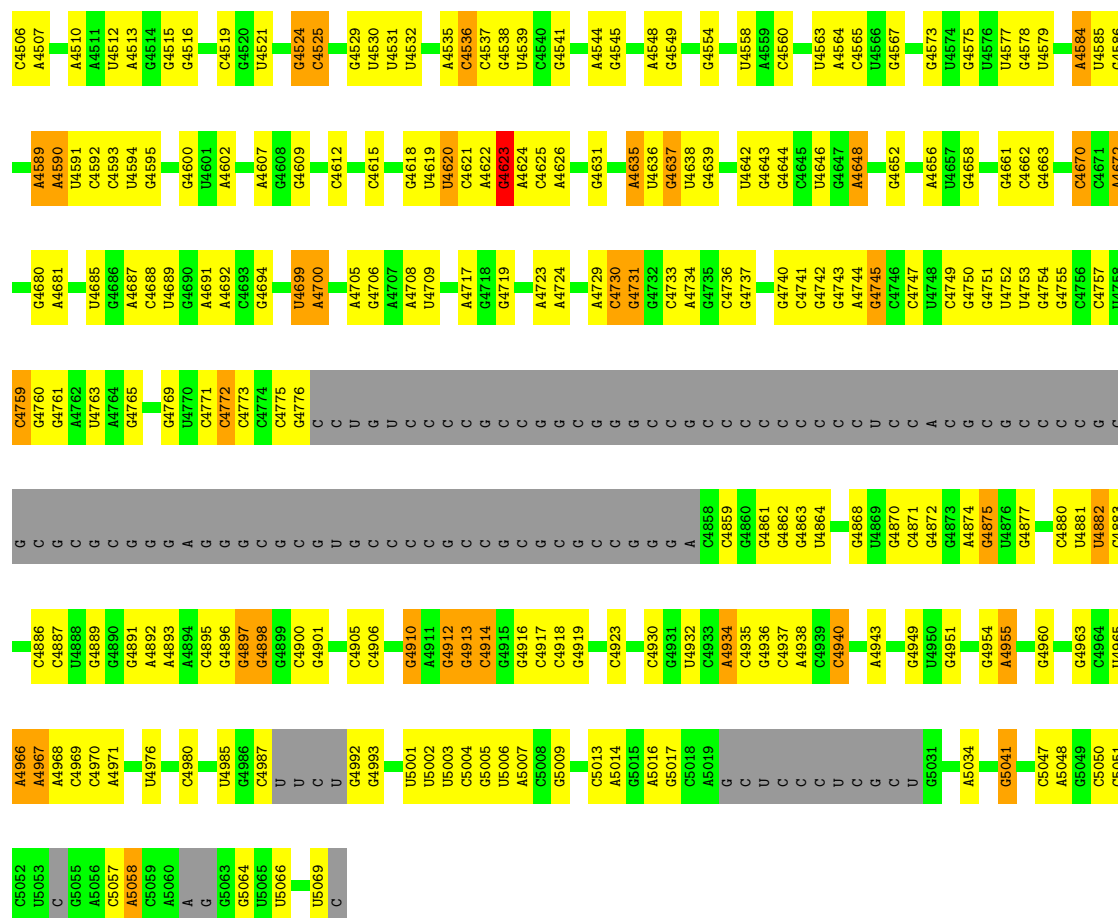
Chain L5:  38% 25% 5% 32%





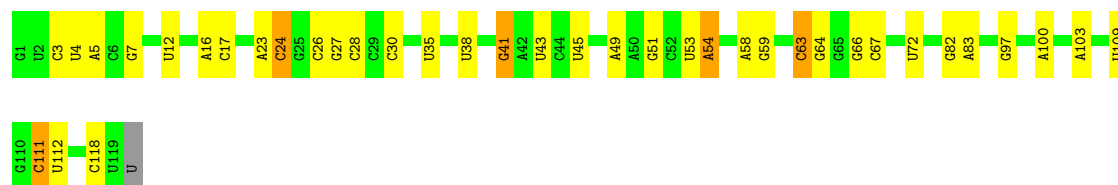






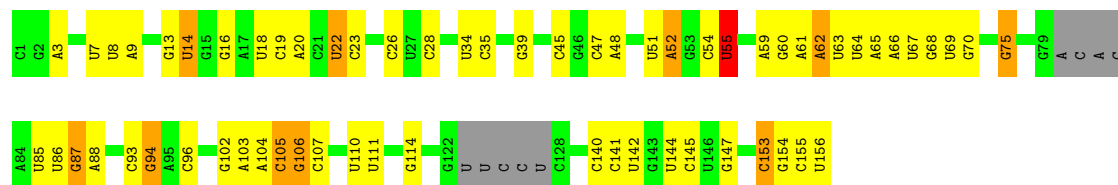
• Molecule 9: 5S rRNA

Chain L7: 68% 28% • •



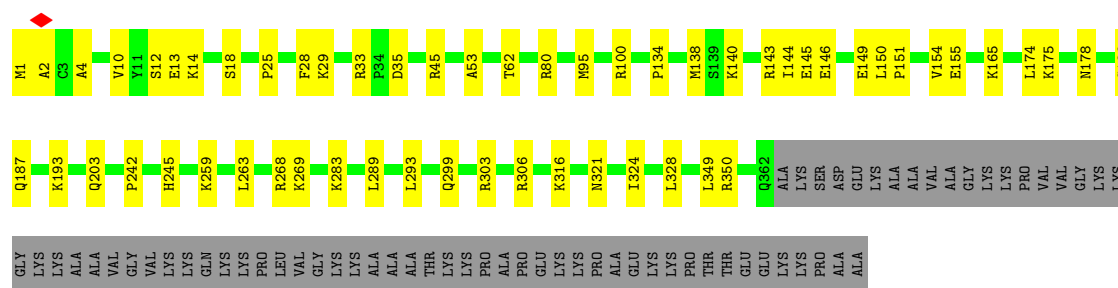
• Molecule 10: 5.8S rRNA

Chain L8: 54% 33% 6% • 6%



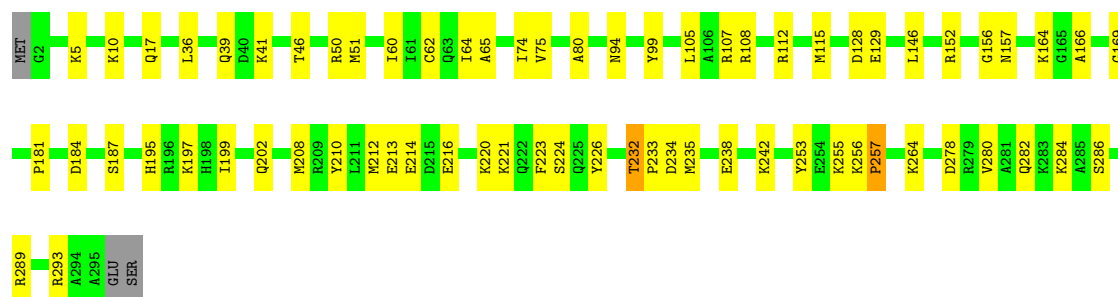
• Molecule 11: 60S ribosomal protein L4

Chain LC: 71% 13% 15%



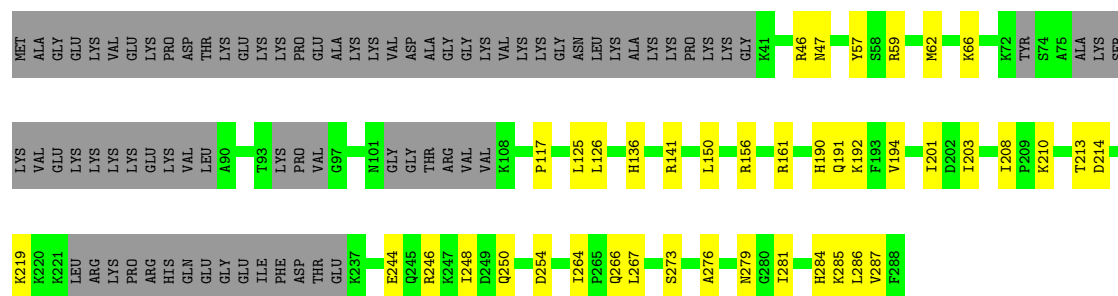
• Molecule 12: 60S ribosomal protein L5

Chain LD: 76% 22% ..



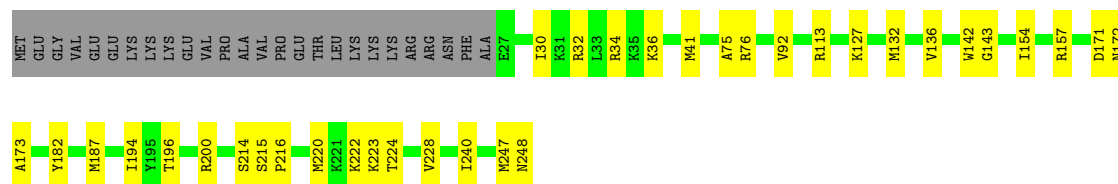
• Molecule 13: Large ribosomal subunit protein eL6

Chain LE: 58% 14% 27%



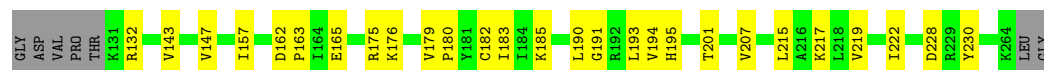
• Molecule 14: Large ribosomal subunit protein uL30

Chain LF: 75% 14% 10%

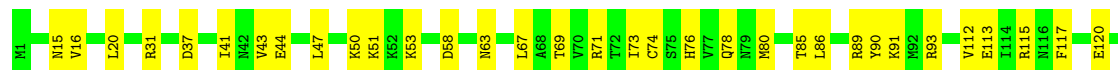


• Molecule 15: 60S ribosomal protein L7a

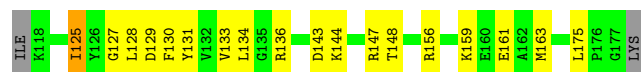
Chain LG: 70% 14% 16%



- Molecule 16: 60S ribosomal protein L9



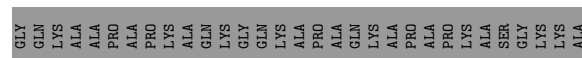
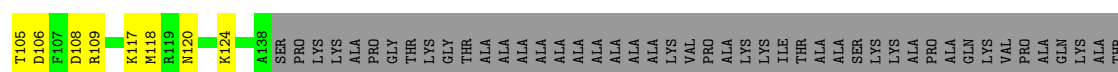
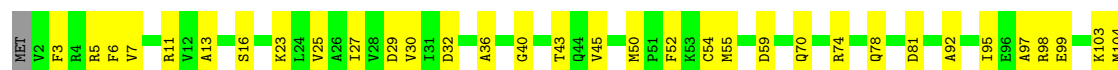
- Molecule 17: 60S ribosomal protein L11



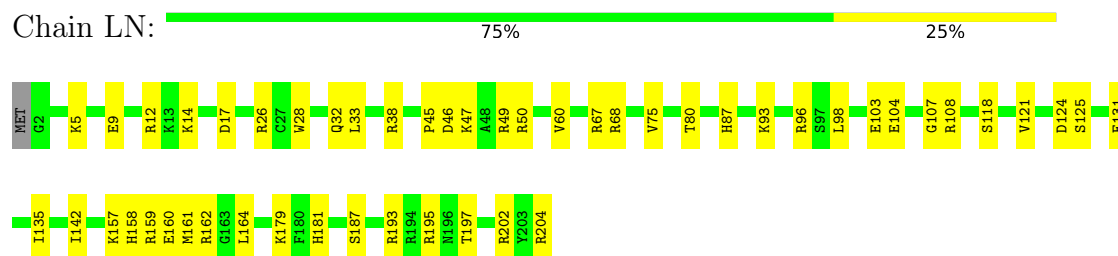
- Molecule 18: 60S ribosomal protein L13



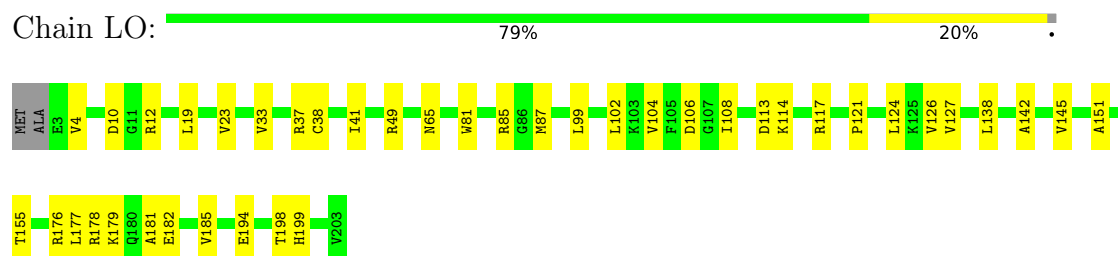
- Molecule 19: 60S ribosomal protein L14



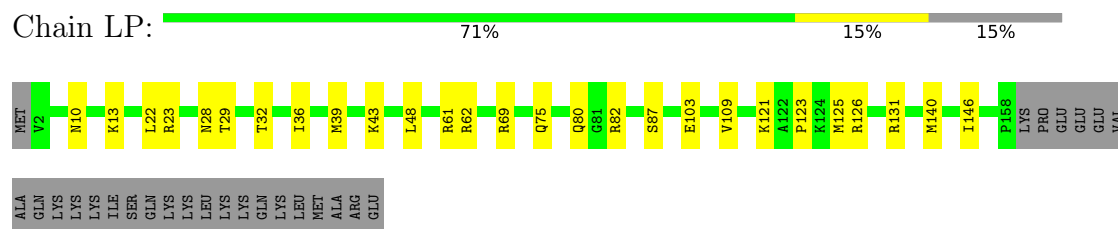
- Molecule 20: 60S ribosomal protein L15



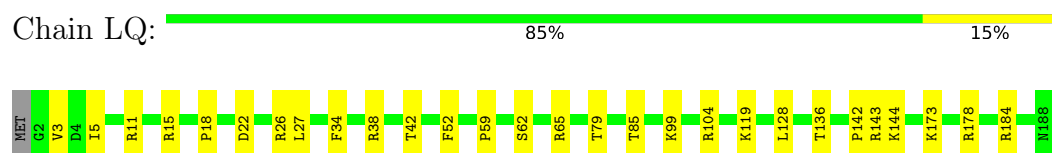
- Molecule 21: 60S ribosomal protein L13a



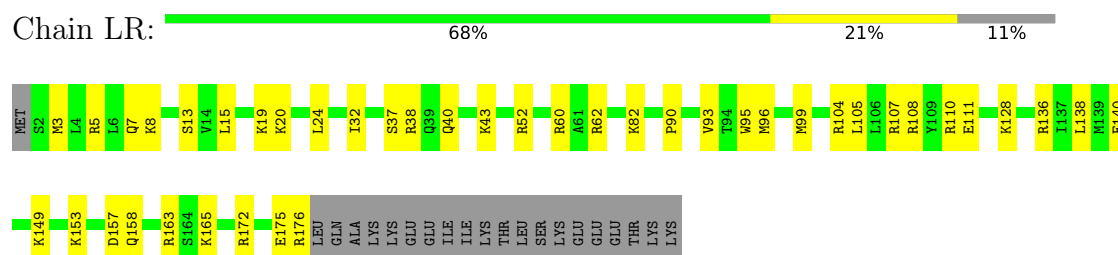
- Molecule 22: 60S ribosomal protein L17



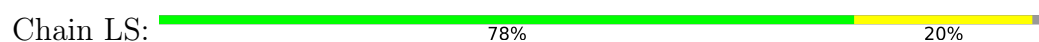
- Molecule 23: 60S ribosomal protein L18



- Molecule 24: 60S ribosomal protein L19

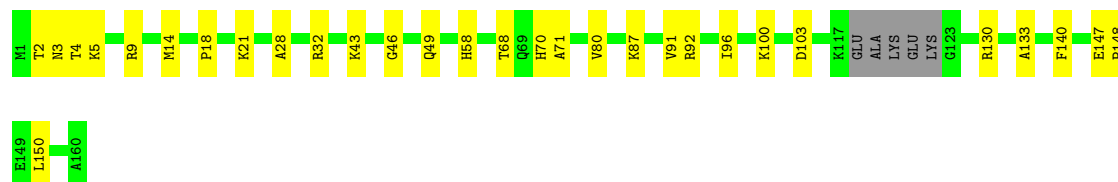
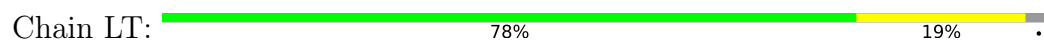


- Molecule 25: 60S ribosomal protein L18a

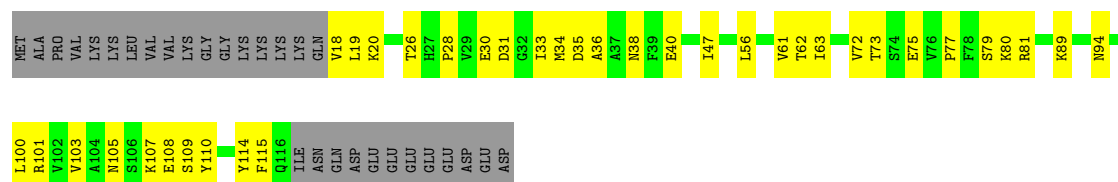




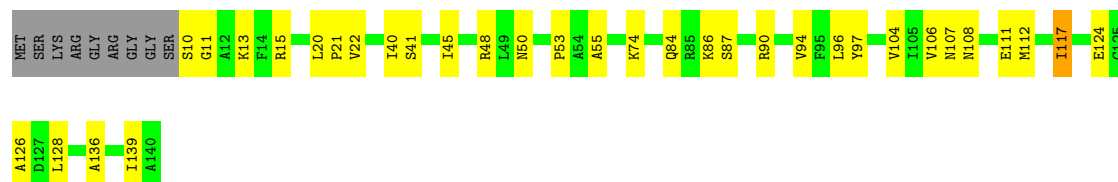
- Molecule 26: 60S ribosomal protein L21



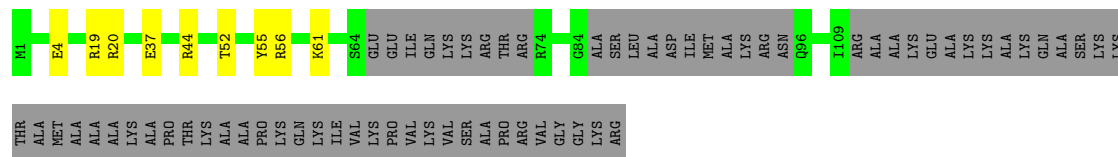
- Molecule 27: 60S ribosomal protein L22



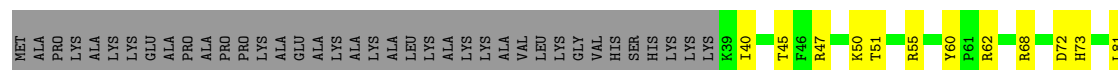
- Molecule 28: 60S ribosomal protein L23



- Molecule 29: 60S ribosomal protein L24

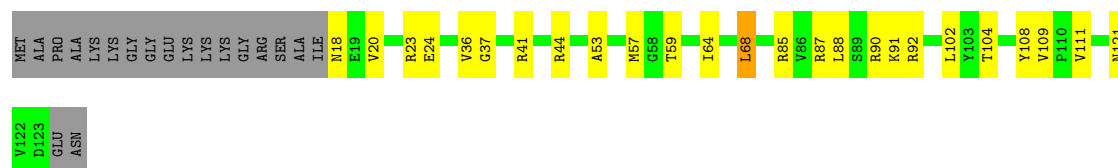


- Molecule 30: 60S ribosomal protein L23a



- Molecule 36: 60S ribosomal protein L31

Chain Ld:  65% 19% 15%



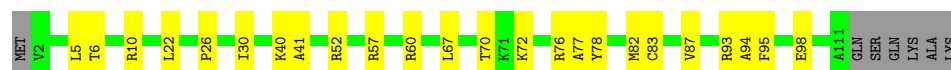
- Molecule 37: 60S ribosomal protein L35a

Chain Lf:  75% 24%



- Molecule 38: 60S ribosomal protein L34

Chain Lg:  74% 21% 6%



- Molecule 39: 60S ribosomal protein L35

Chain Lh:  89% 10%



- Molecule 40: 60S ribosomal protein L36

Chain Li:  84% 10% 5%



- Molecule 41: Large ribosomal subunit protein eL37

Chain Lj:  74% 14% 10%



- Molecule 42: 60S ribosomal protein L38

Chain Lk:  70% 29%



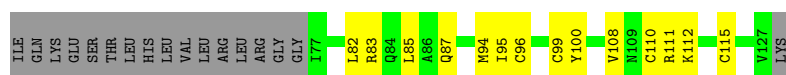
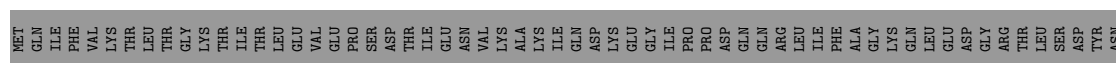
- Molecule 43: 60S ribosomal protein L39

Chain Ll: 71% 25% .



- Molecule 44: Ubiquitin-60S ribosomal protein L40

Chain Lm: 29% 11% 60%



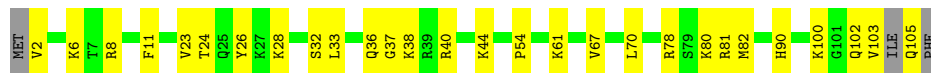
- Molecule 45: 60S ribosomal protein L41

Chain Ln: 88% 12%



- Molecule 46: 60S ribosomal protein L36a

Chain Lo: 71% 26% .



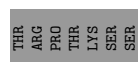
- Molecule 47: 60S ribosomal protein L37a

Chain Lp: 84% 15% .



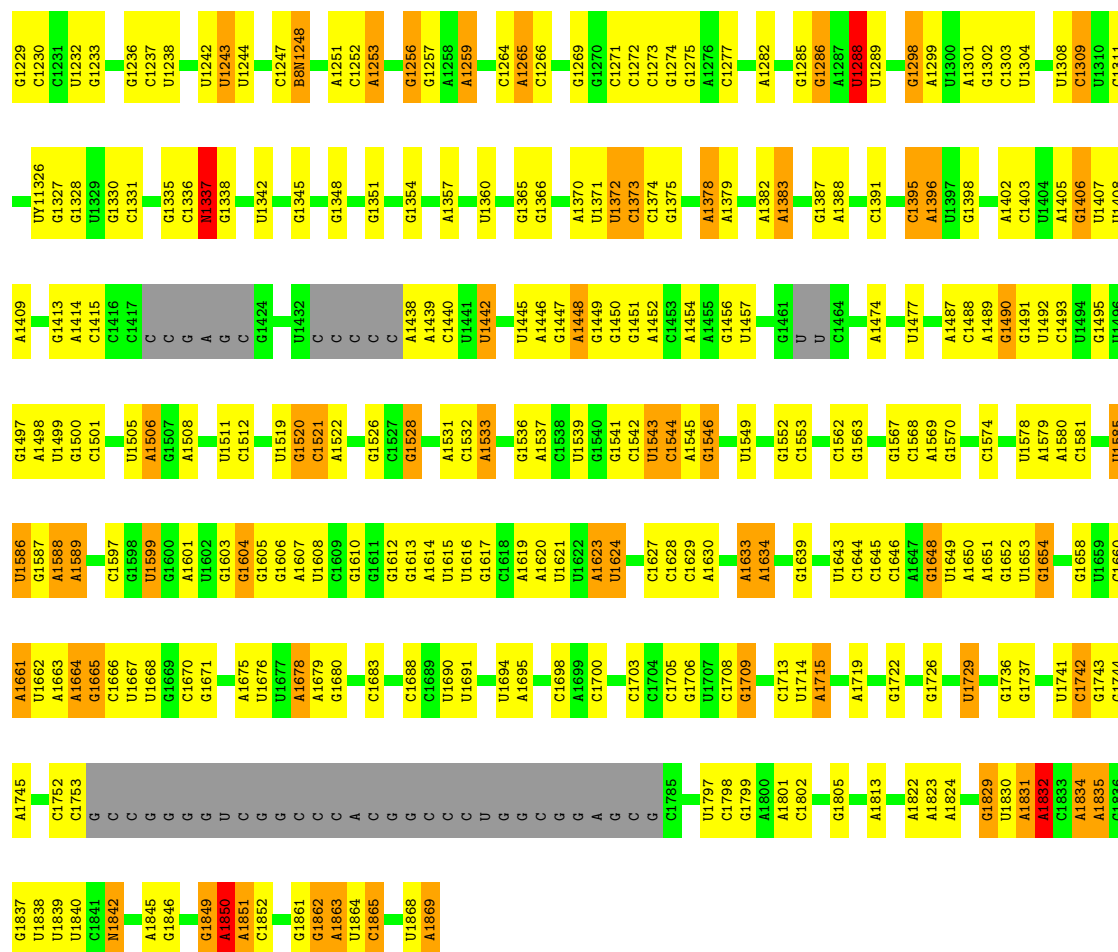
- Molecule 48: 60S ribosomal protein L28

Chain Lr: 69% 22% 9%



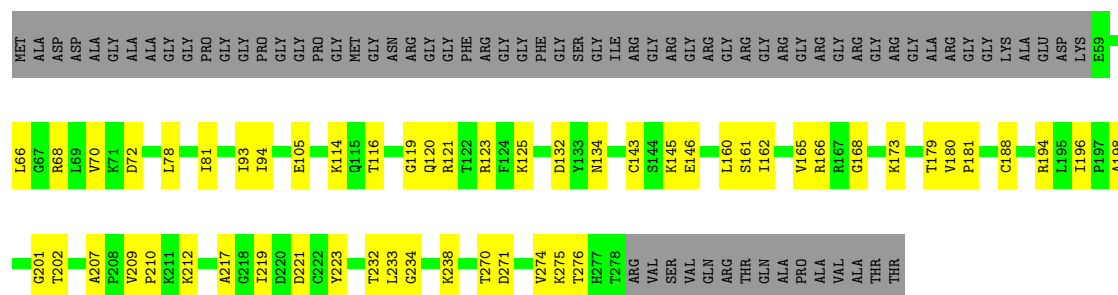
Chain S2:





• Molecule 50: 40S ribosomal protein S2

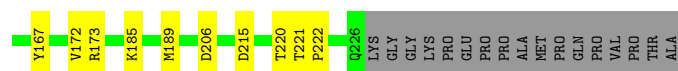
Chain SC: 57% 18% 25%



• Molecule 51: 40S ribosomal protein S3

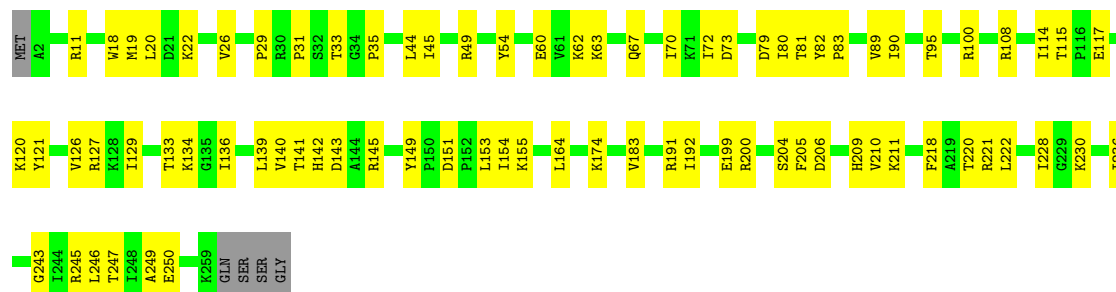
Chain SD: 75% 17% 8%





- Molecule 52: Small ribosomal subunit protein eS4, X isoform

Chain SE: 68% 30%



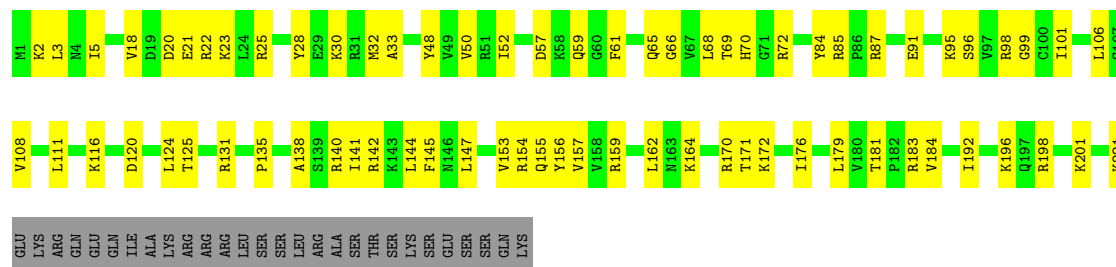
- Molecule 53: 40S ribosomal protein S5

Chain SF: 82% 9% 8%



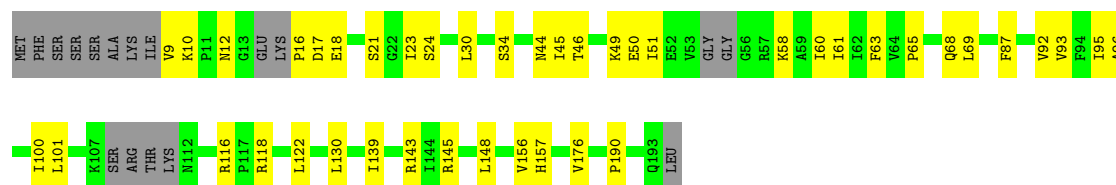
- Molecule 54: 40S ribosomal protein S6

Chain SG: 60% 29% 11%



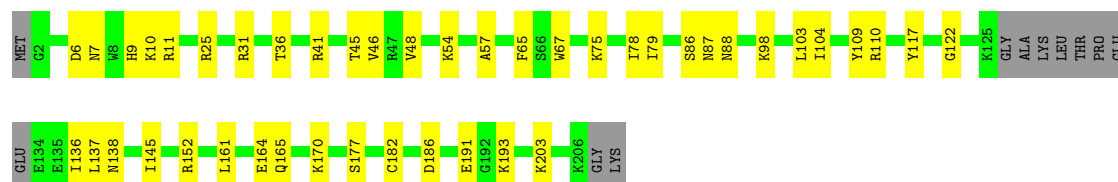
- Molecule 55: 40S ribosomal protein S7

Chain SH: 69% 22% 9%

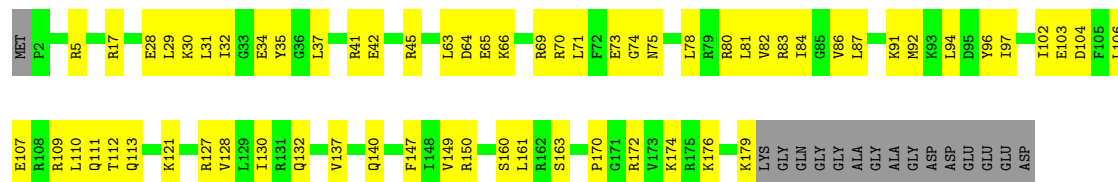


- Molecule 56: 40S ribosomal protein S8

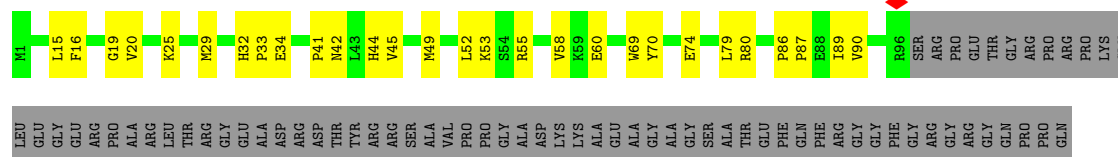
Chain SI: 74% 21% 5%



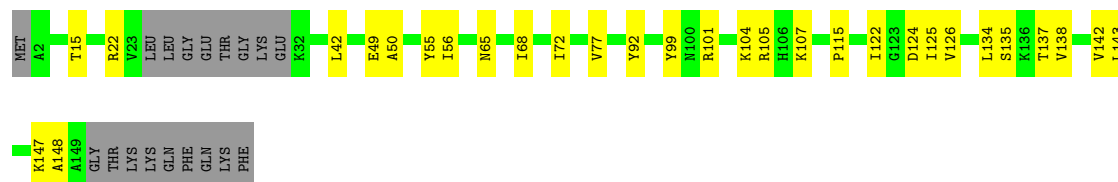
- Molecule 57: 40S ribosomal protein S9



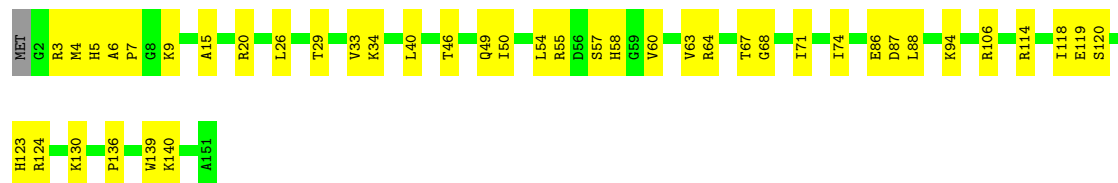
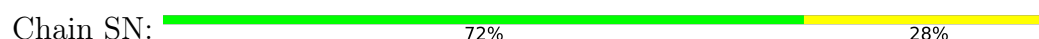
- Molecule 58: 40S ribosomal protein S10



- Molecule 59: 40S ribosomal protein S11

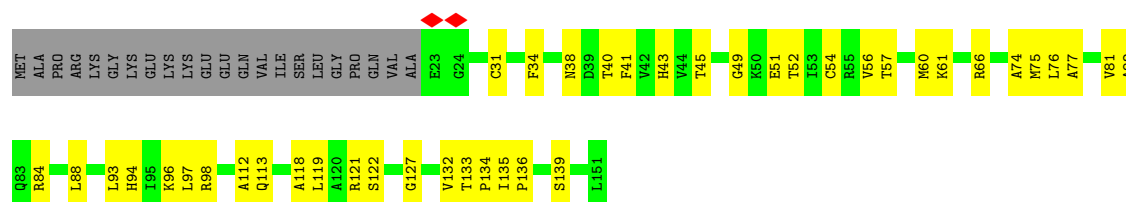


- Molecule 60: 40S ribosomal protein S13



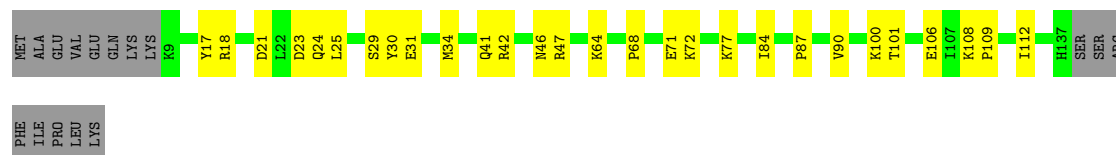
- Molecule 61: 40S ribosomal protein S14





- Molecule 62: 40S ribosomal protein S15

Chain SP: 70% 19% 11%



- Molecule 63: 40S ribosomal protein S16

Chain SQ: 75% 21%



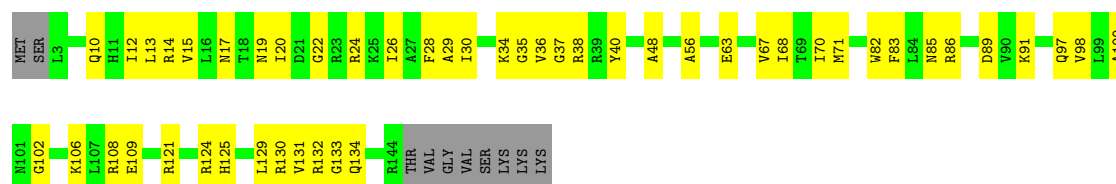
- Molecule 64: 40S ribosomal protein S17

Chain SR: 74% 22%



- Molecule 65: 40S ribosomal protein S18

Chain SS: 61% 32% 7%



- Molecule 66: Small ribosomal subunit protein eS19

Chain ST: 73% 24%





- Molecule 67: 40S ribosomal protein S20

Chain SU: 58% 27% 15%



- Molecule 68: 40S ribosomal protein S21

Chain SV: 83% 17%



- Molecule 69: 40S ribosomal protein S15a

Chain SW: 75% 23% ..



- Molecule 70: 40S ribosomal protein S23

Chain SX: 85% 13% .



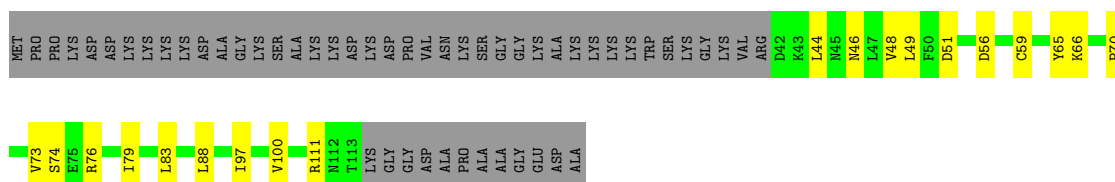
- Molecule 71: 40S ribosomal protein S24

Chain SY: 62% 30% 8%



- Molecule 72: 40S ribosomal protein S25

Chain SZ: 42% 15% 42%



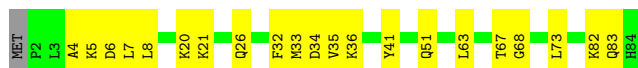
- Molecule 73: 40S ribosomal protein S26

Chain Sa: 70% 17% 14%



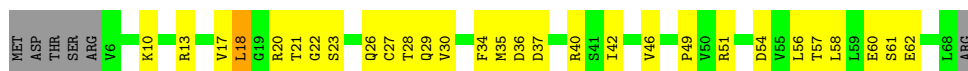
- Molecule 74: 40S ribosomal protein S27

Chain Sb: 74% 25%



- Molecule 75: 40S ribosomal protein S28

Chain Sc: 49% 41% 9%



- Molecule 76: 40S ribosomal protein S29

Chain Sd: 62% 29% 7%



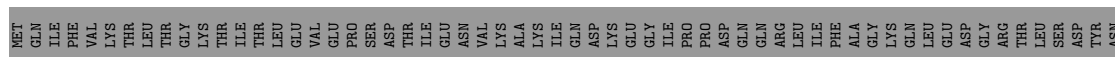
- Molecule 77: 40S ribosomal protein S30

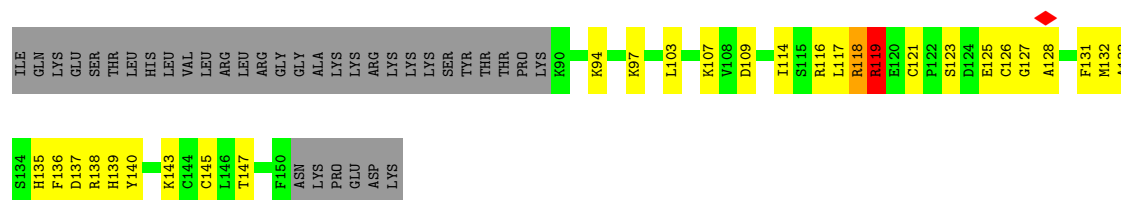
Chain Se: 68% 17% 15%



- Molecule 78: Ubiquitin

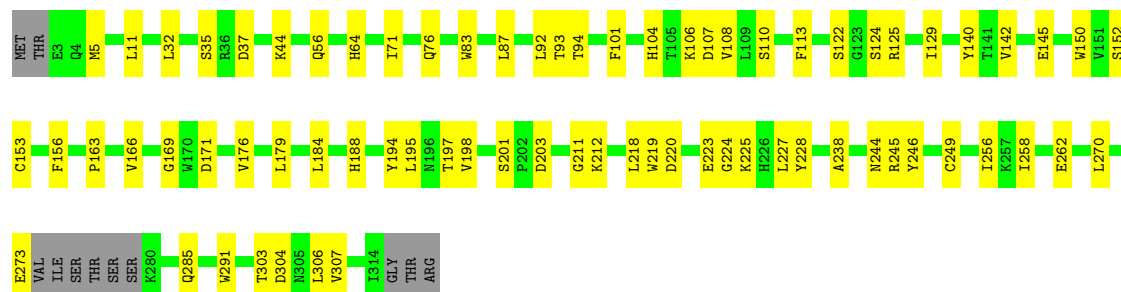
Chain Sf: 21% 17% 61%





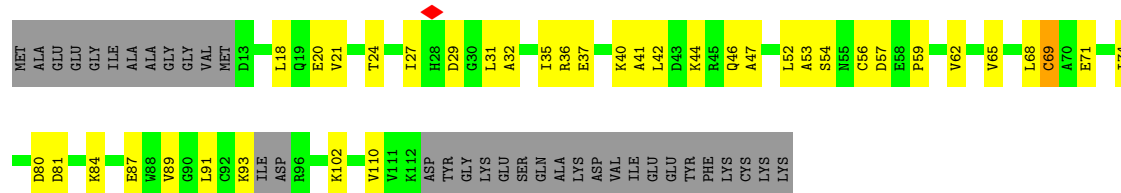
• Molecule 79: Receptor of activated protein C kinase 1

Chain Sg: 74% 23% .



• Molecule 80: 40S ribosomal protein S12

Chain SM: 45% 28% 26% .



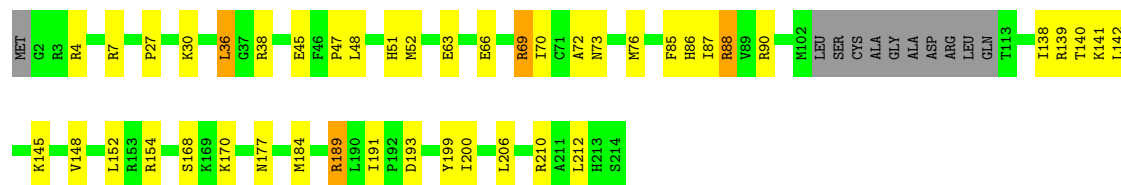
• Molecule 81: 60S ribosomal protein L32

Chain Le: 73% 21% 6% .



• Molecule 82: 60S ribosomal protein L10

Chain LI: 74% 19% 5% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15395	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.022	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, G7M, 4AC, SPD, OMG, A2M, K, 6MZ, MA6, B8N, PSU, UY1, OMU, PUT, ZN, HYG, NA, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	LA	0.23	0/1924	0.35	0/2581
2	SA	0.22	0/1742	0.46	4/2368 (0.2%)
3	LB	0.20	0/3215	0.31	0/4314
4	SB	0.22	0/1754	0.31	0/2347
5	A4	0.32	0/257	0.36	0/397
6	B4	0.22	0/1795	0.30	0/2798
7	D4	0.20	0/1506	0.35	0/2342
8	L5	0.24	0/81933	0.28	0/127773
9	L7	0.23	0/2836	0.24	0/4421
10	L8	0.23	0/3425	0.28	0/5333
11	LC	0.20	0/2928	0.29	0/3933
12	LD	0.72	7/2437 (0.3%)	0.93	8/3263 (0.2%)
13	LE	0.17	0/1677	0.30	0/2250
14	LF	0.22	0/1880	0.30	0/2505
15	LG	0.18	0/1824	0.29	0/2462
16	LH	0.18	0/1545	0.31	0/2077
17	LJ	0.31	1/1352 (0.1%)	0.36	0/1809
18	LL	0.19	0/1616	0.31	0/2163
19	LM	0.20	0/1143	0.35	0/1530
20	LN	0.23	0/1746	0.30	0/2338
21	LO	0.20	0/1678	0.30	0/2245
22	LP	0.20	0/1294	0.29	0/1739
23	LQ	0.20	0/1537	0.28	0/2052
24	LR	0.19	0/1474	0.28	0/1949
25	LS	0.19	0/1469	0.31	0/1970
26	LT	0.20	0/1272	0.28	0/1698
27	LU	0.14	0/822	0.37	0/1103
28	LV	0.23	0/993	0.35	0/1332
29	LW	0.18	0/676	0.26	0/906
30	LX	0.19	0/979	0.30	0/1319
31	LY	0.18	0/1120	0.28	0/1491

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LZ	0.19	0/1141	0.33	0/1521
33	La	0.21	0/1188	0.28	0/1587
34	Lb	0.20	0/759	0.29	0/1003
35	Lc	0.33	0/736	0.52	0/988
36	Ld	0.19	0/886	0.31	0/1194
37	Lf	0.24	0/886	0.38	0/1189
38	Lg	0.22	0/871	0.29	0/1164
39	Lh	0.17	0/1019	0.31	0/1347
40	Li	0.15	0/829	0.28	0/1097
41	Lj	0.29	0/730	0.40	0/965
42	Lk	0.22	0/559	0.51	1/745 (0.1%)
43	Ll	0.19	0/445	0.25	0/588
44	Lm	0.28	0/417	0.53	0/555
45	Ln	0.26	0/240	0.26	0/305
46	Lo	0.20	0/851	0.31	0/1121
47	Lp	0.22	0/717	0.28	0/953
48	Lr	0.20	0/1007	0.28	0/1351
49	S2	0.27	1/37049 (0.0%)	0.30	0/57713
50	SC	0.21	0/1741	0.36	0/2354
51	SD	0.21	0/1715	0.29	0/2313
52	SE	0.22	0/2092	0.34	0/2816
53	SF	0.21	0/1507	0.29	0/2024
54	SG	0.18	0/1772	0.32	0/2366
55	SH	0.16	0/1380	0.34	0/1856
56	SI	0.21	0/1609	0.33	0/2155
57	SJ	0.17	0/1507	0.32	0/2015
58	SK	0.59	2/828 (0.2%)	1.12	5/1118 (0.4%)
59	SL	0.20	0/1167	0.32	0/1563
60	SN	0.35	1/1229 (0.1%)	0.33	1/1652 (0.1%)
61	SO	0.23	0/971	0.32	0/1302
62	SP	0.25	0/1081	0.36	0/1445
63	SQ	0.20	0/1138	0.29	0/1523
64	SR	0.21	0/1067	0.31	0/1433
65	SS	0.22	0/1189	0.32	0/1592
66	ST	0.20	0/1118	0.27	0/1499
67	SU	0.22	0/800	0.39	0/1075
68	SV	0.17	0/643	0.28	0/860
69	SW	0.21	0/1051	0.30	0/1406
70	SX	0.21	0/1100	0.35	0/1471
71	SY	0.15	0/1005	0.28	0/1340
72	SZ	0.20	0/580	0.36	0/780
73	Sa	0.50	2/801 (0.2%)	0.94	3/1074 (0.3%)
74	Sb	0.19	0/647	0.37	0/870

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sc	0.27	0/491	0.39	0/658
76	Sd	0.21	0/446	0.29	0/591
77	Se	0.16	0/403	0.26	0/527
78	Sf	0.34	0/498	0.61	1/661 (0.2%)
79	Sg	0.17	0/2445	0.33	0/3326
80	SM	0.29	0/727	0.51	0/981
81	Le	0.22	0/1062	0.31	0/1417
82	LI	0.25	0/1679	0.41	1/2243 (0.0%)
All	All	0.25	14/219668 (0.0%)	0.33	24/322500 (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
35	Lc	0	1
41	Lj	0	2
78	Sf	0	3
82	LI	0	3
All	All	0	9

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	LD	257	PRO	CB-CG	21.12	2.55	1.49
12	LD	257	PRO	CG-CD	-17.03	0.92	1.50
12	LD	233	PRO	CG-CD	-15.34	0.98	1.50
58	SK	87	PRO	CB-CG	-11.60	0.91	1.49
60	SN	136	PRO	CA-C	-9.20	1.46	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	LD	257	PRO	CB-CG-CD	-32.49	2.13	106.10
12	LD	233	PRO	N-CD-CG	-24.19	66.91	103.20
58	SK	87	PRO	CB-CG-CD	23.08	179.95	106.10
73	Sa	97	PRO	N-CD-CG	-18.80	75.00	103.20
58	SK	87	PRO	CA-CB-CG	-17.06	72.08	104.50

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	Lc	17	ARG	Sidechain
41	Lj	43	ARG	Sidechain
41	Lj	55	ARG	Sidechain
78	Sf	116	ARG	Sidechain
78	Sf	118	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	LA	1886	0	1973	40	0
2	SA	1705	0	1704	35	0
3	LB	3147	0	3237	75	0
4	SB	1727	0	1796	41	0
5	A4	231	0	116	9	0
6	B4	1604	0	816	27	0
7	D4	1349	0	682	34	0
8	L5	74335	0	37632	923	0
9	L7	2538	0	1286	25	0
10	L8	3132	0	1593	48	0
11	LC	2874	0	3043	50	0
12	LD	2391	0	2426	60	0
13	LE	1648	0	1750	31	0
14	LF	1846	0	1976	30	0
15	LG	1793	0	1898	34	0
16	LH	1526	0	1605	37	0
17	LJ	1330	0	1354	38	0
18	LL	1588	0	1682	33	0
19	LM	1121	0	1181	35	0
20	LN	1701	0	1749	40	0
21	LO	1646	0	1790	29	0
22	LP	1267	0	1293	20	0
23	LQ	1513	0	1628	22	0
24	LR	1458	0	1599	38	0
25	LS	1431	0	1461	28	0
26	LT	1247	0	1302	27	0
27	LU	808	0	831	25	0
28	LV	979	0	1039	27	0
29	LW	663	0	612	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	LX	962	0	1029	25	0
31	LY	1103	0	1177	29	0
32	LZ	1115	0	1195	32	0
33	La	1159	0	1209	26	0
34	Lb	747	0	798	21	0
35	Lc	725	0	763	36	0
36	Ld	871	0	915	16	0
37	Lf	867	0	897	19	0
38	Lg	861	0	937	23	0
39	Lh	1011	0	1137	9	0
40	Li	818	0	899	9	0
41	Lj	715	0	751	15	0
42	Lk	553	0	602	13	0
43	Ll	435	0	472	13	0
44	Lm	411	0	438	14	0
45	Ln	239	0	289	2	0
46	Lo	839	0	902	22	0
47	Lp	707	0	756	12	0
48	Lr	992	0	1045	23	0
49	S2	33711	0	17041	450	0
50	SC	1704	0	1784	37	0
51	SD	1689	0	1734	31	0
52	SE	2050	0	2156	64	0
53	SF	1486	0	1538	13	0
54	SG	1749	0	1875	56	0
55	SH	1360	0	1390	33	0
56	SI	1582	0	1607	32	0
57	SJ	1482	0	1591	49	0
58	SK	804	0	825	21	0
59	SL	1147	0	1207	22	0
60	SN	1205	0	1292	30	0
61	SO	959	0	974	27	0
62	SP	1060	0	1104	20	0
63	SQ	1120	0	1189	24	0
64	SR	1053	0	1109	27	0
65	SS	1171	0	1226	33	0
66	ST	1098	0	1120	31	0
67	SU	790	0	847	30	0
68	SV	636	0	637	9	0
69	SW	1034	0	1080	32	0
70	SX	1082	0	1141	17	0
71	SY	988	0	1034	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	SZ	574	0	627	13	0
73	Sa	788	0	837	13	0
74	Sb	633	0	631	19	0
75	Sc	489	0	512	17	0
76	Sd	436	0	430	15	0
77	Se	400	0	440	8	0
78	Sf	489	0	486	32	0
79	Sg	2389	0	2343	54	0
80	SM	722	0	730	32	0
81	Le	1044	0	1136	21	0
82	LI	1641	0	1683	33	0
83	B4	3	0	0	0	0
83	L5	17	0	0	0	0
83	L8	1	0	0	0	0
83	LA	1	0	0	0	0
83	La	1	0	0	0	0
83	Le	1	0	0	0	0
83	S2	15	0	0	0	0
83	SN	1	0	0	0	0
84	A4	2	0	0	0	0
84	B4	4	0	0	0	0
84	D4	1	0	0	0	0
84	L5	157	0	0	0	0
84	L7	2	0	0	0	0
84	L8	3	0	0	0	0
84	LI	1	0	0	0	0
84	LN	1	0	0	0	0
84	LP	1	0	0	0	0
84	LT	1	0	0	0	0
84	Lp	1	0	0	0	0
84	S2	93	0	0	0	0
85	L5	12	0	0	0	0
85	L7	1	0	0	0	0
85	L8	1	0	0	0	0
85	LP	1	0	0	0	0
85	Ll	1	0	0	0	0
85	S2	7	0	0	0	0
86	L5	10	0	19	2	0
87	L5	6	0	12	1	0
88	Lg	1	0	0	0	0
88	Lj	1	0	0	0	0
88	Lo	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	Lp	1	0	0	0	0
88	SM	1	0	0	0	0
88	Sd	1	0	0	0	0
88	Sf	1	0	0	0	0
89	S2	36	0	37	0	0
90	L5	1	0	0	0	0
90	L8	1	0	0	0	0
90	LH	1	0	0	0	0
90	LI	1	0	0	0	0
90	LV	1	0	0	1	0
90	S2	1	0	0	0	0
90	SX	1	0	0	0	0
All	All	206575	0	152689	3039	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 9.

The worst 5 of 3039 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)
12:LD:257:PRO:CG	12:LD:257:PRO:N	1.89	1.33
12:LD:257:PRO:CD	12:LD:257:PRO:HG3	1.69	1.17
78:Sf:119:ARG:HG2	78:Sf:132:MET:HE2	1.18	1.09
12:LD:257:PRO:CD	12:LD:257:PRO:HG2	1.69	1.08
12:LD:257:PRO:CG	12:LD:257:PRO:HD3	1.58	1.07

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LA	246/257 (96%)	225 (92%)	21 (8%)	0	100	100
2	SA	215/295 (73%)	206 (96%)	9 (4%)	0	100	100
3	LB	396/403 (98%)	367 (93%)	29 (7%)	0	100	100
4	SB	211/264 (80%)	207 (98%)	4 (2%)	0	100	100
11	LC	360/427 (84%)	342 (95%)	18 (5%)	0	100	100
12	LD	292/297 (98%)	285 (98%)	7 (2%)	0	100	100
13	LE	197/288 (68%)	181 (92%)	16 (8%)	0	100	100
14	LF	220/248 (89%)	214 (97%)	6 (3%)	0	100	100
15	LG	220/266 (83%)	211 (96%)	9 (4%)	0	100	100
16	LH	189/192 (98%)	181 (96%)	8 (4%)	0	100	100
17	LJ	163/178 (92%)	153 (94%)	10 (6%)	0	100	100
18	LL	192/211 (91%)	171 (89%)	21 (11%)	0	100	100
19	LM	135/215 (63%)	126 (93%)	8 (6%)	1 (1%)	18	49
20	LN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
21	LO	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
22	LP	155/184 (84%)	150 (97%)	5 (3%)	0	100	100
23	LQ	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
24	LR	173/196 (88%)	171 (99%)	2 (1%)	0	100	100
25	LS	169/176 (96%)	158 (94%)	11 (6%)	0	100	100
26	LT	151/160 (94%)	146 (97%)	5 (3%)	0	100	100
27	LU	97/128 (76%)	89 (92%)	8 (8%)	0	100	100
28	LV	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
29	LW	83/157 (53%)	81 (98%)	2 (2%)	0	100	100
30	LX	116/156 (74%)	110 (95%)	6 (5%)	0	100	100
31	LY	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
32	LZ	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
33	La	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
34	Lb	88/159 (55%)	86 (98%)	2 (2%)	0	100	100
35	Lc	91/115 (79%)	83 (91%)	7 (8%)	1 (1%)	11	40
36	Ld	104/125 (83%)	100 (96%)	4 (4%)	0	100	100
37	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
38	Lg	108/117 (92%)	104 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	Lh	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
40	Li	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
41	Lj	85/97 (88%)	82 (96%)	3 (4%)	0	100	100
42	Lk	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
43	Ll	47/51 (92%)	43 (92%)	4 (8%)	0	100	100
44	Lm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
45	Ln	23/25 (92%)	23 (100%)	0	0	100	100
46	Lo	100/106 (94%)	92 (92%)	8 (8%)	0	100	100
47	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
48	Lr	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
50	SC	218/293 (74%)	208 (95%)	10 (5%)	0	100	100
51	SD	219/243 (90%)	211 (96%)	8 (4%)	0	100	100
52	SE	256/263 (97%)	242 (94%)	14 (6%)	0	100	100
53	SF	183/204 (90%)	173 (94%)	10 (6%)	0	100	100
54	SG	219/249 (88%)	204 (93%)	15 (7%)	0	100	100
55	SH	169/194 (87%)	160 (95%)	9 (5%)	0	100	100
56	SI	193/208 (93%)	182 (94%)	11 (6%)	0	100	100
57	SJ	176/194 (91%)	170 (97%)	6 (3%)	0	100	100
58	SK	94/165 (57%)	88 (94%)	6 (6%)	0	100	100
59	SL	136/158 (86%)	127 (93%)	9 (7%)	0	100	100
60	SN	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
61	SO	127/151 (84%)	117 (92%)	10 (8%)	0	100	100
62	SP	127/145 (88%)	123 (97%)	4 (3%)	0	100	100
63	SQ	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
64	SR	128/135 (95%)	122 (95%)	6 (5%)	0	100	100
65	SS	140/152 (92%)	130 (93%)	10 (7%)	0	100	100
66	ST	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
67	SU	99/119 (83%)	90 (91%)	9 (9%)	0	100	100
68	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
69	SW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
70	SX	139/143 (97%)	128 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	SY	121/133 (91%)	118 (98%)	3 (2%)	0	100	100
72	SZ	70/125 (56%)	63 (90%)	7 (10%)	0	100	100
73	Sa	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
74	Sb	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
75	Sc	61/69 (88%)	53 (87%)	8 (13%)	0	100	100
76	Sd	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
77	Se	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
78	Sf	59/156 (38%)	46 (78%)	13 (22%)	0	100	100
79	Sg	302/317 (95%)	279 (92%)	23 (8%)	0	100	100
80	SM	94/132 (71%)	86 (92%)	8 (8%)	0	100	100
81	Le	125/135 (93%)	121 (97%)	4 (3%)	0	100	100
82	LI	199/214 (93%)	194 (98%)	5 (2%)	0	100	100
All	All	10966/12688 (86%)	10396 (95%)	568 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	LM	32	ASP
35	Lc	99	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LA	187/199 (94%)	187 (100%)	0	100	100
2	SA	178/243 (73%)	177 (99%)	1 (1%)	78	81
3	LB	330/349 (95%)	328 (99%)	2 (1%)	78	81
4	SB	193/231 (84%)	192 (100%)	1 (0%)	81	82
11	LC	299/348 (86%)	299 (100%)	0	100	100
12	LD	247/250 (99%)	247 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	LE	175/252 (69%)	175 (100%)	0	100	100
14	LF	192/215 (89%)	192 (100%)	0	100	100
15	LG	189/223 (85%)	189 (100%)	0	100	100
16	LH	170/171 (99%)	170 (100%)	0	100	100
17	LJ	138/149 (93%)	137 (99%)	1 (1%)	76	79
18	LL	161/177 (91%)	161 (100%)	0	100	100
19	LM	115/161 (71%)	115 (100%)	0	100	100
20	LN	171/172 (99%)	170 (99%)	1 (1%)	78	81
21	LO	172/174 (99%)	172 (100%)	0	100	100
22	LP	137/163 (84%)	137 (100%)	0	100	100
23	LQ	164/165 (99%)	164 (100%)	0	100	100
24	LR	153/175 (87%)	153 (100%)	0	100	100
25	LS	152/157 (97%)	152 (100%)	0	100	100
26	LT	132/140 (94%)	132 (100%)	0	100	100
27	LU	89/115 (77%)	89 (100%)	0	100	100
28	LV	101/107 (94%)	99 (98%)	2 (2%)	48	67
29	LW	57/126 (45%)	57 (100%)	0	100	100
30	LX	105/133 (79%)	105 (100%)	0	100	100
31	LY	121/135 (90%)	121 (100%)	0	100	100
32	LZ	118/118 (100%)	118 (100%)	0	100	100
33	La	119/121 (98%)	119 (100%)	0	100	100
34	Lb	75/126 (60%)	75 (100%)	0	100	100
35	Lc	78/97 (80%)	78 (100%)	0	100	100
36	Ld	94/110 (86%)	93 (99%)	1 (1%)	65	75
37	Lf	86/89 (97%)	86 (100%)	0	100	100
38	Lg	91/100 (91%)	91 (100%)	0	100	100
39	Lh	108/110 (98%)	108 (100%)	0	100	100
40	Li	85/89 (96%)	84 (99%)	1 (1%)	63	74
41	Lj	74/80 (92%)	74 (100%)	0	100	100
42	Lk	60/65 (92%)	60 (100%)	0	100	100
43	Ll	46/48 (96%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	Lm	45/116 (39%)	45 (100%)	0	100	100
45	Ln	24/24 (100%)	24 (100%)	0	100	100
46	Lo	90/94 (96%)	89 (99%)	1 (1%)	65	75
47	Lp	74/75 (99%)	73 (99%)	1 (1%)	59	72
48	Lr	105/121 (87%)	104 (99%)	1 (1%)	68	75
50	SC	185/225 (82%)	185 (100%)	0	100	100
51	SD	174/202 (86%)	174 (100%)	0	100	100
52	SE	221/225 (98%)	221 (100%)	0	100	100
53	SF	159/170 (94%)	158 (99%)	1 (1%)	78	81
54	SG	183/218 (84%)	183 (100%)	0	100	100
55	SH	139/174 (80%)	138 (99%)	1 (1%)	76	79
56	SI	162/180 (90%)	161 (99%)	1 (1%)	78	81
57	SJ	158/168 (94%)	157 (99%)	1 (1%)	78	81
58	SK	86/136 (63%)	85 (99%)	1 (1%)	63	74
59	SL	126/142 (89%)	126 (100%)	0	100	100
60	SN	129/131 (98%)	129 (100%)	0	100	100
61	SO	98/119 (82%)	96 (98%)	2 (2%)	48	67
62	SP	114/130 (88%)	114 (100%)	0	100	100
63	SQ	116/121 (96%)	115 (99%)	1 (1%)	70	77
64	SR	117/122 (96%)	117 (100%)	0	100	100
65	SS	121/132 (92%)	121 (100%)	0	100	100
66	ST	111/115 (96%)	111 (100%)	0	100	100
67	SU	89/107 (83%)	89 (100%)	0	100	100
68	SV	67/67 (100%)	66 (98%)	1 (2%)	57	71
69	SW	112/113 (99%)	110 (98%)	2 (2%)	51	69
70	SX	110/115 (96%)	110 (100%)	0	100	100
71	SY	103/115 (90%)	102 (99%)	1 (1%)	68	75
72	SZ	64/103 (62%)	63 (98%)	1 (2%)	55	71
73	Sa	85/98 (87%)	84 (99%)	1 (1%)	63	74
74	Sb	69/76 (91%)	69 (100%)	0	100	100
75	Sc	54/62 (87%)	51 (94%)	3 (6%)	19	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	Sd	46/49 (94%)	45 (98%)	1 (2%)	45	65
77	Se	40/48 (83%)	40 (100%)	0	100	100
78	Sf	52/140 (37%)	52 (100%)	0	100	100
79	Sg	265/275 (96%)	264 (100%)	1 (0%)	84	83
80	SM	74/108 (68%)	73 (99%)	1 (1%)	59	72
81	Le	113/121 (93%)	113 (100%)	0	100	100
82	LI	172/181 (95%)	172 (100%)	0	100	100
All	All	9414/10801 (87%)	9381 (100%)	33 (0%)	81	83

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
75	Sc	57	THR
75	Sc	58	LEU
80	SM	69	CYS
48	Lr	63	VAL
47	Lp	78	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
34	Lb	6	ASN
48	Lr	21	ASN
36	Ld	79	ASN
40	Li	20	ASN
53	SF	118	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	L8	144/156 (92%)	27 (18%)	0
49	S2	1561/1869 (83%)	347 (22%)	6 (0%)
5	A4	10/13 (76%)	0	0
6	B4	74/75 (98%)	18 (24%)	0
7	D4	60/76 (78%)	23 (38%)	0
8	L5	3436/5070 (67%)	666 (19%)	16 (0%)
9	L7	118/120 (98%)	11 (9%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	5403/7379 (73%)	1092 (20%)	22 (0%)

5 of 1092 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B4	8	U
6	B4	10	G
6	B4	11	C
6	B4	12	G
6	B4	17	G

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	L5	4740	G
49	S2	604	A
49	S2	601	OMG
49	S2	1395	C
8	L5	2019	C

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

76 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
49	A2M	S2	27	49,84	22,25,26	3.48	10 (45%)	31,36,39	2.40	10 (32%)
8	A2M	L5	4590	8,84	22,25,26	3.46	9 (40%)	31,36,39	2.47	11 (35%)
49	OMG	S2	644	49	23,26,27	2.40	9 (39%)	33,38,41	2.59	10 (30%)
10	OMU	L8	14	10	19,22,23	3.05	8 (42%)	26,31,34	1.83	7 (26%)
8	OMC	L5	2365	8	19,22,23	2.94	8 (42%)	26,31,34	0.76	0
8	A2M	L5	3825	8	22,25,26	3.49	10 (45%)	31,36,39	2.37	11 (35%)
8	A2M	L5	3724	8	22,25,26	3.46	10 (45%)	31,36,39	2.40	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	OMG	S2	1328	49	23,26,27	2.37	9 (39%)	33,38,41	2.52	10 (30%)
8	OMG	L5	4228	8	23,26,27	2.35	9 (39%)	33,38,41	2.44	12 (36%)
49	OMC	S2	174	49	19,22,23	2.97	8 (42%)	26,31,34	0.75	0
49	OMC	S2	1703	49	19,22,23	2.94	8 (42%)	26,31,34	0.67	0
10	PSU	L8	55	10	18,21,22	4.39	7 (38%)	22,30,33	1.63	4 (18%)
8	OMU	L5	4620	8	19,22,23	2.91	8 (42%)	26,31,34	1.79	5 (19%)
8	OMG	L5	3744	8	23,26,27	2.38	9 (39%)	33,38,41	2.51	11 (33%)
8	OMG	L5	4623	8	23,26,27	2.36	9 (39%)	33,38,41	2.49	11 (33%)
8	OMC	L5	1340	8	19,22,23	2.91	8 (42%)	26,31,34	0.74	0
8	OMG	L5	4494	8	23,26,27	2.42	9 (39%)	33,38,41	2.58	10 (30%)
8	A2M	L5	2401	8	22,25,26	3.45	9 (40%)	31,36,39	2.35	10 (32%)
8	PSU	L5	1782	8	18,21,22	4.43	7 (38%)	22,30,33	1.72	4 (18%)
8	A2M	L5	3723	8	22,25,26	3.48	9 (40%)	31,36,39	2.33	10 (32%)
8	A2M	L5	3760	8	22,25,26	3.48	10 (45%)	31,36,39	2.32	8 (25%)
8	PSU	L5	4353	8	18,21,22	4.41	7 (38%)	22,30,33	1.82	5 (22%)
8	A2M	L5	1871	8	22,25,26	3.51	10 (45%)	31,36,39	2.40	10 (32%)
49	A2M	S2	1678	49	22,25,26	3.52	9 (40%)	31,36,39	2.49	11 (35%)
49	6MZ	S2	1832	49	22,25,26	2.52	4 (18%)	30,36,39	2.27	9 (30%)
8	PSU	L5	3758	8	18,21,22	4.37	7 (38%)	22,30,33	1.81	4 (18%)
8	PSU	L5	3729	8	18,21,22	4.38	7 (38%)	22,30,33	1.77	5 (22%)
49	OMG	S2	683	49	23,26,27	2.39	9 (39%)	33,38,41	2.49	12 (36%)
8	PSU	L5	1683	8	18,21,22	4.37	7 (38%)	22,30,33	1.78	5 (22%)
49	B8N	S2	1248	49	24,29,30	3.07	8 (33%)	29,42,45	2.06	9 (31%)
8	OMC	L5	2422	8,84	19,22,23	2.95	8 (42%)	26,31,34	0.74	0
8	OMG	L5	4637	8	23,26,27	2.41	9 (39%)	33,38,41	2.68	10 (30%)
8	PSU	L5	3734	8	18,21,22	4.53	7 (38%)	22,30,33	1.77	5 (22%)
49	OMU	S2	1288	49	19,22,23	2.98	8 (42%)	26,31,34	1.70	5 (19%)
8	A2M	L5	1326	8	22,25,26	3.46	10 (45%)	31,36,39	2.40	11 (35%)
8	OMG	L5	1625	8	23,26,27	2.40	9 (39%)	33,38,41	2.58	10 (30%)
8	OMG	L5	4370	8	23,26,27	2.37	9 (39%)	33,38,41	2.52	10 (30%)
49	A2M	S2	668	49,84	22,25,26	3.45	10 (45%)	31,36,39	2.43	11 (35%)
49	MA6	S2	1851	49	23,26,27	1.40	4 (17%)	34,38,41	3.44	11 (32%)
8	OMG	L5	4618	8	23,26,27	2.37	9 (39%)	33,38,41	2.48	11 (33%)
49	A2M	S2	1383	49	22,25,26	3.44	9 (40%)	31,36,39	2.40	10 (32%)
49	OMU	S2	1442	49,84	19,22,23	2.94	8 (42%)	26,31,34	1.72	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	OMC	L5	2351	8	19,22,23	2.94	8 (42%)	26,31,34	0.86	0
8	A2M	L5	398	8	22,25,26	3.47	10 (45%)	31,36,39	2.39	10 (32%)
8	OMG	L5	3627	8	23,26,27	2.37	9 (39%)	33,38,41	2.46	11 (33%)
8	OMC	L5	2861	8	19,22,23	2.91	8 (42%)	26,31,34	0.70	0
8	OMC	L5	3701	8,84	19,22,23	2.92	8 (42%)	26,31,34	0.71	0
8	OMG	L5	4499	8	23,26,27	2.38	9 (39%)	33,38,41	2.53	10 (30%)
8	OMC	L5	4536	8	19,22,23	2.88	8 (42%)	26,31,34	0.76	0
8	OMG	L5	2424	8	23,26,27	2.43	9 (39%)	33,38,41	2.56	10 (30%)
8	OMG	L5	3792	8	23,26,27	2.38	9 (39%)	33,38,41	2.61	10 (30%)
49	A2M	S2	159	49	22,25,26	3.49	9 (40%)	31,36,39	2.45	10 (32%)
49	4AC	S2	1842	49	21,24,25	3.37	9 (42%)	29,34,37	1.02	4 (13%)
8	A2M	L5	3718	8	22,25,26	3.46	9 (40%)	31,36,39	2.40	12 (38%)
8	A2M	L5	1524	8	22,25,26	3.48	10 (45%)	31,36,39	2.28	10 (32%)
49	A2M	S2	576	49	22,25,26	3.46	9 (40%)	31,36,39	2.39	12 (38%)
8	OMG	L5	1522	8	23,26,27	2.35	9 (39%)	33,38,41	2.52	11 (33%)
49	OMU	S2	428	49	19,22,23	3.01	8 (42%)	26,31,34	1.68	5 (19%)
8	OMC	L5	1881	8,84	19,22,23	2.90	8 (42%)	26,31,34	0.79	0
49	OMC	S2	1391	49	19,22,23	2.94	8 (42%)	26,31,34	0.76	0
49	G7M	S2	1639	49,6	23,26,27	2.60	9 (39%)	35,39,42	2.50	11 (31%)
49	A2M	S2	1031	49,83	22,25,26	3.48	10 (45%)	31,36,39	2.41	10 (32%)
49	UY1	S2	1326	49,84	19,22,23	4.02	7 (36%)	22,31,34	1.82	5 (22%)
49	4AC	S2	1337	49	21,24,25	3.37	9 (42%)	29,34,37	1.20	4 (13%)
8	OMG	L5	1316	8	23,26,27	2.39	9 (39%)	33,38,41	2.61	10 (30%)
49	MA6	S2	1850	49	23,26,27	1.44	4 (17%)	34,38,41	3.10	11 (32%)
8	OMC	L5	3841	8	19,22,23	2.87	8 (42%)	26,31,34	0.65	0
8	OMG	L5	2364	8	23,26,27	2.37	9 (39%)	33,38,41	2.52	11 (33%)
8	OMG	L5	2876	8	23,26,27	2.35	9 (39%)	33,38,41	2.66	10 (30%)
8	OMC	L5	2804	8	19,22,23	2.87	8 (42%)	26,31,34	0.71	0
8	A2M	L5	2787	8,84	22,25,26	3.43	9 (40%)	31,36,39	2.36	11 (35%)
49	OMG	S2	601	49	23,26,27	2.40	9 (39%)	33,38,41	2.72	9 (27%)
8	OMU	L5	3925	8	19,22,23	2.85	8 (42%)	26,31,34	1.66	5 (19%)
8	A2M	L5	2815	8	22,25,26	3.43	9 (40%)	31,36,39	2.44	10 (32%)
8	A2M	L5	2363	8,84	22,25,26	3.48	10 (45%)	31,36,39	2.38	10 (32%)
10	OMG	L8	75	10	23,26,27	2.39	9 (39%)	33,38,41	2.53	10 (30%)

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
49	A2M	S2	27	49,84	-	1/9/27/28	0/3/3/3
8	A2M	L5	4590	8,84	-	2/9/27/28	0/3/3/3
49	OMG	S2	644	49	-	4/9/27/28	0/3/3/3
10	OMU	L8	14	10	-	5/9/27/28	0/2/2/2
8	OMC	L5	2365	8	-	0/9/27/28	0/2/2/2
8	A2M	L5	3825	8	-	0/9/27/28	0/3/3/3
8	A2M	L5	3724	8	-	1/9/27/28	0/3/3/3
49	OMG	S2	1328	49	-	0/9/27/28	0/3/3/3
8	OMG	L5	4228	8	-	0/9/27/28	0/3/3/3
49	OMC	S2	174	49	-	0/9/27/28	0/2/2/2
49	OMC	S2	1703	49	-	2/9/27/28	0/2/2/2
10	PSU	L8	55	10	-	2/7/25/26	0/2/2/2
8	OMU	L5	4620	8	-	2/9/27/28	0/2/2/2
8	OMG	L5	3744	8	-	0/9/27/28	0/3/3/3
8	OMG	L5	4623	8	-	2/9/27/28	0/3/3/3
8	OMC	L5	1340	8	-	0/9/27/28	0/2/2/2
8	OMG	L5	4494	8	-	0/9/27/28	0/3/3/3
8	A2M	L5	2401	8	-	2/9/27/28	0/3/3/3
8	PSU	L5	1782	8	-	0/7/25/26	0/2/2/2
8	A2M	L5	3723	8	-	1/9/27/28	0/3/3/3
8	A2M	L5	3760	8	-	0/9/27/28	0/3/3/3
8	PSU	L5	4353	8	-	0/7/25/26	0/2/2/2
8	A2M	L5	1871	8	-	0/9/27/28	0/3/3/3
49	A2M	S2	1678	49	-	1/9/27/28	0/3/3/3
49	6MZ	S2	1832	49	-	3/9/27/28	0/3/3/3
8	PSU	L5	3758	8	-	0/7/25/26	0/2/2/2
8	PSU	L5	3729	8	-	2/7/25/26	0/2/2/2
49	OMG	S2	683	49	-	2/9/27/28	0/3/3/3
8	PSU	L5	1683	8	-	0/7/25/26	0/2/2/2
49	B8N	S2	1248	49	-	7/16/34/35	0/2/2/2
8	OMC	L5	2422	8,84	-	2/9/27/28	0/2/2/2
8	OMG	L5	4637	8	-	0/9/27/28	0/3/3/3
8	PSU	L5	3734	8	-	2/7/25/26	0/2/2/2
49	OMU	S2	1288	49	-	2/9/27/28	0/2/2/2
8	A2M	L5	1326	8	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OMG	L5	1625	8	-	2/9/27/28	0/3/3/3
8	OMG	L5	4370	8	-	0/9/27/28	0/3/3/3
49	A2M	S2	668	49,84	-	3/9/27/28	0/3/3/3
49	MA6	S2	1851	49	-	3/11/29/30	0/3/3/3
8	OMG	L5	4618	8	-	0/9/27/28	0/3/3/3
49	A2M	S2	1383	49	-	1/9/27/28	0/3/3/3
49	OMU	S2	1442	49,84	-	1/9/27/28	0/2/2/2
8	OMC	L5	2351	8	-	5/9/27/28	0/2/2/2
8	A2M	L5	398	8	-	2/9/27/28	0/3/3/3
8	OMG	L5	3627	8	-	2/9/27/28	0/3/3/3
8	OMC	L5	2861	8	-	1/9/27/28	0/2/2/2
8	OMC	L5	3701	8,84	-	5/9/27/28	0/2/2/2
8	OMG	L5	4499	8	-	0/9/27/28	0/3/3/3
8	OMC	L5	4536	8	-	0/9/27/28	0/2/2/2
8	OMG	L5	2424	8	-	2/9/27/28	0/3/3/3
8	OMG	L5	3792	8	-	0/9/27/28	0/3/3/3
49	A2M	S2	159	49	-	2/9/27/28	0/3/3/3
49	4AC	S2	1842	49	-	0/11/29/30	0/2/2/2
8	A2M	L5	3718	8	-	0/9/27/28	0/3/3/3
8	A2M	L5	1524	8	-	1/9/27/28	0/3/3/3
49	A2M	S2	576	49	-	2/9/27/28	0/3/3/3
8	OMG	L5	1522	8	-	0/9/27/28	0/3/3/3
49	OMU	S2	428	49	-	6/9/27/28	0/2/2/2
8	OMC	L5	1881	8,84	-	0/9/27/28	0/2/2/2
49	OMC	S2	1391	49	-	0/9/27/28	0/2/2/2
49	G7M	S2	1639	49,6	-	1/7/25/26	0/3/3/3
49	A2M	S2	1031	49,83	-	0/9/27/28	0/3/3/3
49	UY1	S2	1326	49,84	-	2/9/27/28	0/2/2/2
49	4AC	S2	1337	49	-	0/11/29/30	0/2/2/2
8	OMG	L5	1316	8	-	1/9/27/28	0/3/3/3
49	MA6	S2	1850	49	-	1/11/29/30	0/3/3/3
8	OMC	L5	3841	8	-	1/9/27/28	0/2/2/2
8	OMG	L5	2364	8	-	2/9/27/28	0/3/3/3
8	OMG	L5	2876	8	-	2/9/27/28	0/3/3/3
8	OMC	L5	2804	8	-	1/9/27/28	0/2/2/2
8	A2M	L5	2787	8,84	-	3/9/27/28	0/3/3/3
49	OMG	S2	601	49	-	5/9/27/28	0/3/3/3
8	OMU	L5	3925	8	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	A2M	L5	2815	8	-	0/9/27/28	0/3/3/3
8	A2M	L5	2363	8,84	-	0/9/27/28	0/3/3/3
10	OMG	L8	75	10	-	0/9/27/28	0/3/3/3

The worst 5 of 644 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	3734	PSU	C6-C5	11.80	1.49	1.35
8	L5	1782	PSU	C6-C5	11.44	1.48	1.35
10	L8	55	PSU	C6-C5	11.40	1.48	1.35
8	L5	1683	PSU	C6-C5	11.32	1.48	1.35
8	L5	4353	PSU	C6-C5	11.30	1.48	1.35

The worst 5 of 566 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1851	MA6	N1-C6-N6	-13.85	101.94	117.08
49	S2	1850	MA6	N1-C6-N6	-11.56	104.44	117.08
49	S2	601	OMG	C1'-N9-C8	-8.84	101.52	126.70
8	L5	2876	OMG	C1'-N9-C8	-8.55	102.35	126.70
8	L5	4637	OMG	C1'-N9-C8	-8.45	102.64	126.70

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	L8	14	OMU	O4'-C1'-N1-C2
10	L8	14	OMU	O4'-C1'-N1-C6
10	L8	14	OMU	C1'-C2'-O2'-CM2
10	L8	55	PSU	C3'-C4'-C5'-O5'
10	L8	55	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

42 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	S2	27	A2M	2	0
49	S2	644	OMG	2	0
10	L8	14	OMU	4	0
8	L5	3724	A2M	1	0
8	L5	4228	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	S2	174	OMC	1	0
10	L8	55	PSU	3	0
8	L5	3744	OMG	1	0
8	L5	4623	OMG	1	0
8	L5	1340	OMC	2	0
8	L5	3723	A2M	2	0
8	L5	3760	A2M	1	0
8	L5	1871	A2M	1	0
49	S2	1678	A2M	2	0
49	S2	1832	6MZ	1	0
49	S2	1288	OMU	1	0
8	L5	1326	A2M	3	0
8	L5	1625	OMG	1	0
49	S2	1383	A2M	1	0
49	S2	1442	OMU	1	0
8	L5	398	A2M	1	0
8	L5	3627	OMG	1	0
8	L5	2861	OMC	1	0
8	L5	3701	OMC	1	0
8	L5	4536	OMC	3	0
8	L5	2424	OMG	1	0
49	S2	1842	4AC	1	0
8	L5	3718	A2M	3	0
8	L5	1524	A2M	1	0
49	S2	576	A2M	3	0
49	S2	428	OMU	1	0
49	S2	1337	4AC	5	0
8	L5	1316	OMG	1	0
49	S2	1850	MA6	6	0
8	L5	3841	OMC	1	0
8	L5	2876	OMG	2	0
8	L5	2804	OMC	3	0
49	S2	601	OMG	2	0
8	L5	3925	OMU	2	0
8	L5	2815	A2M	1	0
8	L5	2363	A2M	1	0
10	L8	75	OMG	2	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 340 ligands modelled in this entry, 337 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	PUT	L5	5287	-	5,5,5	0.23	0	4,4,4	0.24	0
86	SPD	L5	5286	-	9,9,9	0.43	0	8,8,8	0.39	0
89	HYG	S2	1901	84	35,39,39	2.58	10 (28%)	43,60,60	1.18	4 (9%)

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	PUT	L5	5287	-	-	0/3/3/3	-
86	SPD	L5	5286	-	-	0/7/7/7	-
89	HYG	S2	1901	84	-	3/12/87/87	0/4/4/4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	S2	1901	HYG	O29-C12	8.46	1.57	1.43
89	S2	1901	HYG	O22-C17	6.40	1.53	1.43
89	S2	1901	HYG	O14-C13	5.92	1.56	1.41
89	S2	1901	HYG	C17-C12	-3.71	1.45	1.53
89	S2	1901	HYG	C16-C15	3.40	1.60	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	S2	1901	HYG	O14-C13-C12	-3.51	102.55	109.51
89	S2	1901	HYG	O22-C17-C16	3.30	119.25	111.22
89	S2	1901	HYG	O11-C5-C4	-2.37	104.56	109.47
89	S2	1901	HYG	C23-O28-C27	-2.05	108.08	112.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

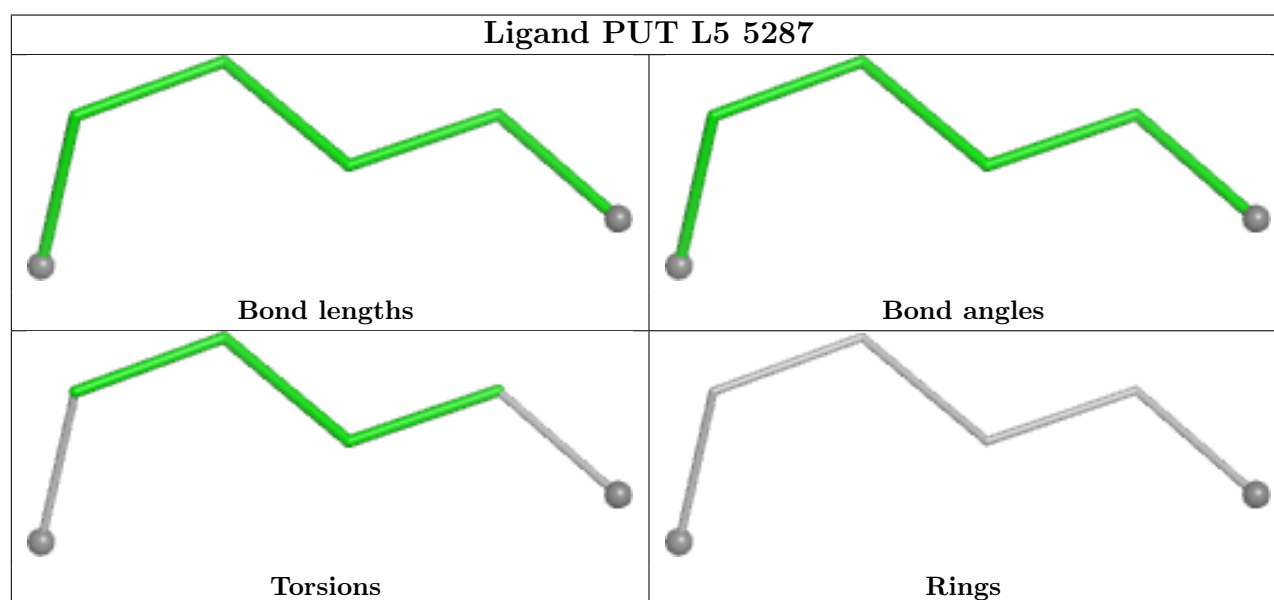
Mol	Chain	Res	Type	Atoms
89	S2	1901	HYG	C26-C27-C33-C34
89	S2	1901	HYG	O28-C27-C33-C34
89	S2	1901	HYG	O14-C13-O18-C6

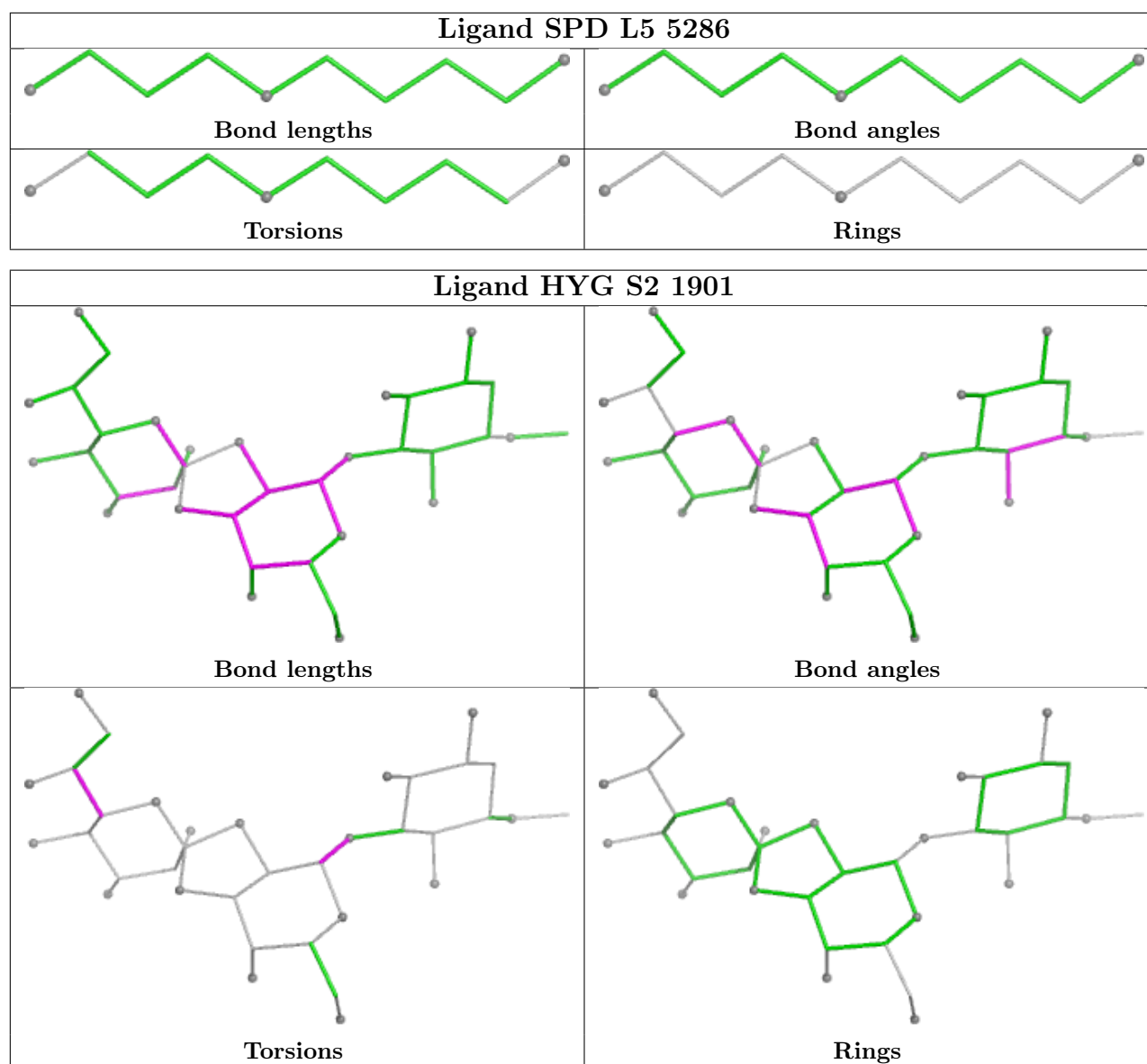
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	L5	5287	PUT	1	0
86	L5	5286	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
49	S2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	1832:6MZ	O3'	1833:C	P	4.54
1	S2	1248:B8N	O3'	1249:C	P	3.93

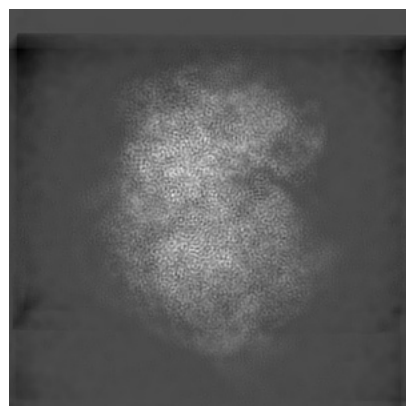
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52565. These allow visual inspection of the internal detail of the map and identification of artifacts.

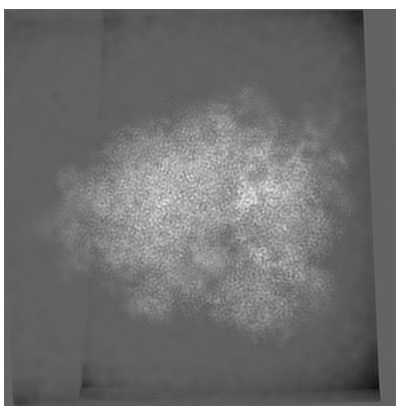
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

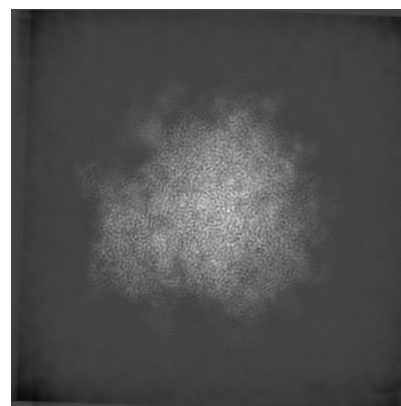
6.1.1 Primary map



X

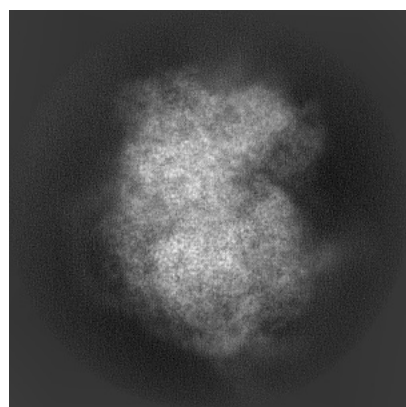


Y

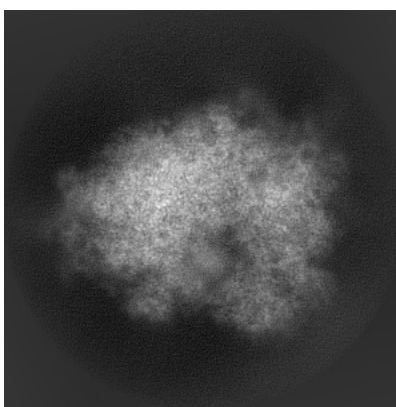


Z

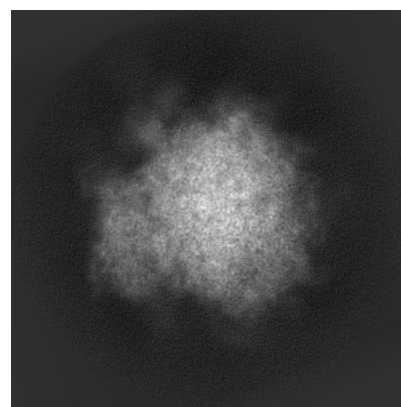
6.1.2 Raw map



X



Y

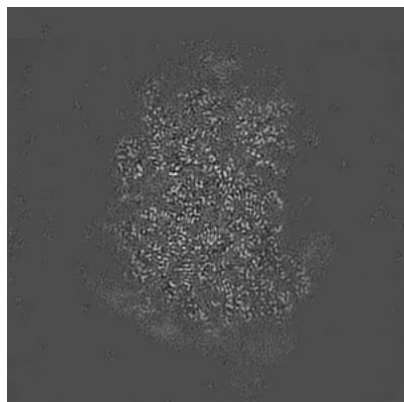


Z

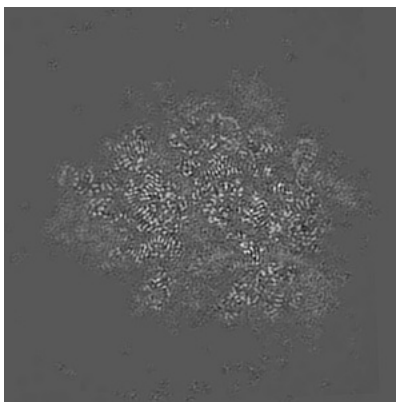
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

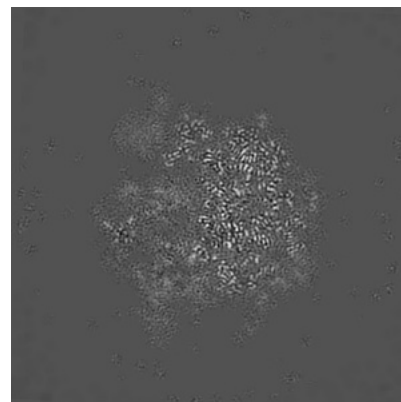
6.2.1 Primary map



X Index: 240

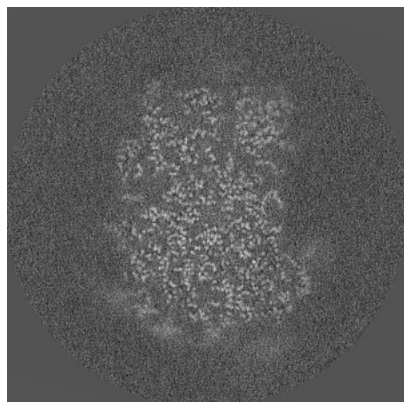


Y Index: 240

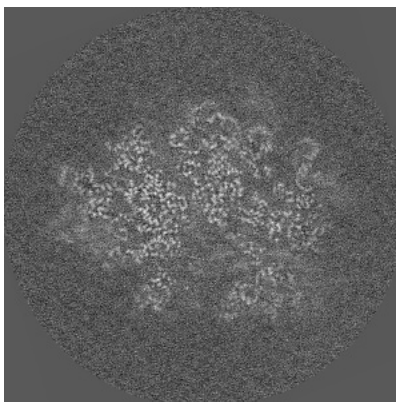


Z Index: 240

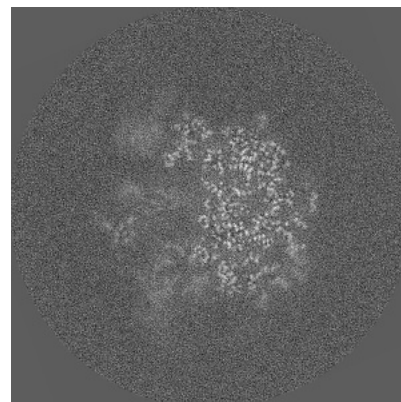
6.2.2 Raw map



X Index: 240



Y Index: 240

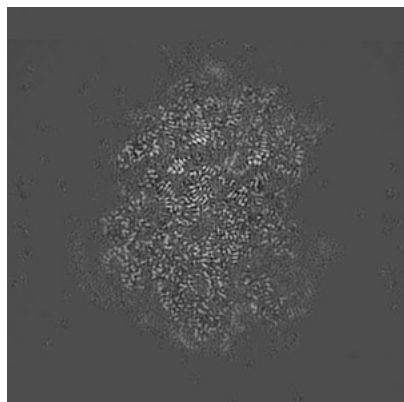


Z Index: 240

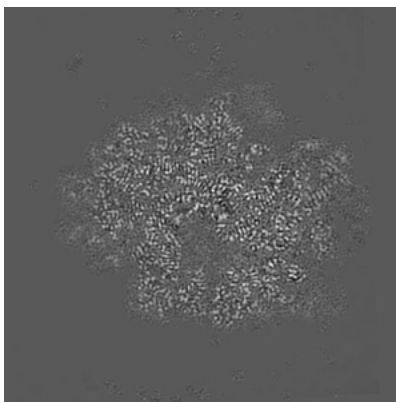
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

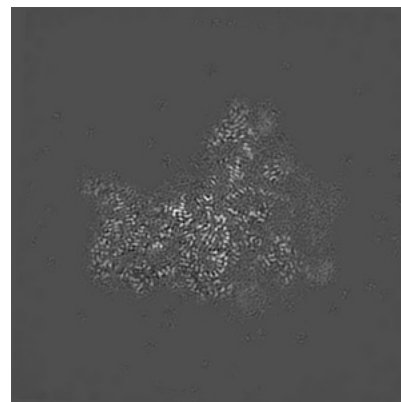
6.3.1 Primary map



X Index: 261

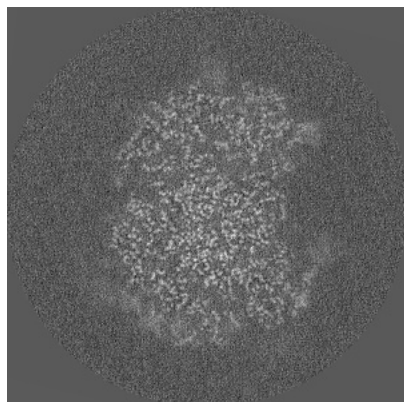


Y Index: 220

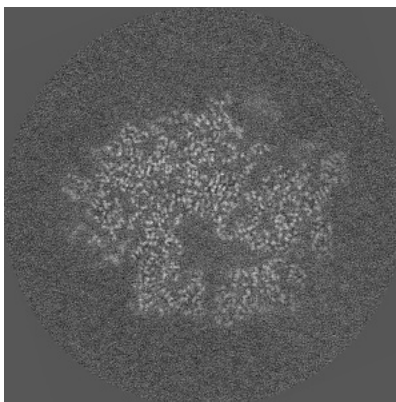


Z Index: 288

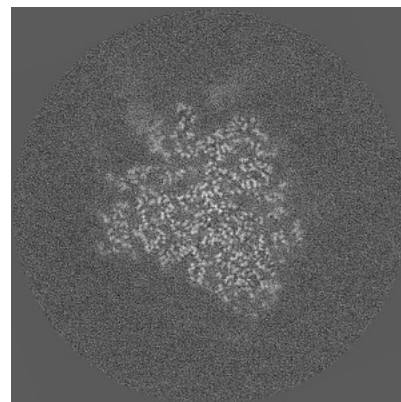
6.3.2 Raw map



X Index: 254



Y Index: 221

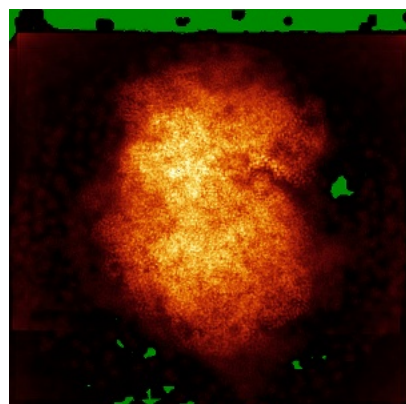


Z Index: 197

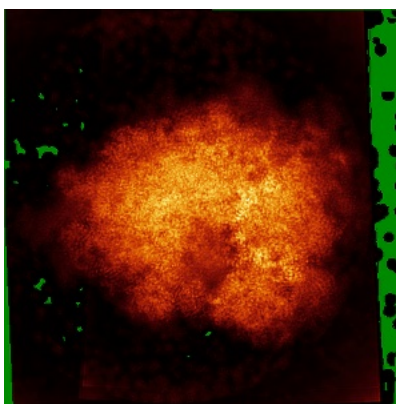
The images above show the largest variance slices of the map in three orthogonal directions.

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

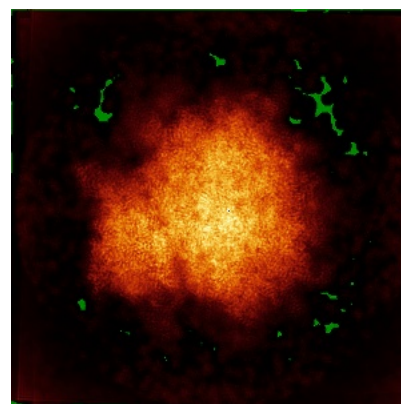
6.4.1 Primary map



X

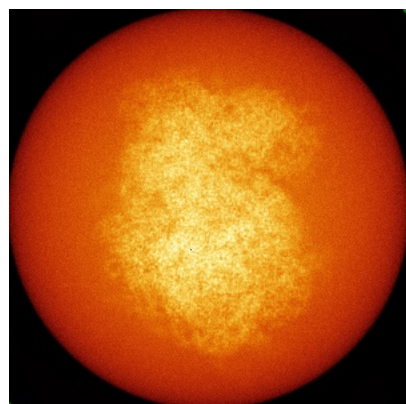


Y

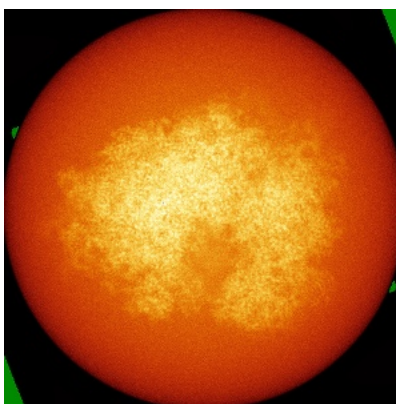


Z

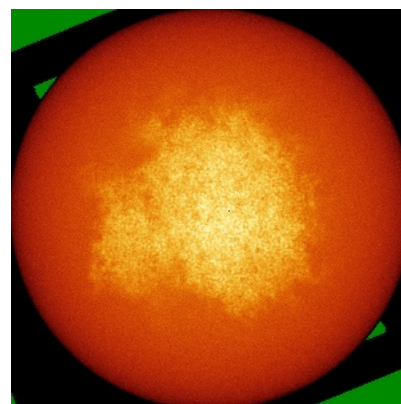
6.4.2 Raw map



X



Y

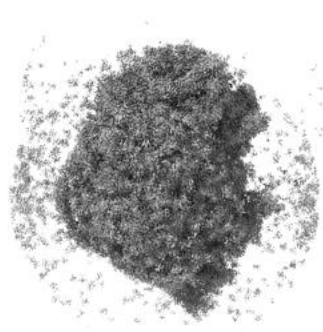


Z

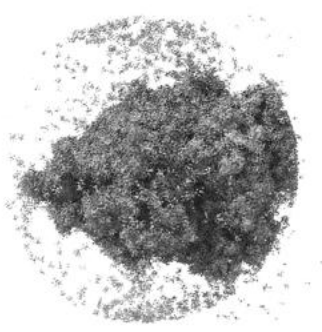
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

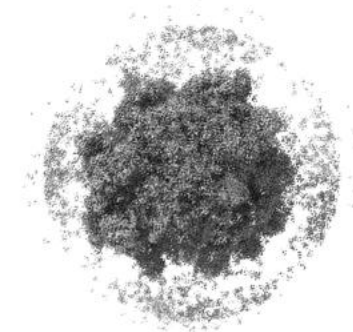
6.5.1 Primary map



X



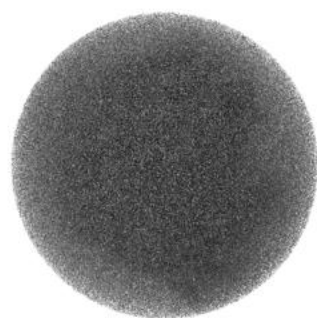
Y



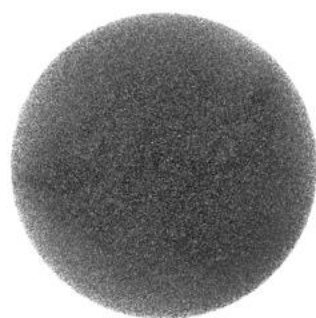
Z

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.

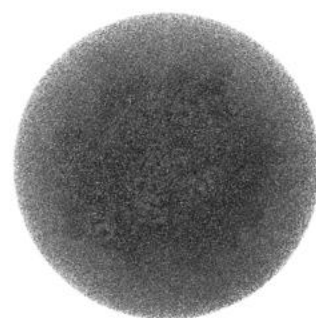
6.5.2 Raw map



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.

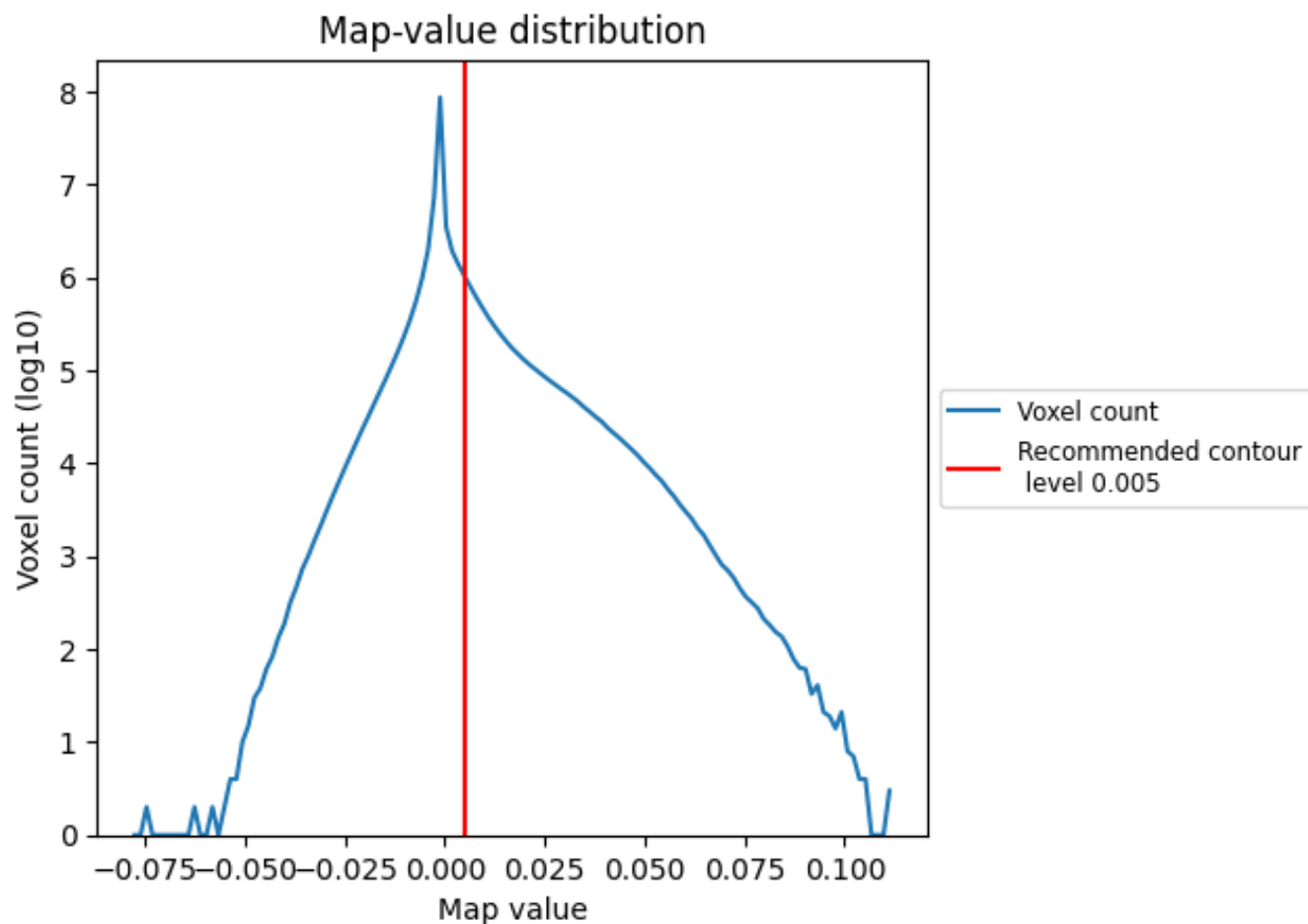
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

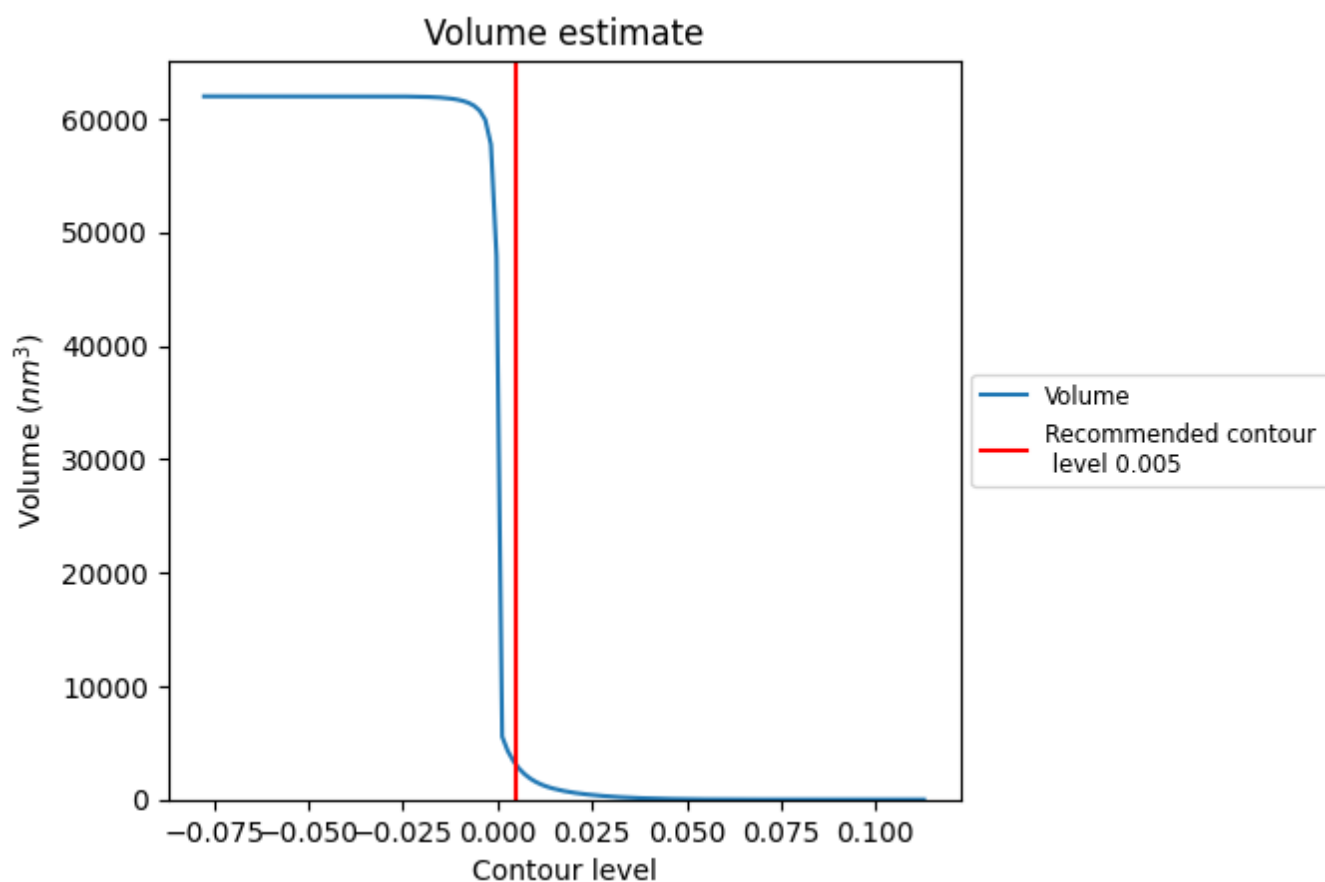
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

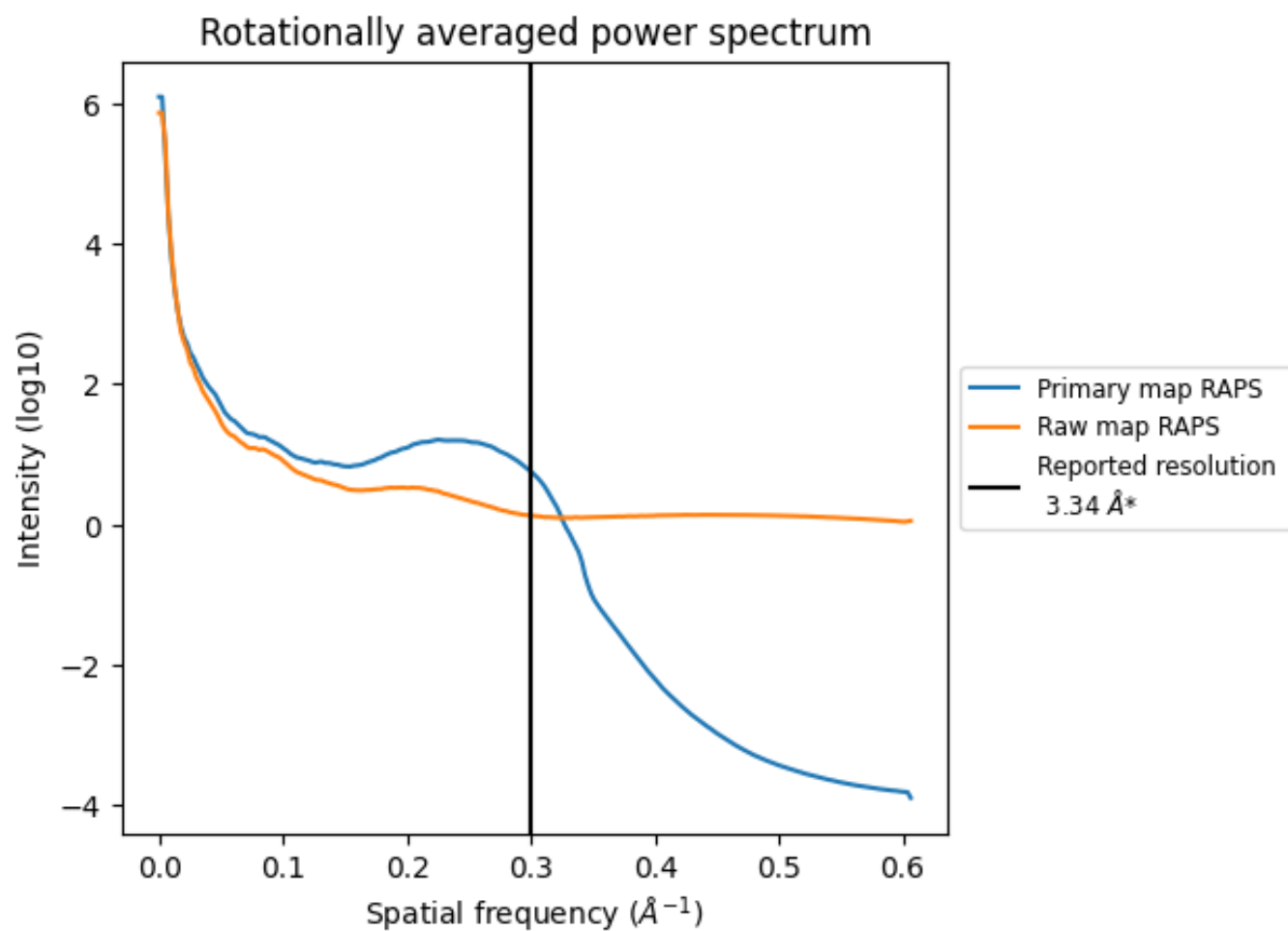
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3036 nm³; this corresponds to an approximate mass of 2742 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

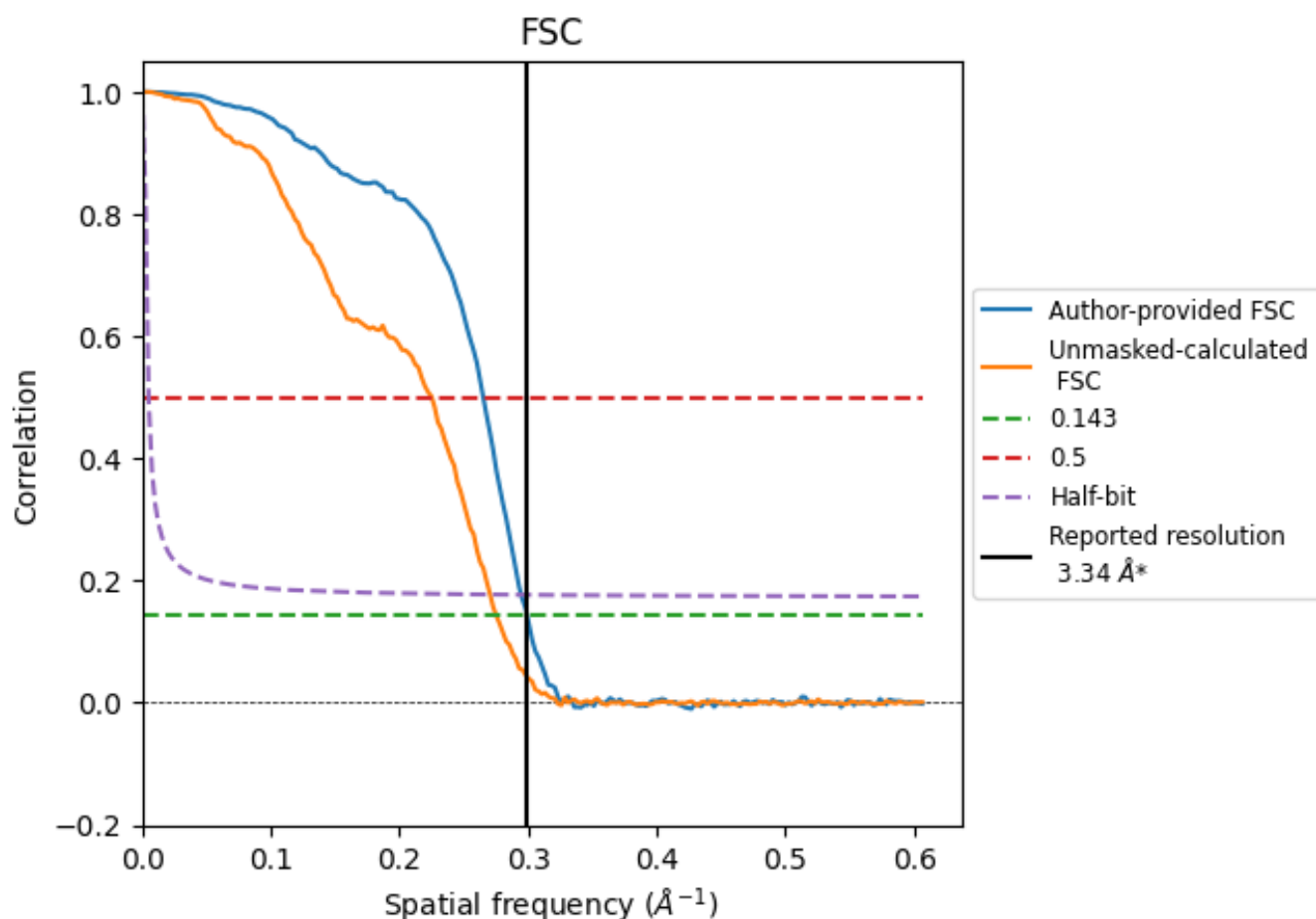


*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8.2 Resolution estimates [i](#)

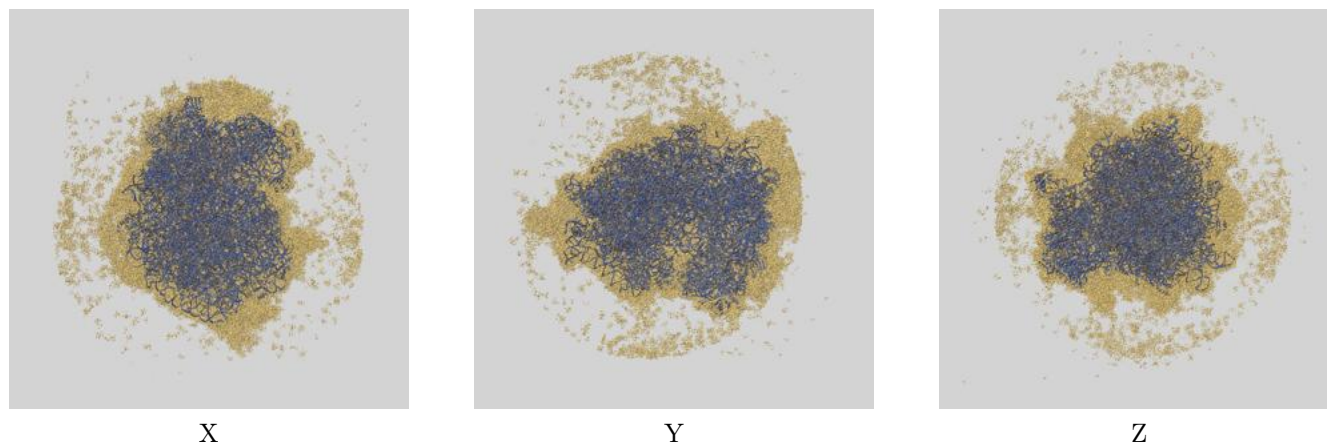
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	3.77	3.39
Unmasked-calculated*	3.63	4.44	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

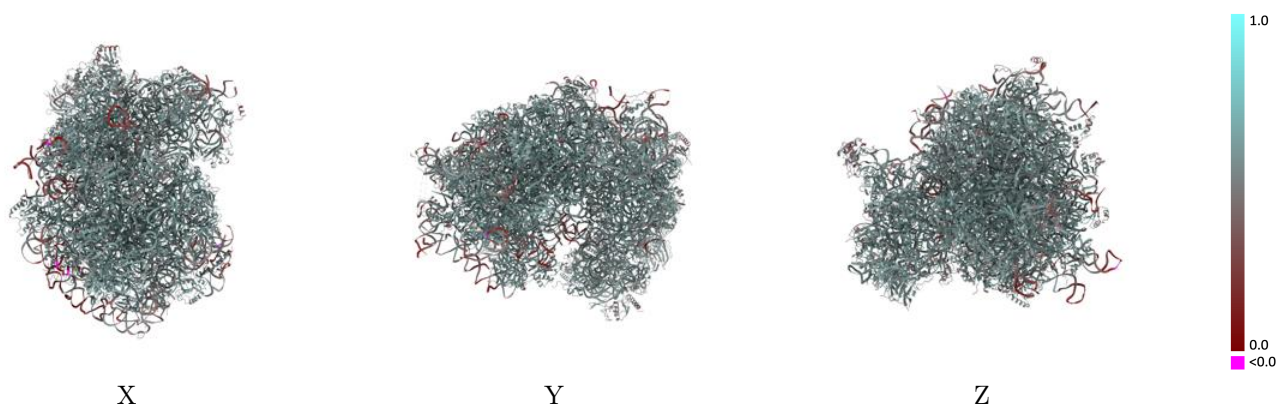
This section contains information regarding the fit between EMDB map EMD-52565 and PDB model 9I14. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



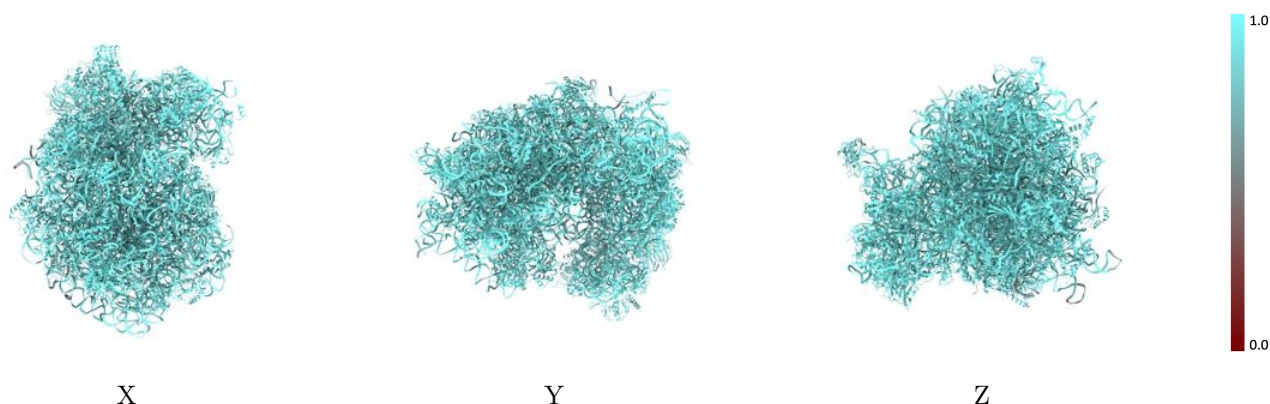
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



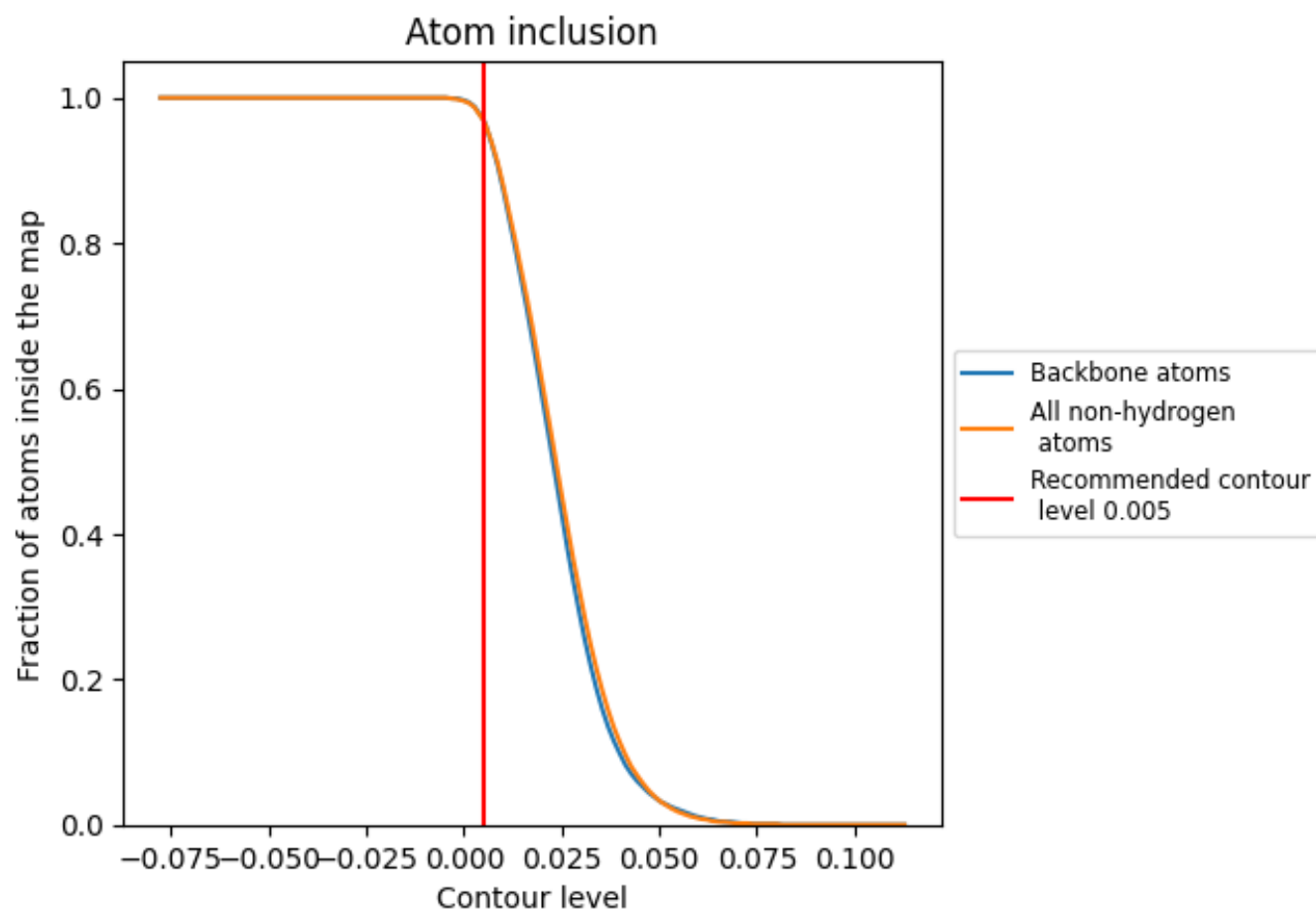
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9690	 0.5510
A4	 0.9790	 0.5320
B4	 0.9500	 0.4080
D4	 0.9110	 0.3570
L5	 0.9660	 0.5340
L7	 0.9930	 0.5760
L8	 0.9860	 0.5630
LA	 0.9840	 0.5980
LB	 0.9760	 0.5860
LC	 0.9720	 0.5850
LD	 0.9590	 0.5690
LE	 0.9680	 0.5660
LF	 0.9690	 0.5850
LG	 0.9560	 0.5580
LH	 0.9590	 0.5740
LI	 0.9660	 0.5810
LJ	 0.9660	 0.5630
LL	 0.9640	 0.5700
LM	 0.9650	 0.5730
LN	 0.9830	 0.6020
LO	 0.9710	 0.5850
LP	 0.9690	 0.5900
LQ	 0.9810	 0.5980
LR	 0.9760	 0.5660
LS	 0.9800	 0.5970
LT	 0.9750	 0.5820
LU	 0.9290	 0.5080
LV	 0.9840	 0.5830
LW	 0.9800	 0.5490
LX	 0.9710	 0.5760
LY	 0.9630	 0.5860
LZ	 0.9710	 0.5710
La	 0.9770	 0.5980
Lb	 0.9670	 0.5600
Lc	 0.9630	 0.5530



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Chain	Atom inclusion	Q-score
Ld	 0.9770	 0.5780
Le	 0.9870	 0.5970
Lf	 0.9860	 0.6000
Lg	 0.9770	 0.5790
Lh	 0.9560	 0.5650
Li	 0.9550	 0.5630
Lj	 0.9870	 0.5950
Lk	 0.9460	 0.5290
Ll	 0.9780	 0.5860
Lm	 0.9750	 0.5720
Ln	 0.9950	 0.5820
Lo	 0.9820	 0.5770
Lp	 0.9910	 0.5870
Lr	 0.9740	 0.5860
S2	 0.9830	 0.5550
SA	 0.9500	 0.5560
SB	 0.9680	 0.5670
SC	 0.9750	 0.5670
SD	 0.9560	 0.5470
SE	 0.9650	 0.5630
SF	 0.9680	 0.5670
SG	 0.9720	 0.5400
SH	 0.9390	 0.5080
SI	 0.9810	 0.5510
SJ	 0.9580	 0.5460
SK	 0.9430	 0.5620
SL	 0.9780	 0.5670
SM	 0.8330	 0.4440
SN	 0.9790	 0.5650
SO	 0.9680	 0.5710
SP	 0.9730	 0.5650
SQ	 0.9610	 0.5770
SR	 0.9340	 0.5310
SS	 0.9650	 0.5680
ST	 0.9640	 0.5780
SU	 0.9280	 0.5270
SV	 0.9410	 0.5610
SW	 0.9770	 0.5750
SX	 0.9630	 0.5640
SY	 0.9660	 0.5580
SZ	 0.9550	 0.5570
Sa	 0.9750	 0.5740

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Chain	Atom inclusion	Q-score
Sb	 0.9440	 0.5090
Sc	 0.9830	 0.5520
Sd	 0.9810	 0.5830
Se	 0.9820	 0.5640
Sf	 0.8910	 0.4750
Sg	 0.9330	 0.5460