



wwPDB EM Validation Summary Report ⓘ

Jun 19, 2026 – 07:43 am BST

PDB ID : 7ZJX / pdb_00007zjx
EMDB ID : EMD-14752
Title : Rabbit 80S ribosome programmed with SECIS and SBP2
Authors : Hilal, T.; Simonovic, M.; Spahn, C.M.T.
Deposited on : 2022-04-12
Resolution : 3.10 Å(reported)
Based on initial model : 7O7Y

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:

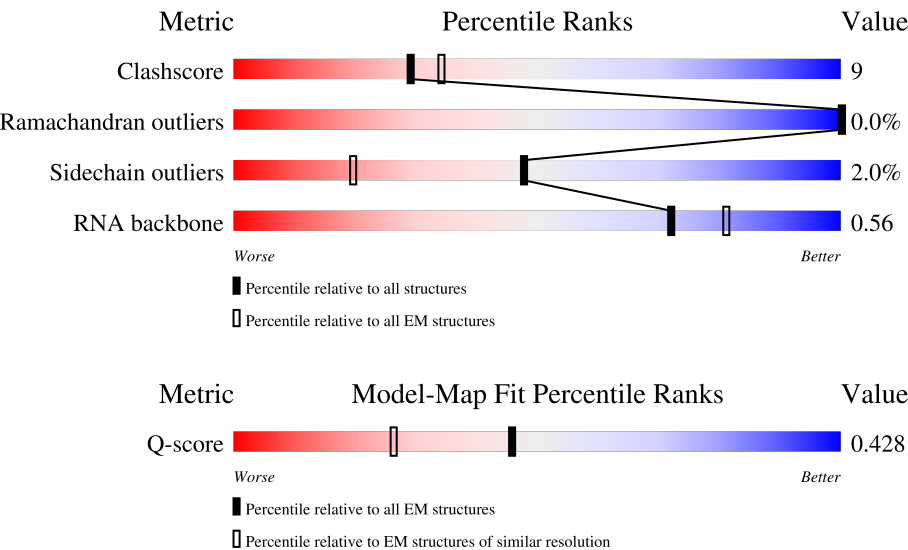
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal 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 i

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

The reported resolution of this entry is 3.10 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.



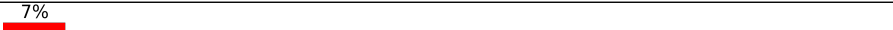
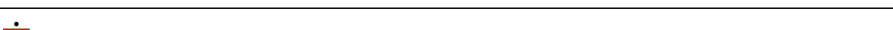
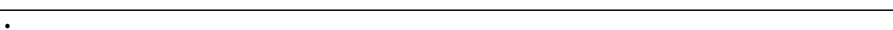
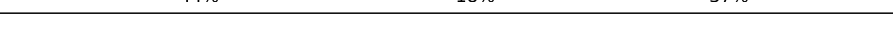
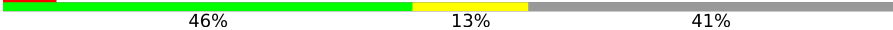
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	B	854	9% 18% 6% 76%
2	I	163	22% 22% 48% 30%
3	L5	4808	46% 26% 5% 22%

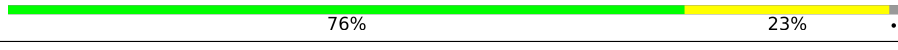
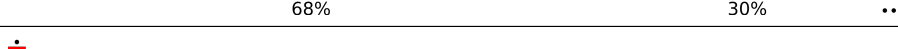
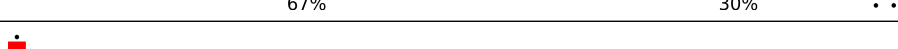
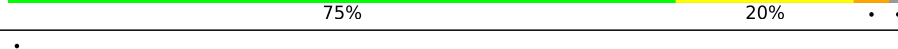
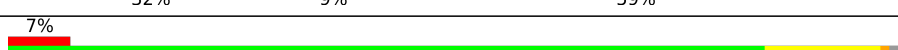
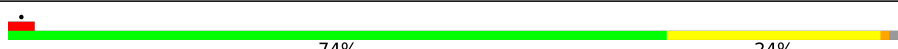
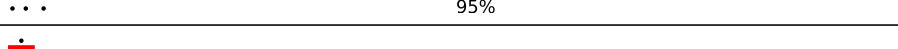
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	158	
6	LD	257	
7	LE	403	
8	LF	413	
9	LG	297	
10	LH	291	
11	LI	247	
12	LJ	266	
13	LK	192	
14	LL	214	
15	LM	178	
16	LO	211	
17	LP	218	
18	LQ	204	
19	LR	203	
20	LS	184	
21	LT	188	
22	LU	196	
23	LV	176	
24	LW	160	
25	LX	128	
26	LY	140	
27	LZ	157	
28	La	156	

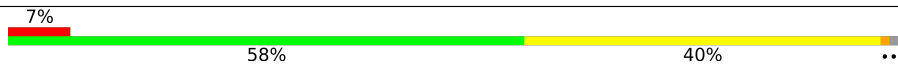
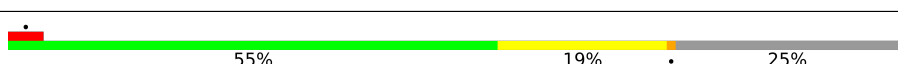
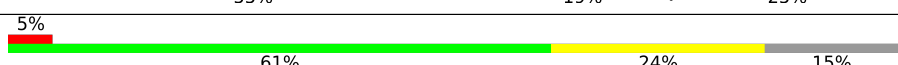
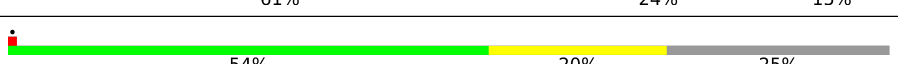
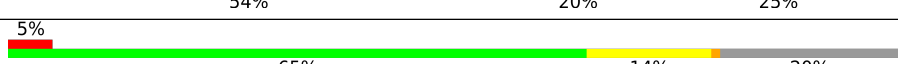
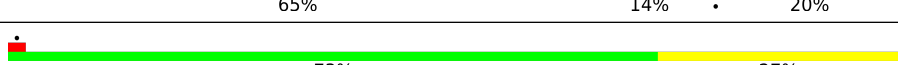
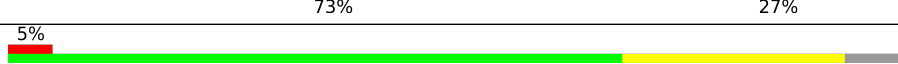
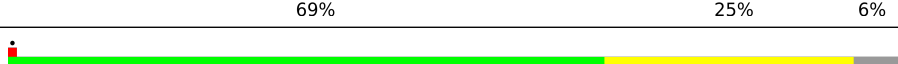
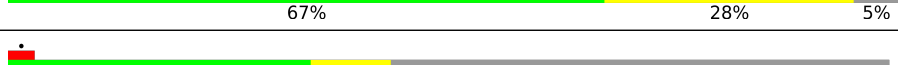
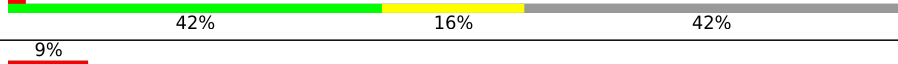
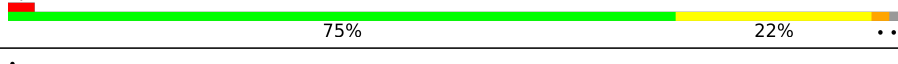
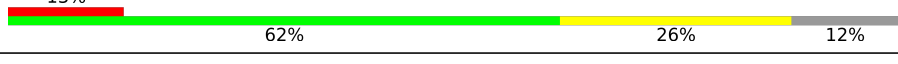
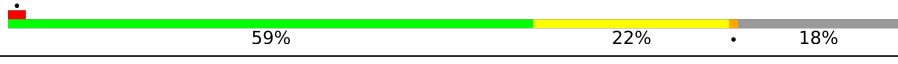
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Mol	Chain	Length	Quality of chain
29	Lb	145	
30	Lc	136	
31	Ld	148	
32	Le	245	
33	Lf	115	
34	Lg	125	
35	Lh	135	
36	Li	110	
37	Lj	117	
38	Lk	123	
39	Ll	105	
40	Lm	97	
41	Ln	70	
42	Lo	51	
43	Lp	128	
44	Lq	106	
45	Lr	92	
46	Ls	137	
47	Lx	217	
48	S	855	
49	S2	1870	
50	SB	84	
51	SC	69	
52	SD	156	
53	SE	133	

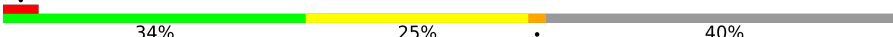
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Mol	Chain	Length	Quality of chain
54	SF	115	
55	SG	317	
56	SH	56	
57	SL	295	
58	SM	264	
59	SN	293	
60	SO	281	
61	SP	263	
62	SQ	204	
63	SR	249	
64	SS	432	
65	ST	208	
66	SU	194	
67	SV	165	
68	SW	158	
69	SX	132	
70	SY	151	
71	SZ	151	
72	Sa	145	
73	Sb	172	
74	Sc	135	
75	Sd	152	
76	Se	145	
77	Sf	119	
78	Sg	83	

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Mol	Chain	Length	Quality of chain
79	Sh	130	
80	Si	143	
81	Sj	130	
82	Sk	124	
83	Sl	25	

2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 222755 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 Selenocysteine insertion sequence-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	204	Total	C	N	O	S	0	0
			1379	881	257	238	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	687	ARG	LYS	conflict	UNP Q96T21
B	692	ILE	VAL	conflict	UNP Q96T21

- Molecule 2 is a RNA chain called CrPV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	163	Total	C	N	O	P	0	0
			3447	1544	588	1152	163		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3732	Total	C	N	O	P	0	0
			80089	35700	14644	26013	3732		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2570	1141	456	851	122		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 6 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LD	253	Total	C	N	O	S	0	0
			1939	1214	396	323	6		

- Molecule 7 is a protein called 60S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LE	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LF	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 9 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LG	294	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LG	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LH	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 11 is a protein called 60S ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LI	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	182	ASN	GLY	conflict	UNP A0A7J8C453
LI	199	HIS	ARG	conflict	UNP A0A7J8C453

- Molecule 12 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LJ	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LJ	184	LEU	ILE	conflict	UNP P62424

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LK	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 14 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

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

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

- Molecule 16 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LO	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LO	74	ARG	HIS	conflict	UNP G1TKB3

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Chain	Residue	Modelled	Actual	Comment	Reference
LO	190	ARG	HIS	conflict	UNP G1TKB3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LP	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 18 is a protein called Ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LR	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LR	174	LEU	ILE	conflict	UNP A0A0N8ETI8
LR	194	ASP	GLU	conflict	UNP A0A0N8ETI8

- Molecule 20 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LS	159	Total	C	N	O	S	0	0
			1288	808	249	222	9		

- Molecule 21 is a protein called 60S ribosomal Protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LT	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LT	134	ARG	CYS	conflict	UNP F6QKI9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LU	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 23 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LV	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LV	36	ASN	ILE	conflict	UNP A0A1Z5LHJ5

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

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

- Molecule 25 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LX	99	Total	C	N	O	S	0	0
			806	516	141	147	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LX	60	ALA	VAL	conflict	UNP Q4R5I3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LY	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LZ	93	Total	C	N	O	S	0	0
			766	480	153	129	4		

- Molecule 28 is a protein called Ribosomal_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	La	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 29 is a protein called Ribosomal protein L26.

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

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ld	147	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Le	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lf	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

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

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

- Molecule 35 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lh	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Li	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lk	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ll	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 40 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lm	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	Ln	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 42 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lo	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 43 is a protein called 60S ribosomal protein L40.

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

- Molecule 44 is a protein called 60S ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lq	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 45 is a protein called 60S ribosomal protein eL43.

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

- Molecule 46 is a protein called 60S ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ls	126	Total	C	N	O	S	0	0
			1014	629	209	170	6		

- Molecule 47 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lx	169	Total	C	N	O		0	0
			840	502	169	169			

- Molecule 48 is a RNA chain called GPX4 SECIS element.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S	46	Total	C	N	O	P	0	0
			983	438	179	320	46		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1118	U	C	conflict	GB 25123295
S	1126	A	C	conflict	GB 25123295
S	1132	A	U	conflict	GB 25123295
S	1133	G	-	insertion	GB 25123295
S	1134	C	-	insertion	GB 25123295
S	1135	C	-	insertion	GB 25123295
S	1136	C	-	insertion	GB 25123295
S	1150	U	A	conflict	GB 25123295

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S2	1770	Total	C	N	O	P	0	0
			37825	16906	6780	12369	1770		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	251	C	U	conflict	GB 37956930
S2	583	U	C	conflict	GB 37956930
S2	584	A	C	conflict	GB 37956930
S2	585	A	G	conflict	GB 37956930
S2	1338	4AC	C	conflict	GB 37956930
S2	1843	4AC	C	conflict	GB 37956930

- Molecule 50 is a protein called 40S ribosomal protein S27.

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

- Molecule 51 is a protein called 40S ribosomal protein S28.

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

- Molecule 52 is a protein called Ubiquitin carboxyl extension protein 80.

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

- Molecule 53 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SE	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 54 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SF	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 55 is a protein called Guanine nucleotide-binding protein subunit beta-2-like 1.

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

- Molecule 56 is a protein called 40S ribosomal protein S29.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SL	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 58 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SM	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 59 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SN	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SN	33	ILE	VAL	conflict	UNP O18789
SN	101	ALA	SER	conflict	UNP O18789

- Molecule 60 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SO	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 61 is a protein called 40S ribosomal protein S4.

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

- Molecule 62 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SQ	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 63 is a protein called 40S ribosomal protein S6.

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

- Molecule 64 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SS	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 65 is a protein called 40S ribosomal protein S8.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SU	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 67 is a protein called S10_ plectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SV	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 68 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SW	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 69 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SX	121	Total	C	N	O	S	0	0
			943	591	167	176	9		

- Molecule 70 is a protein called 40S ribosomal protein S13.

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

- Molecule 71 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SZ	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 72 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Sa	127	Total	C	N	O	S	0	0
			1042	662	196	177	7		

- Molecule 73 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sb	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 74 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sc	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 75 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sd	141	Total	C	N	O	S	0	0
			1171	736	235	199	1		

- Molecule 76 is a protein called 40S Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Se	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 77 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sf	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 78 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sg	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

- Molecule 79 is a protein called 40S ribosomal protein S15a.

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

- Molecule 80 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Si	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 81 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sj	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 82 is a protein called 40S ribosomal protein S25.

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

- Molecule 83 is a protein called 60S ribosomal protein L41.

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

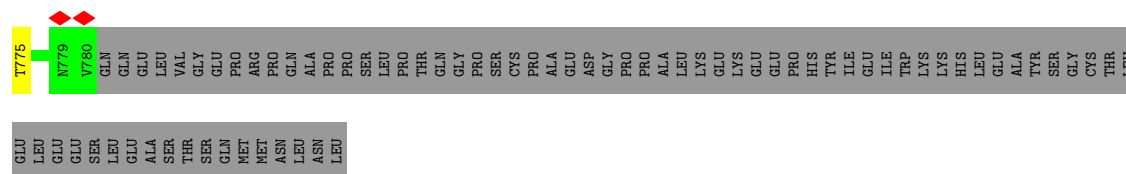
- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	Lj	1	Total	Zn	0
			1	1	
84	Lm	1	Total	Zn	0
			1	1	
84	Lp	1	Total	Zn	0
			1	1	
84	Lq	1	Total	Zn	0
			1	1	
84	Lr	1	Total	Zn	0
			1	1	
84	SD	1	Total	Zn	0
			1	1	

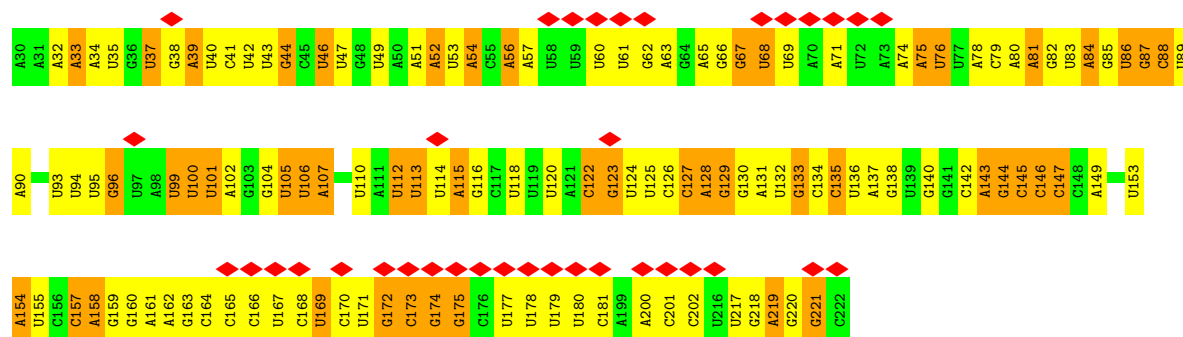
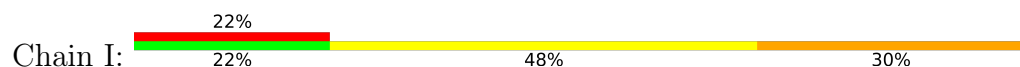
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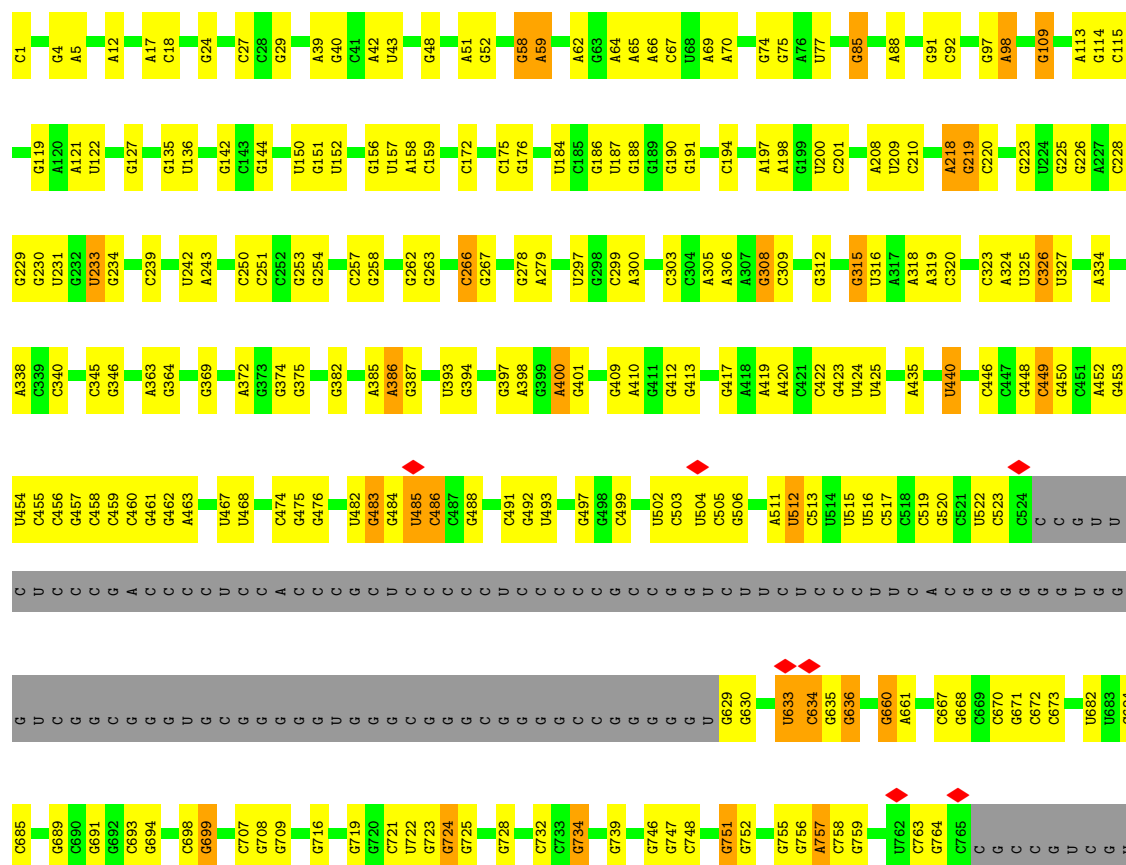
Mol	Chain	Residues	Atoms		AltConf
84	SF	1	Total 1	Zn 1	0
84	SH	1	Total 1	Zn 1	0



• Molecule 2: CrPV IRES

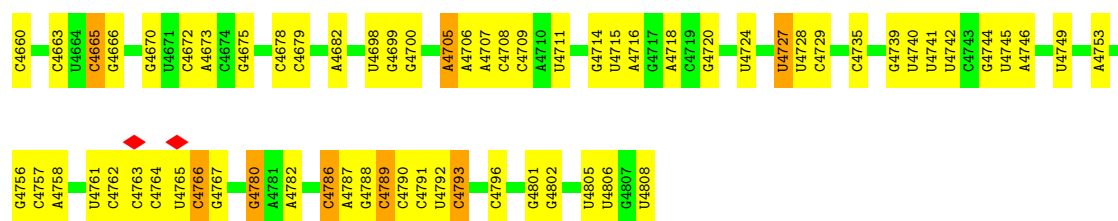


• Molecule 3: 28S rRNA









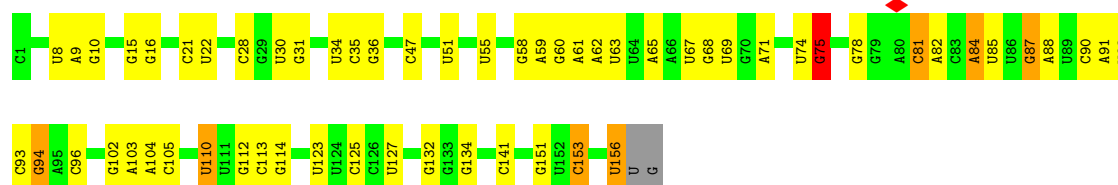
• Molecule 4: 5S rRNA

Chain L7: 70% 27%



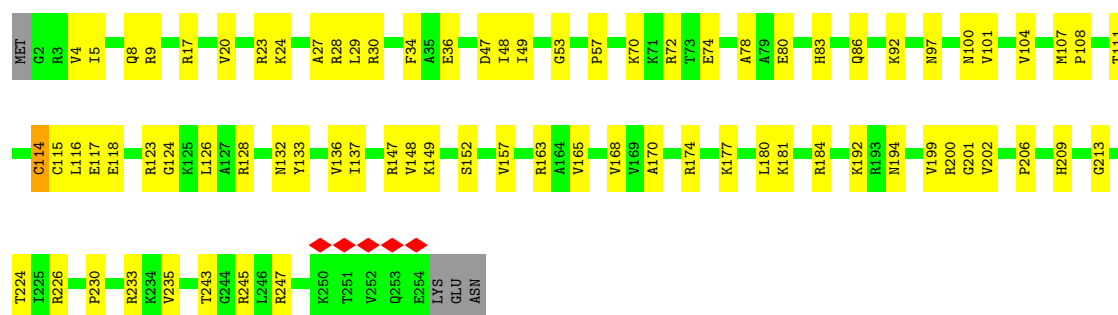
• Molecule 5: 5.8S rRNA

Chain L8: 61% 32%



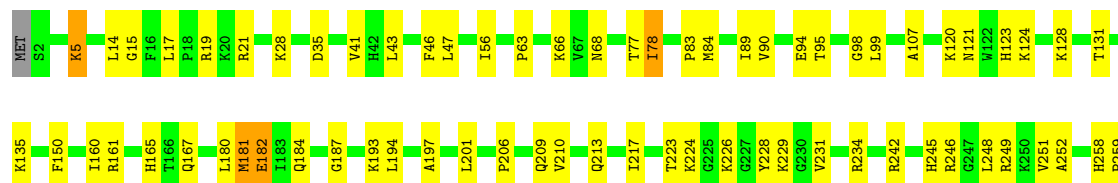
• Molecule 6: 60S ribosomal protein uL2

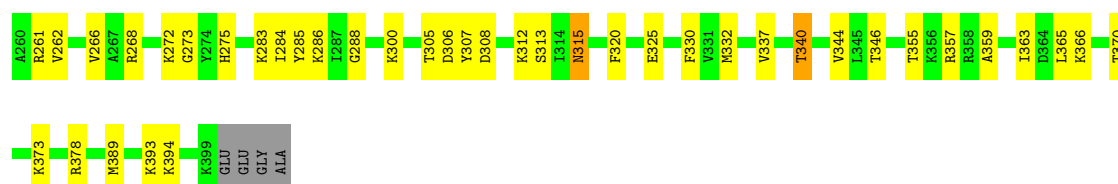
Chain LD: 68% 30%



• Molecule 7: 60S ribosomal protein uL3

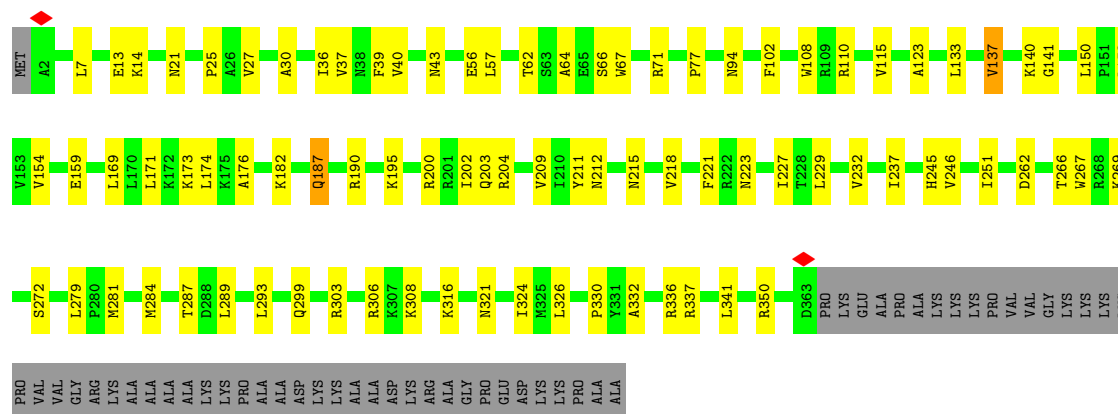
Chain LE: 72% 26%





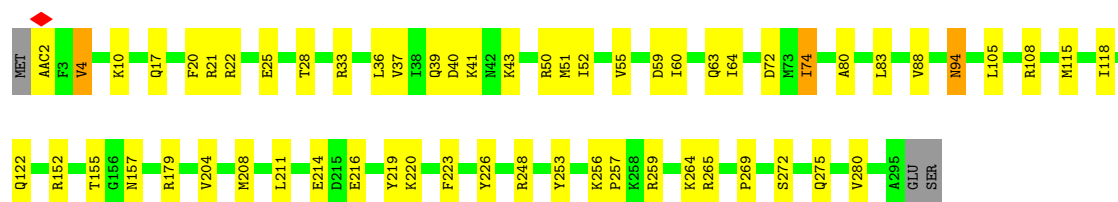
• Molecule 8: 60S ribosomal protein L4

Chain LF: 67% 20% 12%



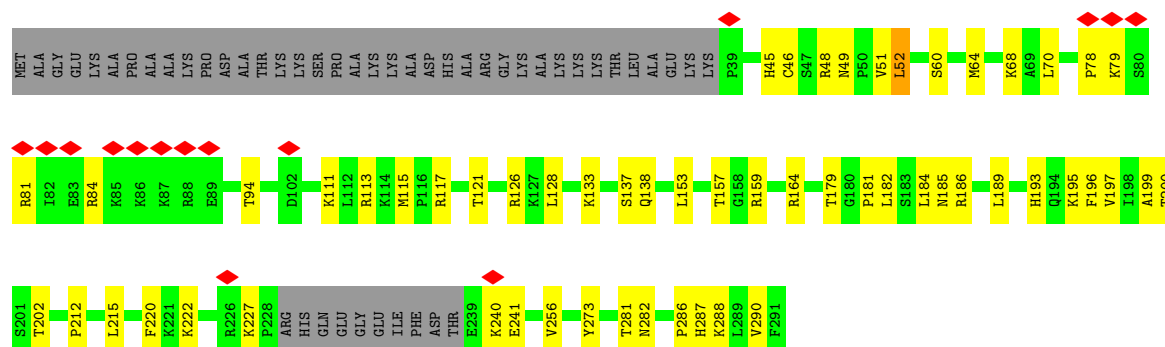
• Molecule 9: Ribosomal_L18_c domain-containing protein

Chain LG: 79% 19% ..



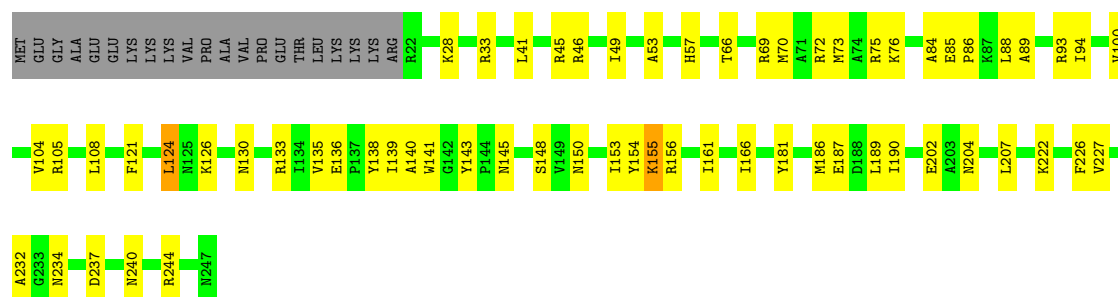
• Molecule 10: 60S ribosomal protein L6

Chain LH: 5% 64% 20% 16%



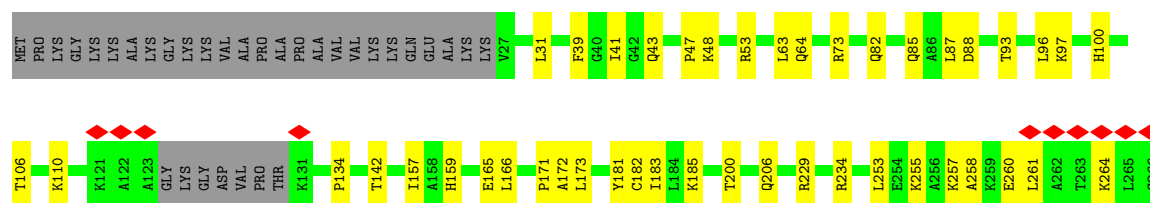
• Molecule 11: 60S ribosomal Protein uL30

Chain LI:  66% 25% 9%



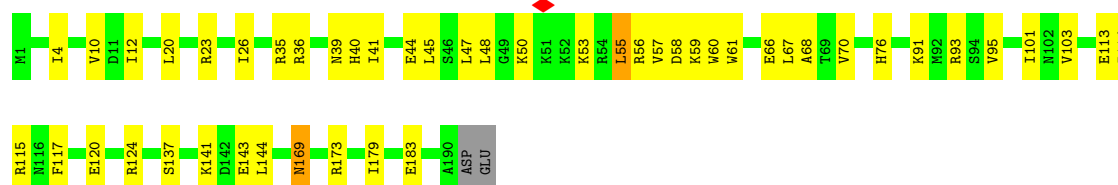
- Molecule 12: 60S ribosomal protein eL8

Chain LJ:  71% 17% 12%



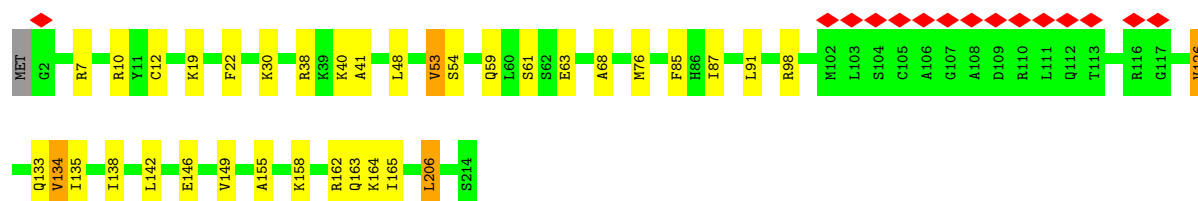
- Molecule 13: 60S ribosomal protein L9

Chain LK:  74% 24% 2%



- Molecule 14: Ribosomal protein L10

Chain LL:  7% 83% 15%



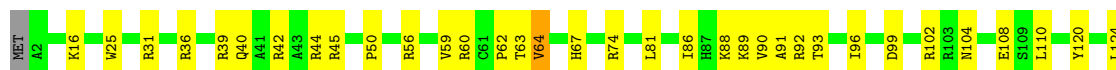
- Molecule 15: 60S ribosomal protein L11

Chain LM:  69% 27% 4%

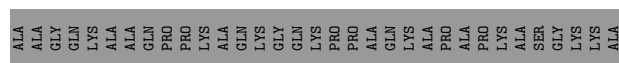
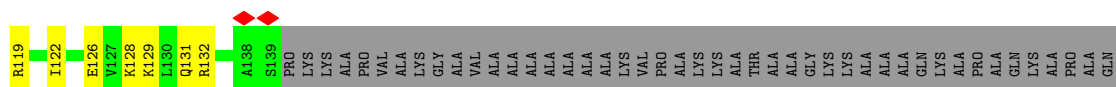




- Molecule 16: 60S ribosomal protein eL13



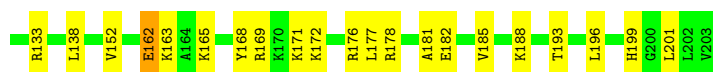
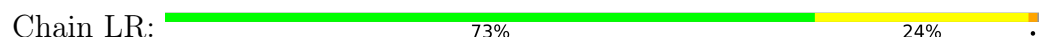
- Molecule 17: 60S ribosomal protein L14



- Molecule 18: Ribosomal protein L15

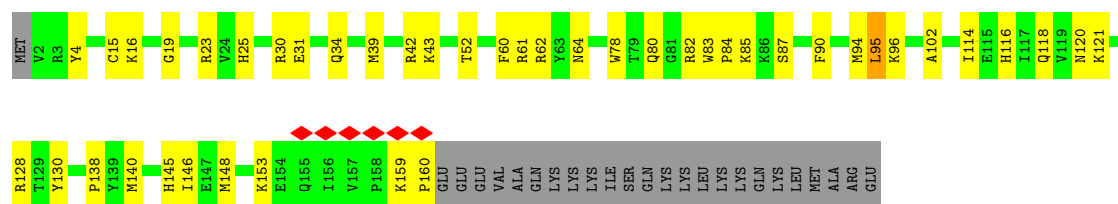


- Molecule 19: 60S ribosomal protein uL13



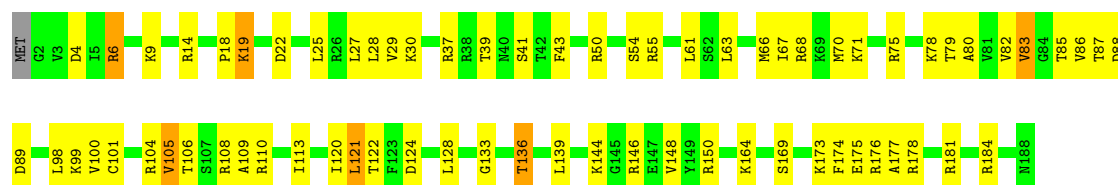
- Molecule 20: 60S ribosomal protein uL22

Chain LS:  62% 23% 14%



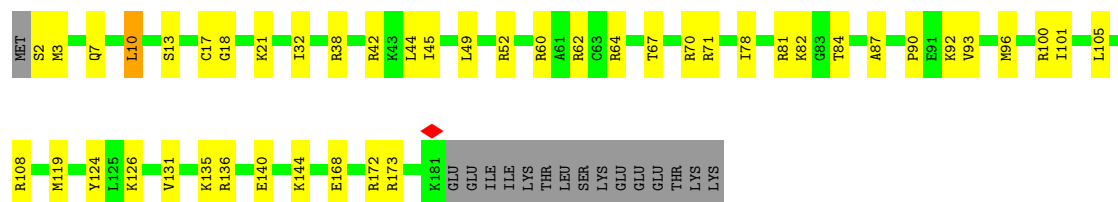
- Molecule 21: 60S ribosomal Protein eL18

Chain LT:  62% 34% 2%



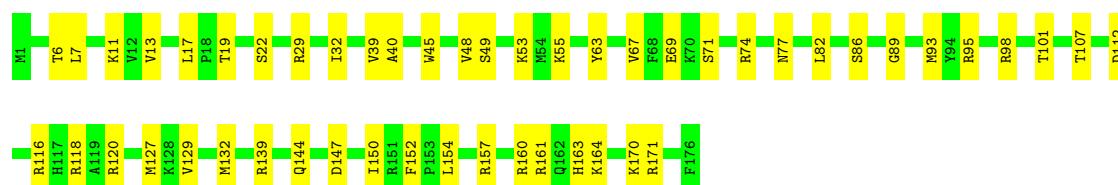
- Molecule 22: 60S ribosomal protein L19

Chain LU:  69% 22% 8%



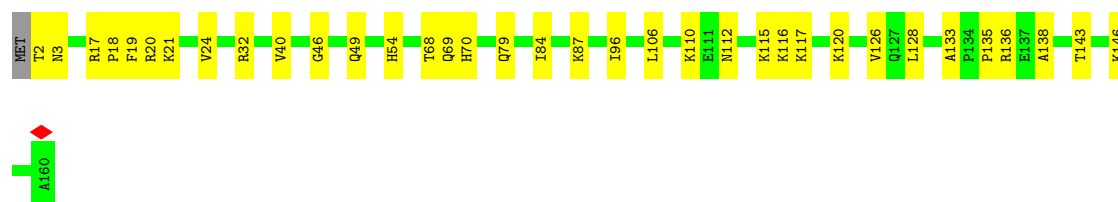
- Molecule 23: 60S ribosomal protein eL20

Chain LV:  72% 28%



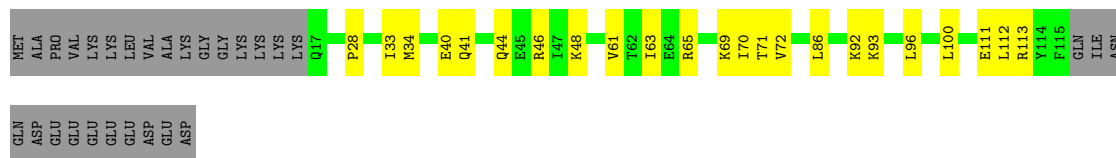
- Molecule 24: 60S ribosomal protein L21

Chain LW:  78% 22%



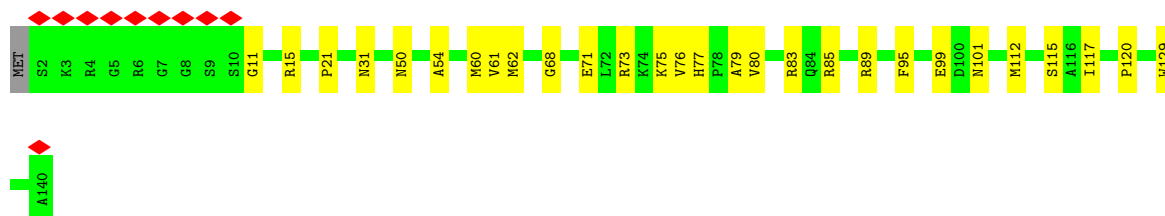
- Molecule 25: 60S ribosomal protein eL22

Chain LX:  59% 18% 23%

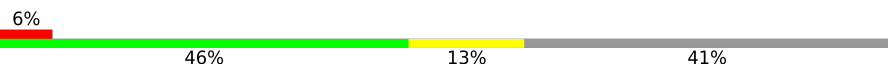


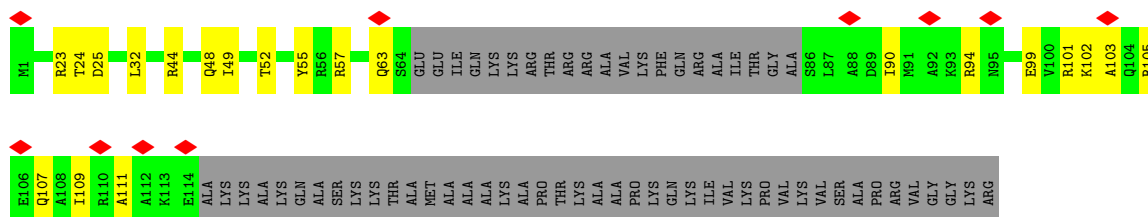
- Molecule 26: 60S ribosomal protein L23

Chain LY:  7% 79% 20%



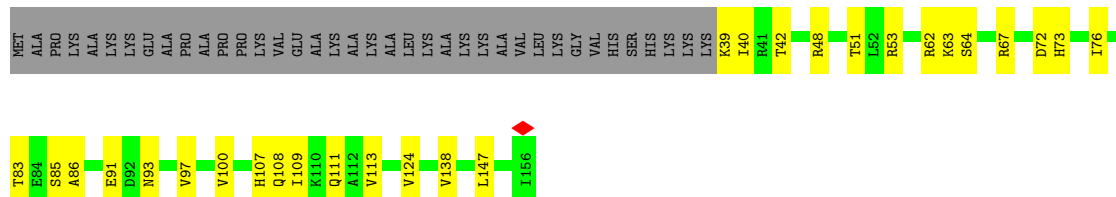
- Molecule 27: Ribosomal protein L24

Chain LZ:  6% 46% 13% 41%



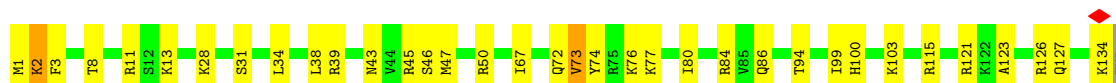
- Molecule 28: Ribosomal_L23eN domain-containing protein

Chain La:  58% 18% 24%

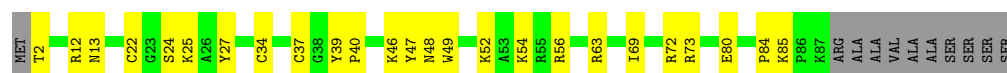


- Molecule 29: Ribosomal protein L26

Chain Lb:  68% 23% 8%



Chain Lm:  63% 26% 11%



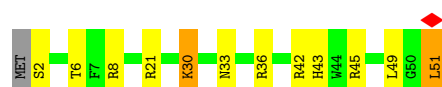
- Molecule 41: 60S ribosomal protein L38

Chain Ln:  84% 14% .



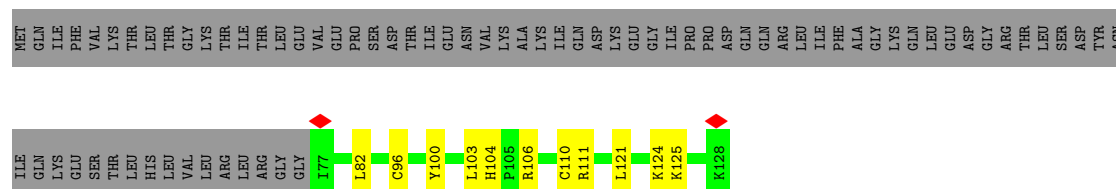
- Molecule 42: 60S ribosomal protein eL39

Chain Lo:  75% 20% . .



- Molecule 43: 60S ribosomal protein L40

Chain Lp:  32% 9% 59%



- Molecule 44: 60S ribosomal protein eL42

Chain Lq:  7% 85% 13% ..



- Molecule 45: 60S ribosomal protein eL43

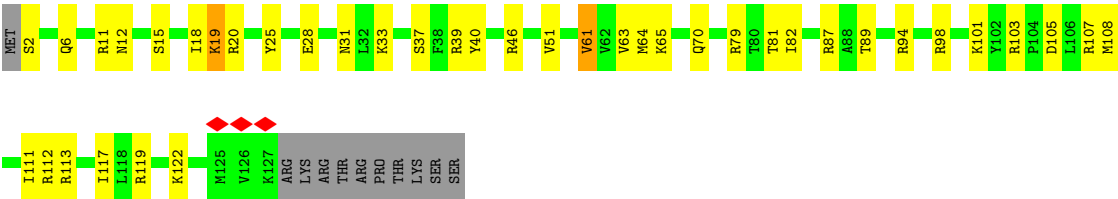
Chain Lr:  74% 24% ..



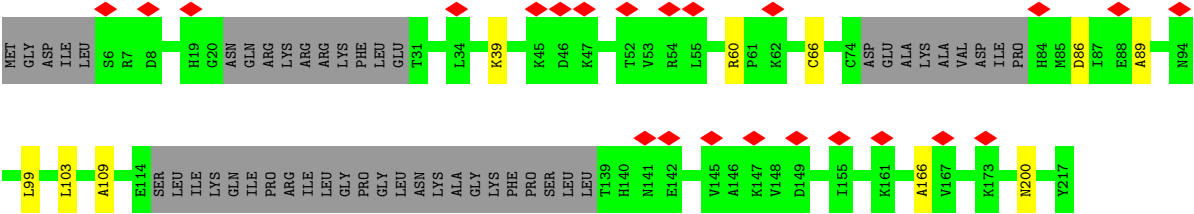
- Molecule 46: 60S ribosomal protein eL28

Chain Ls:  63% 28% . 8%

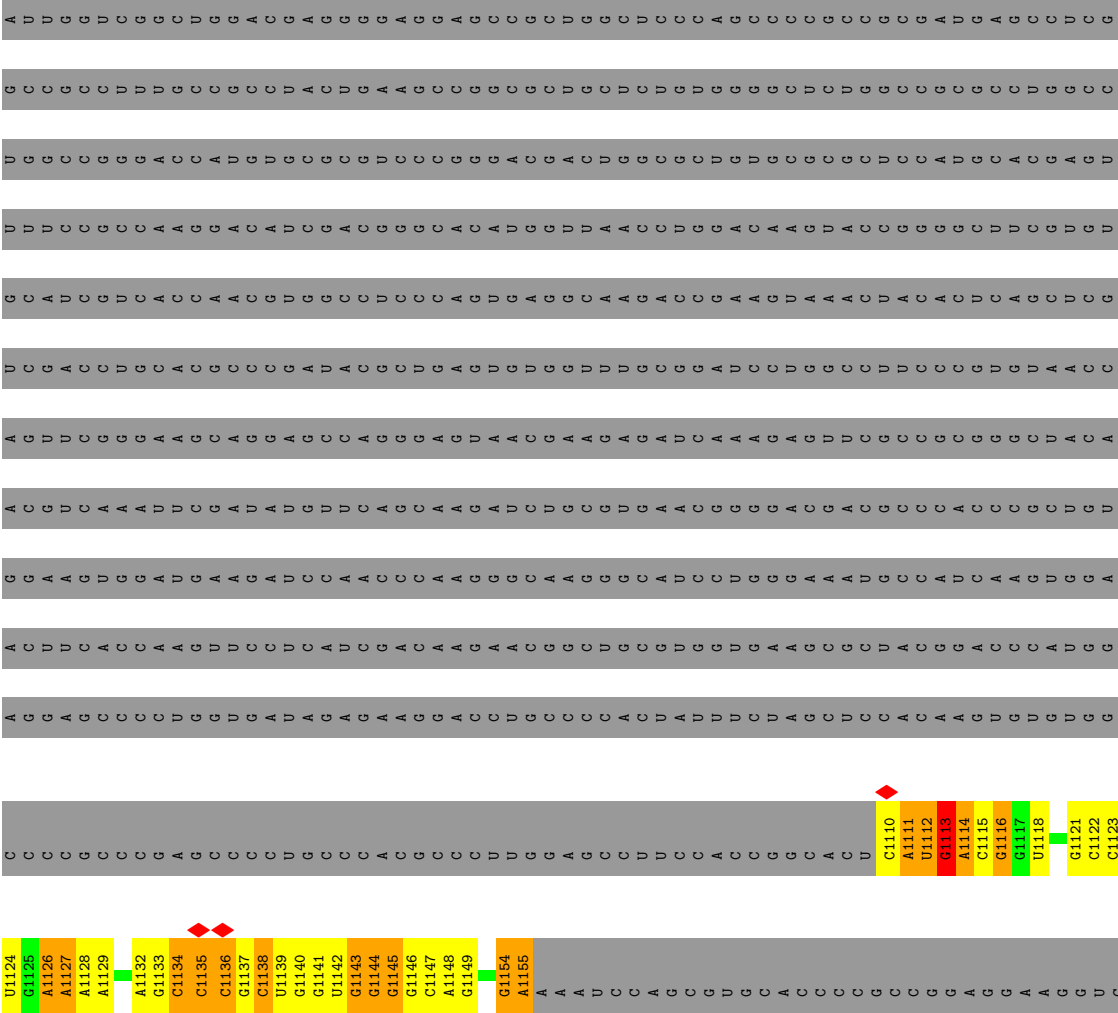




• Molecule 47: Ribosomal protein

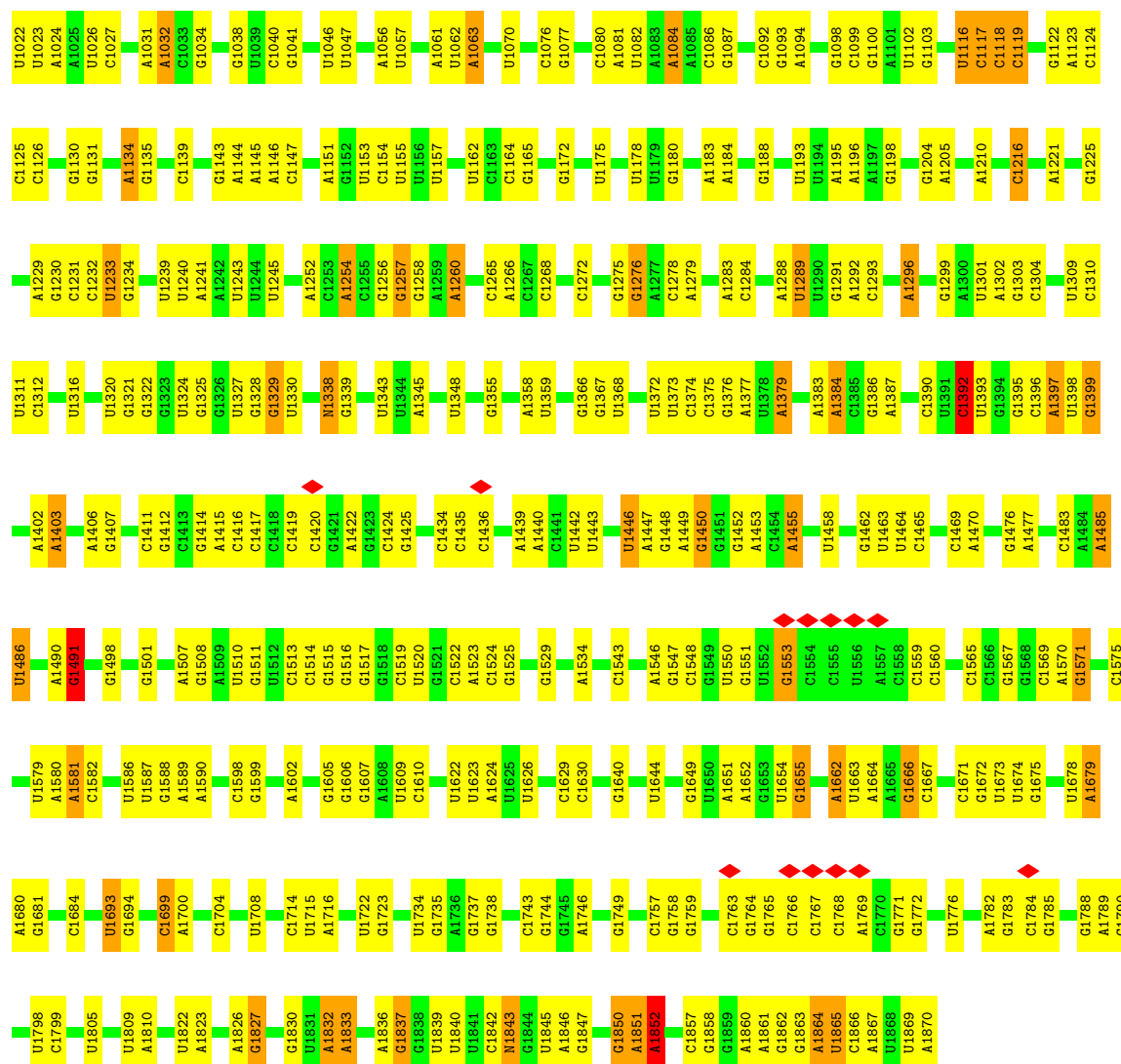


• Molecule 48: GPX4 SECIS element

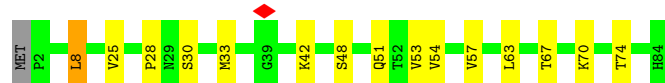
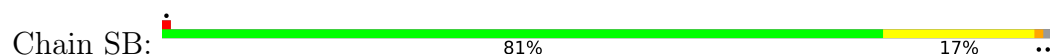


- Molecule 49: 18S rRNA

A921	A922	A923	G926	A927	C928	G929	G930	G934	G935	U944	U945	C949	G950	A956	A963	A964	U967	U969	U970	G972	A982	G983	A984	G985	G987	C990	A991	A993	G1000	U1005	C1008	U1009	A1010	G1011	A1012	A1013	G1014	U1017	U1018	U1019	A1021																																																																																																																																																																																																																																																																																																																																																																				
A827	G828	G829	C830	A831	G832	C836	G837	A838	G839	C840	C841	G842	U845	G846	G847	A848	C852	G853	G861	U864	U867	G868	G869	A870	A871	G872	G873	G874	G875	A876	G879	U886	G892	G893	U894	G895	U898	U899	U900	A909	G910	G911	A914	U915	G916	A917																																																																																																																																																																																																																																																																																																																																																															
C759	U760	C761	C762	G763	C764	U765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156



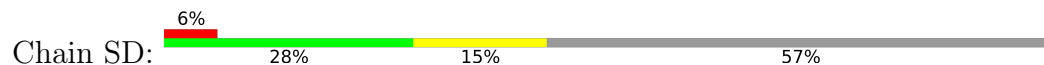
• Molecule 50: 40S ribosomal protein S27

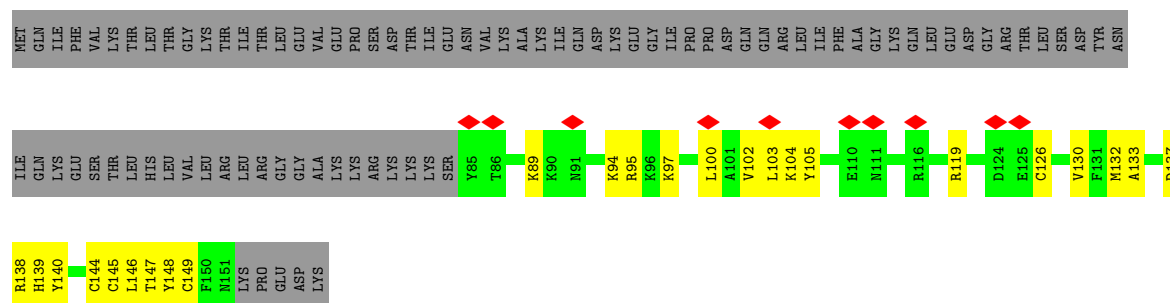


• Molecule 51: 40S ribosomal protein S28

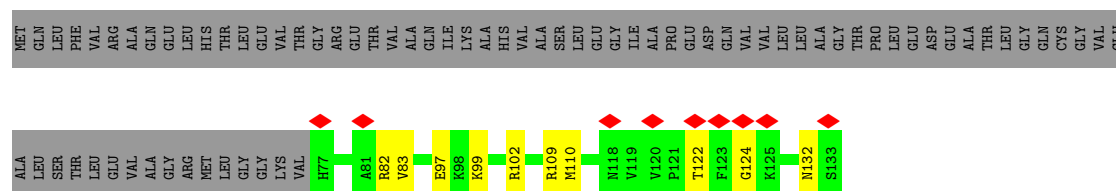
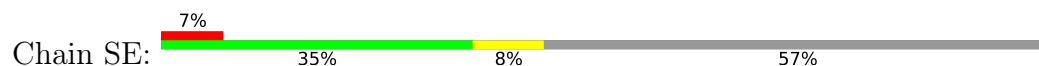


• Molecule 52: Ubiquitin carboxyl extension protein 80

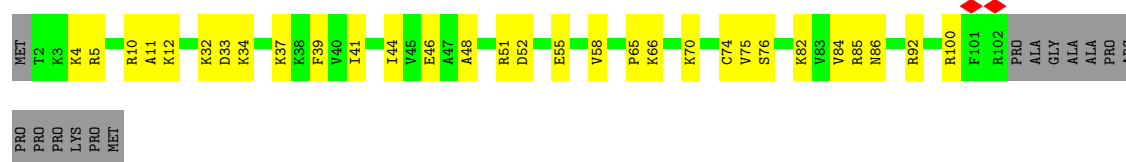




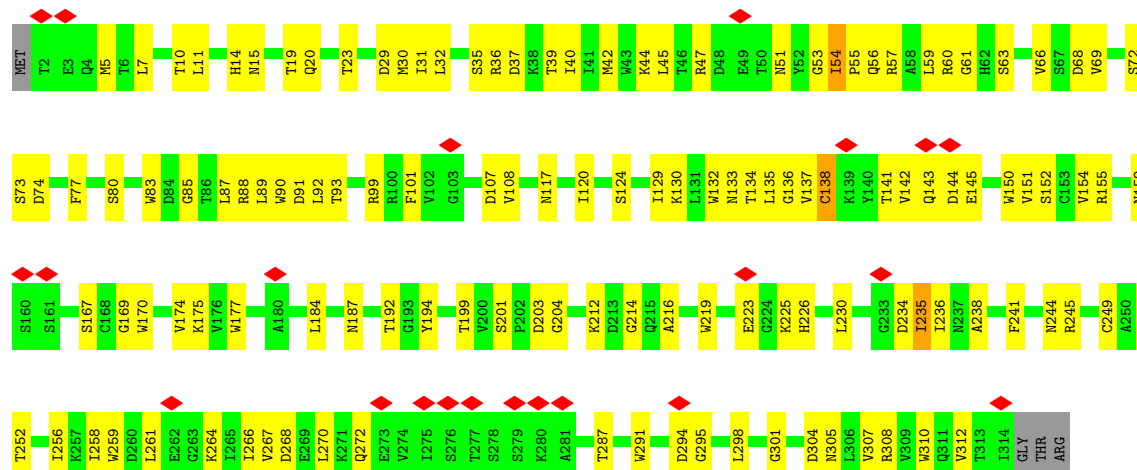
- Molecule 53: 40S ribosomal protein S30



- Molecule 54: 40S ribosomal protein eS26



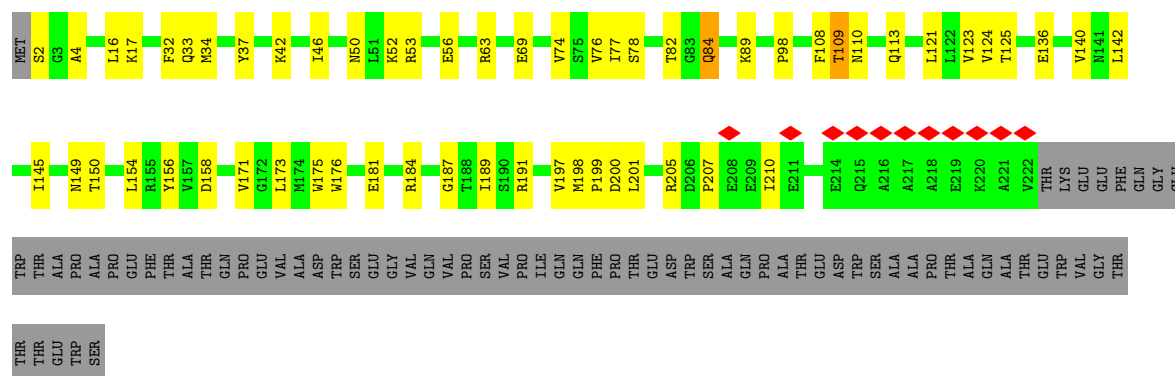
- Molecule 55: Guanine nucleotide-binding protein subunit beta-2-like 1



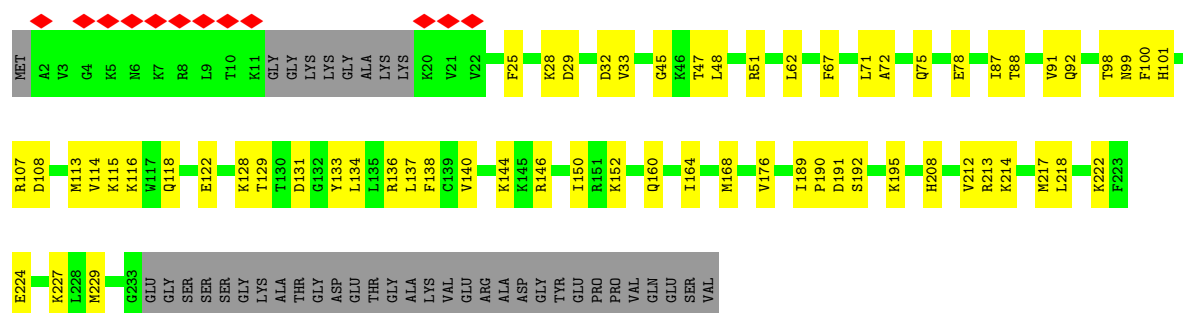
- Molecule 56: 40S ribosomal protein S29



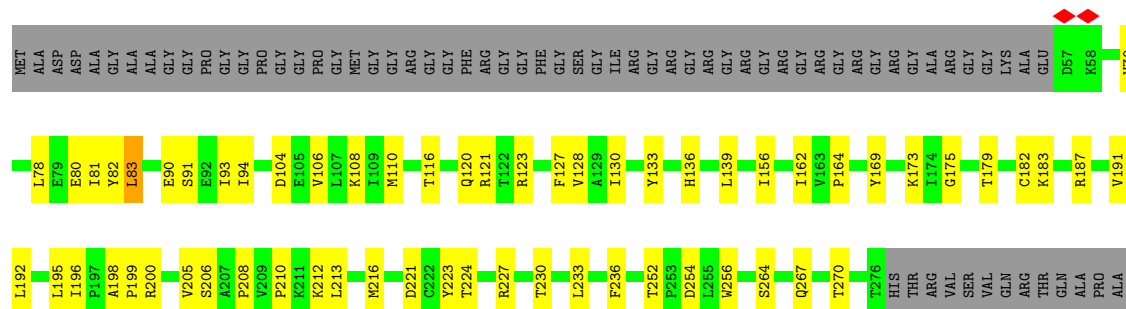
Chain SL: 55% 19% 25%



Chain SM:



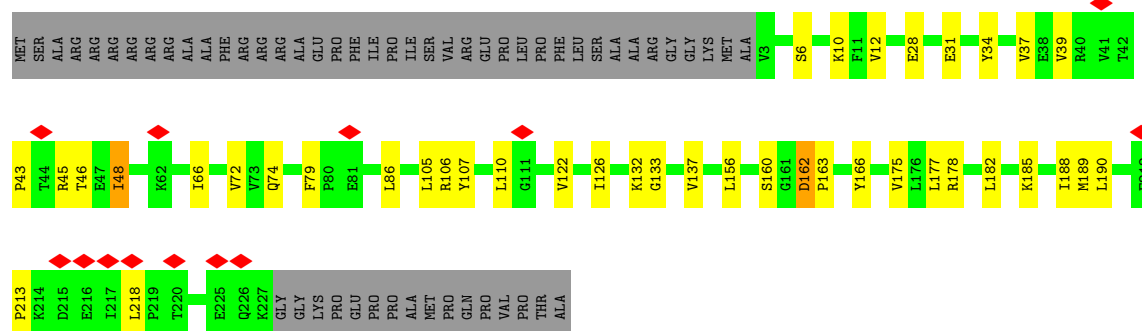
Chain SN:



VAL
ALA
THR
THR

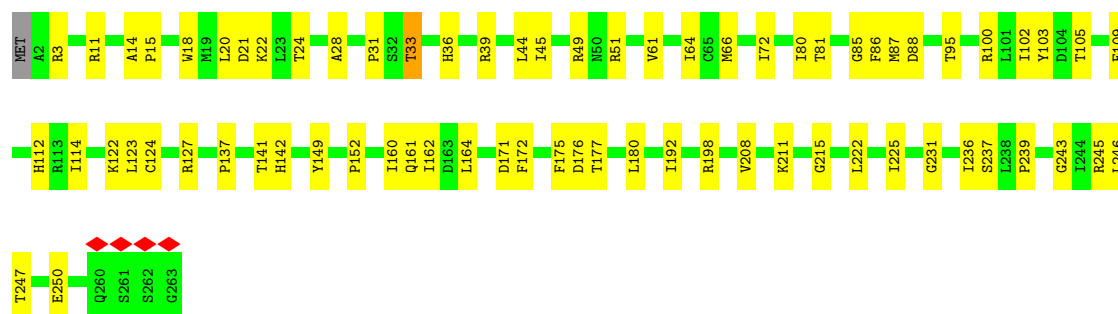
- Molecule 60: 40S ribosomal protein S3

Chain SO: 



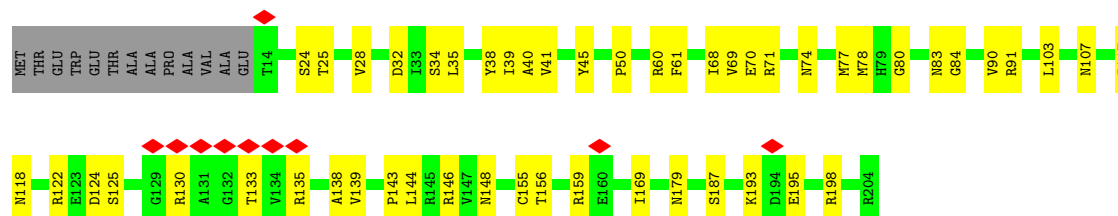
- Molecule 61: 40S ribosomal protein S4

Chain SP: 



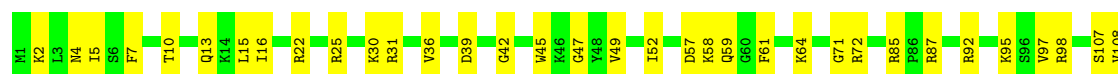
- Molecule 62: Ribosomal protein S5

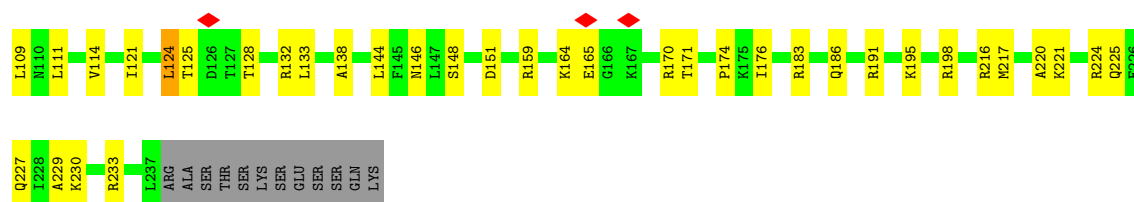
Chain SQ: 



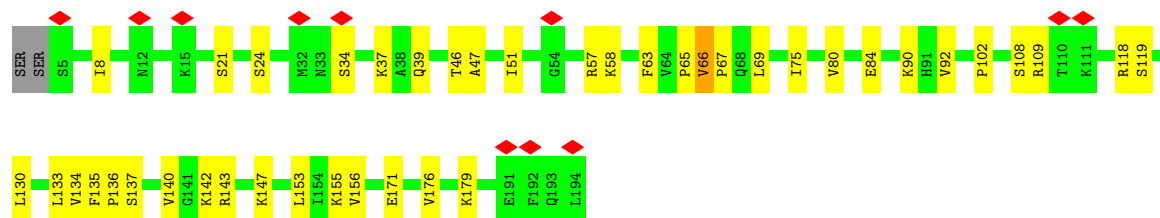
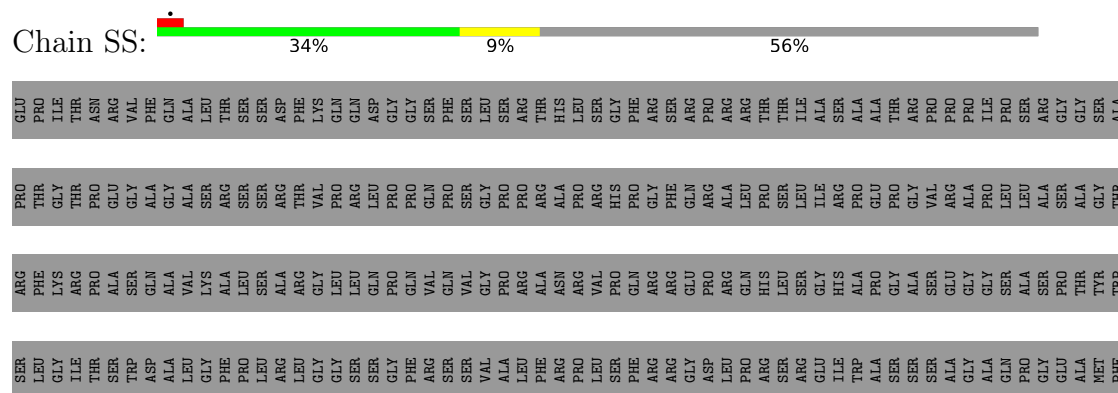
- Molecule 63: 40S ribosomal protein S6

Chain SR: 

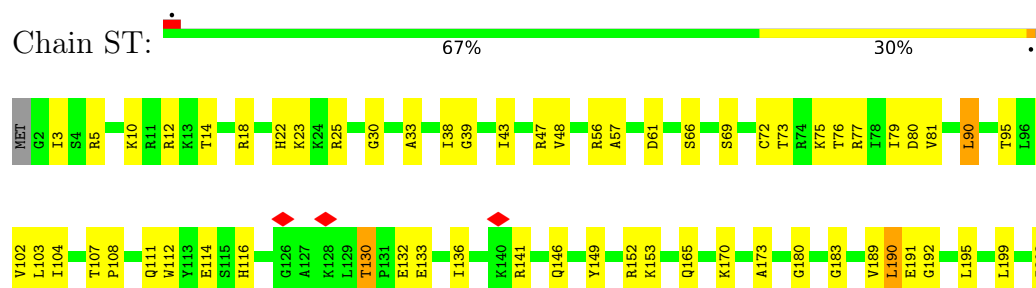




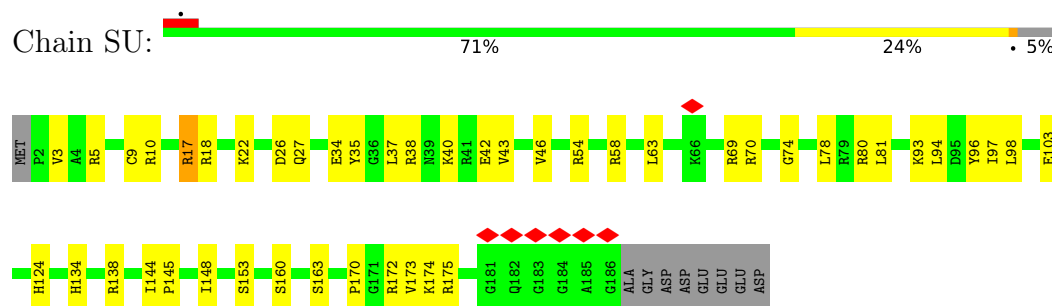
• Molecule 64: 40S ribosomal protein S7



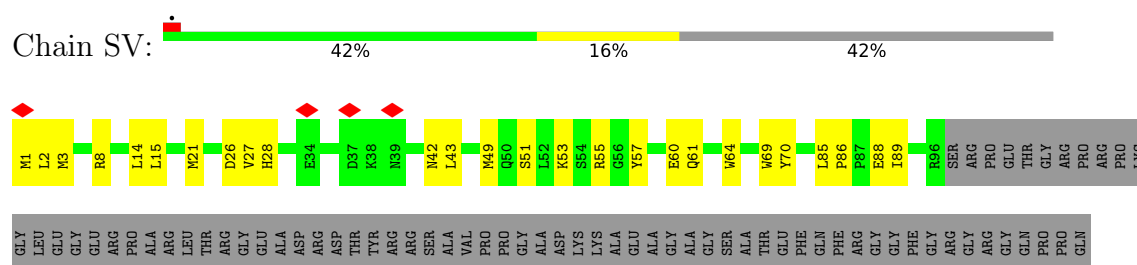
• Molecule 65: 40S ribosomal protein S8



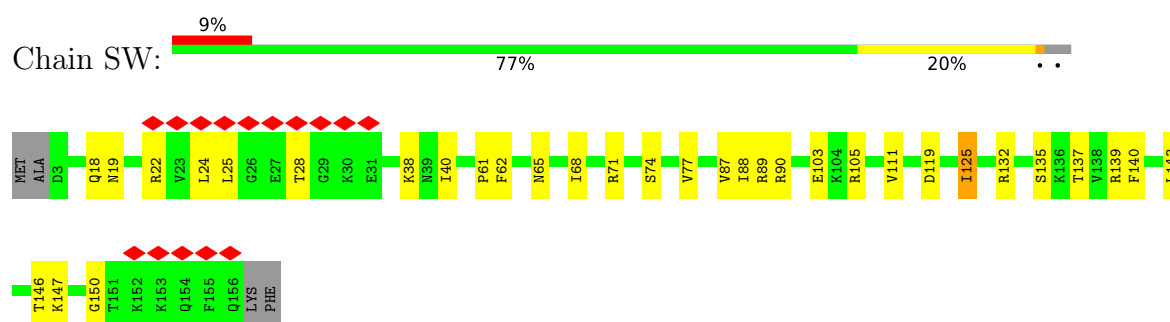
• Molecule 66: 40S ribosomal protein S9



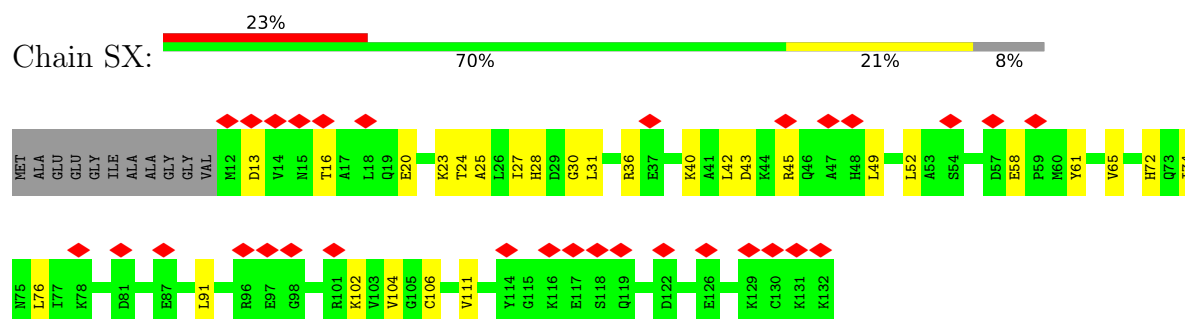
• Molecule 67: S10_ plectin domain-containing protein



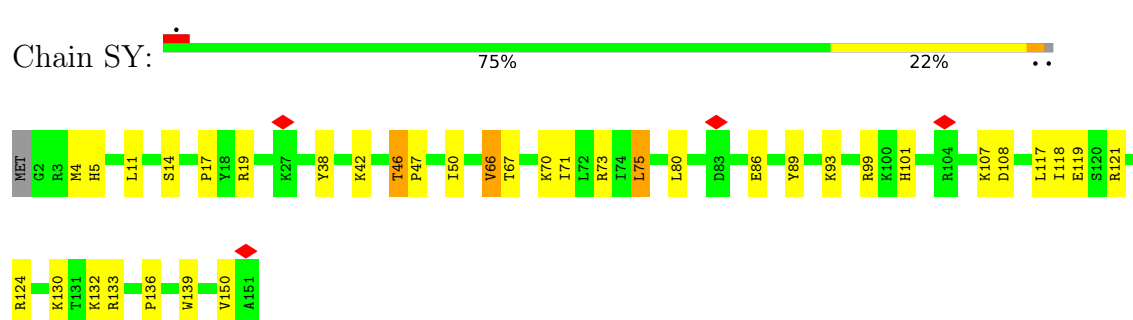
- Molecule 68: 40S ribosomal protein S11



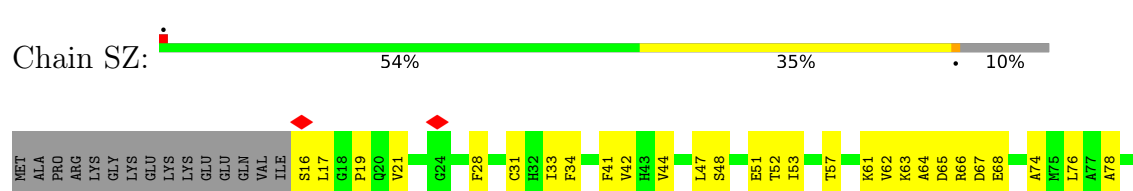
- Molecule 69: 40S ribosomal protein S12



- Molecule 70: 40S ribosomal protein S13

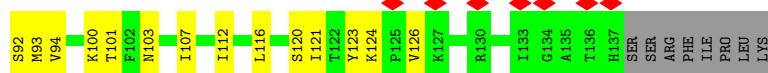
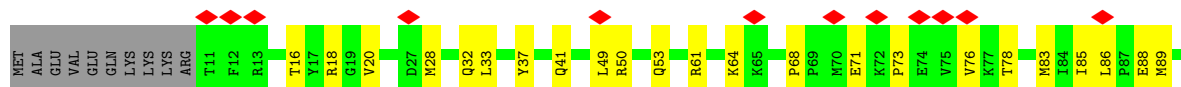


- Molecule 71: 40S ribosomal protein uS11

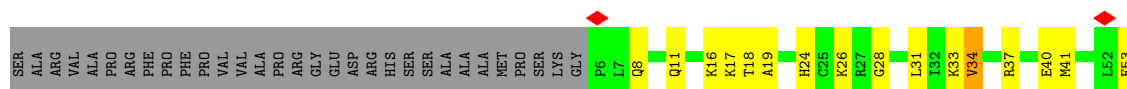




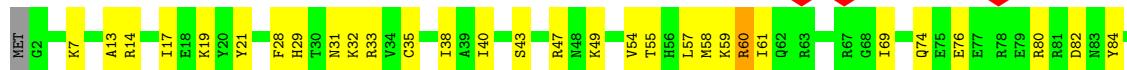
- Molecule 72: 40S ribosomal protein S15



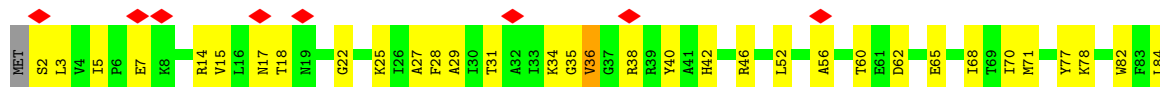
- Molecule 73: 40S ribosomal protein uS9



- Molecule 74: 40S ribosomal protein S17

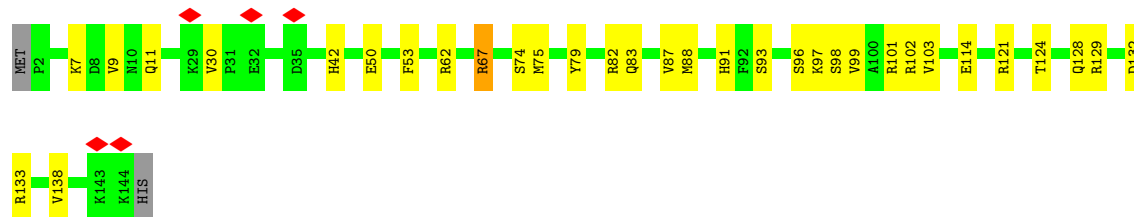


- Molecule 75: 40S ribosomal protein S18



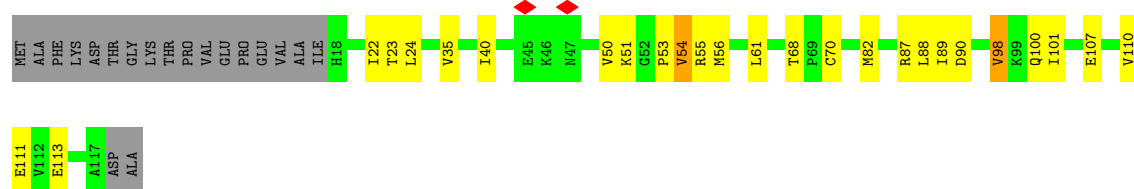
- Molecule 76: 40S Ribosomal protein eS19

Chain Se:  76% 22% ..



- Molecule 77: 40S ribosomal protein S20

Chain Sf:  62% 20% 16%



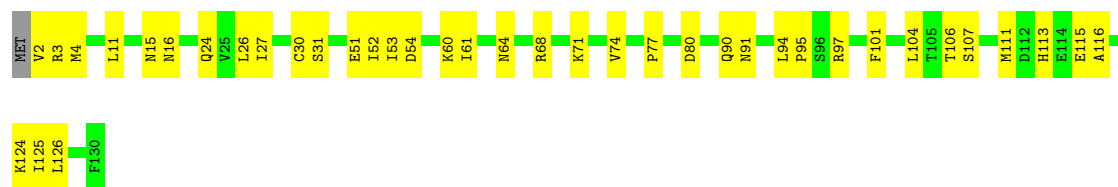
- Molecule 78: 40S ribosomal protein eS21

Chain Sg:  72% 27%



- Molecule 79: 40S ribosomal protein S15a

Chain Sh:  69% 30%



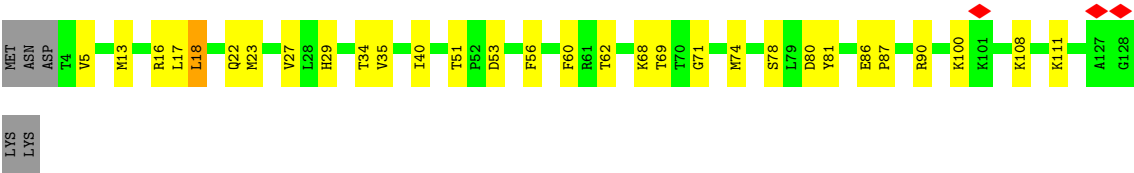
- Molecule 80: 40S ribosomal protein S23

Chain Si:  74% 23% ..

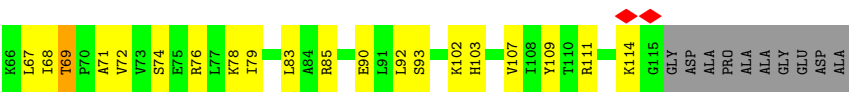
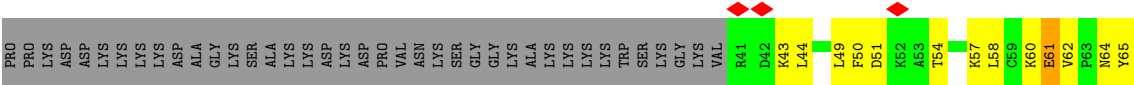
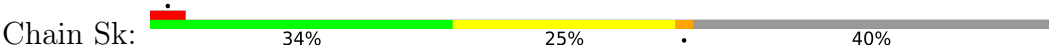


- Molecule 81: 40S ribosomal protein S24

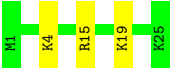
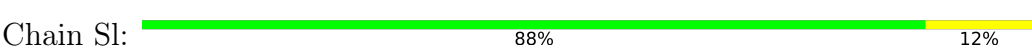
Chain Sj:  73% 22%



• Molecule 82: 40S ribosomal protein S25



• Molecule 83: 60S ribosomal protein L41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39295	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.751	Depositor
Minimum map value	0.000	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	409.2, 409.2, 409.2	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, UR3, OMU, HY3, AYA, ZN, PSU, 5MC, 7MG, A2M, AME, NMM, 6MZ, OMG, OMC, HIC, SAC, 1MA, 4AC, MLZ, M3L, GTP, AAC

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	B	0.15	0/1398	0.34	1/1905 (0.1%)
2	I	0.10	0/3847	0.30	2/5981 (0.0%)
3	L5	0.14	0/86665	0.15	0/135207
4	L7	0.13	0/2835	0.16	0/4418
5	L8	0.12	0/3635	0.14	0/5661
6	LD	0.13	0/1977	0.26	0/2651
7	LE	0.13	0/3261	0.26	0/4364
8	LF	0.13	0/2932	0.24	0/3939
9	LG	0.12	0/2437	0.25	0/3264
10	LH	0.13	0/1998	0.27	0/2673
11	LI	0.13	0/1922	0.26	0/2563
12	LJ	0.11	0/1908	0.24	0/2566
13	LK	0.12	0/1535	0.24	0/2063
14	LL	0.13	0/1756	0.26	0/2346
15	LM	0.11	0/1385	0.26	0/1852
16	LO	0.12	0/1733	0.26	0/2316
17	LP	0.12	0/1158	0.26	0/1547
18	LQ	0.14	0/1746	0.26	0/2338
19	LR	0.13	0/1662	0.24	0/2222
20	LS	0.13	0/1315	0.24	0/1763
21	LT	0.13	0/1539	0.26	0/2054
22	LU	0.11	0/1524	0.21	0/2013
23	LV	0.14	0/1497	0.26	0/2008
24	LW	0.13	0/1326	0.26	0/1770
25	LX	0.10	0/820	0.24	0/1100
26	LY	0.13	0/1048	0.27	0/1402
27	LZ	0.12	0/779	0.24	0/1034
28	La	0.11	0/984	0.23	0/1323
29	Lb	0.12	0/1132	0.25	0/1504
30	Lc	0.11	0/1130	0.21	0/1507
31	Ld	0.13	0/1188	0.27	0/1587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Le	0.11	0/884	0.23	0/1169
33	Lf	0.12	0/847	0.26	0/1134
34	Lg	0.12	0/903	0.23	0/1216
35	Lh	0.13	0/1088	0.25	0/1451
36	Li	0.14	0/903	0.26	0/1208
37	Lj	0.12	0/916	0.26	0/1220
38	Lk	0.10	0/1021	0.23	0/1348
39	Ll	0.11	0/841	0.25	0/1112
40	Lm	0.12	0/720	0.26	0/952
41	Ln	0.10	0/575	0.22	0/761
42	Lo	0.12	0/459	0.27	0/608
43	Lp	0.13	0/426	0.28	0/564
44	Lq	0.11	0/866	0.26	0/1141
45	Lr	0.13	0/718	0.27	0/953
46	Ls	0.12	0/1020	0.26	0/1366
47	Lx	0.10	0/836	0.32	0/1161
48	S	0.18	0/1098	0.40	1/1710 (0.1%)
49	S2	0.15	0/40365	0.16	0/62915
50	SB	0.11	0/665	0.27	0/891
51	SC	0.10	0/497	0.23	0/666
52	SD	0.08	0/560	0.24	0/745
53	SE	0.10	0/462	0.26	0/607
54	SF	0.11	0/828	0.23	0/1109
55	SG	0.09	0/2493	0.24	0/3394
56	SH	0.11	0/470	0.25	0/623
57	SL	0.11	0/1771	0.24	0/2406
58	SM	0.11	0/1841	0.26	0/2459
59	SN	0.11	0/1742	0.25	0/2354
60	SO	0.10	0/1779	0.25	0/2395
61	SP	0.10	0/2118	0.25	0/2849
62	SQ	0.10	0/1531	0.25	0/2059
63	SR	0.09	0/1946	0.24	0/2590
64	SS	0.09	0/1552	0.25	0/2079
65	ST	0.12	0/1715	0.24	0/2287
66	SU	0.10	0/1550	0.25	0/2069
67	SV	0.10	0/834	0.27	0/1125
68	SW	0.10	0/1284	0.25	0/1717
69	SX	0.10	0/953	0.29	0/1276
70	SY	0.11	0/1232	0.25	0/1656
71	SZ	0.11	0/1029	0.27	0/1380
72	Sa	0.09	0/1063	0.24	0/1421
73	Sb	0.10	0/1142	0.28	0/1528
74	Sc	0.10	0/1094	0.23	0/1469

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sd	0.08	0/1180	0.23	0/1581
76	Se	0.08	0/1119	0.21	0/1498
77	Sf	0.10	0/805	0.23	0/1081
78	Sg	0.13	0/636	0.24	0/852
79	Sh	0.12	0/1051	0.26	0/1406
80	Si	0.11	0/1107	0.25	0/1475
81	Sj	0.10	0/1032	0.25	0/1371
82	Sk	0.09	0/604	0.28	0/810
83	Sl	0.10	0/240	0.17	0/305
All	All	0.13	0/234483	0.20	4/344463 (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
47	Lx	0	1
80	Si	0	3
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	219	A	OP1-P-O3'	-8.72	81.84	108.00
2	I	219	A	OP2-P-O3'	-8.68	81.96	108.00
48	S	1113	G	C5'-C4'-C3'	8.21	127.51	115.20
1	B	704	LYS	CB-CA-C	-5.27	110.48	116.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	Lx	60	ARG	Peptide
80	Si	61	GLN	Peptide,Mainchain
80	Si	62	HY3	Mainchain

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	B	1379	0	1207	78	0
2	I	3447	0	1741	75	0
3	L5	80089	0	40554	964	0
4	L7	2570	0	1295	26	0
5	L8	3319	0	1684	46	0
6	LD	1939	0	2036	59	0
7	LE	3206	0	3353	91	0
8	LF	2886	0	3057	65	0
9	LG	2398	0	2430	46	0
10	LH	1960	0	2153	47	0
11	LI	1886	0	2008	50	0
12	LJ	1877	0	2023	30	0
13	LK	1516	0	1597	35	0
14	LL	1717	0	1764	28	0
15	LM	1362	0	1399	34	0
16	LO	1702	0	1820	45	0
17	LP	1137	0	1211	38	0
18	LQ	1701	0	1749	51	0
19	LR	1630	0	1777	47	0
20	LS	1288	0	1326	31	0
21	LT	1515	0	1634	55	0
22	LU	1508	0	1664	39	0
23	LV	1457	0	1492	34	0
24	LW	1298	0	1366	29	0
25	LX	806	0	827	15	0
26	LY	1034	0	1097	18	0
27	LZ	766	0	794	19	0
28	La	967	0	1040	20	0
29	Lb	1115	0	1205	28	0
30	Lc	1107	0	1182	19	0
31	Ld	1159	0	1202	38	0
32	Le	881	0	957	33	0
33	Lf	836	0	888	14	0
34	Lg	888	0	930	16	0
35	Lh	1070	0	1165	34	0
36	Li	884	0	924	18	0
37	Lj	906	0	998	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Lk	1013	0	1147	31	0
39	Ll	830	0	916	20	0
40	Lm	705	0	737	25	0
41	Ln	569	0	637	6	0
42	Lo	447	0	480	15	0
43	Lp	432	0	470	11	0
44	Lq	863	0	927	12	0
45	Lr	708	0	756	20	0
46	Ls	1014	0	1083	28	0
47	Lx	840	0	365	6	0
48	S	983	0	499	32	0
49	S2	37825	0	19178	490	0
50	SB	651	0	672	9	0
51	SC	495	0	523	13	0
52	SD	548	0	554	50	0
53	SE	457	0	502	8	0
54	SF	814	0	863	25	0
55	SG	2436	0	2393	95	0
56	SH	459	0	449	15	0
57	SL	1743	0	1748	43	0
58	SM	1815	0	1908	45	0
59	SN	1706	0	1796	39	0
60	SO	1751	0	1846	28	0
61	SP	2076	0	2177	50	0
62	SQ	1509	0	1563	42	0
63	SR	1923	0	2089	51	0
64	SS	1529	0	1627	27	0
65	ST	1686	0	1772	47	0
66	SU	1525	0	1640	38	0
67	SV	810	0	836	17	0
68	SW	1262	0	1335	23	0
69	SX	943	0	978	17	0
70	SY	1208	0	1294	25	0
71	SZ	1016	0	1039	36	0
72	Sa	1042	0	1088	23	0
73	Sb	1124	0	1193	28	0
74	Sc	1080	0	1135	38	0
75	Sd	1171	0	1230	33	0
76	Se	1113	0	1145	33	0
77	Sf	795	0	862	15	0
78	Sg	640	0	632	20	0
79	Sh	1034	0	1080	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Si	1099	0	1162	26	0
81	Sj	1015	0	1086	23	0
82	Sk	598	0	656	24	0
83	Sl	239	0	289	3	0
84	Lj	1	0	0	0	0
84	Lm	1	0	0	0	0
84	Lp	1	0	0	0	0
84	Lq	1	0	0	0	0
84	Lr	1	0	0	0	0
84	SD	1	0	0	0	0
84	SF	1	0	0	0	0
84	SH	1	0	0	0	0
All	All	222755	0	163906	3197	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 3197 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)
1:B:448:VAL:HG22	52:SD:148:TYR:CB	1.57	1.33
1:B:448:VAL:CG2	52:SD:148:TYR:HB3	1.64	1.28
1:B:658:ARG:HH12	49:S2:1575:C:P	1.61	1.24
1:B:446:LEU:HD21	52:SD:146:LEU:HD23	1.17	1.17
1:B:446:LEU:HD21	52:SD:146:LEU:CD2	1.78	1.11

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	B	200/854 (23%)	171 (86%)	28 (14%)	1 (0%)	24	57
6	LD	251/257 (98%)	238 (95%)	13 (5%)	0	100	100
7	LE	395/403 (98%)	386 (98%)	9 (2%)	0	100	100
8	LF	360/413 (87%)	354 (98%)	6 (2%)	0	100	100
9	LG	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
10	LH	239/291 (82%)	231 (97%)	8 (3%)	0	100	100
11	LI	224/247 (91%)	218 (97%)	6 (3%)	0	100	100
12	LJ	229/266 (86%)	228 (100%)	1 (0%)	0	100	100
13	LK	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
14	LL	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
15	LM	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
16	LO	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
17	LP	136/218 (62%)	133 (98%)	3 (2%)	0	100	100
18	LQ	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
19	LR	197/203 (97%)	197 (100%)	0	0	100	100
20	LS	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
21	LT	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
22	LU	178/196 (91%)	178 (100%)	0	0	100	100
23	LV	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
24	LW	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
25	LX	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
26	LY	137/140 (98%)	137 (100%)	0	0	100	100
27	LZ	89/157 (57%)	89 (100%)	0	0	100	100
28	La	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
29	Lb	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
30	Lc	133/136 (98%)	133 (100%)	0	0	100	100
31	Ld	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	18	49
32	Le	103/245 (42%)	98 (95%)	5 (5%)	0	100	100
33	Lf	106/115 (92%)	106 (100%)	0	0	100	100
34	Lg	105/125 (84%)	105 (100%)	0	0	100	100
35	Lh	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
36	Li	108/110 (98%)	108 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Lj	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
38	Lk	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
39	Ll	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
40	Lm	84/97 (87%)	84 (100%)	0	0	100	100
41	Ln	67/70 (96%)	67 (100%)	0	0	100	100
42	Lo	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	Lp	49/128 (38%)	49 (100%)	0	0	100	100
44	Lq	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
45	Lr	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
46	Ls	124/137 (90%)	121 (98%)	3 (2%)	0	100	100
47	Lx	161/217 (74%)	143 (89%)	18 (11%)	0	100	100
50	SB	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
51	SC	61/69 (88%)	61 (100%)	0	0	100	100
52	SD	65/156 (42%)	64 (98%)	1 (2%)	0	100	100
53	SE	55/133 (41%)	55 (100%)	0	0	100	100
54	SF	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
55	SG	311/317 (98%)	300 (96%)	11 (4%)	0	100	100
56	SH	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
57	SL	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
58	SM	220/264 (83%)	216 (98%)	4 (2%)	0	100	100
59	SN	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
60	SO	223/281 (79%)	220 (99%)	3 (1%)	0	100	100
61	SP	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
62	SQ	189/204 (93%)	183 (97%)	6 (3%)	0	100	100
63	SR	235/249 (94%)	233 (99%)	2 (1%)	0	100	100
64	SS	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
65	ST	204/208 (98%)	203 (100%)	1 (0%)	0	100	100
66	SU	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
67	SV	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
68	SW	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
69	SX	119/132 (90%)	115 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	SY	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
71	SZ	134/151 (89%)	128 (96%)	6 (4%)	0	100	100
72	Sa	125/145 (86%)	124 (99%)	1 (1%)	0	100	100
73	Sb	139/172 (81%)	132 (95%)	7 (5%)	0	100	100
74	Sc	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
75	Sd	139/152 (91%)	136 (98%)	3 (2%)	0	100	100
76	Se	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
77	Sf	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
78	Sg	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
79	Sh	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
80	Si	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
81	Sj	123/130 (95%)	123 (100%)	0	0	100	100
82	Sk	73/124 (59%)	71 (97%)	2 (3%)	0	100	100
83	Sl	23/25 (92%)	23 (100%)	0	0	100	100
All	All	11653/14208 (82%)	11397 (98%)	254 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	703	SER
31	Ld	15	VAL

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	B	102/761 (13%)	99 (97%)	3 (3%)	37	66
6	LD	195/199 (98%)	192 (98%)	3 (2%)	57	75
7	LE	344/347 (99%)	334 (97%)	10 (3%)	37	66
8	LF	302/337 (90%)	297 (98%)	5 (2%)	53	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	LG	247/250 (99%)	242 (98%)	5 (2%)	48	72
10	LH	216/251 (86%)	212 (98%)	4 (2%)	50	73
11	LI	197/215 (92%)	193 (98%)	4 (2%)	48	72
12	LJ	199/223 (89%)	196 (98%)	3 (2%)	57	75
13	LK	169/171 (99%)	166 (98%)	3 (2%)	51	73
14	LL	180/181 (99%)	176 (98%)	4 (2%)	45	71
15	LM	143/149 (96%)	142 (99%)	1 (1%)	76	82
16	LO	175/176 (99%)	171 (98%)	4 (2%)	44	70
17	LP	117/161 (73%)	115 (98%)	2 (2%)	53	74
18	LQ	171/172 (99%)	168 (98%)	3 (2%)	51	73
19	LR	171/173 (99%)	167 (98%)	4 (2%)	44	70
20	LS	139/163 (85%)	138 (99%)	1 (1%)	76	82
21	LT	164/165 (99%)	155 (94%)	9 (6%)	19	50
22	LU	159/175 (91%)	158 (99%)	1 (1%)	78	83
23	LV	154/154 (100%)	149 (97%)	5 (3%)	34	64
24	LW	139/140 (99%)	139 (100%)	0	100	100
25	LX	88/113 (78%)	87 (99%)	1 (1%)	65	78
26	LY	106/107 (99%)	105 (99%)	1 (1%)	70	80
27	LZ	79/126 (63%)	79 (100%)	0	100	100
28	La	106/134 (79%)	104 (98%)	2 (2%)	50	73
29	Lb	124/135 (92%)	122 (98%)	2 (2%)	55	75
30	Lc	117/118 (99%)	115 (98%)	2 (2%)	53	74
31	Ld	118/120 (98%)	113 (96%)	5 (4%)	26	58
32	Le	87/183 (48%)	84 (97%)	3 (3%)	32	63
33	Lf	92/98 (94%)	89 (97%)	3 (3%)	33	63
34	Lg	98/110 (89%)	93 (95%)	5 (5%)	21	52
35	Lh	116/121 (96%)	112 (97%)	4 (3%)	32	63
36	Li	89/89 (100%)	89 (100%)	0	100	100
37	Lj	98/100 (98%)	97 (99%)	1 (1%)	68	79
38	Lk	109/110 (99%)	106 (97%)	3 (3%)	38	66
39	Ll	86/89 (97%)	83 (96%)	3 (4%)	32	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	Lm	73/80 (91%)	73 (100%)	0	100	100
41	Ln	64/65 (98%)	62 (97%)	2 (3%)	35	64
42	Lo	47/48 (98%)	44 (94%)	3 (6%)	16	44
43	Lp	47/115 (41%)	47 (100%)	0	100	100
44	Lq	92/93 (99%)	91 (99%)	1 (1%)	65	78
45	Lr	74/75 (99%)	72 (97%)	2 (3%)	39	67
46	Ls	109/120 (91%)	106 (97%)	3 (3%)	38	66
50	SB	75/76 (99%)	72 (96%)	3 (4%)	28	60
51	SC	56/62 (90%)	56 (100%)	0	100	100
52	SD	60/140 (43%)	60 (100%)	0	100	100
53	SE	47/106 (44%)	46 (98%)	1 (2%)	47	71
54	SF	88/98 (90%)	87 (99%)	1 (1%)	65	78
55	SG	272/275 (99%)	267 (98%)	5 (2%)	51	73
56	SH	48/49 (98%)	48 (100%)	0	100	100
57	SL	182/243 (75%)	179 (98%)	3 (2%)	55	75
58	SM	203/231 (88%)	199 (98%)	4 (2%)	48	72
59	SN	185/223 (83%)	182 (98%)	3 (2%)	55	75
60	SO	189/232 (82%)	186 (98%)	3 (2%)	55	75
61	SP	224/225 (100%)	222 (99%)	2 (1%)	70	80
62	SQ	161/170 (95%)	159 (99%)	2 (1%)	63	78
63	SR	207/218 (95%)	206 (100%)	1 (0%)	81	85
64	SS	170/360 (47%)	167 (98%)	3 (2%)	51	73
65	ST	178/180 (99%)	174 (98%)	4 (2%)	45	71
66	SU	161/168 (96%)	160 (99%)	1 (1%)	78	83
67	SV	87/136 (64%)	86 (99%)	1 (1%)	65	78
68	SW	139/142 (98%)	137 (99%)	2 (1%)	59	76
69	SX	103/108 (95%)	101 (98%)	2 (2%)	50	73
70	SY	130/131 (99%)	125 (96%)	5 (4%)	29	60
71	SZ	106/119 (89%)	101 (95%)	5 (5%)	23	55
72	Sa	113/130 (87%)	110 (97%)	3 (3%)	39	67
73	Sb	117/140 (84%)	115 (98%)	2 (2%)	53	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	Sc	120/121 (99%)	116 (97%)	4 (3%)	33	63
75	Sd	122/131 (93%)	119 (98%)	3 (2%)	42	69
76	Se	112/114 (98%)	111 (99%)	1 (1%)	70	80
77	Sf	92/107 (86%)	89 (97%)	3 (3%)	33	63
78	Sg	67/67 (100%)	63 (94%)	4 (6%)	17	47
79	Sh	112/113 (99%)	109 (97%)	3 (3%)	39	67
80	Si	112/114 (98%)	109 (97%)	3 (3%)	39	67
81	Sj	107/112 (96%)	105 (98%)	2 (2%)	50	73
82	Sk	66/102 (65%)	63 (96%)	3 (4%)	24	56
83	Sl	24/24 (100%)	24 (100%)	0	100	100
All	All	9937/11879 (84%)	9735 (98%)	202 (2%)	48	72

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	Lr	52	VAL
61	SP	33	THR
82	Sk	61	GLU
46	Ls	113	ARG
57	SL	84	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
62	SQ	118	ASN
75	Sd	42	HIS
63	SR	65	GLN
68	SW	11	GLN
79	Sh	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	160/163 (98%)	90 (56%)	6 (3%)
3	L5	3719/4808 (77%)	532 (14%)	3 (0%)
4	L7	118/120 (98%)	8 (6%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
48	S	45/855 (5%)	19 (42%)	4 (8%)
49	S2	1764/1870 (94%)	244 (13%)	2 (0%)
5	L8	155/158 (98%)	18 (11%)	0
All	All	5961/7974 (74%)	911 (15%)	15 (0%)

5 of 911 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	33	A
2	I	37	U
2	I	39	A
2	I	44	G
2	I	46	U

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	3549	A
49	S2	191	A
3	L5	4445	U
49	S2	1485	A
48	S	1113	G

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

219 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	PSU	S2	36	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	5 (22%)
49	A2M	S2	1679	49	22,25,26	1.73	6 (27%)	31,36,39	2.43	15 (48%)
3	PSU	L5	3583	3	18,21,22	1.39	3 (16%)	22,30,33	1.82	4 (18%)
3	A2M	L5	4269	3	22,25,26	1.72	7 (31%)	31,36,39	2.48	15 (48%)
3	PSU	L5	3494	3	18,21,22	1.42	3 (16%)	22,30,33	1.80	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3616	3	18,21,22	1.38	3 (16%)	22,30,33	1.90	5 (22%)
3	PSU	L5	4169	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	3447	3	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
3	A2M	L5	1270	3	22,25,26	1.73	7 (31%)	31,36,39	2.48	15 (48%)
3	PSU	L5	4058	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	5 (22%)
49	PSU	S2	1245	49	18,21,22	1.42	3 (16%)	22,30,33	1.80	4 (18%)
49	A2M	S2	159	49	22,25,26	1.69	6 (27%)	31,36,39	2.42	14 (45%)
49	A2M	S2	577	49	22,25,26	1.71	7 (31%)	31,36,39	2.42	14 (45%)
3	OMG	L5	3476	3	23,26,27	1.18	2 (8%)	33,38,41	1.90	9 (27%)
3	PSU	L5	4322	3	18,21,22	1.39	3 (16%)	22,30,33	1.85	4 (18%)
49	PSU	S2	407	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
3	OMG	L5	4383	3	23,26,27	1.19	3 (13%)	33,38,41	1.90	9 (27%)
3	OMU	L5	3973	3	19,22,23	1.00	2 (10%)	26,31,34	1.83	6 (23%)
3	OMG	L5	3942	3	23,26,27	1.17	2 (8%)	33,38,41	1.89	9 (27%)
49	A2M	S2	1384	49	22,25,26	1.72	6 (27%)	31,36,39	2.45	13 (41%)
3	OMC	L5	2667	3	19,22,23	1.17	2 (10%)	26,31,34	0.87	0
3	OMU	L5	4244	3	19,22,23	1.02	2 (10%)	26,31,34	1.79	5 (19%)
49	A2M	S2	166	49	22,25,26	1.72	6 (27%)	31,36,39	2.46	14 (45%)
49	PSU	S2	1626	49	18,21,22	1.42	3 (16%)	22,30,33	1.77	4 (18%)
49	PSU	S2	210	49	18,21,22	1.45	3 (16%)	22,30,33	1.80	5 (22%)
49	PSU	S2	1178	49	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
3	PSU	L5	4278	3	18,21,22	1.48	2 (11%)	22,30,33	1.65	3 (13%)
49	4AC	S2	1843	49	21,24,25	1.12	2 (9%)	29,34,37	1.30	3 (10%)
49	PSU	S2	1175	49	18,21,22	1.41	3 (16%)	22,30,33	1.80	4 (18%)
3	OMC	L5	2208	3	19,22,23	1.16	2 (10%)	26,31,34	0.95	1 (3%)
49	PSU	S2	687	49	18,21,22	1.41	3 (16%)	22,30,33	1.81	5 (22%)
3	1MA	L5	1266	3	21,25,26	1.82	4 (19%)	31,37,40	1.94	5 (16%)
3	PSU	L5	4325	3	18,21,22	1.37	3 (16%)	22,30,33	1.85	5 (22%)
49	OMG	S2	1491	49	23,26,27	1.16	2 (8%)	33,38,41	1.87	9 (27%)
49	PSU	S2	218	49	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
49	OMU	S2	1805	49	19,22,23	0.99	2 (10%)	26,31,34	1.76	4 (15%)
3	5MC	L5	3514	3	18,22,23	1.34	3 (16%)	26,32,35	1.24	3 (11%)
3	5MC	L5	4193	3	18,22,23	1.29	3 (16%)	26,32,35	1.48	4 (15%)
3	OMC	L5	2647	3	19,22,23	1.15	2 (10%)	26,31,34	1.01	1 (3%)
3	OMC	L5	4202	3	19,22,23	1.16	2 (10%)	26,31,34	0.91	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	HY3	Si	62	80	6,8,9	1.30	1 (16%)	5,10,12	1.40	1 (20%)
3	OMG	L5	2207	3	23,26,27	1.18	3 (13%)	33,38,41	1.86	9 (27%)
46	SAC	Ls	2	46	7,8,9	0.52	0	8,9,11	0.84	1 (12%)
78	AME	Sg	1	78	9,10,11	0.67	0	9,11,13	1.07	1 (11%)
3	PSU	L5	3554	3	18,21,22	1.40	3 (16%)	22,30,33	1.82	5 (22%)
3	OMC	L5	3573	3	19,22,23	1.14	2 (10%)	26,31,34	0.90	0
32	MLZ	Le	5	32	8,9,10	0.49	0	4,9,11	0.19	0
3	OMC	L5	2265	3	19,22,23	1.15	2 (10%)	26,31,34	0.89	0
49	OMC	S2	1392	49	19,22,23	1.17	2 (10%)	26,31,34	0.96	1 (3%)
3	PSU	L5	3652	3	18,21,22	1.37	3 (16%)	22,30,33	1.88	5 (22%)
49	OMG	S2	602	49	23,26,27	1.17	3 (13%)	33,38,41	1.89	9 (27%)
3	PSU	L5	4382	3	18,21,22	1.38	3 (16%)	22,30,33	1.76	4 (18%)
49	PSU	S2	1046	49	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
3	OMC	L5	1284	3	19,22,23	1.18	2 (10%)	26,31,34	0.89	0
3	PSU	L5	4217	3	18,21,22	1.40	3 (16%)	22,30,33	1.80	4 (18%)
3	PSU	L5	4099	3	18,21,22	1.39	3 (16%)	22,30,33	1.86	4 (18%)
49	PSU	S2	1005	49	18,21,22	1.43	3 (16%)	22,30,33	1.82	4 (18%)
3	OMC	L5	2704	3	19,22,23	1.15	2 (10%)	26,31,34	0.87	1 (3%)
5	PSU	L8	55	5	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
3	A2M	L5	4317	3	22,25,26	1.73	6 (27%)	31,36,39	2.43	13 (41%)
3	OMU	L5	4052	3	19,22,23	0.99	2 (10%)	26,31,34	1.78	4 (15%)
3	PSU	L5	4149	3	18,21,22	1.36	3 (16%)	22,30,33	1.90	4 (18%)
3	PSU	L5	4203	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
3	A2M	L5	3456	3	22,25,26	1.72	6 (27%)	31,36,39	2.45	13 (41%)
3	OMG	L5	3631	3	23,26,27	1.19	2 (8%)	33,38,41	1.88	9 (27%)
3	PSU	L5	4045	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
49	PSU	S2	1348	49	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
3	A2M	L5	2244	3	22,25,26	1.73	6 (27%)	31,36,39	2.47	15 (48%)
3	PSU	L5	4188	3	18,21,22	1.37	3 (16%)	22,30,33	1.90	4 (18%)
3	A2M	L5	2630	3	22,25,26	1.72	6 (27%)	31,36,39	2.54	17 (54%)
3	PSU	L5	3585	3	18,21,22	1.39	3 (16%)	22,30,33	1.81	5 (22%)
43	M3L	Lp	98	43	10,11,12	0.51	0	9,14,16	0.47	0
49	PSU	S2	1233	49	18,21,22	1.42	3 (16%)	22,30,33	1.82	5 (22%)
3	PSU	L5	1731	3	18,21,22	1.37	3 (16%)	22,30,33	1.84	4 (18%)
49	PSU	S2	682	49	18,21,22	1.41	3 (16%)	22,30,33	1.85	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4042	3	18,21,22	1.39	3 (16%)	22,30,33	1.86	5 (22%)
49	OMU	S2	628	49	19,22,23	1.01	1 (5%)	26,31,34	1.84	5 (19%)
3	A2M	L5	3557	3	22,25,26	1.72	7 (31%)	31,36,39	2.45	13 (41%)
49	MA6	S2	1852	49	23,26,27	1.46	4 (17%)	34,38,41	2.37	11 (32%)
3	UR3	L5	4276	3	19,22,23	1.29	3 (15%)	26,32,35	1.24	2 (7%)
49	OMU	S2	1443	49	19,22,23	0.99	2 (10%)	26,31,34	1.74	4 (15%)
3	PSU	L5	4749	3	18,21,22	1.42	3 (16%)	22,30,33	1.82	4 (18%)
49	OMG	S2	437	49	23,26,27	1.16	2 (8%)	33,38,41	1.91	9 (27%)
49	A2M	S2	591	49	22,25,26	1.71	6 (27%)	31,36,39	2.60	15 (48%)
3	PSU	L5	2475	3	18,21,22	1.41	3 (16%)	22,30,33	1.87	4 (18%)
3	A2M	L5	400	3	22,25,26	1.72	6 (27%)	31,36,39	2.45	13 (41%)
49	PSU	S2	816	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
3	OMG	L5	1260	3	23,26,27	1.19	3 (13%)	33,38,41	1.92	9 (27%)
3	PSU	L5	4177	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	5 (22%)
49	OMU	S2	355	49	19,22,23	0.99	2 (10%)	26,31,34	1.78	5 (19%)
3	PSU	L5	4246	3	18,21,22	1.39	3 (16%)	22,30,33	1.85	5 (22%)
76	NMM	Se	67	76	9,11,12	1.57	1 (11%)	6,12,14	3.46	2 (33%)
3	A2M	L5	1810	3	22,25,26	1.72	7 (31%)	31,36,39	2.47	15 (48%)
3	PSU	L5	1718	3	18,21,22	1.39	3 (16%)	22,30,33	1.84	5 (22%)
3	PSU	L5	3462	3	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
3	OMG	L5	4240	3	23,26,27	1.18	2 (8%)	33,38,41	1.88	10 (30%)
3	PSU	L5	4711	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	PSU	L5	4740	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	5 (22%)
49	PSU	S2	864	49	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
49	PSU	S2	573	49	18,21,22	1.42	3 (16%)	22,30,33	1.81	4 (18%)
3	OMG	L5	2267	3	23,26,27	1.16	2 (8%)	33,38,41	1.88	9 (27%)
3	PSU	L5	4298	3	18,21,22	1.36	3 (16%)	22,30,33	1.86	5 (22%)
3	OMC	L5	3601	3	19,22,23	1.14	2 (10%)	26,31,34	0.96	2 (7%)
49	PSU	S2	93	49	18,21,22	1.41	3 (16%)	22,30,33	1.79	4 (18%)
49	OMU	S2	1289	49	19,22,23	0.98	2 (10%)	26,31,34	1.74	5 (19%)
3	PSU	L5	4435	3	18,21,22	1.39	3 (16%)	22,30,33	1.89	5 (22%)
49	OMC	S2	174	49	19,22,23	1.17	2 (10%)	26,31,34	0.90	0
8	AYA	LF	2	8	6,7,8	0.73	0	5,8,10	0.33	0
3	PSU	L5	1721	3	18,21,22	1.41	3 (16%)	22,30,33	1.84	4 (18%)
3	OMC	L5	1820	3	19,22,23	1.16	2 (10%)	26,31,34	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PSU	S2	119	49	18,21,22	1.43	3 (16%)	22,30,33	1.84	4 (18%)
49	PSU	S2	1644	49	18,21,22	1.43	3 (16%)	22,30,33	1.83	4 (18%)
49	A2M	S2	99	49	22,25,26	1.72	6 (27%)	31,36,39	2.47	14 (45%)
3	PSU	L5	1683	3	18,21,22	1.40	3 (16%)	22,30,33	1.80	5 (22%)
3	OMC	L5	3619	3	19,22,23	1.17	2 (10%)	26,31,34	0.87	0
49	PSU	S2	1057	49	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
3	OMC	L5	3433	3	19,22,23	1.17	2 (10%)	26,31,34	0.98	1 (3%)
49	A2M	S2	1032	49	22,25,26	1.73	7 (31%)	31,36,39	2.47	13 (41%)
3	OMU	L5	3657	3	19,22,23	0.99	2 (10%)	26,31,34	1.85	5 (19%)
3	A2M	L5	3492	3,49	22,25,26	1.70	6 (27%)	31,36,39	2.68	16 (51%)
49	PSU	S2	815	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
49	OMU	S2	429	49	19,22,23	1.01	2 (10%)	26,31,34	1.82	6 (23%)
3	OMG	L5	4138	3	23,26,27	1.17	3 (13%)	33,38,41	1.93	10 (30%)
49	OMG	S2	645	49	23,26,27	1.16	3 (13%)	33,38,41	1.91	10 (30%)
75	SAC	Sd	2	75	7,8,9	0.54	0	8,9,11	0.85	1 (12%)
3	PSU	L5	3371	3	18,21,22	1.38	3 (16%)	22,30,33	1.83	5 (22%)
3	A2M	L5	3517	3	22,25,26	1.73	7 (31%)	31,36,39	2.59	17 (54%)
49	A2M	S2	485	49	22,25,26	1.70	7 (31%)	31,36,39	2.44	14 (45%)
3	OMC	L5	3540	3	19,22,23	1.14	2 (10%)	26,31,34	0.88	1 (3%)
3	6MZ	L5	3966	3	22,25,26	1.42	4 (18%)	30,36,39	2.22	9 (30%)
3	PSU	L5	1491	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	4 (18%)
3	PSU	L5	4419	3	18,21,22	1.40	3 (16%)	22,30,33	1.82	5 (22%)
3	A2M	L5	2206	3	22,25,26	1.72	6 (27%)	31,36,39	2.43	14 (45%)
49	OMC	S2	1704	49	19,22,23	1.17	2 (10%)	26,31,34	0.88	1 (3%)
49	4AC	S2	1338	49	21,24,25	1.10	2 (9%)	29,34,37	1.19	3 (10%)
49	OMG	S2	684	49	23,26,27	1.17	2 (8%)	33,38,41	1.87	10 (30%)
3	PSU	L5	4374	3	18,21,22	1.40	3 (16%)	22,30,33	1.88	5 (22%)
3	A2M	L5	3450	3	22,25,26	1.71	6 (27%)	31,36,39	2.41	13 (41%)
3	OMG	L5	3676	3	23,26,27	1.16	2 (8%)	33,38,41	1.92	10 (30%)
49	OMG	S2	1448	49	23,26,27	1.15	2 (8%)	33,38,41	1.88	9 (27%)
49	PSU	S2	650	49	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
49	PSU	S2	1693	49	18,21,22	1.41	3 (16%)	22,30,33	1.84	5 (22%)
49	MA6	S2	1851	49	23,26,27	1.44	4 (17%)	34,38,41	2.37	13 (38%)
3	OMU	L5	2258	3	19,22,23	1.01	2 (10%)	26,31,34	1.75	5 (19%)
49	PSU	S2	610	49	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PSU	S2	802	49	18,21,22	1.43	3 (16%)	22,30,33	1.80	5 (22%)
49	A2M	S2	513	49	22,25,26	1.71	6 (27%)	31,36,39	2.46	14 (45%)
3	PSU	L5	3576	3	18,21,22	1.39	3 (16%)	22,30,33	1.71	4 (18%)
3	A2M	L5	3599	3	22,25,26	1.73	7 (31%)	31,36,39	2.51	15 (48%)
3	PSU	L5	3427	3	18,21,22	1.39	3 (16%)	22,30,33	1.84	5 (22%)
49	PSU	S2	652	49	18,21,22	1.42	3 (16%)	22,30,33	1.85	5 (22%)
3	A2M	L5	4336	3	22,25,26	1.72	6 (27%)	31,36,39	2.48	15 (48%)
3	A2M	L5	2658	3	22,25,26	1.72	6 (27%)	31,36,39	2.49	13 (41%)
49	OMG	S2	1329	49	23,26,27	1.15	2 (8%)	33,38,41	1.90	9 (27%)
5	PSU	L8	69	5	18,21,22	1.38	3 (16%)	22,30,33	1.85	4 (18%)
49	OMU	S2	116	49	19,22,23	1.00	2 (10%)	26,31,34	1.73	6 (23%)
49	OMG	S2	510	49	23,26,27	1.16	2 (8%)	33,38,41	1.92	10 (30%)
49	OMU	S2	1327	49	19,22,23	1.00	2 (10%)	26,31,34	1.81	5 (19%)
3	PSU	L5	1801	3	18,21,22	1.38	3 (16%)	22,30,33	1.86	4 (18%)
49	OMU	S2	172	49	19,22,23	0.99	2 (10%)	26,31,34	1.82	4 (15%)
49	PSU	S2	1239	49	18,21,22	1.42	3 (16%)	22,30,33	1.80	4 (18%)
3	A2M	L5	1489	3	22,25,26	1.72	6 (27%)	31,36,39	2.49	13 (41%)
3	OMC	L5	2194	3	19,22,23	1.15	2 (10%)	26,31,34	0.94	1 (3%)
49	PSU	S2	105	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	5 (22%)
3	OMG	L5	3974	3	23,26,27	1.16	3 (13%)	33,38,41	1.89	11 (33%)
3	OMG	L5	4116	3	23,26,27	1.18	3 (13%)	33,38,41	1.89	9 (27%)
49	7MG	S2	1640	49	22,26,27	1.18	2 (9%)	29,39,42	2.13	9 (31%)
5	OMG	L8	75	5	23,26,27	1.20	3 (13%)	33,38,41	1.85	9 (27%)
49	PSU	S2	34	49	18,21,22	1.41	3 (16%)	22,30,33	1.85	4 (18%)
3	A2M	L5	3562	3	22,25,26	1.72	7 (31%)	31,36,39	2.44	14 (45%)
44	MLZ	Lq	53	44	8,9,10	0.48	0	4,9,11	0.16	0
49	PSU	S2	109	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	PSU	L5	4166	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
49	OMC	S2	463	49	19,22,23	1.18	2 (10%)	26,31,34	0.88	0
49	PSU	S2	967	49	18,21,22	1.41	3 (16%)	22,30,33	1.82	4 (18%)
3	OMC	L5	4282	3	19,22,23	1.16	2 (10%)	26,31,34	0.94	1 (3%)
3	PSU	L5	1638	3	18,21,22	1.38	3 (16%)	22,30,33	1.84	5 (22%)
3	PSU	L5	3466	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
49	PSU	S2	1368	49	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
3	PSU	L5	3490	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4107	3	18,21,22	1.38	3 (16%)	22,30,33	1.80	4 (18%)
49	A2M	S2	469	49	22,25,26	1.71	6 (27%)	31,36,39	2.48	14 (45%)
3	OMU	L5	4366	3	19,22,23	0.99	2 (10%)	26,31,34	1.80	5 (19%)
49	A2M	S2	27	49	22,25,26	1.70	7 (31%)	31,36,39	2.47	13 (41%)
3	PSU	L5	1632	3	18,21,22	1.44	4 (22%)	22,30,33	1.70	4 (18%)
3	PSU	L5	4267	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
49	OMG	S2	868	49	23,26,27	1.16	2 (8%)	33,38,41	1.86	9 (27%)
3	PSU	L5	3496	3	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)
3	OMG	L5	2719	3	23,26,27	1.16	2 (8%)	33,38,41	2.08	11 (33%)
49	OMU	S2	121	49	19,22,23	1.01	2 (10%)	26,31,34	1.77	6 (23%)
3	A2M	L5	1479	3	22,25,26	1.73	7 (31%)	31,36,39	2.48	14 (45%)
49	PSU	S2	1082	49	18,21,22	1.36	3 (16%)	22,30,33	1.84	4 (18%)
3	PSU	L5	1799	3	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
3	PSU	L5	3369	3	18,21,22	1.35	3 (16%)	22,30,33	1.85	4 (18%)
3	PSU	L5	3500	3	18,21,22	1.42	3 (16%)	22,30,33	1.84	5 (22%)
4	GTP	L7	1	4	30,34,34	1.21	3 (10%)	46,54,54	1.39	4 (8%)
3	OMG	L5	1580	3	23,26,27	1.17	2 (8%)	33,38,41	1.94	10 (30%)
49	PSU	S2	1446	49	18,21,22	1.44	3 (16%)	22,30,33	1.81	4 (18%)
57	SAC	SL	2	57	7,8,9	0.52	0	8,9,11	0.89	1 (12%)
3	A2M	L5	398	3	22,25,26	1.72	6 (27%)	31,36,39	2.43	13 (41%)
3	PSU	L5	1720	3	18,21,22	1.38	3 (16%)	22,30,33	1.83	5 (22%)
49	PSU	S2	823	49	18,21,22	1.39	3 (16%)	22,30,33	1.80	5 (22%)
3	PSU	L5	1537	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
3	OMG	L5	4364	3	23,26,27	1.17	2 (8%)	33,38,41	1.90	9 (27%)
7	HIC	LE	245	7	10,11,12	0.63	0	8,14,16	0.35	0
3	OMG	L5	3359	3	23,26,27	1.17	2 (8%)	33,38,41	1.92	10 (30%)
3	OMG	L5	4245	3	23,26,27	1.17	3 (13%)	33,38,41	1.87	9 (27%)
49	PSU	S2	867	49	18,21,22	1.42	3 (16%)	22,30,33	1.84	4 (18%)
49	PSU	S2	1047	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	OMG	L5	3524	3	23,26,27	1.18	2 (8%)	33,38,41	1.89	9 (27%)
3	PSU	L5	3502	3	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	2351	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
3	OMU	L5	2680	3	19,22,23	1.01	2 (10%)	26,31,34	1.81	6 (23%)
3	OMG	L5	1477	3	23,26,27	1.18	3 (13%)	33,38,41	1.91	10 (30%)
3	OMG	L5	4369	3	23,26,27	1.18	3 (13%)	33,38,41	1.89	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	OMC	S2	518	49	19,22,23	1.15	2 (10%)	26,31,34	0.92	1 (3%)
3	PSU	L5	4039	3	18,21,22	1.39	3 (16%)	22,30,33	1.82	5 (22%)
49	6MZ	S2	1833	49	22,25,26	1.41	4 (18%)	30,36,39	2.16	9 (30%)
49	A2M	S2	669	49	22,25,26	1.73	7 (31%)	31,36,39	2.64	17 (54%)

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	PSU	S2	36	49	-	0/7/25/26	0/2/2/2
49	A2M	S2	1679	49	-	0/9/27/28	0/3/3/3
3	PSU	L5	3583	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4269	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3494	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3616	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4169	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3447	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1270	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4058	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1245	49	-	0/7/25/26	0/2/2/2
49	A2M	S2	159	49	-	0/9/27/28	0/3/3/3
49	A2M	S2	577	49	-	2/9/27/28	0/3/3/3
3	OMG	L5	3476	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4322	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	407	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	4383	3	-	2/9/27/28	0/3/3/3
3	OMU	L5	3973	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3942	3	-	0/9/27/28	0/3/3/3
49	A2M	S2	1384	49	-	0/9/27/28	0/3/3/3
3	OMC	L5	2667	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	4244	3	-	0/9/27/28	0/2/2/2
49	A2M	S2	166	49	-	0/9/27/28	0/3/3/3
49	PSU	S2	1626	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	210	49	-	2/7/25/26	0/2/2/2
49	PSU	S2	1178	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4278	3	-	0/7/25/26	0/2/2/2
49	4AC	S2	1843	49	-	2/11/29/30	0/2/2/2
49	PSU	S2	1175	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	2208	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PSU	S2	687	49	-	0/7/25/26	0/2/2/2
3	1MA	L5	1266	3	-	0/7/25/26	0/3/3/3
3	PSU	L5	4325	3	-	0/7/25/26	0/2/2/2
49	OMG	S2	1491	49	-	1/9/27/28	0/3/3/3
49	PSU	S2	218	49	-	0/7/25/26	0/2/2/2
49	OMU	S2	1805	49	-	0/9/27/28	0/2/2/2
3	5MC	L5	3514	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4193	3	-	4/7/25/26	0/2/2/2
3	OMC	L5	2647	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	4202	3	-	0/9/27/28	0/2/2/2
80	HY3	Si	62	80	-	0/1/12/14	0/1/1/1
3	OMG	L5	2207	3	-	0/9/27/28	0/3/3/3
46	SAC	Ls	2	46	-	0/7/8/10	-
78	AME	Sg	1	78	-	2/9/10/12	-
3	PSU	L5	3554	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3573	3	-	0/9/27/28	0/2/2/2
32	MLZ	Le	5	32	-	1/7/8/10	-
3	OMC	L5	2265	3	-	2/9/27/28	0/2/2/2
49	OMC	S2	1392	49	-	1/9/27/28	0/2/2/2
3	PSU	L5	3652	3	-	0/7/25/26	0/2/2/2
49	OMG	S2	602	49	-	0/9/27/28	0/3/3/3
3	PSU	L5	4382	3	-	4/7/25/26	0/2/2/2
49	PSU	S2	1046	49	-	2/7/25/26	0/2/2/2
3	OMC	L5	1284	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4217	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4099	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1005	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	2704	3	-	0/9/27/28	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	A2M	L5	4317	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4052	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4149	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4203	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3456	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	3631	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4045	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1348	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	2244	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4188	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2630	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	3585	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	M3L	Lp	98	43	-	0/9/10/12	-
49	PSU	S2	1233	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1731	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	682	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4042	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	628	49	-	2/9/27/28	0/2/2/2
3	A2M	L5	3557	3	-	0/9/27/28	0/3/3/3
49	MA6	S2	1852	49	-	2/11/29/30	0/3/3/3
3	UR3	L5	4276	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	1443	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	4749	3	-	0/7/25/26	0/2/2/2
49	OMG	S2	437	49	-	0/9/27/28	0/3/3/3
49	A2M	S2	591	49	-	1/9/27/28	0/3/3/3
3	PSU	L5	2475	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
49	PSU	S2	816	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	1260	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4177	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	355	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	4246	3	-	2/7/25/26	0/2/2/2
76	NMM	Se	67	76	-	2/9/11/13	-
3	A2M	L5	1810	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1718	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3462	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4240	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4711	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4740	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	864	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	573	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	2267	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4298	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3601	3	-	0/9/27/28	0/2/2/2
49	PSU	S2	93	49	-	0/7/25/26	0/2/2/2
49	OMU	S2	1289	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	4435	3	-	0/7/25/26	0/2/2/2
49	OMC	S2	174	49	-	0/9/27/28	0/2/2/2
8	AYA	LF	2	8	-	2/4/6/8	-
3	PSU	L5	1721	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	1820	3	-	0/9/27/28	0/2/2/2
49	PSU	S2	119	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1644	49	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	A2M	S2	99	49	-	1/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3619	3	-	1/9/27/28	0/2/2/2
49	PSU	S2	1057	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	3433	3	-	4/9/27/28	0/2/2/2
49	A2M	S2	1032	49	-	0/9/27/28	0/3/3/3
3	OMU	L5	3657	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3492	3,49	-	0/9/27/28	0/3/3/3
49	PSU	S2	815	49	-	0/7/25/26	0/2/2/2
49	OMU	S2	429	49	-	4/9/27/28	0/2/2/2
3	OMG	L5	4138	3	-	0/9/27/28	0/3/3/3
49	OMG	S2	645	49	-	3/9/27/28	0/3/3/3
75	SAC	Sd	2	75	-	0/7/8/10	-
3	PSU	L5	3371	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3517	3	-	5/9/27/28	0/3/3/3
49	A2M	S2	485	49	-	0/9/27/28	0/3/3/3
3	OMC	L5	3540	3	-	0/9/27/28	0/2/2/2
3	6MZ	L5	3966	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1491	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4419	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2206	3	-	0/9/27/28	0/3/3/3
49	OMC	S2	1704	49	-	0/9/27/28	0/2/2/2
49	4AC	S2	1338	49	-	4/11/29/30	0/2/2/2
49	OMG	S2	684	49	-	2/9/27/28	0/3/3/3
3	PSU	L5	4374	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3450	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	3676	3	-	0/9/27/28	0/3/3/3
49	OMG	S2	1448	49	-	1/9/27/28	0/3/3/3
49	PSU	S2	650	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1693	49	-	0/7/25/26	0/2/2/2
49	MA6	S2	1851	49	-	1/11/29/30	0/3/3/3
3	OMU	L5	2258	3	-	0/9/27/28	0/2/2/2
49	PSU	S2	610	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	802	49	-	2/7/25/26	0/2/2/2
49	A2M	S2	513	49	-	0/9/27/28	0/3/3/3
3	PSU	L5	3576	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	3599	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3427	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	652	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	4336	3	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	2658	3	-	1/9/27/28	0/3/3/3
49	OMG	S2	1329	49	-	0/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
49	OMU	S2	116	49	-	0/9/27/28	0/2/2/2
49	OMG	S2	510	49	-	0/9/27/28	0/3/3/3
49	OMU	S2	1327	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	1801	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	172	49	-	0/9/27/28	0/2/2/2
49	PSU	S2	1239	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	1489	3	-	3/9/27/28	0/3/3/3
3	OMC	L5	2194	3	-	2/9/27/28	0/2/2/2
49	PSU	S2	105	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	3974	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4116	3	-	0/9/27/28	0/3/3/3
49	7MG	S2	1640	49	-	0/7/37/38	0/3/3/3
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
49	PSU	S2	34	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	3562	3	-	0/9/27/28	0/3/3/3
44	MLZ	Lq	53	44	-	0/7/8/10	-
49	PSU	S2	109	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4166	3	-	0/7/25/26	0/2/2/2
49	OMC	S2	463	49	-	0/9/27/28	0/2/2/2
49	PSU	S2	967	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	4282	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1638	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3466	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1368	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	3490	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4107	3	-	0/7/25/26	0/2/2/2
49	A2M	S2	469	49	-	0/9/27/28	0/3/3/3
3	OMU	L5	4366	3	-	0/9/27/28	0/2/2/2
49	A2M	S2	27	49	-	0/9/27/28	0/3/3/3
3	PSU	L5	1632	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4267	3	-	2/7/25/26	0/2/2/2
49	OMG	S2	868	49	-	0/9/27/28	0/3/3/3
3	PSU	L5	3496	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2719	3	-	0/9/27/28	0/3/3/3
49	OMU	S2	121	49	-	0/9/27/28	0/2/2/2
3	A2M	L5	1479	3	-	1/9/27/28	0/3/3/3
49	PSU	S2	1082	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1799	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3369	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3500	3	-	0/7/25/26	0/2/2/2
4	GTP	L7	1	4	-	0/22/38/38	0/3/3/3
3	OMG	L5	1580	3	-	2/9/27/28	0/3/3/3
49	PSU	S2	1446	49	-	0/7/25/26	0/2/2/2
57	SAC	SL	2	57	-	1/7/8/10	-
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1720	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	823	49	-	2/7/25/26	0/2/2/2
3	PSU	L5	1537	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4364	3	-	0/9/27/28	0/3/3/3
7	HIC	LE	245	7	-	2/5/6/8	0/1/1/1
3	OMG	L5	3359	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4245	3	-	0/9/27/28	0/3/3/3
49	PSU	S2	867	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1047	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	3524	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3502	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2351	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2680	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	1477	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4369	3	-	0/9/27/28	0/3/3/3
49	OMC	S2	518	49	-	2/9/27/28	0/2/2/2
3	PSU	L5	4039	3	-	0/7/25/26	0/2/2/2
49	6MZ	S2	1833	49	-	0/9/27/28	0/3/3/3
49	A2M	S2	669	49	-	4/9/27/28	0/3/3/3

The worst 5 of 684 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1266	1MA	C2-N3	4.92	1.39	1.30
49	S2	1852	MA6	C5-C4	4.50	1.47	1.39
49	S2	1851	MA6	C5-C4	4.39	1.47	1.39
49	S2	1833	6MZ	C5-C4	4.38	1.47	1.39
3	L5	3966	6MZ	C5-C4	4.35	1.47	1.39

The worst 5 of 1361 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	Se	67	NMM	NE-CZ-NH2	-7.43	112.67	119.48
3	L5	1266	1MA	N1-C2-N3	-7.03	117.65	126.00
3	L5	4269	A2M	N3-C2-N1	-6.83	117.91	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1270	A2M	N3-C2-N1	-6.80	117.97	128.60
3	L5	2630	A2M	N3-C2-N1	-6.80	117.97	128.60

There are no chirality outliers.

5 of 101 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	S2	429	OMU	C2'-C1'-N1-C2
49	S2	429	OMU	C2'-C1'-N1-C6
49	S2	577	A2M	C3'-C4'-C5'-O5'
49	S2	645	OMG	O4'-C4'-C5'-O5'
49	S2	645	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

70 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	S2	1679	A2M	1	0
3	L5	4269	A2M	3	0
3	L5	4383	OMG	2	0
3	L5	3973	OMU	1	0
3	L5	3942	OMG	1	0
49	S2	1384	A2M	1	0
3	L5	2667	OMC	1	0
49	S2	166	A2M	1	0
3	L5	4278	PSU	1	0
49	S2	1843	4AC	2	0
49	S2	687	PSU	1	0
3	L5	4325	PSU	1	0
49	S2	1491	OMG	1	0
3	L5	4193	5MC	2	0
3	L5	2207	OMG	2	0
78	Sg	1	AME	2	0
3	L5	2265	OMC	2	0
49	S2	1392	OMC	1	0
49	S2	602	OMG	2	0
3	L5	4382	PSU	2	0
3	L5	4099	PSU	1	0
3	L5	4052	OMU	1	0
3	L5	4203	PSU	2	0
3	L5	3456	A2M	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3585	PSU	1	0
49	S2	1233	PSU	1	0
49	S2	682	PSU	1	0
49	S2	1852	MA6	2	0
3	L5	400	A2M	1	0
3	L5	1260	OMG	1	0
49	S2	355	OMU	2	0
76	Se	67	NMM	1	0
3	L5	1810	A2M	2	0
3	L5	3601	OMC	1	0
49	S2	1289	OMU	2	0
49	S2	1032	A2M	1	0
3	L5	3657	OMU	1	0
49	S2	815	PSU	1	0
3	L5	4138	OMG	1	0
3	L5	3517	A2M	1	0
3	L5	3540	OMC	1	0
49	S2	1338	4AC	2	0
49	S2	684	OMG	1	0
49	S2	1693	PSU	1	0
49	S2	1851	MA6	2	0
3	L5	2258	OMU	1	0
3	L5	3599	A2M	2	0
49	S2	1329	OMG	1	0
49	S2	116	OMU	2	0
49	S2	172	OMU	1	0
3	L5	1489	A2M	1	0
3	L5	4116	OMG	1	0
5	L8	75	OMG	2	0
3	L5	4166	PSU	1	0
3	L5	3466	PSU	1	0
3	L5	4366	OMU	1	0
49	S2	27	A2M	3	0
49	S2	868	OMG	1	0
3	L5	2719	OMG	1	0
3	L5	1479	A2M	1	0
3	L5	3369	PSU	1	0
4	L7	1	GTP	1	0
3	L5	1580	OMG	1	0
49	S2	1446	PSU	1	0
3	L5	4364	OMG	1	0
7	LE	245	HIC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3359	OMG	1	0
3	L5	3524	OMG	1	0
49	S2	1833	6MZ	2	0
49	S2	669	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
2	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	181:C	O3'	199:A	P	24.04
1	I	202:C	O3'	216:U	P	23.09

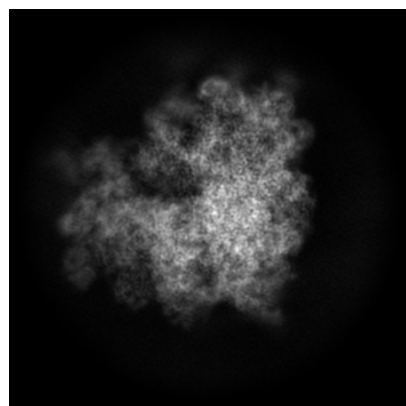
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14752. These allow visual inspection of the internal detail of the map and identification of artifacts.

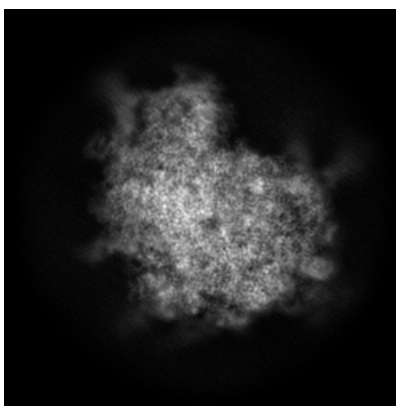
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

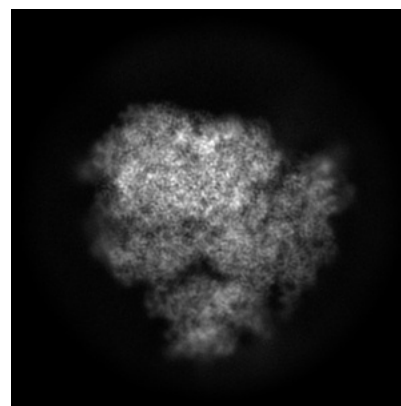
6.1.1 Primary map



X

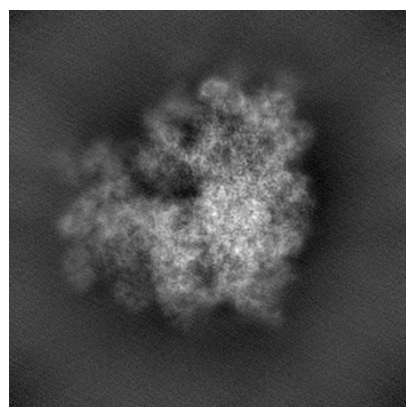


Y

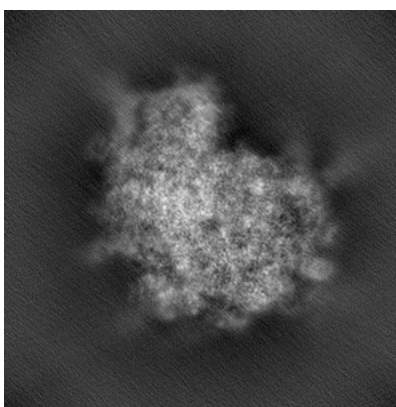


Z

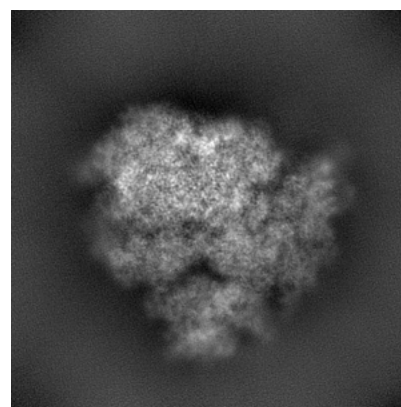
6.1.2 Raw map



X



Y

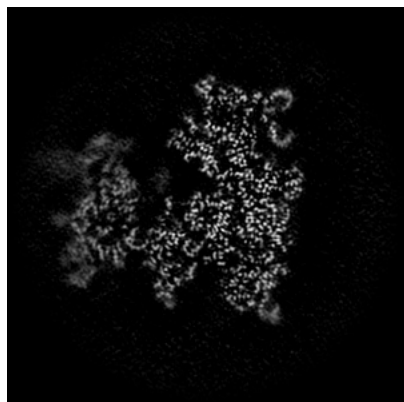


Z

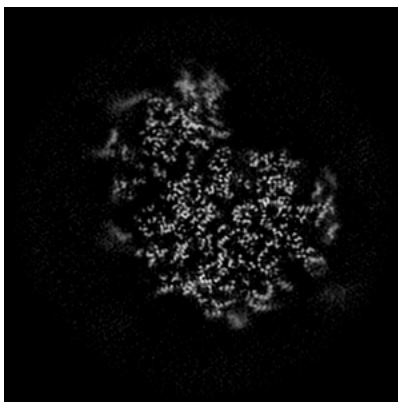
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

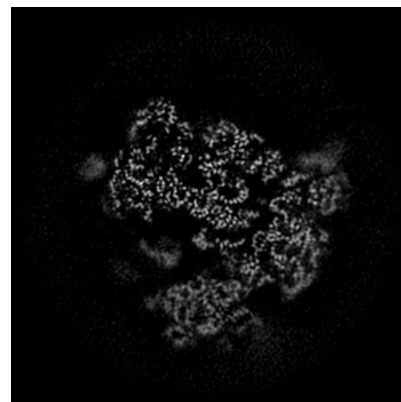
6.2.1 Primary map



X Index: 165

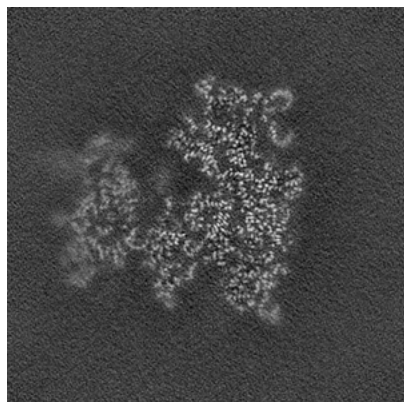


Y Index: 165

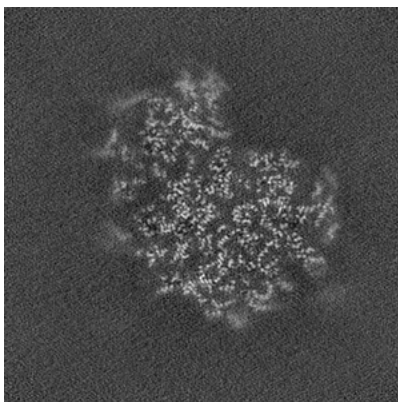


Z Index: 165

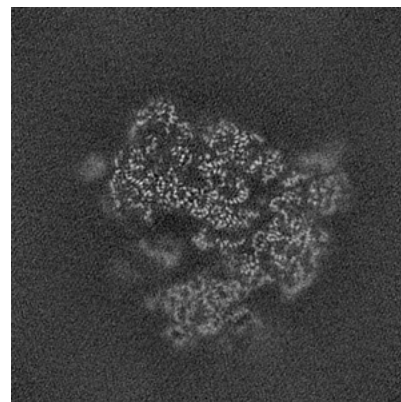
6.2.2 Raw map



X Index: 165



Y Index: 165

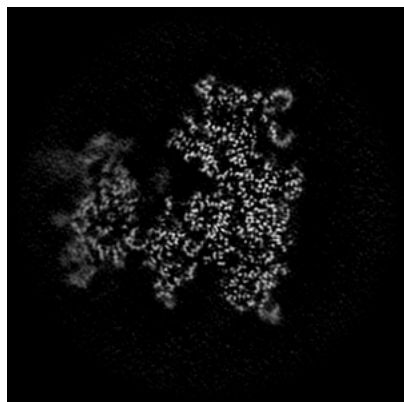


Z Index: 165

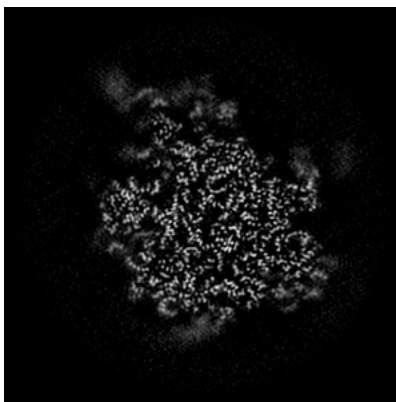
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

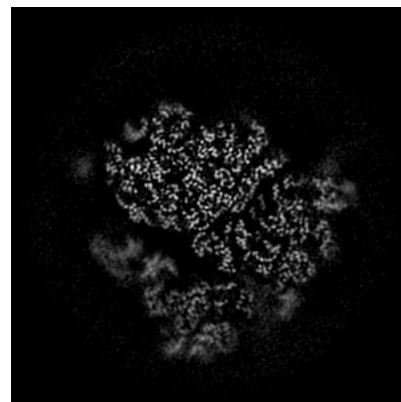
6.3.1 Primary map



X Index: 165

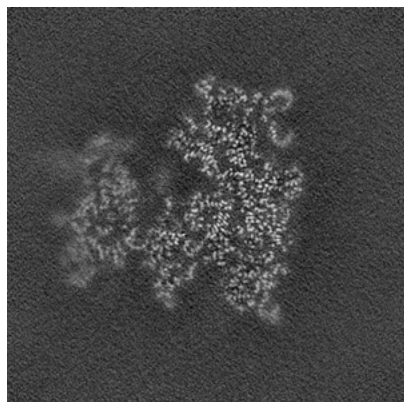


Y Index: 194

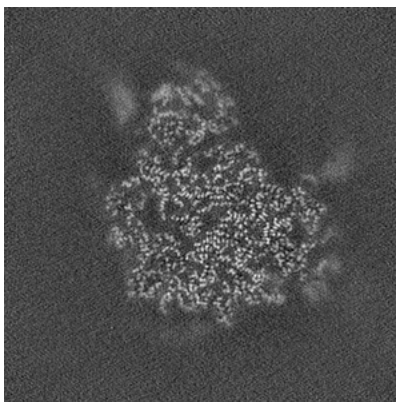


Z Index: 150

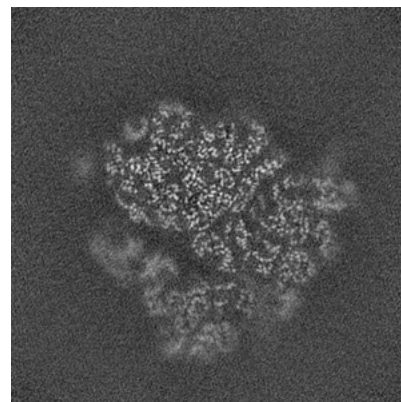
6.3.2 Raw map



X Index: 165



Y Index: 186

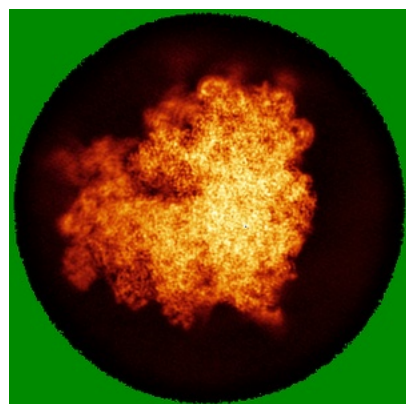


Z Index: 150

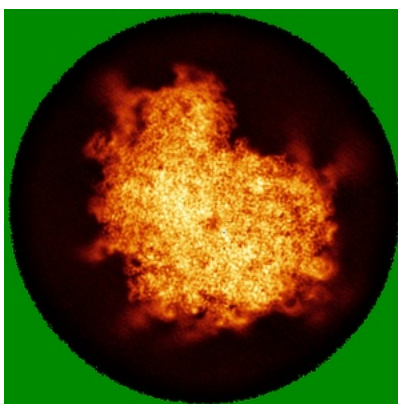
The images above show the largest variance slices of the map in three orthogonal directions.

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

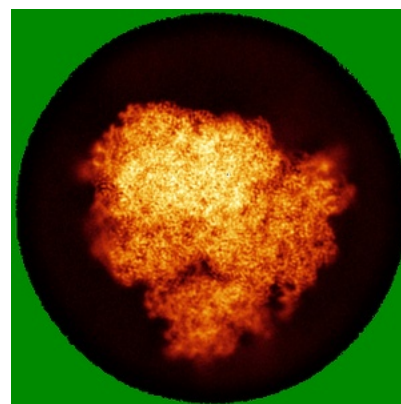
6.4.1 Primary map



X

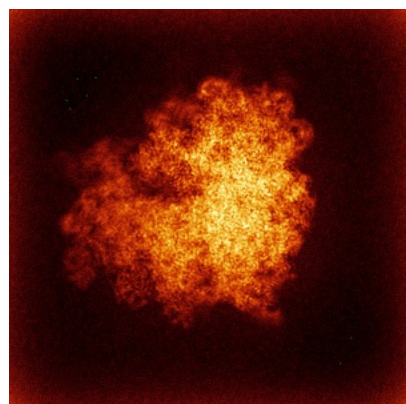


Y

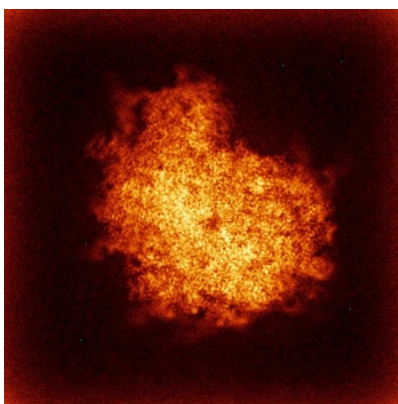


Z

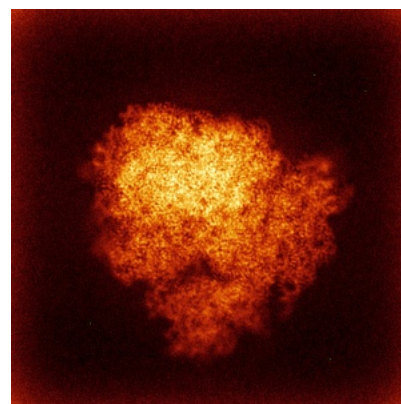
6.4.2 Raw map



X



Y

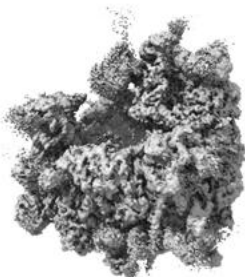


Z

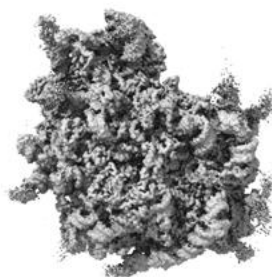
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



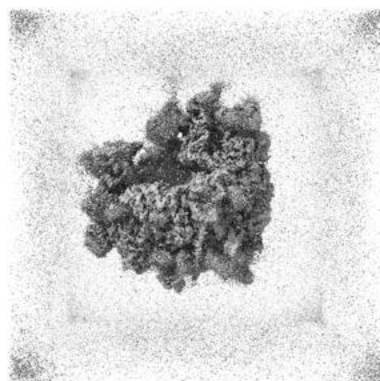
Y



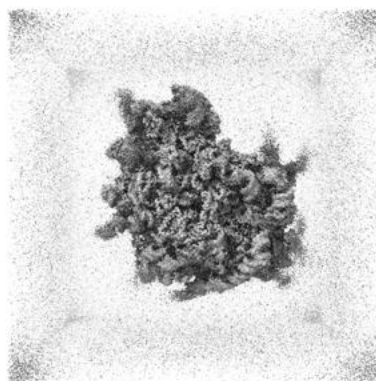
Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

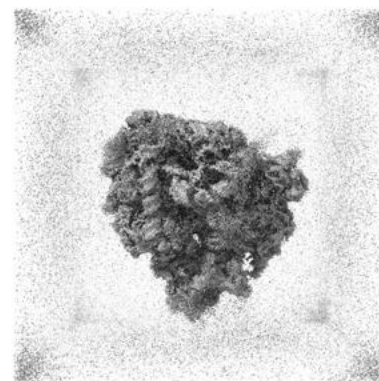
6.5.2 Raw map



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.

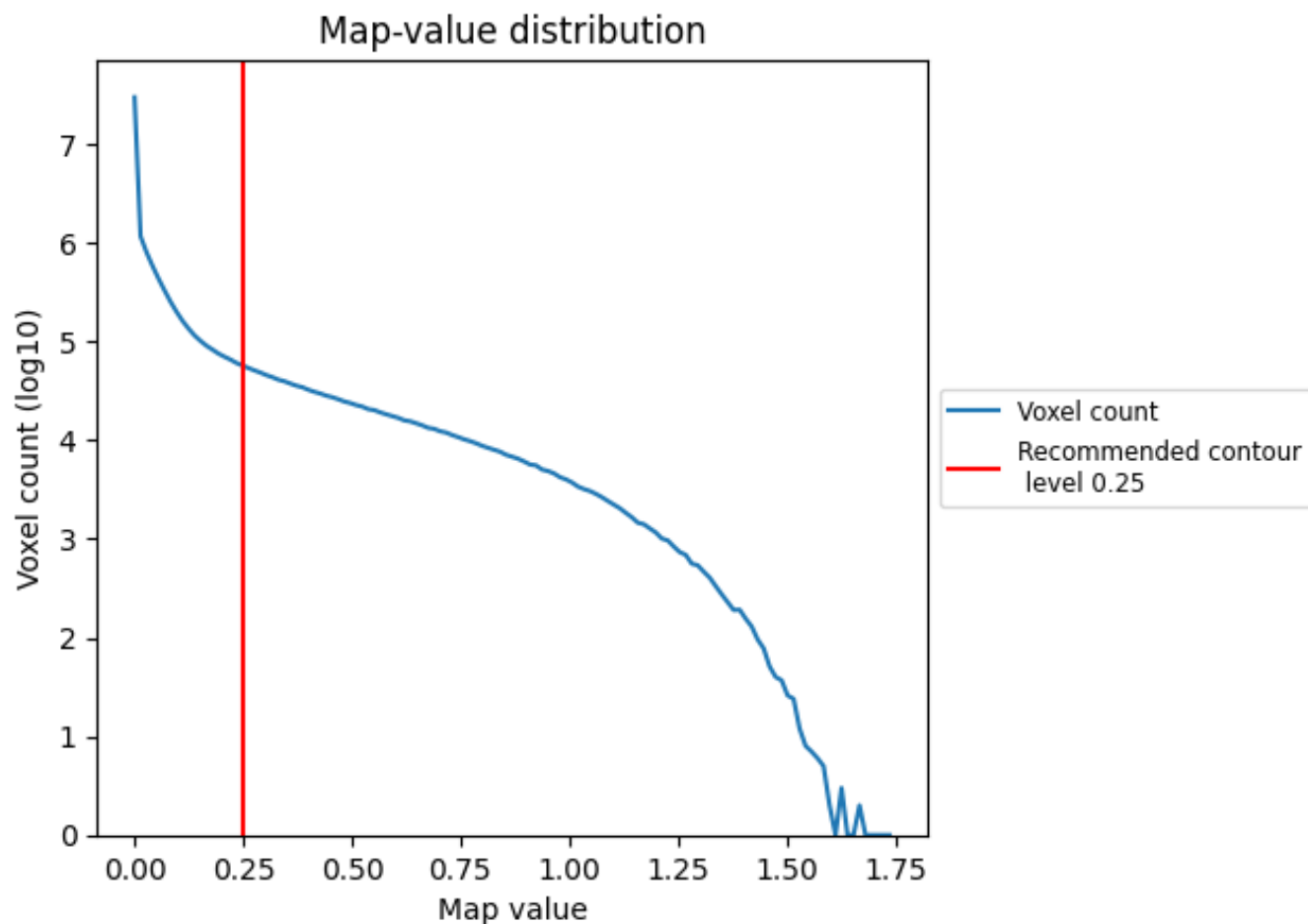
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

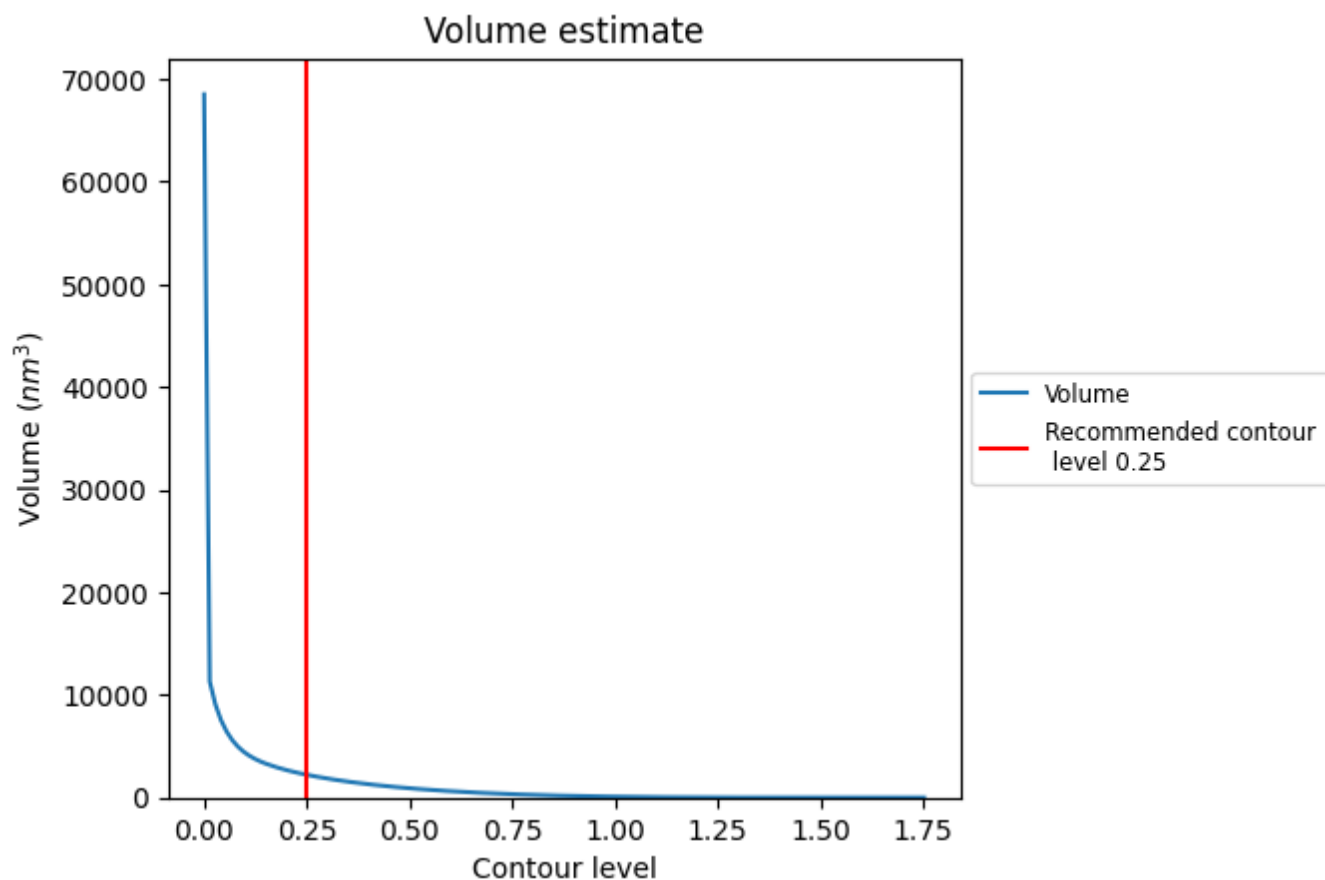
This section contains the results of statistical analysis of the map.

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.

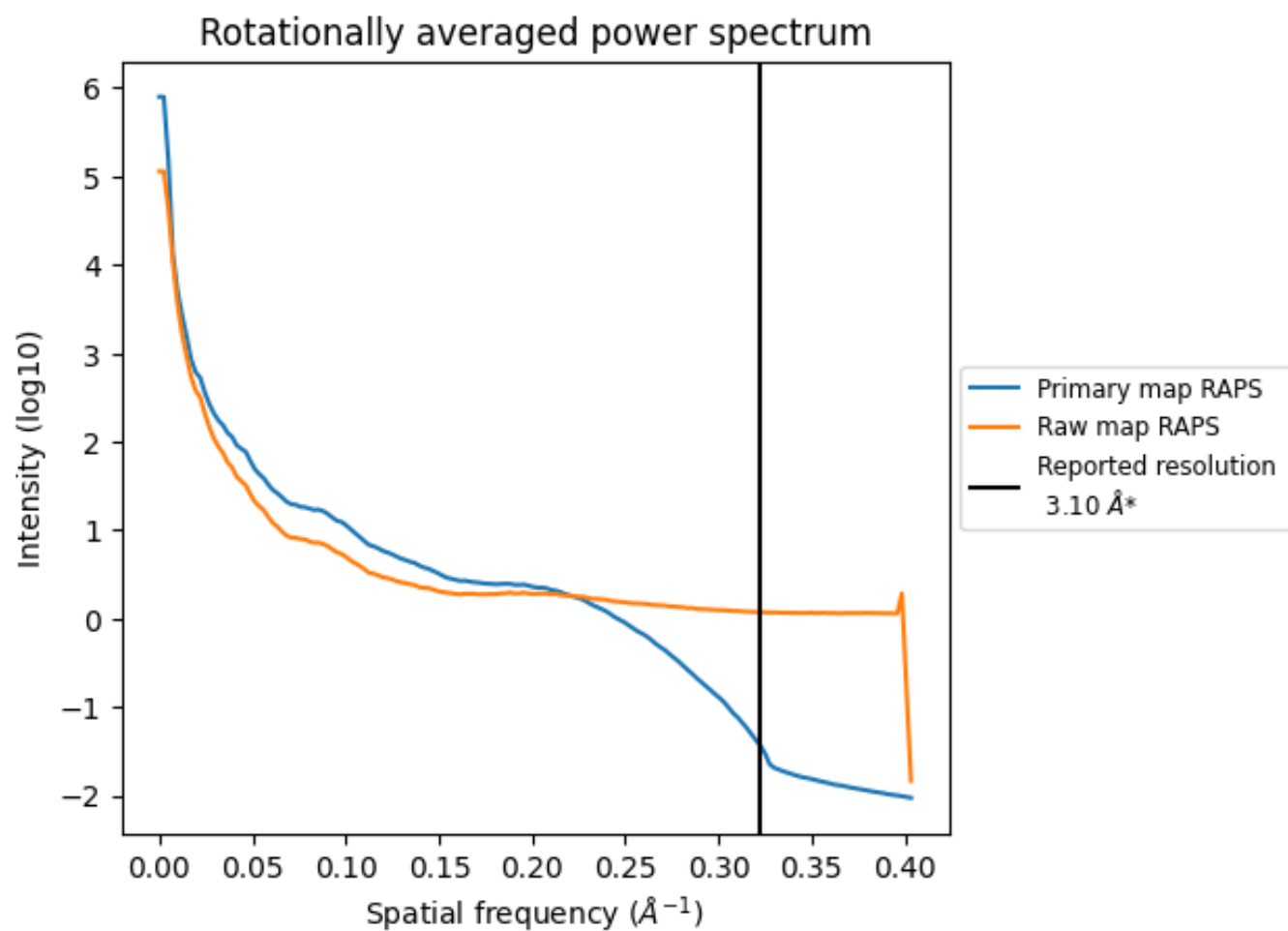
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2219 nm³; this corresponds to an approximate mass of 2005 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 ⓘ

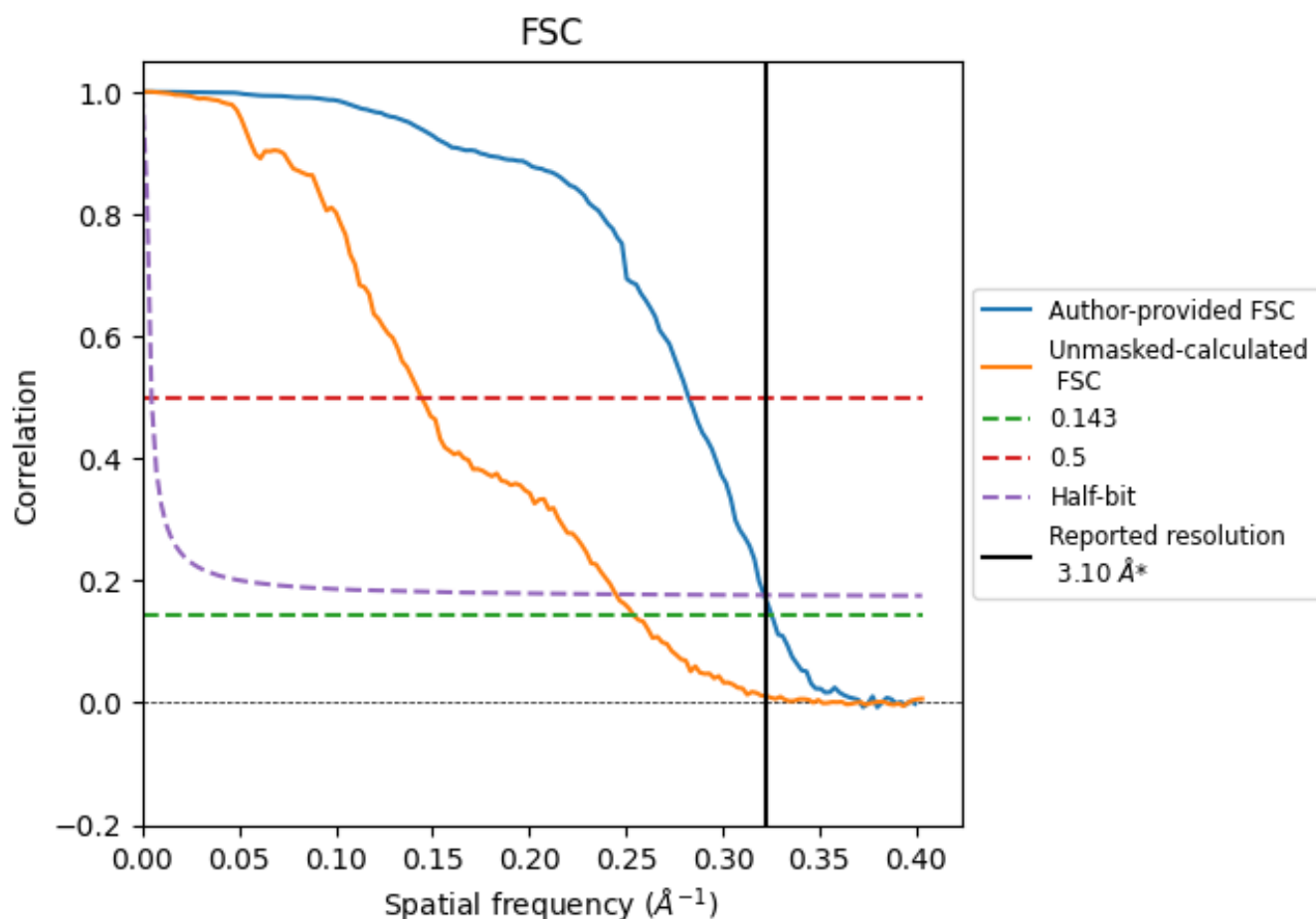


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

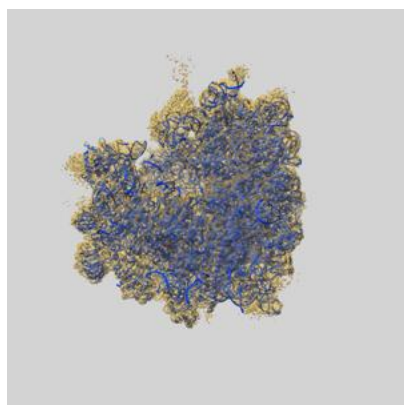
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.54	3.11
Unmasked-calculated*	3.94	6.93	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.1 by more than 10 %

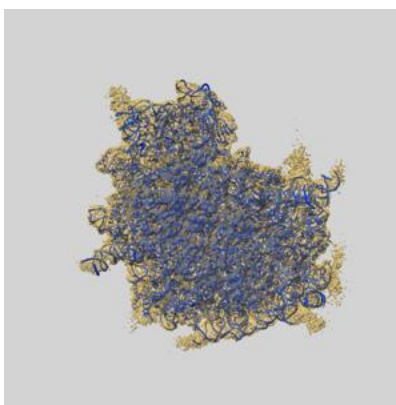
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14752 and PDB model 7ZJX. Per-residue inclusion information can be found in section [3](#) on page [22](#).

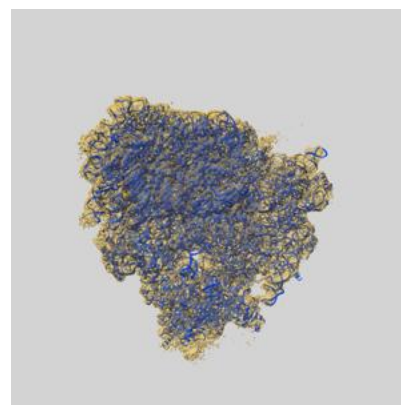
9.1 Map-model overlay [i](#)



X



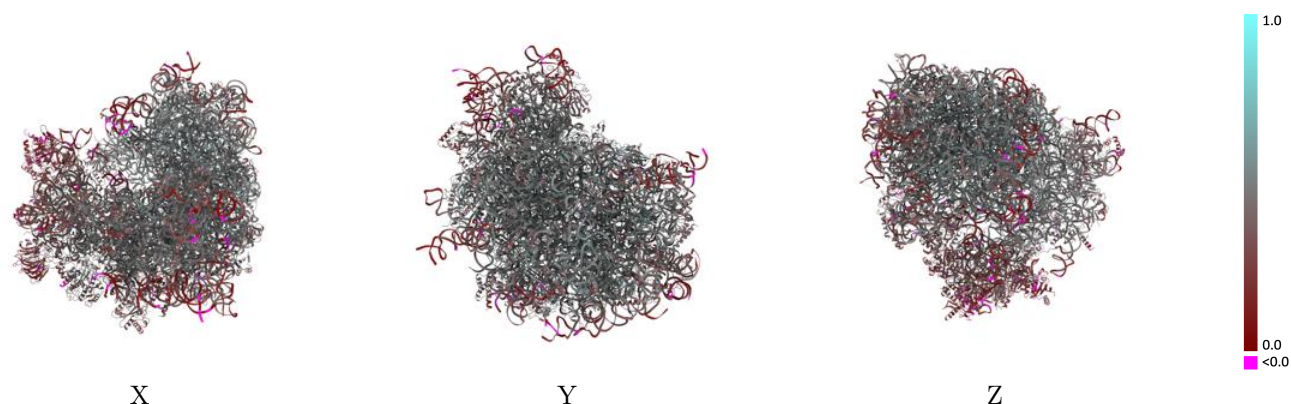
Y



Z

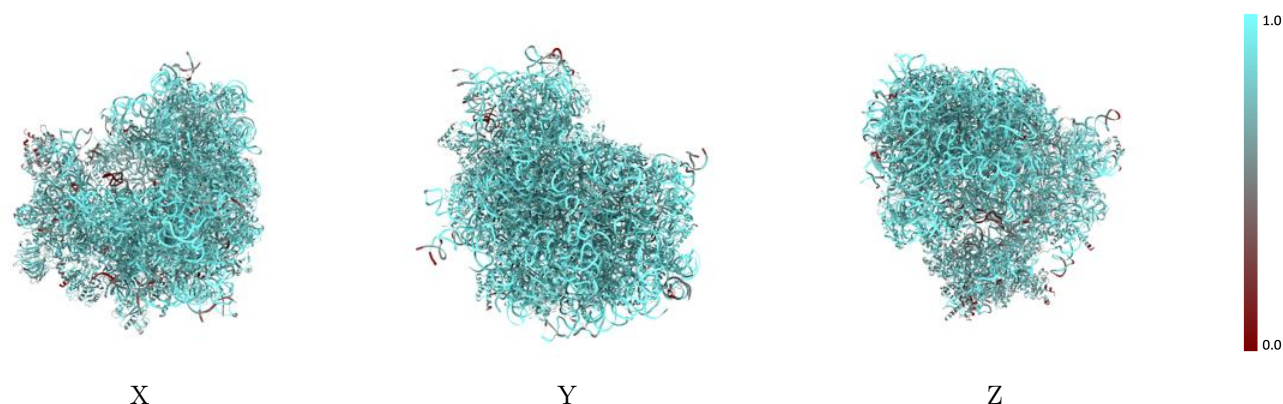
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



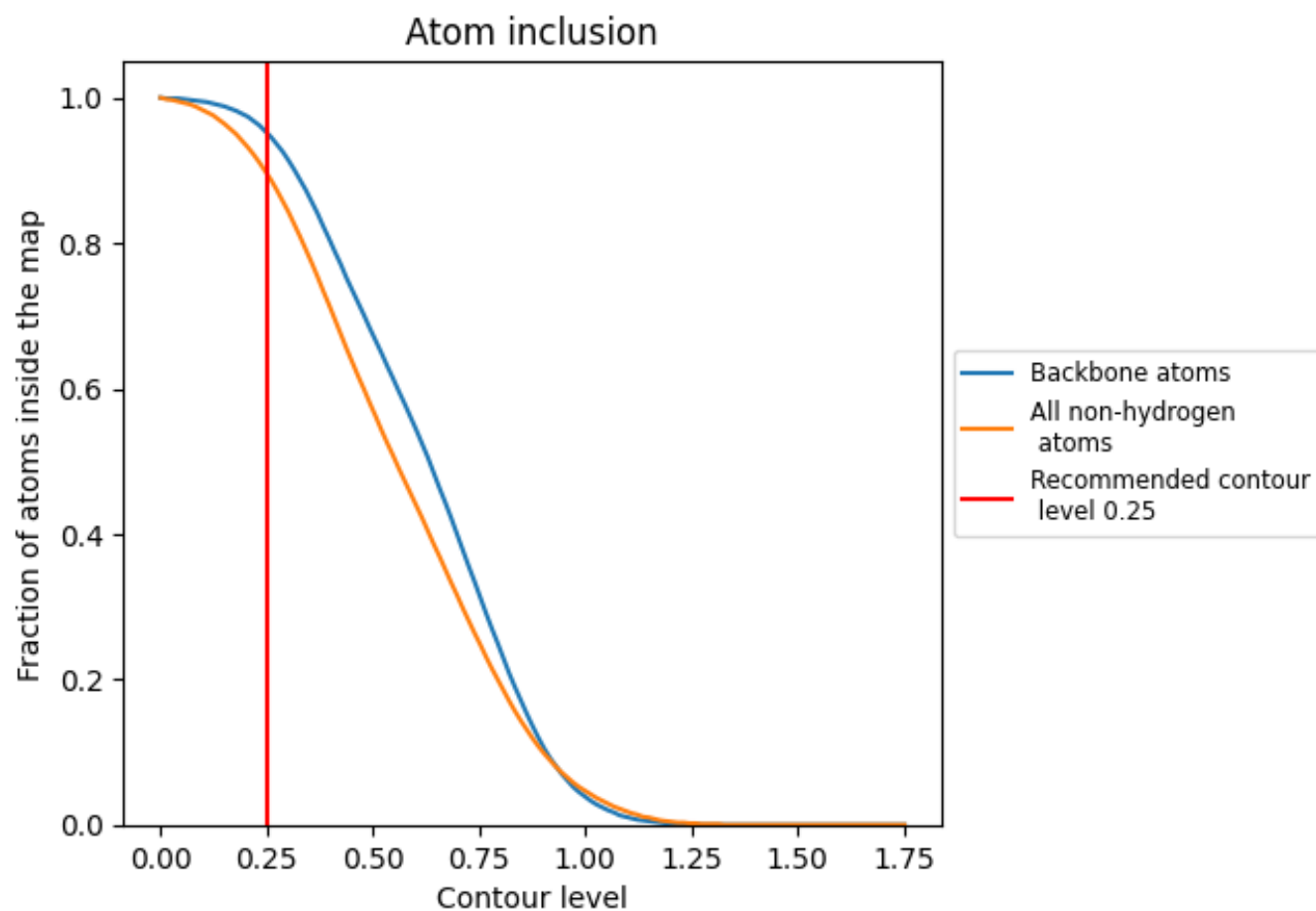
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.4280
B	 0.5320	 0.1750
I	 0.6960	 0.1580
L5	 0.9580	 0.4480
L7	 0.9920	 0.4880
L8	 0.9680	 0.4730
LD	 0.8600	 0.5080
LE	 0.8940	 0.4970
LF	 0.8860	 0.4920
LG	 0.8860	 0.4490
LH	 0.8290	 0.4210
LI	 0.8610	 0.4830
LJ	 0.8620	 0.4420
LK	 0.8690	 0.4790
LL	 0.8030	 0.4740
LM	 0.8070	 0.4090
LO	 0.8570	 0.4520
LP	 0.8970	 0.4600
LQ	 0.9190	 0.5190
LR	 0.8740	 0.4890
LS	 0.8720	 0.4930
LT	 0.8770	 0.4920
LU	 0.8710	 0.4630
LV	 0.8880	 0.5030
LW	 0.8370	 0.4790
LX	 0.8900	 0.4380
LY	 0.8280	 0.4910
LZ	 0.7810	 0.3950
La	 0.8560	 0.4730
Lb	 0.8720	 0.4800
Lc	 0.9230	 0.4830
Ld	 0.9300	 0.5100
Le	 0.7920	 0.3950
Lf	 0.7950	 0.4400
Lg	 0.8910	 0.4910



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Chain	Atom inclusion	Q-score
Lh	 0.8630	 0.4970
Li	 0.8920	 0.5140
Lj	 0.8630	 0.4790
Lk	 0.8660	 0.4640
Ll	 0.8440	 0.4370
Lm	 0.9050	 0.5140
Ln	 0.8420	 0.4420
Lo	 0.8530	 0.4670
Lp	 0.8740	 0.4850
Lq	 0.7960	 0.4680
Lr	 0.8240	 0.4830
Ls	 0.8960	 0.4910
Lx	 0.8010	 0.1730
S	 0.7810	 0.1380
S2	 0.9450	 0.4130
SB	 0.8330	 0.4410
SC	 0.6650	 0.3490
SD	 0.6800	 0.2290
SE	 0.7000	 0.3620
SF	 0.8240	 0.4520
SG	 0.7540	 0.2530
SH	 0.8170	 0.3830
SL	 0.8010	 0.4180
SM	 0.8140	 0.4400
SN	 0.8200	 0.4540
SO	 0.7080	 0.3550
SP	 0.8460	 0.4500
SQ	 0.7410	 0.3230
SR	 0.8400	 0.3770
SS	 0.7700	 0.3820
ST	 0.8460	 0.4560
SU	 0.8380	 0.4240
SV	 0.7630	 0.3430
SW	 0.7640	 0.4440
SX	 0.5510	 0.1750
SY	 0.8290	 0.4600
SZ	 0.8410	 0.4580
Sa	 0.6580	 0.3070
Sb	 0.7780	 0.3230
Sc	 0.7350	 0.3580
Sd	 0.6990	 0.2790
Se	 0.8020	 0.3240

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Chain	Atom inclusion	Q-score
Sf	 0.7700	 0.3470
Sg	 0.8360	 0.4270
Sh	 0.8330	 0.4650
Si	 0.8390	 0.4840
Sj	 0.8450	 0.3800
Sk	 0.7560	 0.2420
Sl	 0.8490	 0.4840