



wwPDB EM Validation Summary Report ⓘ

Jun 20, 2026 – 08:29 pm BST

PDB ID : 9SYR / pdb_00009syr
EMDB ID : EMD-55351
Title : Human quaternary complex of a translating 80S ribosome, NAC, MetAP1 and NatD
Authors : Yudin, D.; Jaskolowski, M.; Scaiola, A.; Ban, N.
Deposited on : 2025-10-13
Resolution : 3.55 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

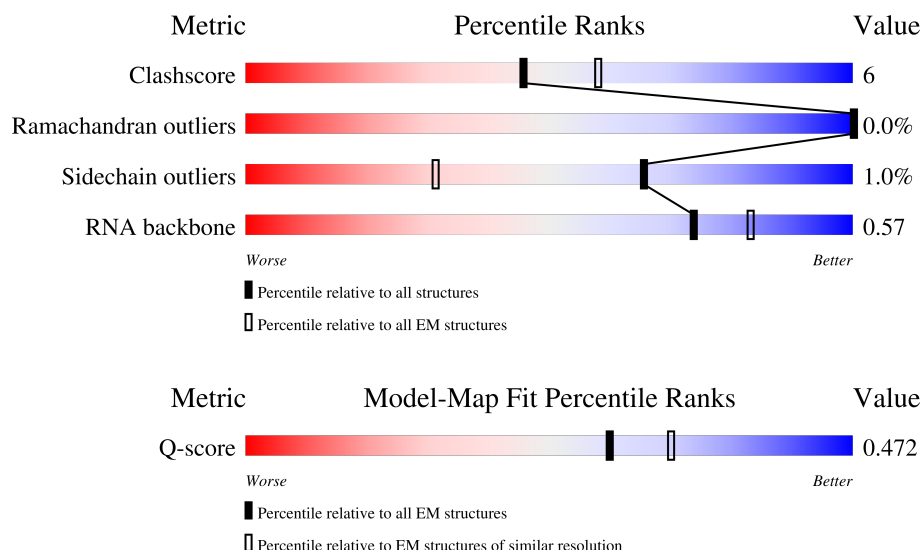
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.55 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.



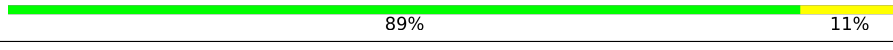
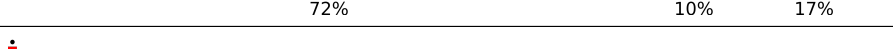
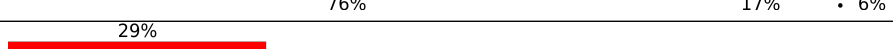
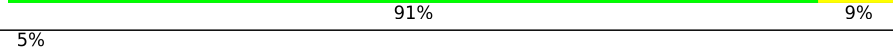
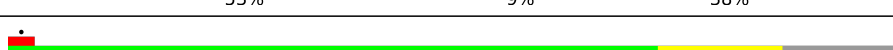
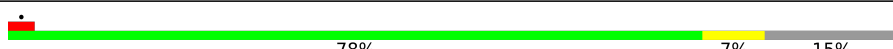
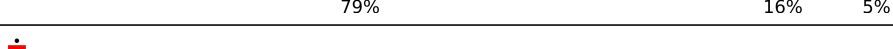
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12819 (3.05 - 4.05)

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	L1	5070	
2	Lc	427	
3	Ld	297	

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Mol	Chain	Length	Quality of chain
4	Le	288	
5	Lf	199	
6	Lg	184	
7	Lh	188	
8	Li	196	
9	Lj	176	
10	Lk	160	
11	Ll	128	
12	Lm	140	
13	Ln	157	
14	Lo	156	
15	Lp	145	
16	Lq	136	
17	Lr	148	
18	Ls	159	
19	Lt	115	
20	Lu	125	
21	Lv	135	
22	Lw	110	
23	Lx	117	
24	Ly	123	
25	Lz	105	
26	Na	238	
27	Nb	162	
28	Nd	365	

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Mol	Chain	Length	Quality of chain
29	Nm	386	
30	S1	1869	
31	S2	1824	
32	S3	76	
33	SA	208	
34	SB	194	
35	SC	204	
36	SD	158	
37	SE	165	
38	SF	151	
39	SG	151	
40	SH	132	
41	Sa	152	
42	Sb	135	
43	Sc	146	
44	Sd	152	
45	Se	84	
46	Sf	130	
47	Sg	143	
48	L2	121	
49	Sh	131	
50	Si	145	
51	Sj	115	
52	Sk	84	
53	Sl	119	

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Mol	Chain	Length	Quality of chain
54	Sm	125	
55	Sn	133	
56	So	69	
57	Sp	56	
58	Sq	25	
59	Sr	156	
60	Ss	317	
61	St	295	
62	Su	264	
63	Sv	293	
64	Sw	263	
65	Sx	243	
66	Sy	249	
67	Sz	194	
68	L3	157	
69	LA	97	
70	LB	70	
71	LC	51	
72	LD	99	
73	LE	106	
74	LF	92	
75	LG	137	
76	LH	204	
77	LI	248	
78	LJ	266	

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Mol	Chain	Length	Quality of chain
79	LK	192	 86% 12%
80	LM	214	 5% 83% 16%
81	LN	414	 7% 91%
82	LO	178	 78% 17%
83	LP	211	 87% 10%
84	LQ	215	 55% 9% 35%
85	La	257	 82% 14%
86	Lb	403	 86% 12%

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 217377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	3403	Total	C	N	O	P	1	0
			73061	32575	13368	23714	3404		

- Molecule 2 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Lc	363	Total	C	N	O	S	0	0
			2890	1818	577	482	13		

- Molecule 3 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ld	292	Total	C	N	O	S	0	0
			2372	1503	431	424	14		

- Molecule 4 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Le	218	Total	C	N	O	S	0	0
			1752	1128	333	287	4		

- Molecule 5 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Lf	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 6 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Lg	152	Total	C	N	O	S	0	0
			1233	771	240	213	9		

- Molecule 7 is a protein called 60S ribosomal protein L18.

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

- Molecule 8 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Li	180	Total	C	N	O	S	0	0
			1501	929	327	236	9		

- Molecule 9 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Lj	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 10 is a protein called 60S ribosomal protein L21.

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

- Molecule 11 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ll	102	Total	C	N	O	S	0	0
			833	533	146	152	2		

- Molecule 12 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Lm	132	Total	C	N	O	S	0	0
			985	621	185	174	5		

- Molecule 13 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Ln	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 14 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Lo	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 15 is a protein called 60S ribosomal protein L26.

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

- Molecule 16 is a protein called 60S ribosomal protein L27.

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

- Molecule 17 is a protein called 60S ribosomal protein L27a.

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

- Molecule 18 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ls	99	Total	C	N	O	S	0	0
			806	500	177	125	4		

- Molecule 19 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Lt	100	Total	C	N	O	S	0	0
			772	490	136	139	7		

- Molecule 20 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Lu	106	Total	C	N	O	S	0	0
			868	551	170	145	2		

- Molecule 21 is a protein called 60S ribosomal protein L32.

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

- Molecule 22 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Lw	109	Total	C	N	O	S	1	0
			879	557	174	144	4		

- Molecule 23 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Lx	111	Total	C	N	O	S	0	0
			882	552	182	142	6		

- Molecule 24 is a protein called 60S ribosomal protein L35.

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

- Molecule 25 is a protein called 60S ribosomal protein L36.

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

- Molecule 26 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Na	108	Total	C	N	O	S	0	0
			840	524	153	159	4		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Na	-22	MET	-	initiating methionine	UNP Q13765
Na	-21	GLY	-	expression tag	UNP Q13765
Na	-20	SER	-	expression tag	UNP Q13765
Na	-19	SER	-	expression tag	UNP Q13765
Na	-18	HIS	-	expression tag	UNP Q13765
Na	-17	HIS	-	expression tag	UNP Q13765

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Chain	Residue	Modelled	Actual	Comment	Reference
Na	-16	HIS	-	expression tag	UNP Q13765
Na	-15	HIS	-	expression tag	UNP Q13765
Na	-14	HIS	-	expression tag	UNP Q13765
Na	-13	HIS	-	expression tag	UNP Q13765
Na	-12	SER	-	expression tag	UNP Q13765
Na	-11	SER	-	expression tag	UNP Q13765
Na	-10	GLY	-	expression tag	UNP Q13765
Na	-9	LEU	-	expression tag	UNP Q13765
Na	-8	GLU	-	expression tag	UNP Q13765
Na	-7	VAL	-	expression tag	UNP Q13765
Na	-6	LEU	-	expression tag	UNP Q13765
Na	-5	PHE	-	expression tag	UNP Q13765
Na	-4	GLN	-	expression tag	UNP Q13765
Na	-3	GLY	-	expression tag	UNP Q13765
Na	-2	PRO	-	expression tag	UNP Q13765
Na	-1	SER	-	expression tag	UNP Q13765
Na	0	GLY	-	expression tag	UNP Q13765

- Molecule 27 is a protein called Isoform 2 of Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Nb	120	Total	C	N	O	S	0	0
			934	580	168	182	4		

- Molecule 28 is a protein called Ubiquitin-like protein SMT3,N-alpha-acetyltransferase 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Nd	236	Total	C	N	O	S	0	0
			1890	1182	337	353	18		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Nd	-127	MET	-	initiating methionine	UNP Q12306
Nd	-126	GLY	-	expression tag	UNP Q12306
Nd	-125	SER	-	expression tag	UNP Q12306
Nd	-124	SER	-	expression tag	UNP Q12306
Nd	-123	HIS	-	expression tag	UNP Q12306
Nd	-122	HIS	-	expression tag	UNP Q12306
Nd	-121	HIS	-	expression tag	UNP Q12306
Nd	-120	HIS	-	expression tag	UNP Q12306
Nd	-119	HIS	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
Nd	-118	HIS	-	expression tag	UNP Q12306
Nd	-117	SER	-	expression tag	UNP Q12306
Nd	-116	SER	-	expression tag	UNP Q12306
Nd	-115	GLY	-	expression tag	UNP Q12306
Nd	-114	LEU	-	expression tag	UNP Q12306
Nd	-113	VAL	-	expression tag	UNP Q12306
Nd	-112	PRO	-	expression tag	UNP Q12306
Nd	-111	ARG	-	expression tag	UNP Q12306
Nd	-110	GLY	-	expression tag	UNP Q12306
Nd	-109	SER	-	expression tag	UNP Q12306
Nd	-108	HIS	-	expression tag	UNP Q12306
Nd	-107	MET	-	expression tag	UNP Q12306
Nd	-106	ALA	-	expression tag	UNP Q12306
Nd	-105	SER	-	expression tag	UNP Q12306
Nd	-104	MET	-	expression tag	UNP Q12306
Nd	-103	THR	-	expression tag	UNP Q12306
Nd	-102	GLY	-	expression tag	UNP Q12306
Nd	-101	GLY	-	expression tag	UNP Q12306
Nd	-100	GLN	-	expression tag	UNP Q12306
Nd	-99	GLN	-	expression tag	UNP Q12306
Nd	-98	MET	-	expression tag	UNP Q12306
Nd	-97	GLY	-	expression tag	UNP Q12306
Nd	-96	ARG	-	expression tag	UNP Q12306
Nd	-95	GLY	-	expression tag	UNP Q12306
Nd	-94	SER	-	expression tag	UNP Q12306

- Molecule 29 is a protein called Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Nm	380	Total	C	N	O	S	0	0
			2984	1870	532	558	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Nm	220	ASN	ASP	engineered mutation	UNP P53582

- Molecule 30 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S1	1771	Total	C	N	O	P	0	0
			37855	16922	6786	12376	1771		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S2	7	Total	C	N	O	P	0	0
			148	66	24	51	7		

- Molecule 32 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S3	74	Total	C	N	O	P	0	0
			1579	704	284	517	74		

- Molecule 33 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SA	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 34 is a protein called 40S ribosomal protein S9.

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

- Molecule 35 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SC	192	Total	C	N	O	S	0	0
			1517	948	287	275	7		

- Molecule 36 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SD	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 37 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SE	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 38 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SF	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 39 is a protein called 40S ribosomal protein S14.

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SH	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 41 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Sa	124	Total	C	N	O	S	0	0
			1016	644	192	173	7		

- Molecule 42 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Sb	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 43 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Sc	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 44 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Sd	146	Total	C	N	O	S	0	0
			1200	753	242	204	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Sd	2	ACE	-	acetylation	UNP P62269

- Molecule 45 is a protein called Small ribosomal subunit protein eS21.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 46 is a protein called 40S ribosomal protein S15a.

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

- Molecule 47 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 48 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L2	118	Total	C	N	O	P	0	0
			2518	1122	449	829	118		

- Molecule 49 is a protein called Isoform 3 of Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Sh	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 50 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Si	144	Total	C	N	O	S	0	0
			1123	704	217	199	3		

- Molecule 51 is a protein called 40S ribosomal protein S26.

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

- Molecule 52 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Sk	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 53 is a protein called 40S ribosomal protein S20.

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

- Molecule 54 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Sm	83	Total	C	N	O	S	0	0
			670	431	125	113	1		

- Molecule 55 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Sn	59	Total	C	N	O	S	0	0
			467	290	102	74	1		

- Molecule 56 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	So	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 57 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Sp	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 58 is a protein called 60S ribosomal protein L41.

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

- Molecule 59 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Sr	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 60 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Ss	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 61 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	St	223	Total	C	N	O	S	0	0
			1750	1111	306	325	8		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 62 is a protein called 40S ribosomal protein S3a.

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

- Molecule 63 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sv	223	Total	C	N	O	S	1	0
			1741	1124	300	307	10		

- Molecule 64 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 65 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Sx	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 66 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sy	240	Total	C	N	O	S	0	0
			1945	1212	393	333	7		

- Molecule 67 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Sz	189	Total	C	N	O	S	0	0
			1523	972	280	270	1		

- Molecule 68 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	L3	148	Total	C	N	O	P	0	0
			3156	1408	563	1037	148		

- Molecule 69 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	LA	86	Total	C	N	O	S	1	0
			713	442	155	111	5		

- Molecule 70 is a protein called 60S ribosomal protein L38.

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

- Molecule 71 is a protein called 60S ribosomal protein L39.

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

- Molecule 72 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	LD	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 73 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	LE	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 74 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	LF	92	Total	C	N	O	S	0	0
			716	450	137	121	8		

- Molecule 75 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	LG	124	Total	C	N	O	S	0	0
			992	615	206	167	4		

- Molecule 76 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	LH	203	Total	C	N	O	S	1	0
			1708	1077	360	267	4		

- Molecule 77 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	LI	223	Total	C	N	O	S	0	0
			1851	1189	355	298	9		

- Molecule 78 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	LJ	223	Total	C	N	O	S	0	0
			1809	1153	349	303	4		

- Molecule 79 is a protein called 60S ribosomal protein L9.

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

- Molecule 80 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	LM	213	Total	C	N	O	S	0	0
			1716	1086	331	285	14		

- Molecule 81 is a protein called Green fluorescent protein,Small ubiquitin-related modifier 1,Green fluorescent protein,Small ubiquitin-related modifier 1,Histone H4,X-box-binding protein 1,X-box-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	LN	39	Total	C	N	O	S	0	0
			316	203	62	48	3		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LN	-4	MET	-	initiating methionine	UNP P42212
LN	-3	ALA	-	expression tag	UNP P42212
LN	-2	ALA	-	expression tag	UNP P42212
LN	-1	ALA	-	expression tag	UNP P42212
LN	0	THR	-	expression tag	UNP P42212
LN	1	MET	-	expression tag	UNP P42212
LN	2	VAL	-	expression tag	UNP P42212
LN	65	LEU	PHE	conflict	UNP P42212
LN	66	THR	SER	conflict	UNP P42212
LN	222	LYS	LEU	conflict	UNP P42212

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Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LN	232	GLY	-	linker	UNP P42212
LN	233	SER	-	linker	UNP P42212
LN	234	GLY	-	linker	UNP P42212
LN	235	SER	-	linker	UNP P42212
LN	236	GLY	-	linker	UNP P42212
LN	237	SER	-	linker	UNP P42212
LN	238	GLY	-	linker	UNP P42212
LN	239	SER	-	linker	UNP P42212
LN	240	GLY	-	linker	UNP P42212
LN	241	SER	-	linker	UNP P42212
LN	242	GLY	-	linker	UNP P42212
LN	243	SER	-	linker	UNP P42212
LN	244	GLY	-	linker	UNP P42212
LN	245	SER	-	linker	UNP P42212
LN	246	GLY	-	linker	UNP P42212
LN	247	SER	-	linker	UNP P42212
LN	248	GLY	-	linker	UNP P42212
LN	249	SER	-	linker	UNP P42212
LN	250	GLY	-	linker	UNP P42212
LN	251	SER	-	linker	UNP P42212
LN	252	GLY	-	linker	UNP P42212
LN	253	SER	-	linker	UNP P42212
LN	254	SER	-	linker	UNP P42212
LN	255	ALA	-	linker	UNP P42212
LN	256	ALA	-	linker	UNP P42212
LN	257	GLY	-	linker	UNP P42212
LN	312	LYS	ASN	conflict	UNP P55857
LN	319	LYS	ASP	conflict	UNP P55857
LN	325	ALA	GLY	conflict	UNP P55857
LN	327	ARG	GLN	conflict	UNP P55857
LN	403	CYS	PRO	conflict	UNP B1AHH2
LN	404	ALA	SER	conflict	UNP B1AHH2

- Molecule 82 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	LO	170	Total	C	N	O	S	0	0
			1358	858	253	241	6		

- Molecule 83 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	LP	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 84 is a protein called 60S ribosomal protein L14.

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

- Molecule 85 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	La	246	Total	C	N	O	S	0	0
			1887	1183	387	311	6		

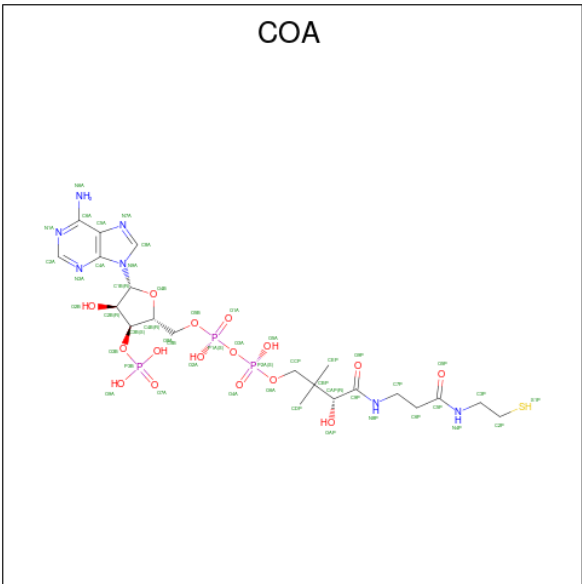
- Molecule 86 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Lb	395	Total	C	N	O	S	1	0
			3194	2034	600	545	15		

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

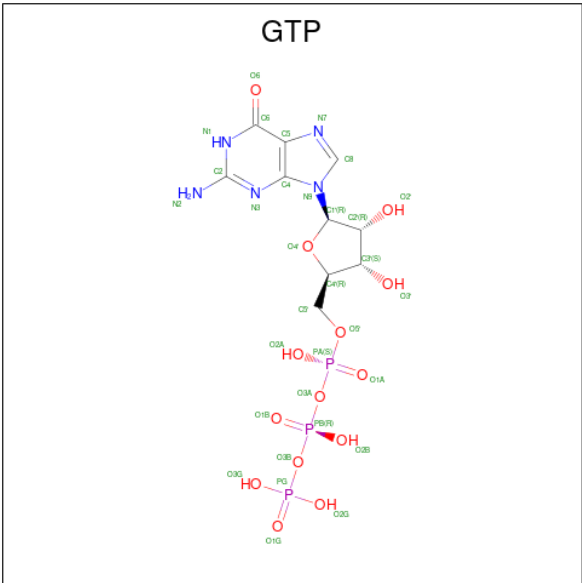
Mol	Chain	Residues	Atoms		AltConf
87	Lx	1	Total	Zn	0
			1	1	
87	Nm	2	Total	Zn	0
			2	2	
87	Sj	1	Total	Zn	0
			1	1	
87	Sp	1	Total	Zn	0
			1	1	
87	Sr	1	Total	Zn	0
			1	1	
87	LA	1	Total	Zn	0
			1	1	
87	LD	1	Total	Zn	0
			1	1	
87	LE	1	Total	Zn	0
			1	1	
87	LF	1	Total	Zn	0
			1	1	

- Molecule 88 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						AltConf
88	Nd	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

- Molecule 89 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

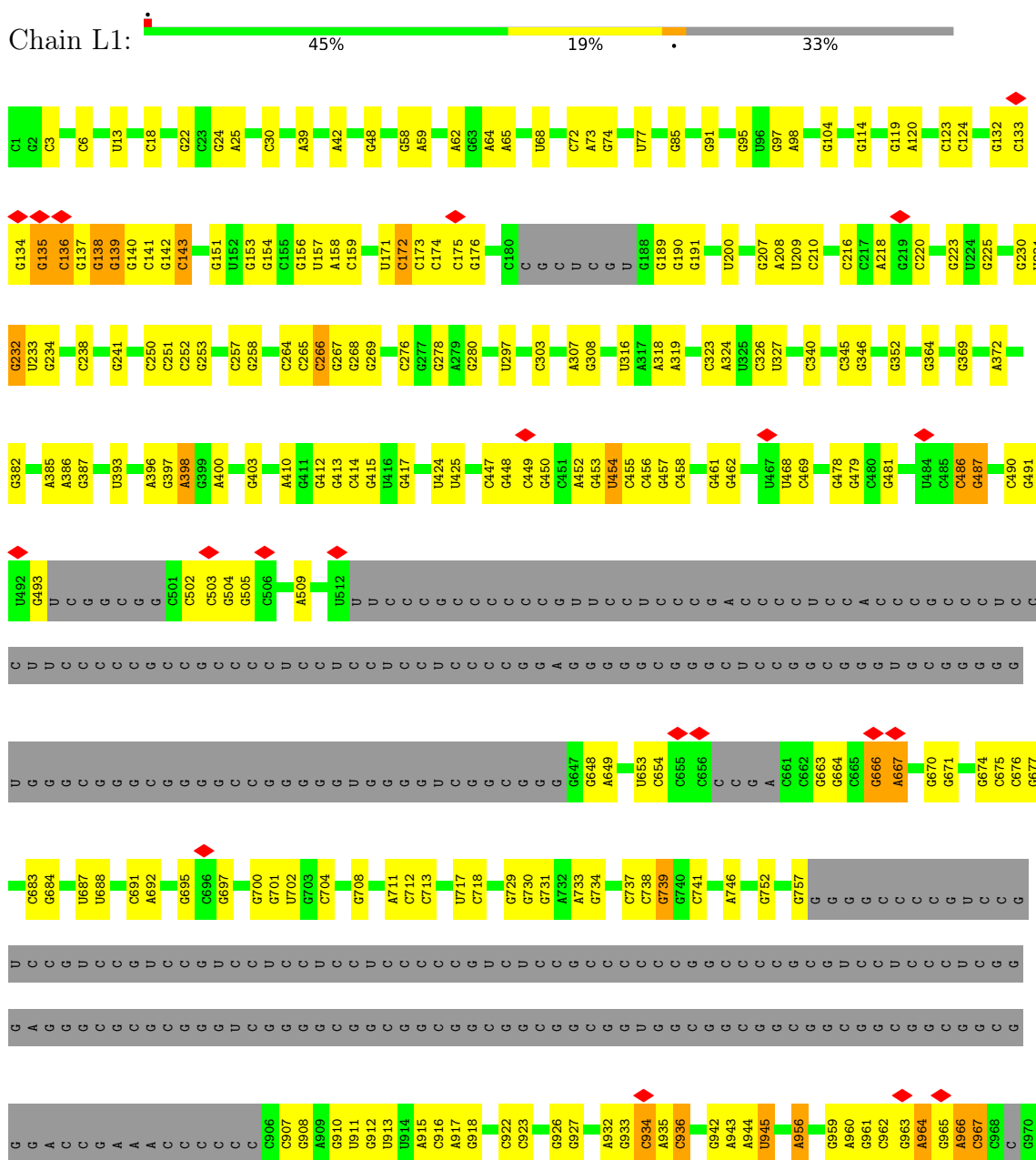


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
89	L2	1	32	10	5	14	3	0

3 Residue-property plots [i](#)

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

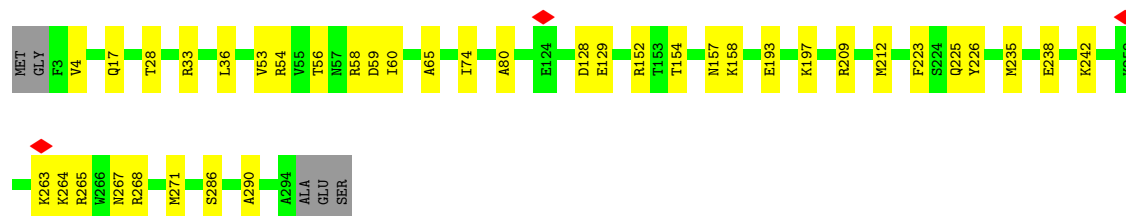
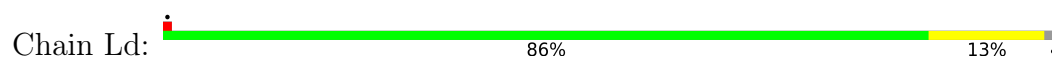
• Molecule 1: 28S rRNA



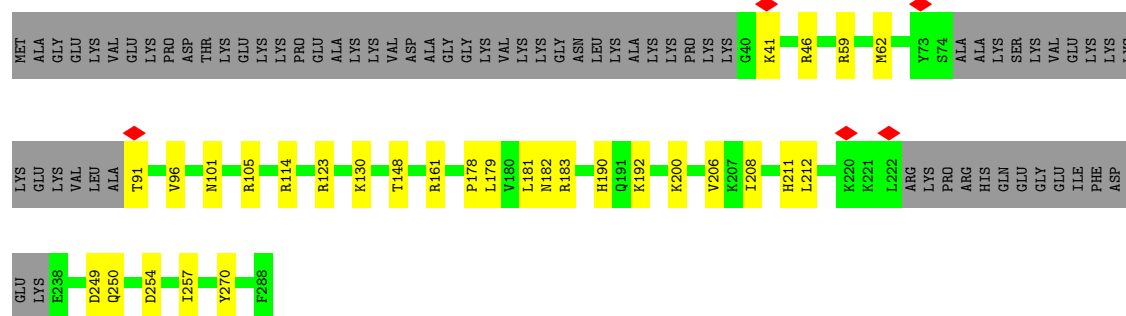




- Molecule 3: 60S ribosomal protein L5



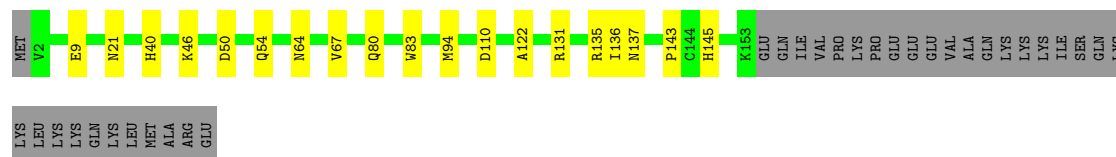
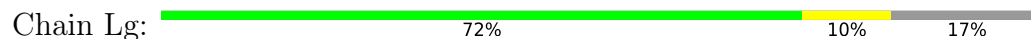
- Molecule 4: Large ribosomal subunit protein eL6



- Molecule 5: Large ribosomal subunit protein uL13



- Molecule 6: 60S ribosomal protein L17



- Molecule 7: 60S ribosomal protein L18

Chain Lh:  87% 12% ..



- Molecule 8: 60S ribosomal protein L19

Chain Li:  81% 11% . 8%



- Molecule 9: 60S ribosomal protein L18a

Chain Lj:  89% 11%



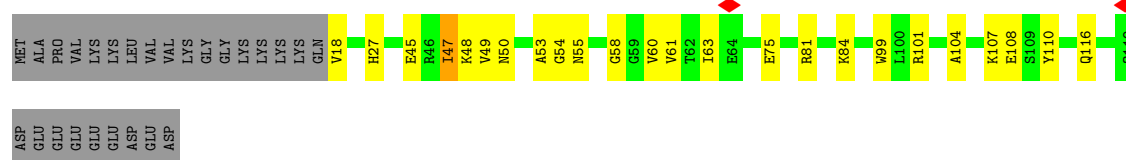
- Molecule 10: 60S ribosomal protein L21

Chain Lk:  82% 17% .



- Molecule 11: 60S ribosomal protein L22

Chain Ll:  61% 18% . 20%



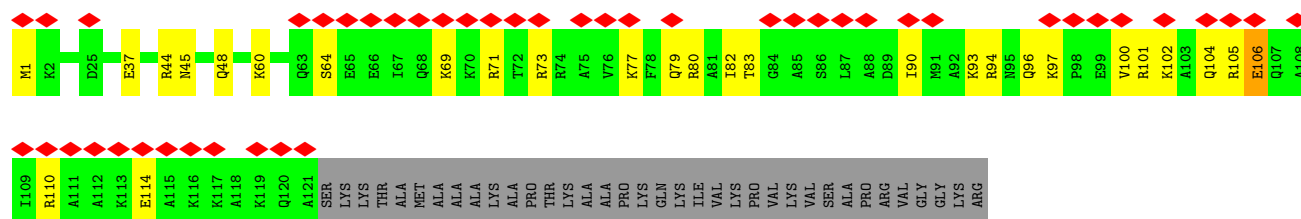
- Molecule 12: 60S ribosomal protein L23

Chain Lm:  76% 17% . 6%

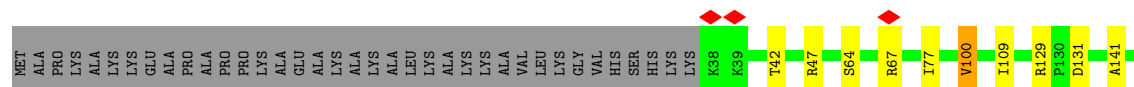


- Molecule 13: 60S ribosomal protein L24

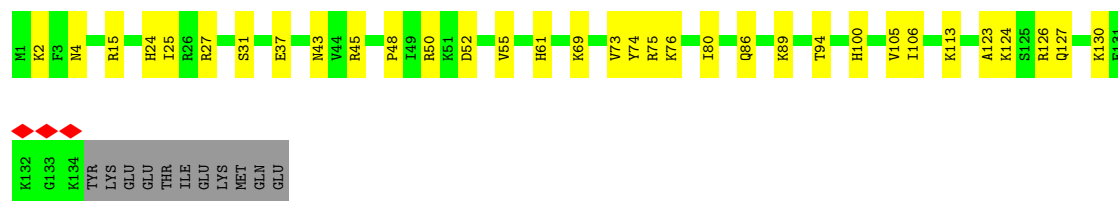
Chain Ln:  29% 59% 17% 23%



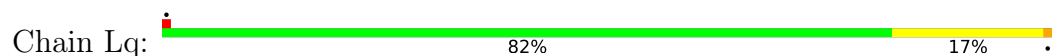
- Molecule 14: 60S ribosomal protein L23a



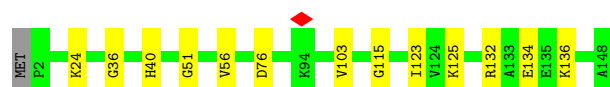
- Molecule 15: 60S ribosomal protein L26



- Molecule 16: 60S ribosomal protein L27

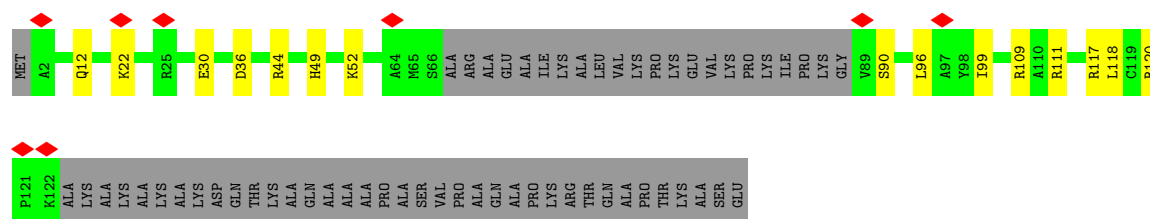


- Molecule 17: 60S ribosomal protein L27a

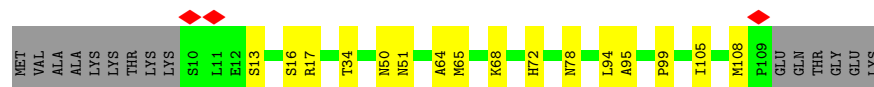
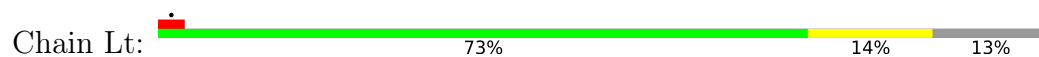


- Molecule 18: 60S ribosomal protein L29

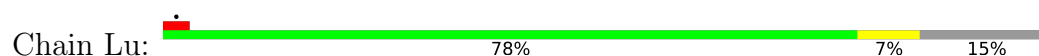




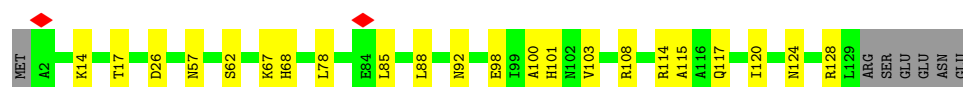
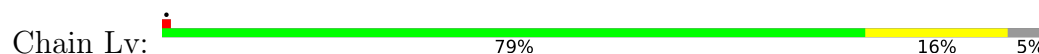
- Molecule 19: 60S ribosomal protein L30



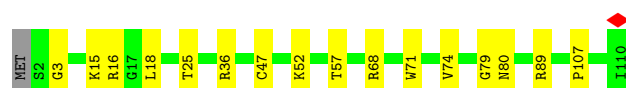
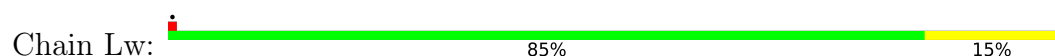
- Molecule 20: 60S ribosomal protein L31



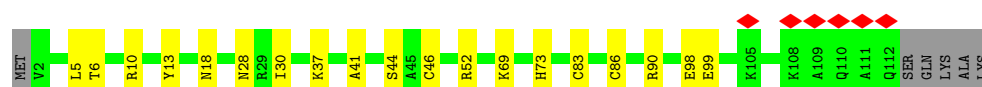
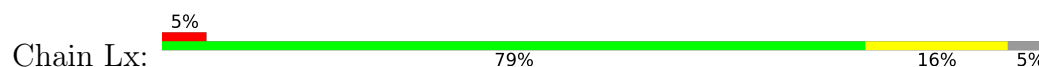
- Molecule 21: 60S ribosomal protein L32



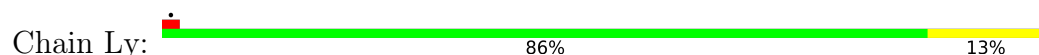
- Molecule 22: 60S ribosomal protein L35a



- Molecule 23: 60S ribosomal protein L34

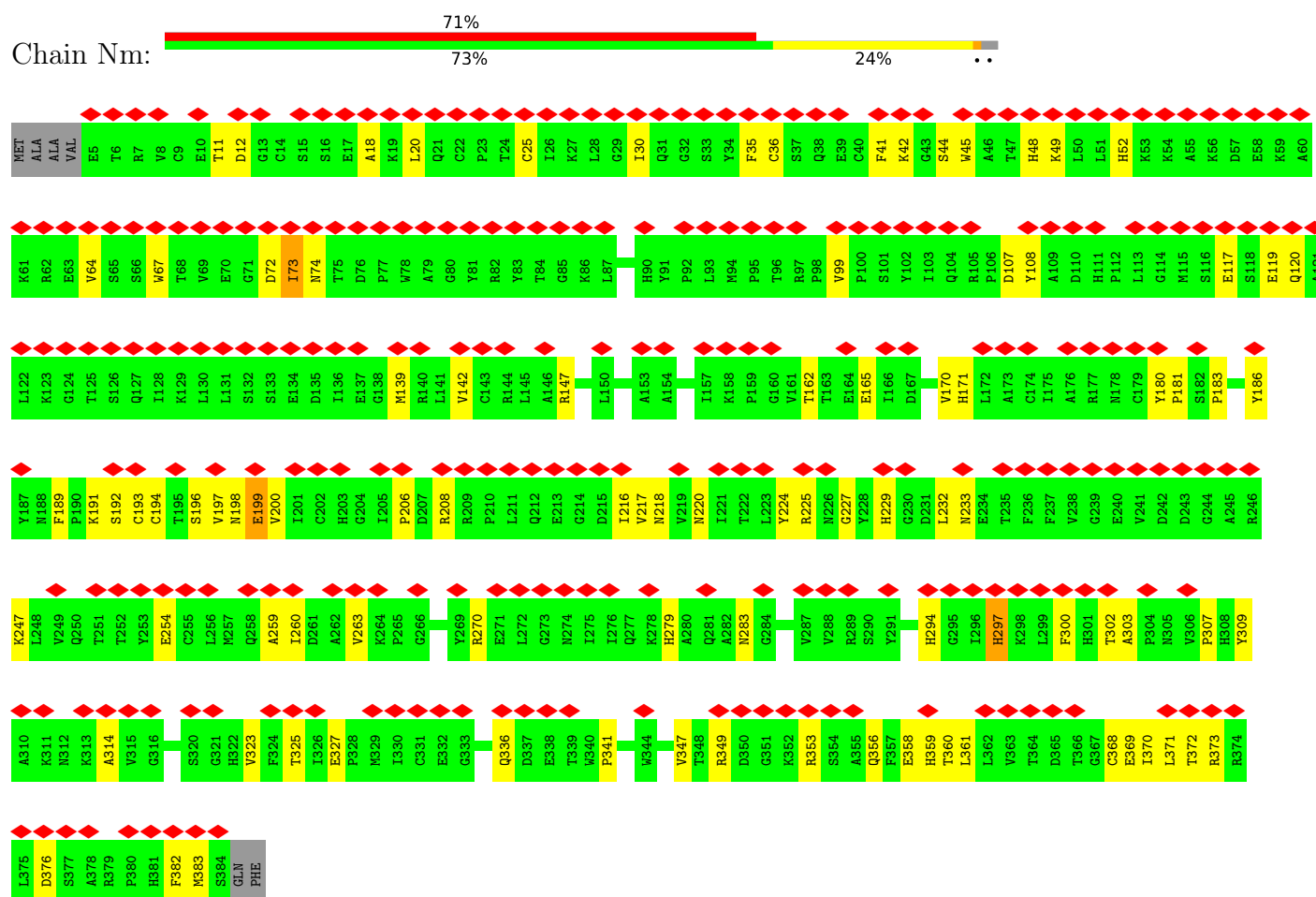


- Molecule 24: 60S ribosomal protein L35

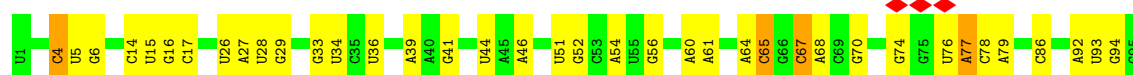


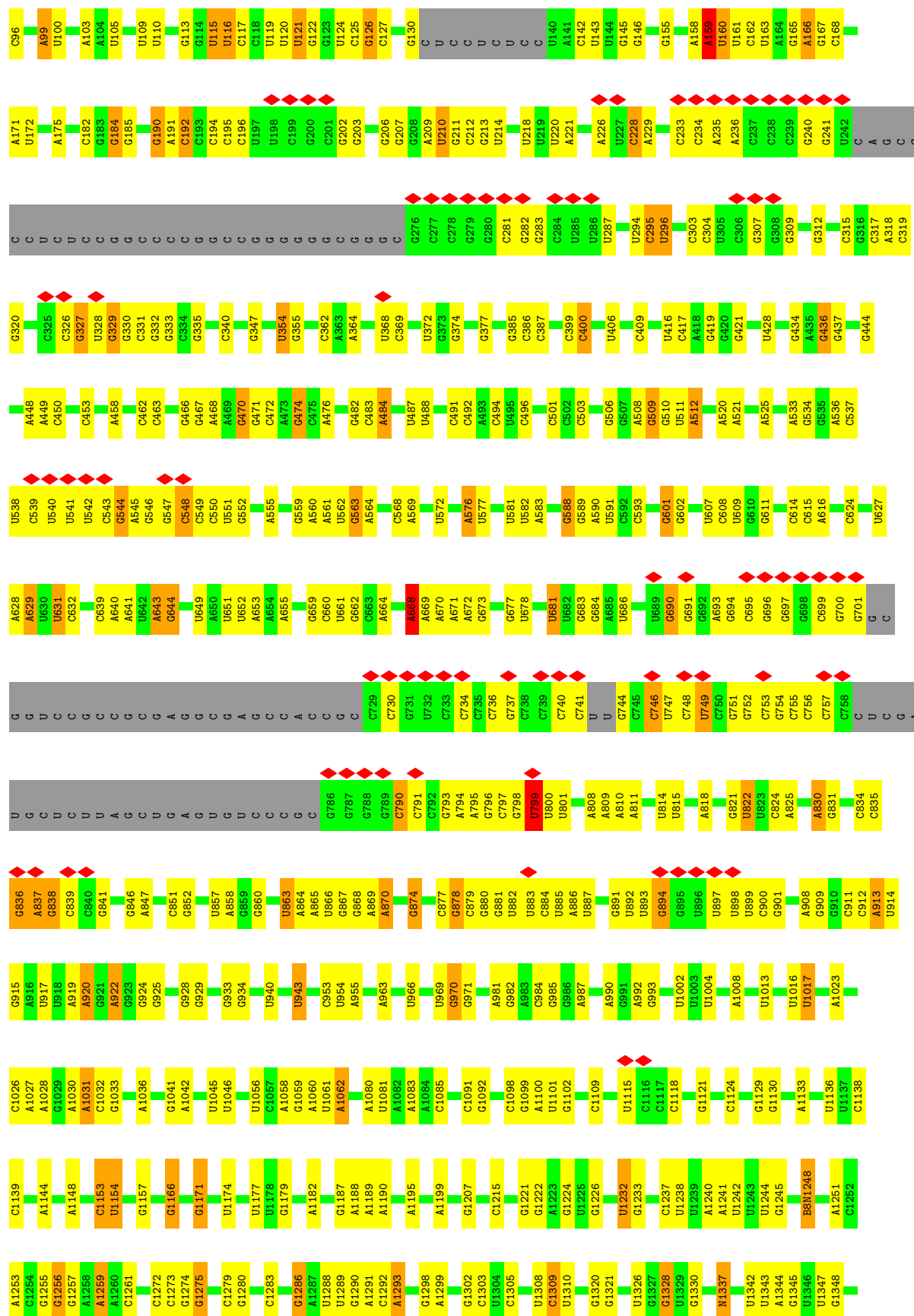


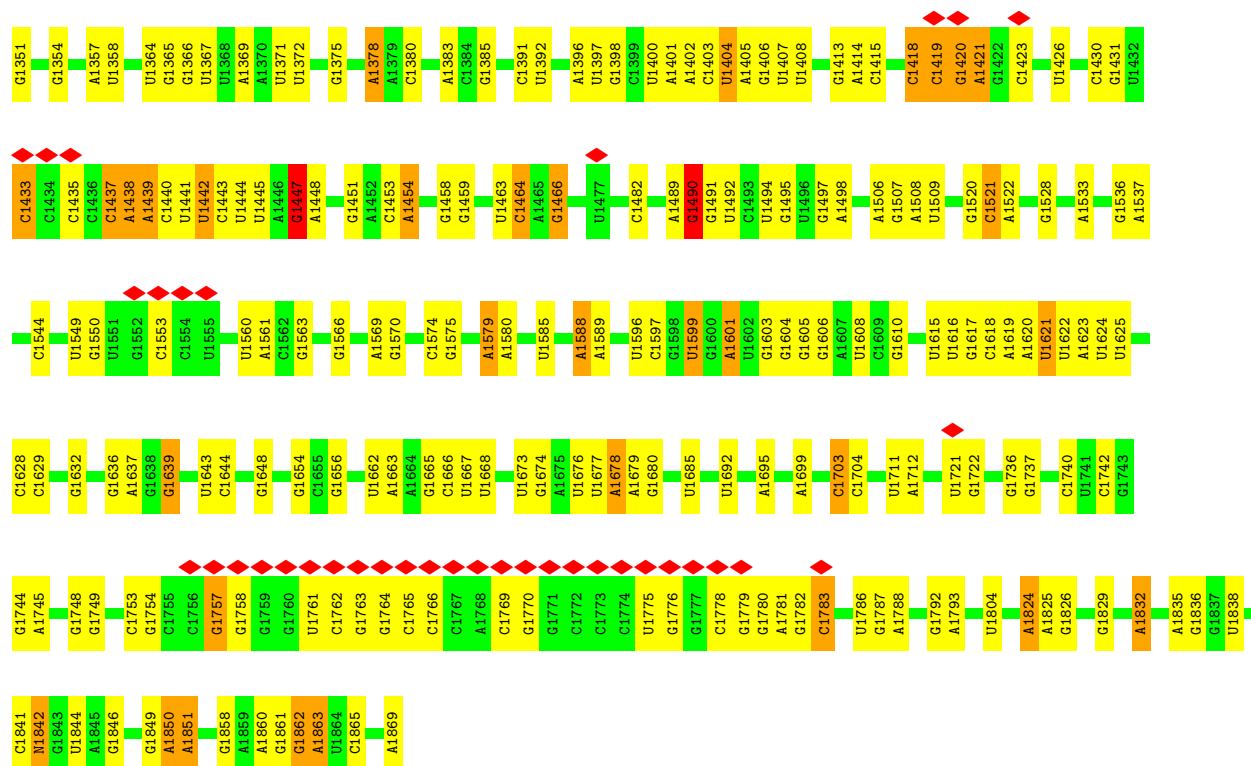
- Molecule 29: Methionine aminopeptidase 1



- Molecule 30: 18S rRNA



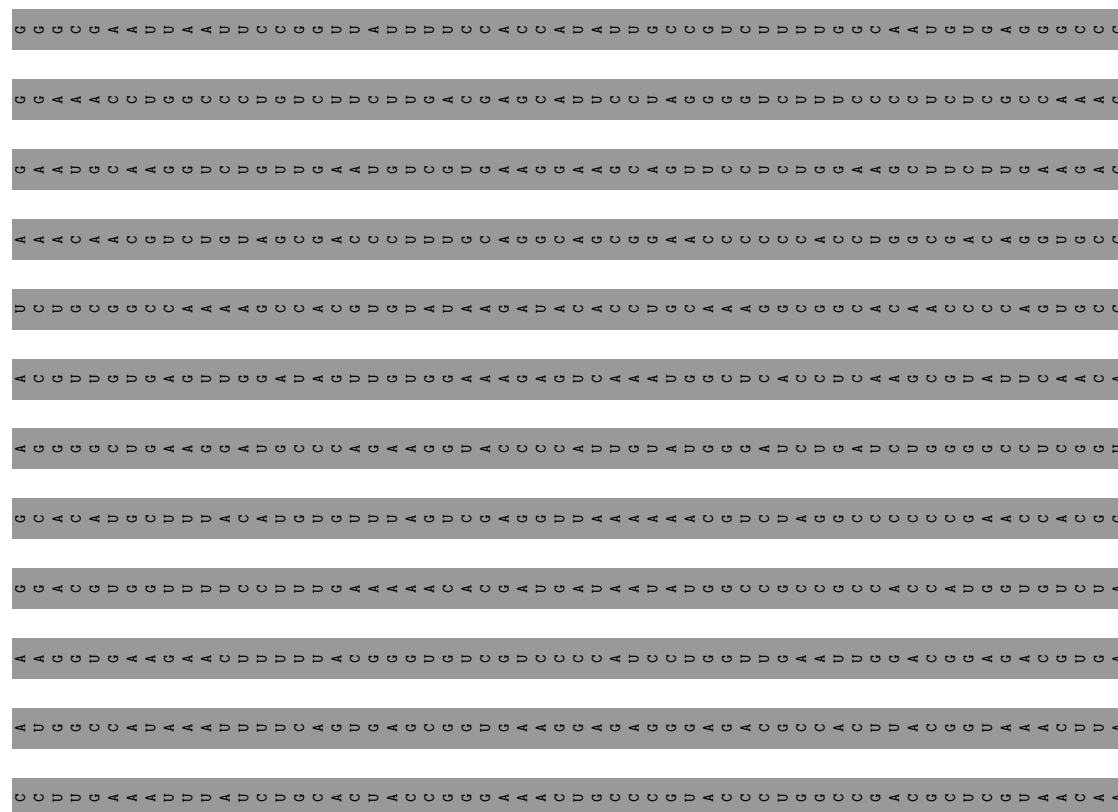


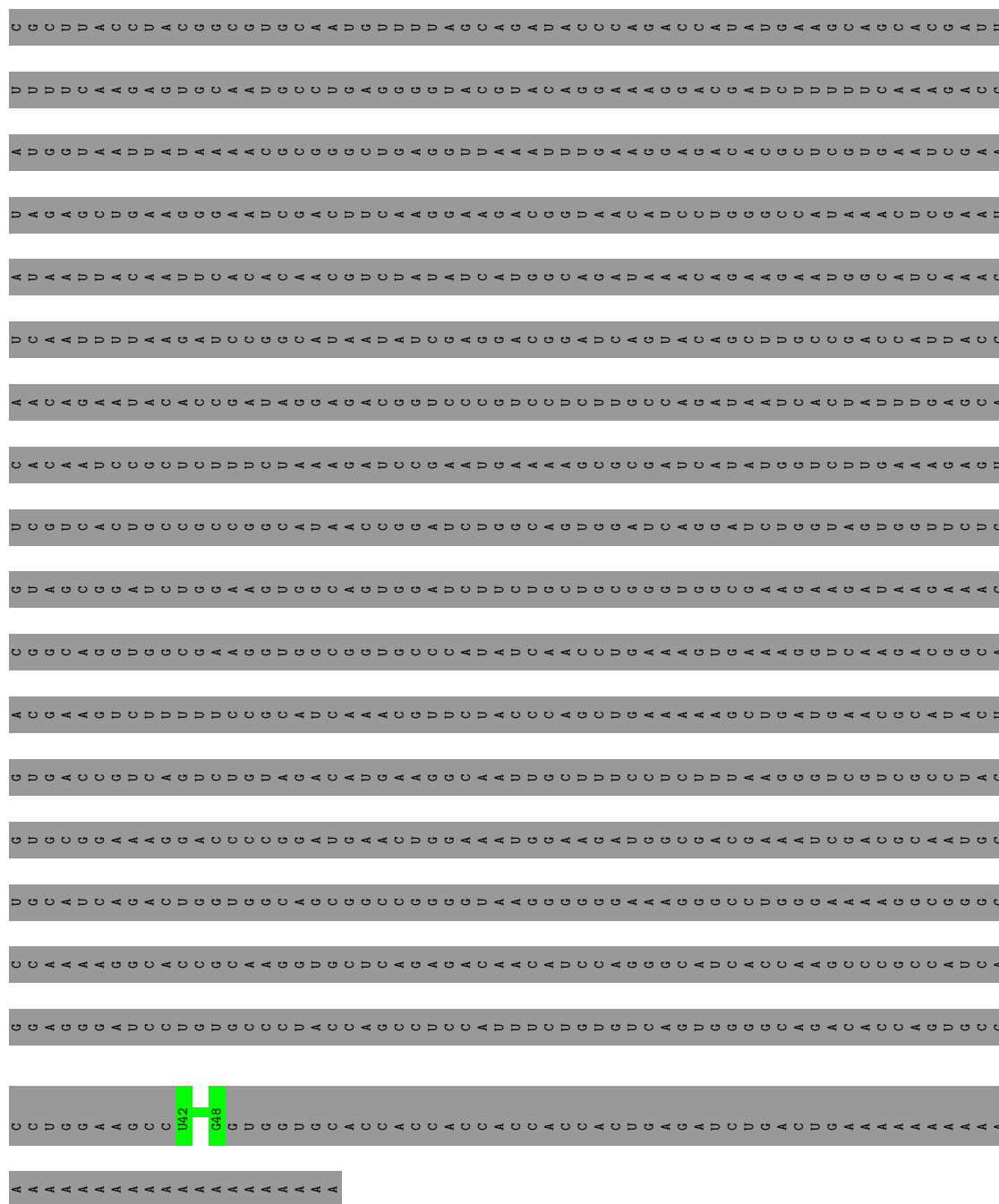


• Molecule 31: mRNA

Chain S2:

100%

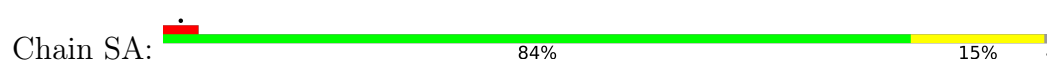




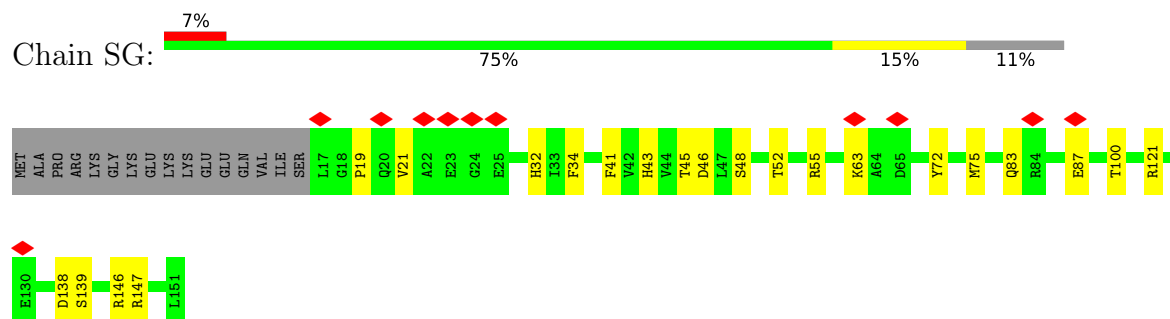
- Molecule 32: tRNA



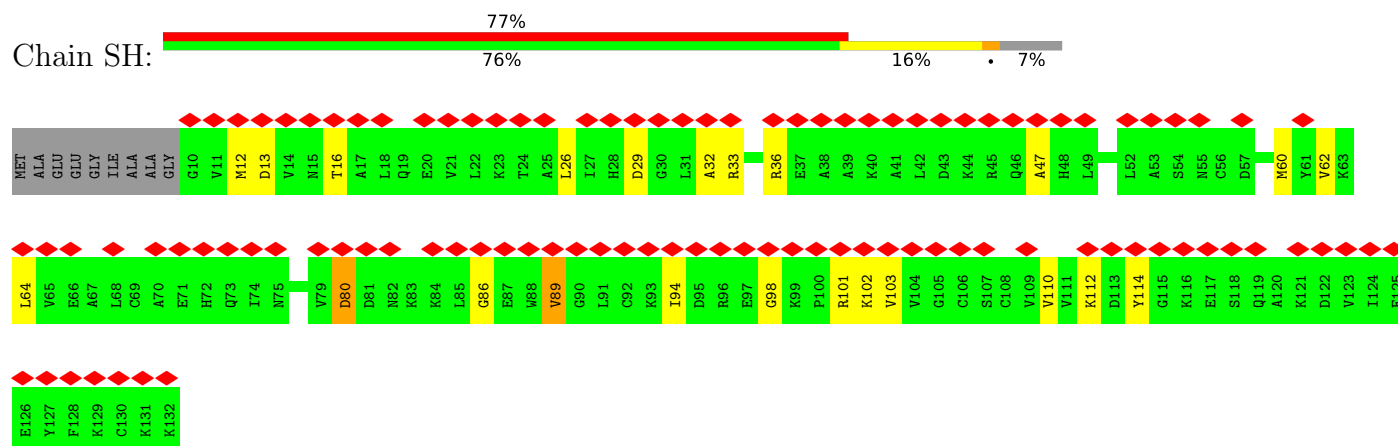
- Molecule 33: 40S ribosomal protein S8



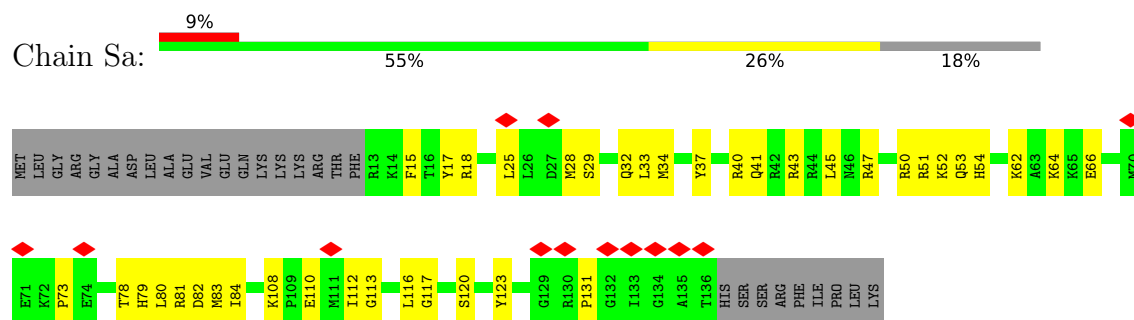
- Molecule 39: 40S ribosomal protein S14



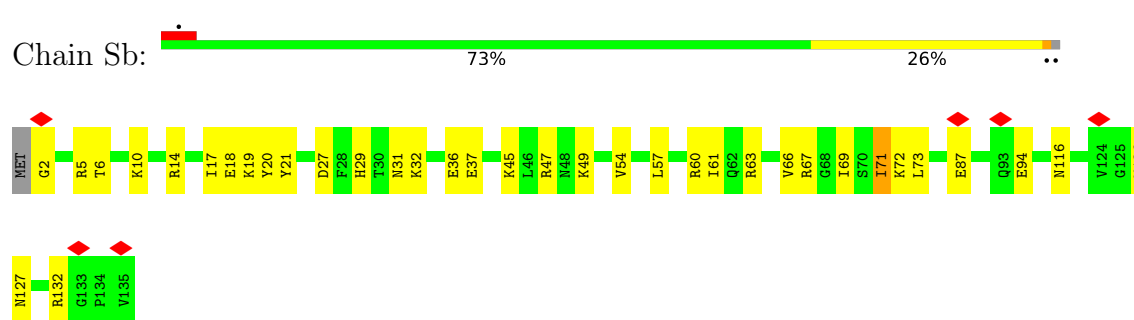
- Molecule 40: 40S ribosomal protein S12



- Molecule 41: 40S ribosomal protein S15

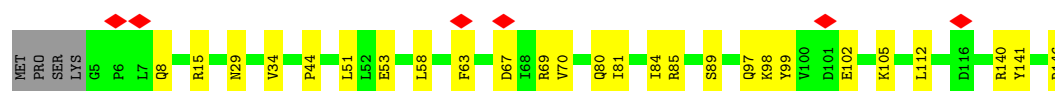


- Molecule 42: 40S ribosomal protein S17



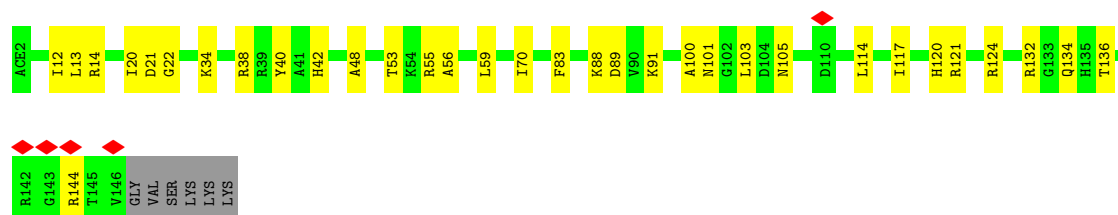
- Molecule 43: 40S ribosomal protein S16

Chain Sc:  79% 18%



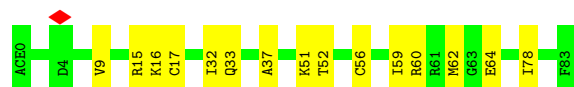
- Molecule 44: Small ribosomal subunit protein uS13

Chain Sd:  74% 22%



- Molecule 45: Small ribosomal subunit protein eS21

Chain Se:  82% 18%



- Molecule 46: 40S ribosomal protein S15a

Chain Sf:  81% 18%



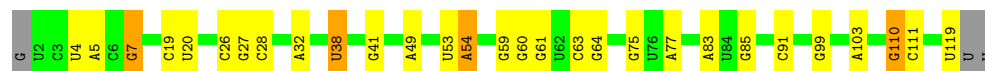
- Molecule 47: Small ribosomal subunit protein uS12

Chain Sg:  88% 10%



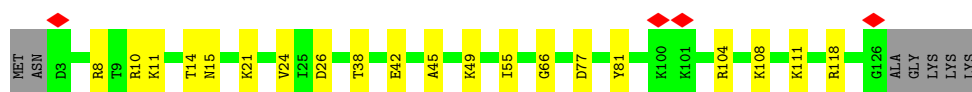
- Molecule 48: 5S rRNA

Chain L2:  74% 21%

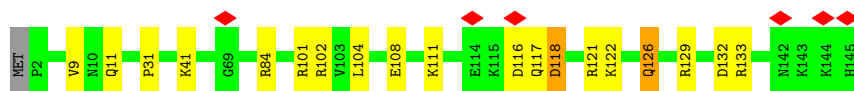
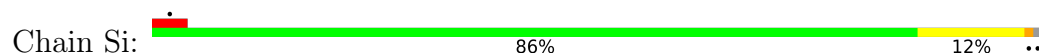


- Molecule 49: Isoform 3 of Small ribosomal subunit protein eS24

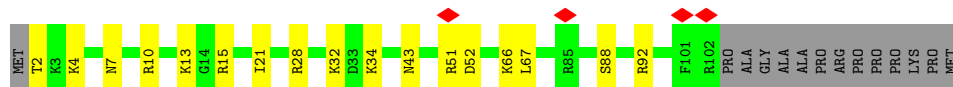
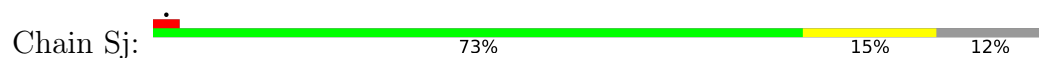
Chain Sh:  79% 15% 5%



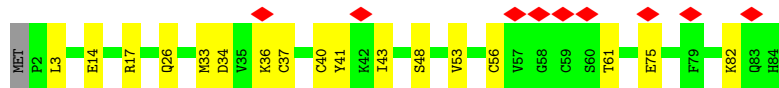
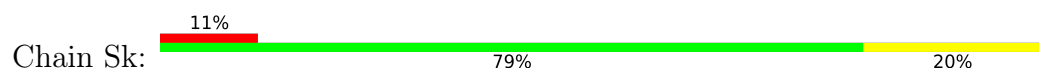
- Molecule 50: Small ribosomal subunit protein eS19



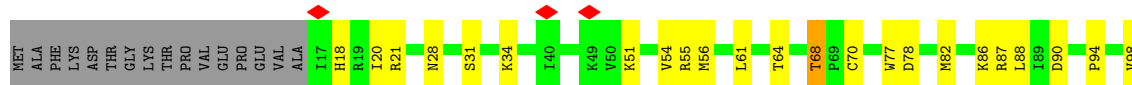
- Molecule 51: 40S ribosomal protein S26



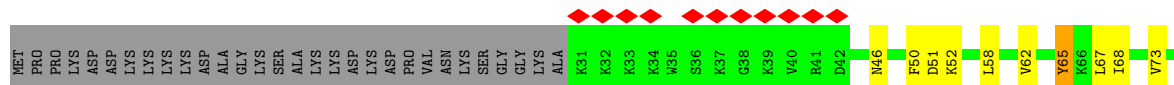
- Molecule 52: 40S ribosomal protein S27



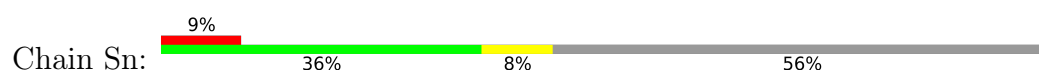
- Molecule 53: 40S ribosomal protein S20



- Molecule 54: 40S ribosomal protein S25



- Molecule 55: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



MET GLN LEU PHE VAL ARG ALA GLN LEU HIS THR PHE GLU VAL THR GLY GLN GLU THR VAL ALA GLN ILE LYS ALA HIS VAL SER LEU GLY ILE ALA PRO GLU ASP VAL VAL LEU LEU ALA GLY ALA PRO LEU ASP GLU THR GLY CYS GLY VAL GLU

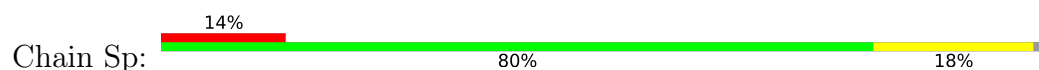
ALA LEU THR THR LEU VAL ALA GLY ARG MET LEU GLY GLY K75 K76 K77 K78 R82 K85 V86 K102 A106 Y112 N113 N118 V119 V120 P121 T122 F123 G124 K125 K126 K127 S133

- Molecule 56: 40S ribosomal protein S28



MET ASP THR S4 R5 V6 Q7 K10 R13 V17 L18 G19 R20 G25 Q29 V30 R31 V32 D37 T38 S39 R44 G53 D54 V55 E60 R63 E64 A65 R66 R67 L68 ARG

- Molecule 57: 40S ribosomal protein S29



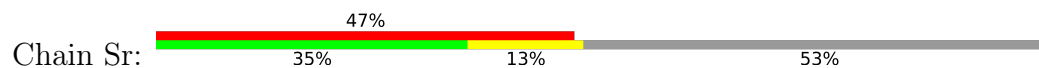
MET G2 H3 Q4 Q5 L6 Y7 W8 S9 H10 K13 G17 C21 R27 L30 K33 Y34 G35 L36 C39 R44 K54 L55 D56

- Molecule 58: 60S ribosomal protein L41



M1 R2 A3 K4 W5 R6 K7 K8 M10 R11 R18 R23 S24 K25

- Molecule 59: Ubiquitin

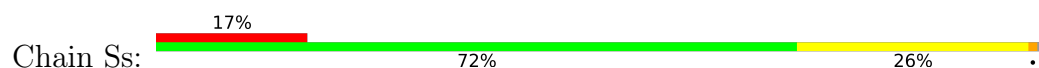


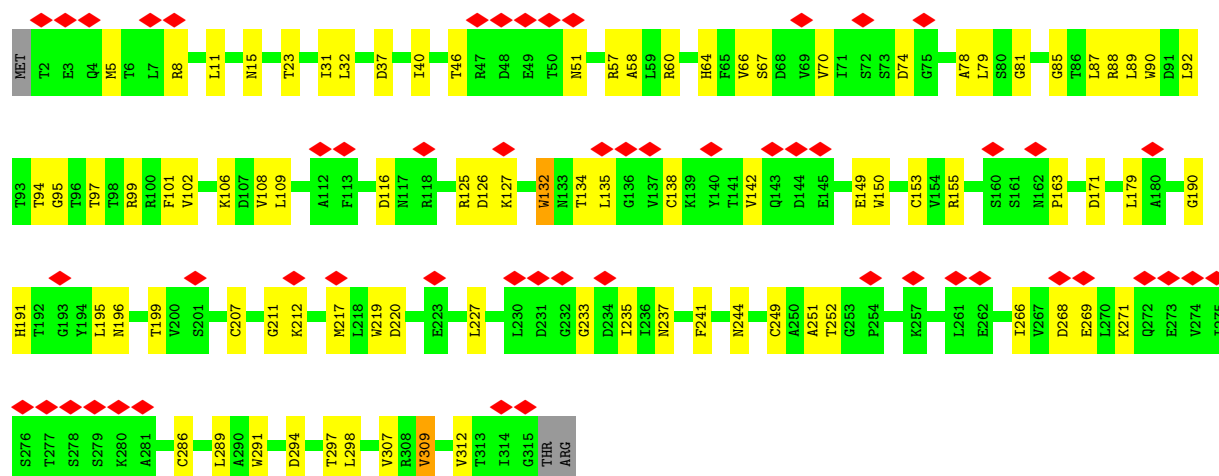
MET GLN ILE PHE VAL LYS THR LEU THR LEU GLY LYS THR ILE THR THR GLY VAL PRO SER ASP THR THR ILE ASN VAL VAL LYS ALA LYS ILE GLN ASP LYS GLY GLY ILE PRO PRO ASP GLN GLN ARG LEU LEU THR PHE ALA GLY LYS GLN LEU LEU ASP GLY ARG THR LEU SER ASP TYR ASN

ILE GLN LYS GLU PHE THR LEU HIS VAL LEU LEU ARG ARG GLY GLY VAL K78 K79 R80 R81 K82 K83 S84 Y85 T86 T87 P88 K89 K90 N91 K92 H93 K94 R95 K96 K97 V98 K99 L100 A101 V102 L103 K104 Y105 Y106 K107 V108 D109 E110 N111 G112 K113 I114 S115 R116 L117 R118 R119 E120

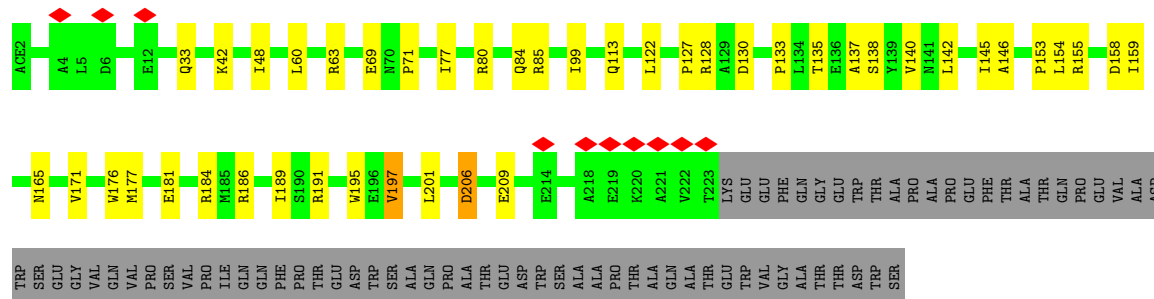
C121 P122 S123 D124 E125 C126 G127 A128 G129 V130 F131 M132 A133 S134 H135 F136 D137 R138 H139 Y140 C141 G142 K143 C144 C145 L146 T147 Y148 C149 F150 M151 LYS PRO GLU ASP LYS

- Molecule 60: Receptor of activated protein C kinase 1

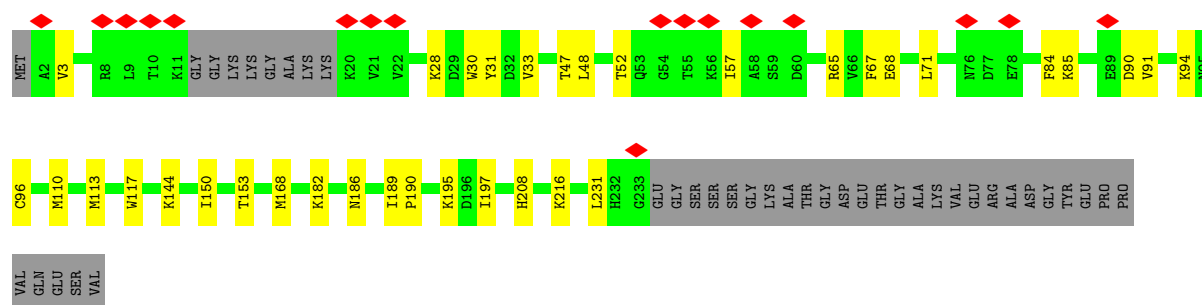




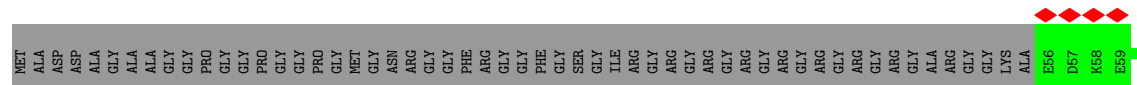
- Molecule 61: Small ribosomal subunit protein uS2

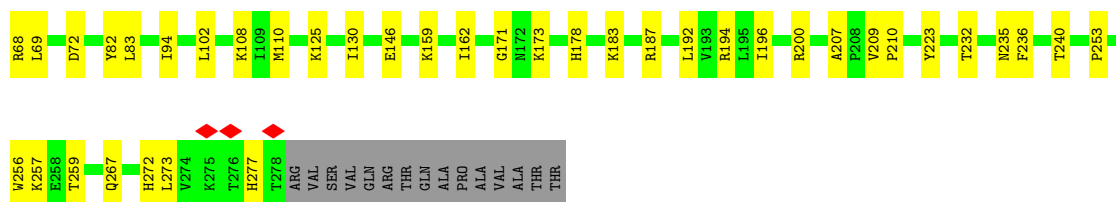


- Molecule 62: 40S ribosomal protein S3a



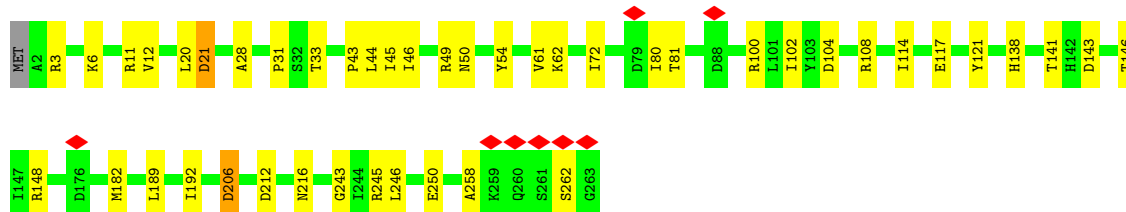
- Molecule 63: 40S ribosomal protein S2





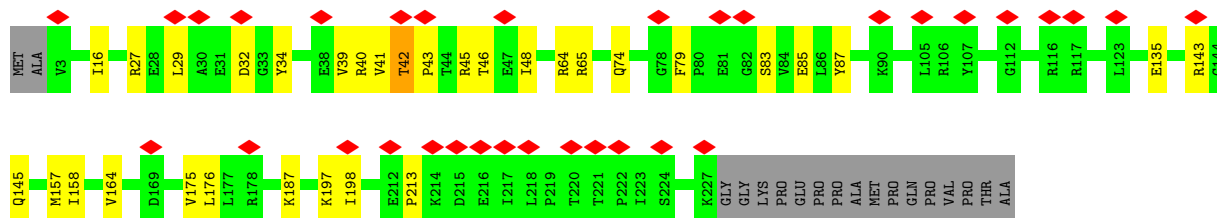
- Molecule 64: Small ribosomal subunit protein eS4, X isoform

Chain Sw: 83% 16%



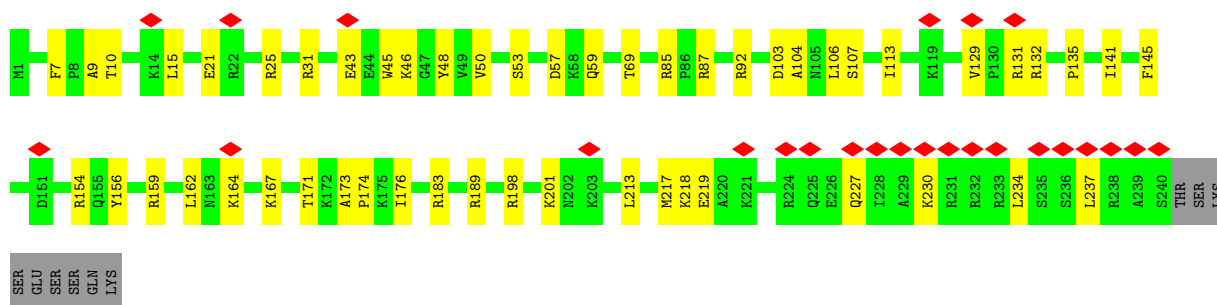
- Molecule 65: 40S ribosomal protein S3

Chain Sx: 14% 79% 13% 7%



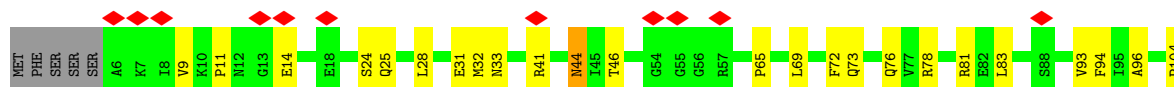
- Molecule 66: 40S ribosomal protein S6

Chain Sy: 10% 76% 21%

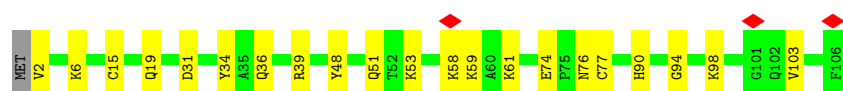


- Molecule 67: 40S ribosomal protein S7

Chain Sz: 10% 77% 20%



Chain LE:  79% 20%



- Molecule 74: 60S ribosomal protein L37a

Chain LF:  5% 87% 13%



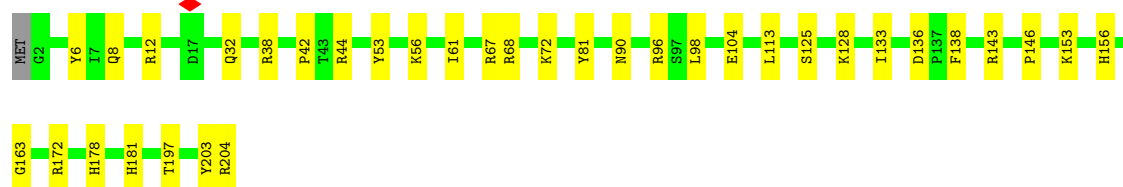
- Molecule 75: 60S ribosomal protein L28

Chain LG:  82% 9% 9%



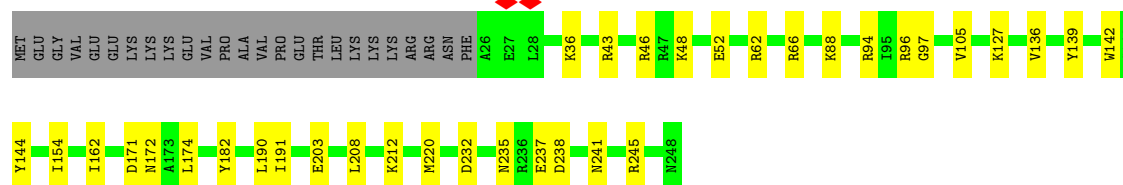
- Molecule 76: 60S ribosomal protein L15

Chain LH:  82% 17%



- Molecule 77: Large ribosomal subunit protein uL30

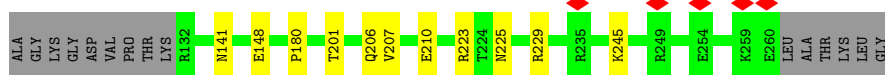
Chain LI:  76% 14% 10%



- Molecule 78: 60S ribosomal protein L7a

Chain LJ:  74% 10% 16%





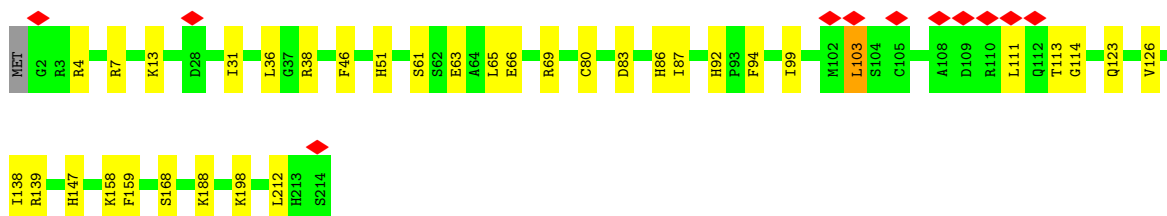
- Molecule 79: 60S ribosomal protein L9

Chain LK: 86% 12%



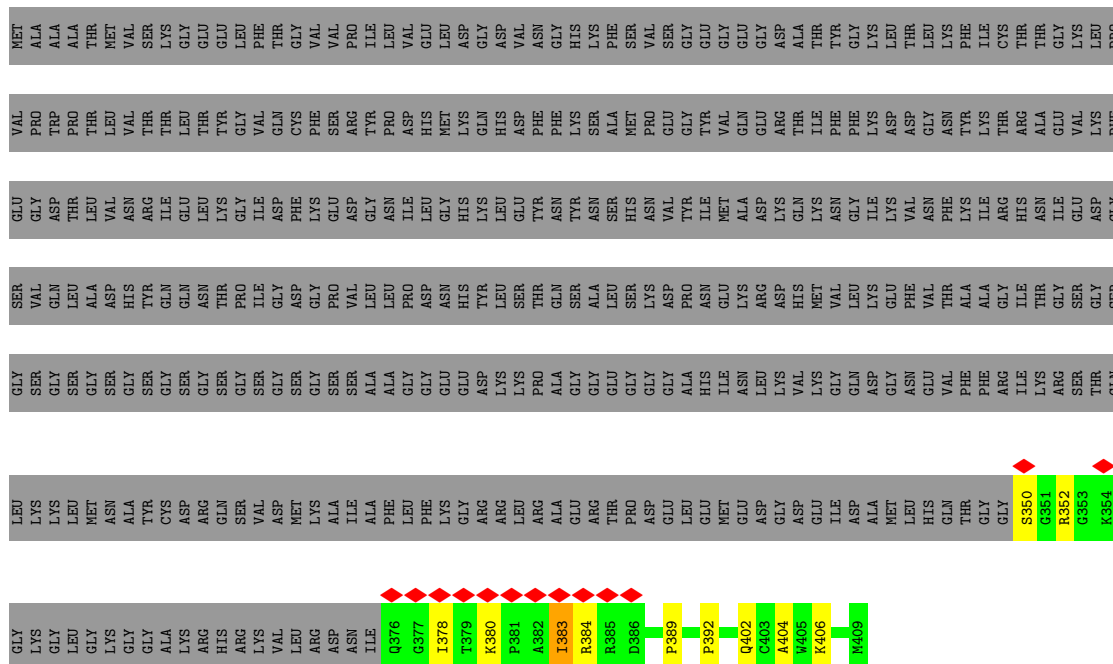
- Molecule 80: 60S ribosomal protein L10

Chain LM: 5% 83% 16%



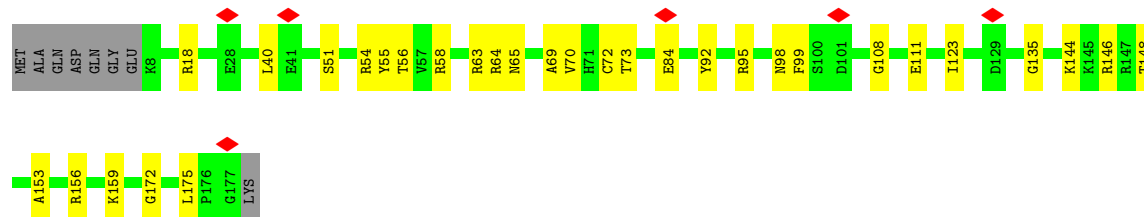
- Molecule 81: Green fluorescent protein, Small ubiquitin-related modifier 1, Green fluorescent protein, Small ubiquitin-related modifier 1, Histone H4, X-box-binding protein 1, X-box-binding protein 1

Chain LN: 7% 91%



- Molecule 82: 60S ribosomal protein L11

Chain LO:  78% 17%



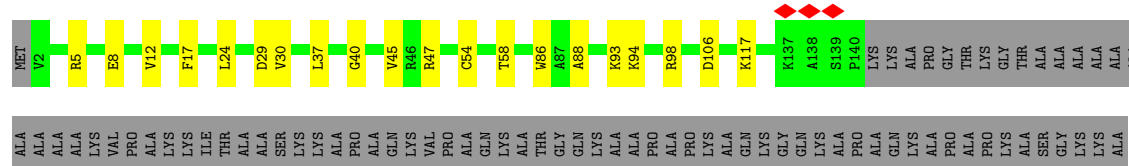
- Molecule 83: Large ribosomal subunit protein eL13

Chain LP:  87% 10%



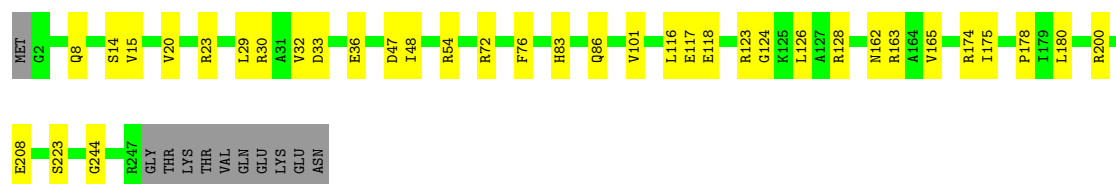
- Molecule 84: 60S ribosomal protein L14

Chain LQ:  55% 9% 35%



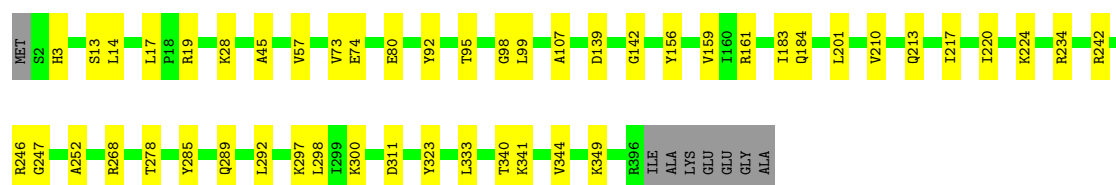
- Molecule 85: 60S ribosomal protein L8

Chain La:  82% 14%



- Molecule 86: 60S ribosomal protein L3

Chain Lb:  86% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.022	Depositor
Minimum map value	-0.502	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	596.4, 596.4, 596.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HY3, ACE, 4AC, ZN, COA, NMM, UY1, MA6, OMC, A2M, PSU, 1MA, IAS, OMG, 5MC, GTP, G7M, 6MZ, OMU, UR3, B8N

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	L1	0.19	1/78858 (0.0%)	0.19	0/122991
2	Lc	0.16	0/2944	0.24	0/3954
3	Ld	0.14	0/2418	0.22	0/3239
4	Le	0.14	0/1786	0.25	0/2395
5	Lf	0.17	0/1666	0.23	0/2228
6	Lg	0.16	0/1259	0.24	0/1689
7	Lh	0.17	0/1537	0.25	0/2052
8	Li	0.14	0/1517	0.21	0/2005
9	Lj	0.16	0/1501	0.23	0/2013
10	Lk	0.16	0/1326	0.23	0/1770
11	Ll	0.16	0/847	0.29	0/1137
12	Lm	0.17	0/999	0.23	0/1340
13	Ln	0.13	0/1006	0.23	0/1334
14	Lo	0.15	0/993	0.21	0/1334
15	Lp	0.15	0/1132	0.24	0/1504
16	Lq	0.15	0/1130	0.22	0/1507
17	Lr	0.16	0/1191	0.24	0/1591
18	Ls	0.13	0/819	0.22	0/1081
19	Lt	0.15	0/783	0.21	0/1052
20	Lu	0.15	0/883	0.23	0/1190
21	Lv	0.17	0/1071	0.24	0/1429
22	Lw	0.17	0/901	0.24	0/1206
23	Lx	0.16	0/892	0.25	0/1189
24	Ly	0.14	0/1023	0.19	0/1351
25	Lz	0.12	0/843	0.20	0/1115
26	Na	0.10	0/844	0.23	0/1128
27	Nb	0.13	0/942	0.30	0/1264
28	Nd	0.10	0/1931	0.26	0/2589
29	Nm	0.10	0/3057	0.26	0/4144
30	S1	0.19	1/40280 (0.0%)	0.18	0/62782
31	S2	0.13	0/164	0.22	0/253

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	S3	0.12	0/1763	0.20	0/2742
33	SA	0.14	0/1711	0.25	0/2282
34	SB	0.13	0/1524	0.21	0/2035
35	SC	0.13	0/1539	0.27	0/2071
36	SD	0.15	0/1250	0.22	0/1673
37	SE	0.11	0/840	0.23	0/1133
38	SF	0.15	0/1226	0.24	0/1649
39	SG	0.15	0/1014	0.23	0/1358
40	SH	0.10	0/963	0.28	0/1291
41	Sa	0.12	0/1035	0.22	0/1383
42	Sb	0.31	0/1097	0.40	0/1474
43	Sc	0.13	0/1146	0.24	0/1534
44	Sd	0.14	0/1216	0.25	0/1630
45	Se	0.15	0/644	0.24	0/862
46	Sf	0.16	0/1051	0.25	0/1406
47	Sg	0.19	0/1107	0.26	0/1475
48	L2	0.16	0/2813	0.16	0/4384
49	Sh	0.12	0/1031	0.21	0/1370
50	Si	0.12	0/1130	0.22	0/1513
51	Sj	0.15	0/828	0.24	0/1109
52	Sk	0.13	0/664	0.26	0/891
53	Sl	0.13	0/813	0.26	0/1092
54	Sm	0.13	0/678	0.26	0/906
55	Sn	0.12	0/473	0.24	0/623
56	So	0.12	0/514	0.21	0/688
57	Sp	0.13	0/469	0.22	0/623
58	Sq	0.15	0/240	0.22	0/305
59	Sr	0.09	0/622	0.26	0/822
60	Ss	0.12	0/2497	0.27	0/3399
61	St	0.15	0/1785	0.25	0/2426
62	Su	0.14	0/1841	0.25	0/2459
63	Sv	0.15	0/1781	0.24	0/2405
64	Sw	0.13	0/2118	0.23	0/2849
65	Sx	0.13	0/1780	0.24	0/2397
66	Sy	0.11	0/1968	0.22	0/2619
67	Sz	0.13	0/1546	0.25	0/2071
68	L3	0.17	0/3453	0.16	0/5376
69	LA	0.17	0/732	0.25	0/968
70	LB	0.13	0/575	0.22	0/761
71	LC	0.17	0/454	0.22	0/599
72	LD	0.13	0/435	0.25	0/575
73	LE	0.14	0/876	0.23	0/1156
74	LF	0.16	0/726	0.25	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	LG	0.16	0/1007	0.23	0/1351
76	LH	0.18	0/1753	0.24	0/2348
77	LI	0.17	0/1885	0.23	0/2512
78	LJ	0.14	0/1840	0.23	0/2476
79	LK	0.15	0/1537	0.23	0/2066
80	LM	0.16	0/1755	0.26	0/2344
81	LN	0.17	0/327	0.34	0/441
82	LO	0.14	0/1381	0.28	0/1848
83	LP	0.15	0/1695	0.24	0/2270
84	LQ	0.14	0/1161	0.20	0/1554
85	La	0.17	0/1925	0.26	0/2581
86	Lb	0.16	0/3265	0.24	0/4369
All	All	0.17	2/228042 (0.0%)	0.21	0/333363

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
42	Sb	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S1	1288	OMU	O3'-P	5.06	1.61	1.56
1	L1	3785	A2M	O3'-P	5.03	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	Sb	67	ARG	Sidechain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	73061	0	37008	588	0
2	Lc	2890	0	3063	42	0
3	Ld	2372	0	2403	28	0
4	Le	1752	0	1904	21	0
5	Lf	1634	0	1779	13	0
6	Lg	1233	0	1263	13	0
7	Lh	1513	0	1628	16	0
8	Li	1501	0	1651	19	0
9	Lj	1461	0	1502	14	0
10	Lk	1298	0	1366	20	0
11	Ll	833	0	856	21	0
12	Lm	985	0	1044	16	0
13	Ln	991	0	1048	27	0
14	Lo	976	0	1053	10	0
15	Lp	1115	0	1205	24	0
16	Lq	1107	0	1182	17	0
17	Lr	1162	0	1213	11	0
18	Ls	806	0	865	13	0
19	Lt	772	0	808	10	0
20	Lu	868	0	913	6	0
21	Lv	1053	0	1147	18	0
22	Lw	879	0	917	10	0
23	Lx	882	0	972	13	0
24	Ly	1015	0	1148	14	0
25	Lz	832	0	917	7	0
26	Na	840	0	898	28	0
27	Nb	934	0	963	40	0
28	Nd	1890	0	1819	55	0
29	Nm	2984	0	2908	63	0
30	S1	37855	0	19186	432	0
31	S2	148	0	75	0	0
32	S3	1579	0	801	20	0
33	SA	1682	0	1769	25	0
34	SB	1499	0	1618	19	0
35	SC	1517	0	1569	18	0
36	SD	1229	0	1302	15	0
37	SE	816	0	841	10	0
38	SF	1202	0	1289	11	0
39	SG	1010	0	1033	14	0
40	SH	953	0	990	14	0
41	Sa	1016	0	1066	32	0
42	Sb	1082	0	1137	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	Sc	1128	0	1195	21	0
44	Sd	1200	0	1262	23	0
45	Se	639	0	638	13	0
46	Sf	1034	0	1080	17	0
47	Sg	1099	0	1162	11	0
48	L2	2518	0	1274	22	0
49	Sh	1014	0	1082	18	0
50	Si	1123	0	1152	15	0
51	Sj	814	0	863	11	0
52	Sk	650	0	672	9	0
53	Sl	803	0	873	17	0
54	Sm	670	0	745	11	0
55	Sn	467	0	516	8	0
56	So	512	0	541	13	0
57	Sp	458	0	448	8	0
58	Sq	239	0	289	8	0
59	Sr	610	0	634	17	0
60	Ss	2440	0	2396	51	0
61	St	1750	0	1755	28	0
62	Su	1815	0	1908	22	0
63	Sv	1741	0	1827	31	0
64	Sw	2076	0	2177	31	0
65	Sx	1752	0	1848	20	0
66	Sy	1945	0	2112	42	0
67	Sz	1523	0	1622	26	0
68	L3	3156	0	1602	20	0
69	LA	713	0	746	11	0
70	LB	569	0	637	6	0
71	LC	444	0	483	9	0
72	LD	429	0	465	8	0
73	LE	862	0	929	13	0
74	LF	716	0	768	9	0
75	LG	992	0	1052	8	0
76	LH	1708	0	1757	29	0
77	LI	1851	0	1981	26	0
78	LJ	1809	0	1941	21	0
79	LK	1518	0	1601	16	0
80	LM	1716	0	1765	23	0
81	LN	316	0	318	12	0
82	LO	1358	0	1388	18	0
83	LP	1664	0	1773	19	0
84	LQ	1138	0	1204	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	La	1887	0	1983	27	0
86	Lb	3194	0	3336	33	0
87	LA	1	0	0	0	0
87	LD	1	0	0	0	0
87	LE	1	0	0	0	0
87	LF	1	0	0	0	0
87	Lx	1	0	0	0	0
87	Nm	2	0	0	0	0
87	Sj	1	0	0	0	0
87	Sp	1	0	0	0	0
87	Sr	1	0	0	0	0
88	Nd	48	0	32	5	0
89	L2	32	0	11	1	0
All	All	217377	0	163962	2122	0

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

The worst 5 of 2122 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:L1:3642:A:HO2'	69:LA:2:THR:N	1.54	1.06
88:Nd:301:COA:HS1	81:LN:350:SER:N	1.59	0.97
42:Sb:71:ILE:HD11	42:Sb:73:LEU:HG	1.54	0.88
30:S1:1757:G:H1	30:S1:1775:U:H3	1.21	0.87
27:Nb:53:VAL:HG12	27:Nb:80:GLN:HB3	1.59	0.83

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	
2	Lc	361/427 (84%)	351 (97%)	10 (3%)	0	100	100
3	Ld	290/297 (98%)	284 (98%)	6 (2%)	0	100	100
4	Le	212/288 (74%)	202 (95%)	10 (5%)	0	100	100
5	Lf	197/199 (99%)	195 (99%)	2 (1%)	0	100	100
6	Lg	150/184 (82%)	147 (98%)	3 (2%)	0	100	100
7	Lh	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
8	Li	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
9	Lj	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
10	Lk	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
11	Ll	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
12	Lm	130/140 (93%)	127 (98%)	3 (2%)	0	100	100
13	Ln	119/157 (76%)	115 (97%)	4 (3%)	0	100	100
14	Lo	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
15	Lp	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
16	Lq	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
17	Lr	145/148 (98%)	141 (97%)	4 (3%)	0	100	100
18	Ls	95/159 (60%)	94 (99%)	1 (1%)	0	100	100
19	Lt	98/115 (85%)	98 (100%)	0	0	100	100
20	Lu	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
21	Lv	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
22	Lw	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
23	Lx	109/117 (93%)	107 (98%)	2 (2%)	0	100	100
24	Ly	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
25	Lz	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
26	Na	104/238 (44%)	100 (96%)	4 (4%)	0	100	100
27	Nb	116/162 (72%)	115 (99%)	1 (1%)	0	100	100
28	Nd	234/365 (64%)	226 (97%)	8 (3%)	0	100	100
29	Nm	378/386 (98%)	369 (98%)	8 (2%)	1 (0%)	36	65
33	SA	203/208 (98%)	198 (98%)	5 (2%)	0	100	100
34	SB	178/194 (92%)	174 (98%)	4 (2%)	0	100	100
35	SC	190/204 (93%)	183 (96%)	7 (4%)	0	100	100
36	SD	149/158 (94%)	145 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	SE	95/165 (58%)	93 (98%)	2 (2%)	0	100	100
38	SF	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
39	SG	131/151 (87%)	127 (97%)	4 (3%)	0	100	100
40	SH	121/132 (92%)	113 (93%)	8 (7%)	0	100	100
41	Sa	122/152 (80%)	117 (96%)	5 (4%)	0	100	100
42	Sb	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
43	Sc	140/146 (96%)	136 (97%)	4 (3%)	0	100	100
44	Sd	144/152 (95%)	138 (96%)	6 (4%)	0	100	100
45	Se	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
46	Sf	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
47	Sg	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
49	Sh	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
50	Si	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
51	Sj	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
52	Sk	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
53	Sl	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
54	Sm	81/125 (65%)	78 (96%)	3 (4%)	0	100	100
55	Sn	57/133 (43%)	54 (95%)	3 (5%)	0	100	100
56	So	63/69 (91%)	60 (95%)	3 (5%)	0	100	100
57	Sp	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
58	Sq	23/25 (92%)	23 (100%)	0	0	100	100
59	Sr	72/156 (46%)	65 (90%)	7 (10%)	0	100	100
60	Ss	312/317 (98%)	295 (95%)	17 (5%)	0	100	100
61	St	221/295 (75%)	216 (98%)	5 (2%)	0	100	100
62	Su	220/264 (83%)	215 (98%)	5 (2%)	0	100	100
63	Sv	222/293 (76%)	218 (98%)	4 (2%)	0	100	100
64	Sw	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
65	Sx	223/243 (92%)	214 (96%)	8 (4%)	1 (0%)	30	61
66	Sy	238/249 (96%)	234 (98%)	4 (2%)	0	100	100
67	Sz	187/194 (96%)	184 (98%)	3 (2%)	0	100	100
69	LA	85/97 (88%)	85 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	LB	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
71	LC	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
72	LD	50/99 (50%)	50 (100%)	0	0	100	100
73	LE	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
74	LF	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
75	LG	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
76	LH	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
77	LI	221/248 (89%)	214 (97%)	7 (3%)	0	100	100
78	LJ	219/266 (82%)	213 (97%)	6 (3%)	0	100	100
79	LK	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
80	LM	211/214 (99%)	203 (96%)	7 (3%)	1 (0%)	24	57
81	LN	35/414 (8%)	32 (91%)	3 (9%)	0	100	100
82	LO	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
83	LP	204/211 (97%)	200 (98%)	4 (2%)	0	100	100
84	LQ	137/215 (64%)	135 (98%)	2 (2%)	0	100	100
85	La	244/257 (95%)	229 (94%)	15 (6%)	0	100	100
86	Lb	394/403 (98%)	385 (98%)	9 (2%)	0	100	100
All	All	12133/14300 (85%)	11816 (97%)	314 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	Nm	297	HIS
65	Sx	42	THR
80	LM	103	LEU

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	
2	Lc	302/348 (87%)	301 (100%)	1 (0%)	86	82
3	Ld	245/250 (98%)	243 (99%)	2 (1%)	73	77
4	Le	193/252 (77%)	192 (100%)	1 (0%)	81	80
5	Lf	171/171 (100%)	170 (99%)	1 (1%)	78	79
6	Lg	133/163 (82%)	133 (100%)	0	100	100
7	Lh	164/165 (99%)	162 (99%)	2 (1%)	63	73
8	Li	157/175 (90%)	156 (99%)	1 (1%)	78	79
9	Lj	157/157 (100%)	157 (100%)	0	100	100
10	Lk	139/140 (99%)	137 (99%)	2 (1%)	59	71
11	Ll	92/115 (80%)	89 (97%)	3 (3%)	33	58
12	Lm	102/107 (95%)	101 (99%)	1 (1%)	68	75
13	Ln	100/126 (79%)	98 (98%)	2 (2%)	48	66
14	Lo	107/133 (80%)	105 (98%)	2 (2%)	50	67
15	Lp	124/135 (92%)	123 (99%)	1 (1%)	73	77
16	Lq	117/118 (99%)	116 (99%)	1 (1%)	70	76
17	Lr	120/121 (99%)	120 (100%)	0	100	100
18	Ls	82/126 (65%)	82 (100%)	0	100	100
19	Lt	84/97 (87%)	83 (99%)	1 (1%)	63	73
20	Lu	93/110 (84%)	93 (100%)	0	100	100
21	Lv	114/121 (94%)	114 (100%)	0	100	100
22	Lw	89/89 (100%)	89 (100%)	0	100	100
23	Lx	95/100 (95%)	95 (100%)	0	100	100
24	Ly	109/110 (99%)	109 (100%)	0	100	100
25	Lz	86/89 (97%)	85 (99%)	1 (1%)	63	73
26	Na	95/202 (47%)	94 (99%)	1 (1%)	65	74
27	Nb	104/136 (76%)	99 (95%)	5 (5%)	23	50
28	Nd	200/314 (64%)	198 (99%)	2 (1%)	68	75
29	Nm	326/330 (99%)	323 (99%)	3 (1%)	70	76
33	SA	178/180 (99%)	177 (99%)	1 (1%)	78	79
34	SB	160/168 (95%)	160 (100%)	0	100	100
35	SC	162/170 (95%)	160 (99%)	2 (1%)	63	73
36	SD	135/142 (95%)	134 (99%)	1 (1%)	76	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	SE	88/136 (65%)	87 (99%)	1 (1%)	65	74
38	SF	130/131 (99%)	129 (99%)	1 (1%)	73	77
39	SG	104/118 (88%)	101 (97%)	3 (3%)	37	60
40	SH	104/108 (96%)	98 (94%)	6 (6%)	18	45
41	Sa	110/134 (82%)	110 (100%)	0	100	100
42	Sb	121/122 (99%)	119 (98%)	2 (2%)	53	69
43	Sc	117/121 (97%)	117 (100%)	0	100	100
44	Sd	126/131 (96%)	123 (98%)	3 (2%)	43	63
45	Se	67/67 (100%)	66 (98%)	1 (2%)	57	70
46	Sf	112/113 (99%)	111 (99%)	1 (1%)	70	76
47	Sg	112/114 (98%)	112 (100%)	0	100	100
49	Sh	108/113 (96%)	108 (100%)	0	100	100
50	Si	113/114 (99%)	111 (98%)	2 (2%)	51	68
51	Sj	88/98 (90%)	86 (98%)	2 (2%)	44	64
52	Sk	75/76 (99%)	73 (97%)	2 (3%)	39	61
53	Sl	93/107 (87%)	92 (99%)	1 (1%)	65	74
54	Sm	74/103 (72%)	73 (99%)	1 (1%)	59	71
55	Sn	48/104 (46%)	48 (100%)	0	100	100
56	So	58/62 (94%)	57 (98%)	1 (2%)	53	69
57	Sp	48/49 (98%)	48 (100%)	0	100	100
58	Sq	24/24 (100%)	24 (100%)	0	100	100
59	Sr	67/140 (48%)	67 (100%)	0	100	100
60	Ss	272/275 (99%)	264 (97%)	8 (3%)	37	60
61	St	184/242 (76%)	182 (99%)	2 (1%)	65	74
62	Su	203/231 (88%)	202 (100%)	1 (0%)	81	80
63	Sv	190/225 (84%)	189 (100%)	1 (0%)	81	80
64	Sw	224/225 (100%)	220 (98%)	4 (2%)	51	68
65	Sx	189/202 (94%)	186 (98%)	3 (2%)	55	69
66	Sy	209/218 (96%)	207 (99%)	2 (1%)	68	75
67	Sz	169/174 (97%)	165 (98%)	4 (2%)	43	63
69	LA	74/80 (92%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	LB	64/65 (98%)	63 (98%)	1 (2%)	55	69
71	LC	47/48 (98%)	45 (96%)	2 (4%)	26	51
72	LD	48/91 (53%)	48 (100%)	0	100	100
73	LE	93/94 (99%)	92 (99%)	1 (1%)	65	74
74	LF	75/75 (100%)	73 (97%)	2 (3%)	39	61
75	LG	107/121 (88%)	107 (100%)	0	100	100
76	LH	172/172 (100%)	172 (100%)	0	100	100
77	LI	192/215 (89%)	192 (100%)	0	100	100
78	LJ	193/223 (86%)	192 (100%)	1 (0%)	81	80
79	LK	169/171 (99%)	169 (100%)	0	100	100
80	LM	180/181 (99%)	179 (99%)	1 (1%)	78	79
81	LN	33/336 (10%)	30 (91%)	3 (9%)	9	33
82	LO	142/149 (95%)	141 (99%)	1 (1%)	76	78
83	LP	172/177 (97%)	172 (100%)	0	100	100
84	LQ	118/161 (73%)	118 (100%)	0	100	100
85	La	189/199 (95%)	186 (98%)	3 (2%)	55	69
86	Lb	345/349 (99%)	343 (99%)	2 (1%)	78	79
All	All	10575/12144 (87%)	10469 (99%)	106 (1%)	65	75

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	Sj	21	ILE
60	Ss	309	VAL
81	LN	384	ARG
52	Sk	3	LEU
60	Ss	94	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
71	LC	33	ASN
86	Lb	289	GLN
74	LF	33	GLN
79	LK	98	HIS

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Mol	Chain	Res	Type
29	Nm	356	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	3376/5070 (66%)	462 (13%)	5 (0%)
30	S1	1765/1869 (94%)	255 (14%)	0
31	S2	6/1824 (0%)	0	0
32	S3	72/76 (94%)	9 (12%)	0
48	L2	117/121 (96%)	9 (7%)	0
68	L3	145/157 (92%)	16 (11%)	0
All	All	5481/9117 (60%)	751 (13%)	5 (0%)

5 of 751 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	6	C
1	L1	13	U
1	L1	25	A
1	L1	30	C
1	L1	39	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	486	C
1	L1	964	A
1	L1	1365	C
1	L1	1633	G
1	L1	2091	C

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

212 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
1	6MZ	L1	4220	1	22,25,26	1.40	4 (18%)	30,36,39	2.24	10 (33%)
30	B8N	S1	1248	30	24,29,30	1.31	3 (12%)	29,42,45	1.31	4 (13%)
30	OMU	S1	799	30	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
1	UR3	L1	4530	1	19,22,23	0.94	0	26,32,35	1.36	1 (3%)
30	OMU	S1	1804	30	19,22,23	1.24	3 (15%)	26,31,34	1.68	4 (15%)
1	OMG	L1	4623	1	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
1	OMC	L1	4456	1	19,22,23	0.83	0	26,31,34	0.78	0
1	A2M	L1	1326	1	22,25,26	1.41	4 (18%)	31,36,39	2.10	10 (32%)
1	OMC	L1	1881	1	19,22,23	0.86	0	26,31,34	1.30	1 (3%)
1	PSU	L1	4689	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	UY1	L1	3818	1	19,22,23	0.91	1 (5%)	22,31,34	1.71	3 (13%)
30	PSU	S1	105	30	18,21,22	1.40	2 (11%)	22,30,33	1.89	3 (13%)
30	PSU	S1	966	30	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	L1	3830	1	22,25,26	1.45	4 (18%)	31,36,39	2.15	10 (32%)
30	A2M	S1	512	30	22,25,26	1.44	4 (18%)	31,36,39	2.22	10 (32%)
30	A2M	S1	1383	30	22,25,26	1.45	4 (18%)	31,36,39	2.21	9 (29%)
30	OMG	S1	509	30	23,26,27	1.23	3 (13%)	33,38,41	1.90	6 (18%)
1	OMG	L1	4370	1	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
30	PSU	S1	1177	30	18,21,22	1.37	3 (16%)	22,30,33	1.89	3 (13%)
30	4AC	S1	1337	30	21,24,25	1.11	2 (9%)	29,34,37	1.05	2 (6%)
30	OMC	S1	174	30	19,22,23	0.81	0	26,31,34	0.78	0
1	A2M	L1	1524	1	22,25,26	1.43	4 (18%)	31,36,39	2.11	10 (32%)
1	PSU	L1	4442	1	18,21,22	1.38	3 (16%)	22,30,33	1.95	5 (22%)
1	PSU	L1	5010	1	18,21,22	1.38	3 (16%)	22,30,33	1.94	4 (18%)
30	PSU	S1	36	30	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
30	A2M	S1	484	30	22,25,26	1.44	4 (18%)	31,36,39	2.08	9 (29%)
1	OMU	L1	3925	1	19,22,23	1.24	3 (15%)	26,31,34	1.74	5 (19%)
30	OMC	S1	1272	30	19,22,23	0.82	0	26,31,34	0.82	0
1	OMG	L1	3627	1	23,26,27	1.22	3 (13%)	33,38,41	1.91	6 (18%)
1	OMG	L1	2364	1	23,26,27	1.20	3 (13%)	33,38,41	1.89	6 (18%)
1	PSU	L1	1744	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	OMG	L1	2876	1	23,26,27	1.23	3 (13%)	33,38,41	1.95	6 (18%)
1	OMG	L1	1625	1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
50	NMM	Si	67	50	9,11,12	0.59	0	6,12,14	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	S1	609	30	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	L1	3869	1	19,22,23	0.82	0	26,31,34	0.78	0
30	OMG	S1	601	30	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
30	OMG	S1	1490	30	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
30	OMU	S1	627	30	19,22,23	1.22	3 (15%)	26,31,34	1.62	4 (15%)
1	PSU	L1	4457	1	18,21,22	1.39	3 (16%)	22,30,33	1.85	3 (13%)
1	A2M	L1	400	1	22,25,26	1.45	4 (18%)	31,36,39	2.03	8 (25%)
1	PSU	L1	4628	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
1	A2M	L1	1871	1	22,25,26	1.46	4 (18%)	31,36,39	2.16	10 (32%)
68	PSU	L3	55	68	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	L1	4299	1	18,21,22	1.37	3 (16%)	22,30,33	1.87	3 (13%)
1	PSU	L1	1792	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	L1	1323	1	22,25,26	1.44	4 (18%)	31,36,39	2.08	9 (29%)
1	PSU	L1	1582	1	18,21,22	1.36	3 (16%)	22,30,33	1.96	4 (18%)
30	A2M	S1	576	30	22,25,26	1.47	4 (18%)	31,36,39	2.14	9 (29%)
1	PSU	L1	4293	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	OMU	L1	4306	1	19,22,23	1.25	3 (15%)	26,31,34	1.70	4 (15%)
30	OMU	S1	121	30	19,22,23	1.24	3 (15%)	26,31,34	1.75	5 (19%)
30	PSU	S1	1625	30	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	L1	4493	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
1	PSU	L1	3768	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
30	PSU	S1	1238	30	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
30	A2M	S1	166	30	22,25,26	1.46	4 (18%)	31,36,39	2.12	8 (25%)
30	A2M	S1	1678	30	22,25,26	1.45	4 (18%)	31,36,39	2.14	9 (29%)
1	PSU	L1	3695	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	L1	4590	1	22,25,26	1.45	4 (18%)	31,36,39	2.14	10 (32%)
1	OMC	L1	1340	1	19,22,23	0.82	0	26,31,34	0.79	0
30	PSU	S1	1347	30	18,21,22	1.36	3 (16%)	22,30,33	1.93	4 (18%)
1	OMG	L1	3792	1	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	L1	3899	1	23,26,27	1.22	3 (13%)	33,38,41	1.90	6 (18%)
1	PSU	L1	4423	1	18,21,22	1.37	2 (11%)	22,30,33	1.82	3 (13%)
1	OMC	L1	2351	1	19,22,23	0.83	0	26,31,34	0.97	2 (7%)
1	OMG	L1	3744	1	23,26,27	1.22	3 (13%)	33,38,41	1.93	6 (18%)
1	OMG	L1	4228	1	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
30	PSU	S1	296	30	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	S1	822	30	18,21,22	1.39	2 (11%)	22,30,33	1.91	3 (13%)
30	PSU	S1	686	30	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	L1	4637	1	23,26,27	1.22	3 (13%)	33,38,41	1.97	6 (18%)
30	PSU	S1	1232	30	18,21,22	1.35	3 (16%)	22,30,33	1.91	4 (18%)
30	PSU	S1	1046	30	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	L1	2632	1	18,21,22	1.36	3 (16%)	22,30,33	1.87	3 (13%)
30	PSU	S1	1174	30	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
30	PSU	S1	681	30	18,21,22	1.38	2 (11%)	22,30,33	1.93	3 (13%)
1	PSU	L1	4673	1	18,21,22	1.39	3 (16%)	22,30,33	1.90	3 (13%)
30	A2M	S1	468	30	22,25,26	1.45	4 (18%)	31,36,39	2.16	10 (32%)
1	PSU	L1	1862	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
30	PSU	S1	1004	30	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
1	PSU	L1	4431	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
30	OMC	S1	462	30	19,22,23	0.81	0	26,31,34	0.78	0
1	PSU	L1	2508	1	18,21,22	1.36	2 (11%)	22,30,33	1.94	4 (18%)
30	PSU	S1	649	30	18,21,22	1.36	2 (11%)	22,30,33	1.94	4 (18%)
30	G7M	S1	1639	30,32	23,26,27	3.08	8 (34%)	35,39,42	3.37	14 (40%)
30	PSU	S1	866	30	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	OMG	L1	4392	1	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	L1	4552	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
30	OMU	S1	1326	30	19,22,23	1.20	3 (15%)	26,31,34	1.71	5 (19%)
1	PSU	L1	4579	1	18,21,22	1.36	3 (16%)	22,30,33	1.93	4 (18%)
1	PSU	L1	4521	1	18,21,22	1.36	3 (16%)	22,30,33	1.90	5 (22%)
30	6MZ	S1	1832	30	22,25,26	1.41	4 (18%)	30,36,39	2.16	9 (30%)
1	PSU	L1	4420	1	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	L1	3730	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
1	PSU	L1	1536	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
1	OMC	L1	2365	1	19,22,23	0.82	0	26,31,34	0.74	0
1	OMG	L1	2424	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	OMU	L1	2837	1	19,22,23	1.23	3 (15%)	26,31,34	1.76	5 (19%)
1	PSU	L1	3637	1	18,21,22	1.38	3 (16%)	22,30,33	1.94	3 (13%)
1	A2M	L1	2401	1	22,25,26	1.44	4 (18%)	31,36,39	2.15	9 (29%)
1	OMG	L1	4499	1	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
39	IAS	SG	138	39	6,7,8	0.97	0	6,8,10	1.31	1 (16%)
1	OMG	L1	4618	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMC	S1	797	30	19,22,23	0.82	0	26,31,34	0.83	0
30	A2M	S1	99	30	22,25,26	1.46	4 (18%)	31,36,39	2.12	8 (25%)
30	OMC	S1	1703	30	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	OMG	L1	1316	1	23,26,27	1.23	3 (13%)	33,38,41	1.96	6 (18%)
1	A2M	L1	2815	1	22,25,26	1.44	4 (18%)	31,36,39	2.15	10 (32%)
1	5MC	L1	3782	1	18,22,23	0.96	2 (11%)	26,32,35	1.22	3 (11%)
1	OMU	L1	4620	1	19,22,23	1.24	3 (15%)	26,31,34	1.74	5 (19%)
1	PSU	L1	3920	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
30	OMG	S1	1447	30	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
30	A2M	S1	590	30	22,25,26	1.45	4 (18%)	31,36,39	2.08	7 (22%)
30	PSU	S1	1136	30	18,21,22	1.37	2 (11%)	22,30,33	1.89	4 (18%)
30	PSU	S1	1081	30	18,21,22	1.43	4 (22%)	22,30,33	1.86	4 (18%)
30	PSU	S1	406	30	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
30	PSU	S1	572	30	18,21,22	1.37	2 (11%)	22,30,33	1.93	4 (18%)
30	MA6	S1	1851	30	23,26,27	2.27	5 (21%)	34,38,41	3.69	13 (38%)
1	A2M	L1	3867	1	22,25,26	1.45	4 (18%)	31,36,39	2.11	9 (29%)
1	PSU	L1	4576	1	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
1	A2M	L1	4523	1	22,25,26	1.45	4 (18%)	31,36,39	2.17	10 (32%)
30	PSU	S1	210	30	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	L1	1683	1	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	L1	1782	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
30	PSU	S1	814	30	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	L1	4196	1,32	23,26,27	1.23	3 (13%)	33,38,41	1.93	6 (18%)
30	A2M	S1	1031	30	22,25,26	1.44	4 (18%)	31,36,39	2.16	9 (29%)
1	OMC	L1	3887	1	19,22,23	0.81	0	26,31,34	0.79	0
1	PSU	L1	4532	1	18,21,22	1.40	3 (16%)	22,30,33	1.88	3 (13%)
1	A2M	L1	2363	1	22,25,26	1.44	4 (18%)	31,36,39	2.15	10 (32%)
1	5MC	L1	4447	1	18,22,23	1.00	2 (11%)	26,32,35	1.18	2 (7%)
1	OMU	L1	4498	1	19,22,23	1.22	3 (15%)	26,31,34	1.70	5 (19%)
30	MA6	S1	1850	30	23,26,27	2.27	5 (21%)	34,38,41	3.70	13 (38%)
30	OMU	S1	172	30	19,22,23	1.21	3 (15%)	26,31,34	1.71	4 (15%)
1	A2M	L1	3724	1	22,25,26	1.44	4 (18%)	31,36,39	2.12	9 (29%)
30	PSU	S1	119	30	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	1MA	L1	1322	1	21,25,26	1.37	3 (14%)	31,37,40	1.61	6 (19%)
30	PSU	S1	801	30	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	S1	1692	30	18,21,22	1.38	2 (11%)	22,30,33	1.96	4 (18%)
1	OMC	L1	2824	1	19,22,23	0.82	0	26,31,34	0.79	0
1	PSU	L1	4296	1	18,21,22	1.36	3 (16%)	22,30,33	1.92	4 (18%)
30	OMU	S1	116	30	19,22,23	1.22	3 (15%)	26,31,34	1.71	4 (15%)
30	OMU	S1	428	30	19,22,23	1.22	2 (10%)	26,31,34	1.67	4 (15%)
1	PSU	L1	5001	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
30	PSU	S1	651	30	18,21,22	1.38	2 (11%)	22,30,33	1.92	3 (13%)
1	OMC	L1	2804	1	19,22,23	0.83	0	26,31,34	0.80	0
68	OMG	L3	75	68	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
1	A2M	L1	1534	1	22,25,26	1.41	4 (18%)	31,36,39	2.13	9 (29%)
30	OMG	S1	436	30	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
30	PSU	S1	863	30	18,21,22	1.37	2 (11%)	22,30,33	1.95	3 (13%)
1	OMU	L1	4227	1	19,22,23	1.26	2 (10%)	26,31,34	1.73	4 (15%)
30	OMU	S1	354	30	19,22,23	1.25	3 (15%)	26,31,34	1.76	5 (19%)
30	A2M	S1	27	30	22,25,26	1.45	4 (18%)	31,36,39	2.14	10 (32%)
1	A2M	L1	398	1	22,25,26	1.44	4 (18%)	31,36,39	2.19	10 (32%)
1	OMC	L1	2861	1	19,22,23	0.82	0	26,31,34	0.82	0
1	PSU	L1	3844	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	L1	4500	1	18,21,22	1.34	2 (11%)	22,30,33	1.95	5 (22%)
30	A2M	S1	159	30	22,25,26	1.46	4 (18%)	31,36,39	2.24	10 (32%)
30	OMU	S1	1442	30	19,22,23	1.25	3 (15%)	26,31,34	1.73	4 (15%)
30	OMG	S1	644	30	23,26,27	1.22	3 (13%)	33,38,41	1.91	6 (18%)
1	PSU	L1	3639	1	18,21,22	1.39	3 (16%)	22,30,33	1.85	3 (13%)
1	PSU	L1	4361	1	18,21,22	1.39	3 (16%)	22,30,33	1.90	3 (13%)
1	PSU	L1	1781	1	18,21,22	1.34	2 (11%)	22,30,33	1.94	4 (18%)
1	OMG	L1	3944	1	23,26,27	1.21	3 (13%)	33,38,41	1.87	6 (18%)
30	PSU	S1	1045	30	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
30	PSU	S1	1643	30	18,21,22	1.37	3 (16%)	22,30,33	1.88	3 (13%)
1	A2M	L1	2787	1	22,25,26	1.43	4 (18%)	31,36,39	2.11	9 (29%)
1	OMG	L1	4494	1	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
30	A2M	S1	668	30	22,25,26	1.45	4 (18%)	31,36,39	2.13	10 (32%)
1	PSU	L1	1677	1	18,21,22	1.38	2 (11%)	22,30,33	1.88	4 (18%)
30	PSU	S1	1445	30	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	OMC	L1	2422	1	19,22,23	0.83	0	26,31,34	0.86	1 (3%)
1	OMU	L1	2415	1	19,22,23	1.24	3 (15%)	26,31,34	1.68	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L1	4353	1	18,21,22	1.37	3 (16%)	22,30,33	1.91	4 (18%)
30	OMC	S1	1391	30	19,22,23	0.81	0	26,31,34	0.82	0
1	PSU	L1	3770	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
47	HY3	Sg	62	47	6,8,9	0.82	0	5,10,12	1.30	1 (20%)
1	PSU	L1	3715	1	18,21,22	1.40	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	L1	3785	1	22,25,26	1.41	4 (18%)	31,36,39	2.26	11 (35%)
1	OMG	L1	1522	1	23,26,27	1.22	3 (13%)	33,38,41	1.93	5 (15%)
1	A2M	L1	3825	1	22,25,26	1.44	4 (18%)	31,36,39	2.15	8 (25%)
1	A2M	L1	4571	1	22,25,26	1.44	4 (18%)	31,36,39	2.09	10 (32%)
1	PSU	L1	4972	1	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
30	PSU	S1	109	30	18,21,22	1.39	3 (16%)	22,30,33	1.89	3 (13%)
30	PSU	S1	1244	30	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
30	4AC	S1	1842	30	21,24,25	1.12	2 (9%)	29,34,37	1.16	3 (10%)
30	PSU	S1	34	30	18,21,22	1.39	2 (11%)	22,30,33	1.86	3 (13%)
30	OMG	S1	683	30	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
1	OMC	L1	4536	1	19,22,23	0.83	0	26,31,34	0.84	0
1	PSU	L1	4312	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
30	OMC	S1	517	30	19,22,23	0.81	0	26,31,34	0.80	0
30	PSU	S1	1056	30	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	L1	3884	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
1	OMC	L1	3701	1	19,22,23	0.80	0	26,31,34	0.75	0
30	PSU	S1	218	30	18,21,22	1.36	2 (11%)	22,30,33	1.86	4 (18%)
1	PSU	L1	1860	1	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	L1	3851	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	L1	4403	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
30	OMG	S1	1328	30	23,26,27	1.22	3 (13%)	33,38,41	1.93	5 (15%)
1	OMC	L1	3841	1	19,22,23	0.83	0	26,31,34	0.85	1 (3%)
1	PSU	L1	3734	1	18,21,22	1.35	3 (16%)	22,30,33	1.92	4 (18%)
30	PSU	S1	93	30	18,21,22	1.38	3 (16%)	22,30,33	1.86	3 (13%)
1	PSU	L1	2839	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	L1	3853	1	18,21,22	1.37	3 (16%)	22,30,33	1.91	3 (13%)
30	PSU	S1	815	30	18,21,22	1.37	2 (11%)	22,30,33	1.93	3 (13%)
68	PSU	L3	69	68	18,21,22	1.38	2 (11%)	22,30,33	1.93	4 (18%)
1	PSU	L1	4471	1	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
30	PSU	S1	1367	30	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	L1	3808	1	19,22,23	0.83	0	26,31,34	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMU	S1	1288	30	19,22,23	1.22	2 (10%)	26,31,34	1.70	4 (15%)
1	A2M	L1	3718	1	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)

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
1	6MZ	L1	4220	1	-	0/9/27/28	0/3/3/3
30	B8N	S1	1248	30	-	4/16/34/35	0/2/2/2
30	OMU	S1	799	30	-	2/9/27/28	0/2/2/2
1	UR3	L1	4530	1	-	0/7/25/26	0/2/2/2
30	OMU	S1	1804	30	-	1/9/27/28	0/2/2/2
1	OMG	L1	4623	1	-	1/9/27/28	0/3/3/3
1	OMC	L1	4456	1	-	0/9/27/28	0/2/2/2
1	A2M	L1	1326	1	-	1/9/27/28	0/3/3/3
1	OMC	L1	1881	1	-	4/9/27/28	0/2/2/2
1	PSU	L1	4689	1	-	0/7/25/26	0/2/2/2
1	UY1	L1	3818	1	-	3/9/27/28	0/2/2/2
30	PSU	S1	105	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	966	30	-	0/7/25/26	0/2/2/2
1	A2M	L1	3830	1	-	0/9/27/28	0/3/3/3
30	A2M	S1	512	30	-	0/9/27/28	0/3/3/3
30	A2M	S1	1383	30	-	0/9/27/28	0/3/3/3
30	OMG	S1	509	30	-	1/9/27/28	0/3/3/3
1	OMG	L1	4370	1	-	0/9/27/28	0/3/3/3
30	PSU	S1	1177	30	-	0/7/25/26	0/2/2/2
30	4AC	S1	1337	30	-	2/11/29/30	0/2/2/2
30	OMC	S1	174	30	-	0/9/27/28	0/2/2/2
1	A2M	L1	1524	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	4442	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	5010	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	36	30	-	0/7/25/26	0/2/2/2
30	A2M	S1	484	30	-	2/9/27/28	0/3/3/3
1	OMU	L1	3925	1	-	0/9/27/28	0/2/2/2
30	OMC	S1	1272	30	-	0/9/27/28	0/2/2/2
1	OMG	L1	3627	1	-	0/9/27/28	0/3/3/3
1	OMG	L1	2364	1	-	2/9/27/28	0/3/3/3
1	PSU	L1	1744	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	2876	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	L1	1625	1	-	0/9/27/28	0/3/3/3
50	NMM	Si	67	50	-	0/9/11/13	-
30	PSU	S1	609	30	-	0/7/25/26	0/2/2/2
1	OMC	L1	3869	1	-	0/9/27/28	0/2/2/2
30	OMG	S1	601	30	-	0/9/27/28	0/3/3/3
30	OMG	S1	1490	30	-	1/9/27/28	0/3/3/3
30	OMU	S1	627	30	-	1/9/27/28	0/2/2/2
1	PSU	L1	4457	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	400	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	4628	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	1871	1	-	0/9/27/28	0/3/3/3
68	PSU	L3	55	68	-	0/7/25/26	0/2/2/2
1	PSU	L1	4299	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	1792	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	1323	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	1582	1	-	0/7/25/26	0/2/2/2
30	A2M	S1	576	30	-	2/9/27/28	0/3/3/3
1	PSU	L1	4293	1	-	0/7/25/26	0/2/2/2
1	OMU	L1	4306	1	-	0/9/27/28	0/2/2/2
30	OMU	S1	121	30	-	1/9/27/28	0/2/2/2
30	PSU	S1	1625	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	4493	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	3768	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	1238	30	-	0/7/25/26	0/2/2/2
30	A2M	S1	166	30	-	0/9/27/28	0/3/3/3
30	A2M	S1	1678	30	-	0/9/27/28	0/3/3/3
1	PSU	L1	3695	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	4590	1	-	1/9/27/28	0/3/3/3
1	OMC	L1	1340	1	-	1/9/27/28	0/2/2/2
30	PSU	S1	1347	30	-	0/7/25/26	0/2/2/2
1	OMG	L1	3792	1	-	0/9/27/28	0/3/3/3
1	OMG	L1	3899	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	4423	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	2351	1	-	2/9/27/28	0/2/2/2
1	OMG	L1	3744	1	-	0/9/27/28	0/3/3/3
1	OMG	L1	4228	1	-	0/9/27/28	0/3/3/3
30	PSU	S1	296	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	822	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	686	30	-	0/7/25/26	0/2/2/2
1	OMG	L1	4637	1	-	2/9/27/28	0/3/3/3
30	PSU	S1	1232	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	1046	30	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L1	2632	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	1174	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	681	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	4673	1	-	0/7/25/26	0/2/2/2
30	A2M	S1	468	30	-	0/9/27/28	0/3/3/3
1	PSU	L1	1862	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	1004	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	4431	1	-	0/7/25/26	0/2/2/2
30	OMC	S1	462	30	-	0/9/27/28	0/2/2/2
1	PSU	L1	2508	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	649	30	-	0/7/25/26	0/2/2/2
30	G7M	S1	1639	30,32	-	0/7/25/26	0/3/3/3
30	PSU	S1	866	30	-	0/7/25/26	0/2/2/2
1	OMG	L1	4392	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	4552	1	-	0/7/25/26	0/2/2/2
30	OMU	S1	1326	30	-	0/9/27/28	0/2/2/2
1	PSU	L1	4579	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	4521	1	-	0/7/25/26	0/2/2/2
30	6MZ	S1	1832	30	-	0/9/27/28	0/3/3/3
1	PSU	L1	4420	1	-	3/7/25/26	0/2/2/2
1	PSU	L1	3730	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	1536	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	2365	1	-	0/9/27/28	0/2/2/2
1	OMG	L1	2424	1	-	0/9/27/28	0/3/3/3
1	OMU	L1	2837	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	3637	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	2401	1	-	0/9/27/28	0/3/3/3
1	OMG	L1	4499	1	-	0/9/27/28	0/3/3/3
39	IAS	SG	138	39	-	1/7/7/8	-
1	OMG	L1	4618	1	-	1/9/27/28	0/3/3/3
30	OMC	S1	797	30	-	0/9/27/28	0/2/2/2
30	A2M	S1	99	30	-	1/9/27/28	0/3/3/3
30	OMC	S1	1703	30	-	1/9/27/28	0/2/2/2
1	OMG	L1	1316	1	-	2/9/27/28	0/3/3/3
1	A2M	L1	2815	1	-	0/9/27/28	0/3/3/3
1	5MC	L1	3782	1	-	0/7/25/26	0/2/2/2
1	OMU	L1	4620	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	3920	1	-	0/7/25/26	0/2/2/2
30	OMG	S1	1447	30	-	2/9/27/28	0/3/3/3
30	A2M	S1	590	30	-	1/9/27/28	0/3/3/3
30	PSU	S1	1136	30	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PSU	S1	1081	30	-	3/7/25/26	0/2/2/2
30	PSU	S1	406	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	572	30	-	0/7/25/26	0/2/2/2
30	MA6	S1	1851	30	-	2/11/29/30	0/3/3/3
1	A2M	L1	3867	1	-	1/9/27/28	0/3/3/3
1	PSU	L1	4576	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	4523	1	-	1/9/27/28	0/3/3/3
30	PSU	S1	210	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	1683	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	1782	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	814	30	-	0/7/25/26	0/2/2/2
1	OMG	L1	4196	1,32	-	0/9/27/28	0/3/3/3
30	A2M	S1	1031	30	-	1/9/27/28	0/3/3/3
1	OMC	L1	3887	1	-	2/9/27/28	0/2/2/2
1	PSU	L1	4532	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	2363	1	-	0/9/27/28	0/3/3/3
1	5MC	L1	4447	1	-	4/7/25/26	0/2/2/2
1	OMU	L1	4498	1	-	0/9/27/28	0/2/2/2
30	MA6	S1	1850	30	-	0/11/29/30	0/3/3/3
30	OMU	S1	172	30	-	0/9/27/28	0/2/2/2
1	A2M	L1	3724	1	-	0/9/27/28	0/3/3/3
30	PSU	S1	119	30	-	0/7/25/26	0/2/2/2
1	1MA	L1	1322	1	-	0/7/25/26	0/3/3/3
30	PSU	S1	801	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	1692	30	-	0/7/25/26	0/2/2/2
1	OMC	L1	2824	1	-	1/9/27/28	0/2/2/2
1	PSU	L1	4296	1	-	0/7/25/26	0/2/2/2
30	OMU	S1	116	30	-	0/9/27/28	0/2/2/2
30	OMU	S1	428	30	-	4/9/27/28	0/2/2/2
1	PSU	L1	5001	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	651	30	-	0/7/25/26	0/2/2/2
1	OMC	L1	2804	1	-	0/9/27/28	0/2/2/2
68	OMG	L3	75	68	-	0/9/27/28	0/3/3/3
1	A2M	L1	1534	1	-	2/9/27/28	0/3/3/3
30	OMG	S1	436	30	-	0/9/27/28	0/3/3/3
30	PSU	S1	863	30	-	0/7/25/26	0/2/2/2
1	OMU	L1	4227	1	-	1/9/27/28	0/2/2/2
30	OMU	S1	354	30	-	0/9/27/28	0/2/2/2
30	A2M	S1	27	30	-	0/9/27/28	0/3/3/3
1	A2M	L1	398	1	-	1/9/27/28	0/3/3/3
1	OMC	L1	2861	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L1	3844	1	-	1/7/25/26	0/2/2/2
1	PSU	L1	4500	1	-	1/7/25/26	0/2/2/2
30	A2M	S1	159	30	-	1/9/27/28	0/3/3/3
30	OMU	S1	1442	30	-	0/9/27/28	0/2/2/2
30	OMG	S1	644	30	-	4/9/27/28	0/3/3/3
1	PSU	L1	3639	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	4361	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	1781	1	-	2/7/25/26	0/2/2/2
1	OMG	L1	3944	1	-	0/9/27/28	0/3/3/3
30	PSU	S1	1045	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	1643	30	-	0/7/25/26	0/2/2/2
1	A2M	L1	2787	1	-	3/9/27/28	0/3/3/3
1	OMG	L1	4494	1	-	0/9/27/28	0/3/3/3
30	A2M	S1	668	30	-	3/9/27/28	0/3/3/3
1	PSU	L1	1677	1	-	3/7/25/26	0/2/2/2
30	PSU	S1	1445	30	-	0/7/25/26	0/2/2/2
1	OMC	L1	2422	1	-	0/9/27/28	0/2/2/2
1	OMU	L1	2415	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	4353	1	-	0/7/25/26	0/2/2/2
30	OMC	S1	1391	30	-	0/9/27/28	0/2/2/2
1	PSU	L1	3770	1	-	0/7/25/26	0/2/2/2
47	HY3	Sg	62	47	-	1/1/12/14	0/1/1/1
1	PSU	L1	3715	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	3785	1	-	3/9/27/28	0/3/3/3
1	OMG	L1	1522	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	3825	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	4571	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	4972	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	109	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	1244	30	-	0/7/25/26	0/2/2/2
30	4AC	S1	1842	30	-	4/11/29/30	0/2/2/2
30	PSU	S1	34	30	-	0/7/25/26	0/2/2/2
30	OMG	S1	683	30	-	0/9/27/28	0/3/3/3
1	OMC	L1	4536	1	-	1/9/27/28	0/2/2/2
1	PSU	L1	4312	1	-	0/7/25/26	0/2/2/2
30	OMC	S1	517	30	-	0/9/27/28	0/2/2/2
30	PSU	S1	1056	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	3884	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	3701	1	-	6/9/27/28	0/2/2/2
30	PSU	S1	218	30	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L1	1860	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	3851	1	-	3/7/25/26	0/2/2/2
1	PSU	L1	4403	1	-	0/7/25/26	0/2/2/2
30	OMG	S1	1328	30	-	0/9/27/28	0/3/3/3
1	OMC	L1	3841	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	3734	1	-	4/7/25/26	0/2/2/2
30	PSU	S1	93	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	2839	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	3853	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	815	30	-	0/7/25/26	0/2/2/2
68	PSU	L3	69	68	-	0/7/25/26	0/2/2/2
1	PSU	L1	4471	1	-	2/7/25/26	0/2/2/2
30	PSU	S1	1367	30	-	0/7/25/26	0/2/2/2
1	OMC	L1	3808	1	-	1/9/27/28	0/2/2/2
30	OMU	S1	1288	30	-	0/9/27/28	0/2/2/2
1	A2M	L1	3718	1	-	0/9/27/28	0/3/3/3

The worst 5 of 524 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S1	1639	G7M	C4-N9	7.73	1.58	1.38
30	S1	1639	G7M	O6-C6	7.57	1.38	1.23
30	S1	1851	MA6	C5-N7	6.64	1.51	1.39
30	S1	1850	MA6	C5-N7	6.61	1.51	1.39
30	S1	1639	G7M	C5-C4	6.09	1.53	1.38

The worst 5 of 965 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	S1	1851	MA6	C4-N9-C8	14.63	121.58	105.73
30	S1	1850	MA6	C4-N9-C8	14.60	121.55	105.73
30	S1	1639	G7M	C8-N7-C5	11.63	122.33	107.78
30	S1	1851	MA6	N3-C4-N9	6.87	138.39	127.08
30	S1	1850	MA6	N3-C4-N9	6.81	138.30	127.08

There are no chirality outliers.

5 of 113 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	Sg	62	HY3	O-C-CA-C3
1	L1	1326	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
1	L1	1677	PSU	C2'-C1'-C5-C4
1	L1	1881	OMC	O4'-C1'-N1-C2
1	L1	1881	OMC	O4'-C1'-N1-C6

There are no ring outliers.

70 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	S1	799	OMU	2	0
1	L1	4456	OMC	1	0
1	L1	1326	A2M	2	0
1	L1	3818	UY1	1	0
1	L1	3830	A2M	1	0
30	S1	512	A2M	1	0
30	S1	509	OMG	2	0
30	S1	1337	4AC	1	0
30	S1	484	A2M	1	0
30	S1	1272	OMC	1	0
1	L1	1625	OMG	1	0
30	S1	601	OMG	1	0
30	S1	1490	OMG	2	0
1	L1	4457	PSU	2	0
1	L1	1871	A2M	1	0
30	S1	576	A2M	1	0
1	L1	4293	PSU	1	0
1	L1	4306	OMU	1	0
30	S1	121	OMU	2	0
30	S1	166	A2M	2	0
30	S1	1678	A2M	3	0
1	L1	4590	A2M	1	0
1	L1	1340	OMC	1	0
1	L1	3899	OMG	1	0
1	L1	2351	OMC	1	0
1	L1	3744	OMG	1	0
30	S1	296	PSU	1	0
30	S1	1232	PSU	2	0
30	S1	681	PSU	1	0
30	S1	462	OMC	1	0
30	S1	1639	G7M	1	0
30	S1	1832	6MZ	1	0
1	L1	4420	PSU	1	0
30	S1	797	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	S1	99	A2M	1	0
30	S1	1703	OMC	1	0
1	L1	1316	OMG	1	0
1	L1	2815	A2M	2	0
1	L1	3782	5MC	1	0
1	L1	4620	OMU	3	0
30	S1	1447	OMG	1	0
1	L1	4523	A2M	1	0
30	S1	210	PSU	2	0
30	S1	1031	A2M	2	0
1	L1	3887	OMC	1	0
1	L1	4447	5MC	1	0
30	S1	1850	MA6	1	0
1	L1	3724	A2M	2	0
30	S1	116	OMU	3	0
1	L1	2804	OMC	1	0
68	L3	75	OMG	1	0
1	L1	1534	A2M	1	0
30	S1	436	OMG	2	0
30	S1	863	PSU	1	0
30	S1	354	OMU	1	0
1	L1	398	A2M	1	0
1	L1	2861	OMC	1	0
30	S1	159	A2M	2	0
30	S1	1442	OMU	1	0
30	S1	668	A2M	2	0
1	L1	2415	OMU	2	0
30	S1	1391	OMC	1	0
1	L1	3785	A2M	1	0
1	L1	3825	A2M	2	0
1	L1	4571	A2M	2	0
30	S1	1842	4AC	2	0
1	L1	4536	OMC	1	0
30	S1	1328	OMG	1	0
1	L1	3808	OMC	1	0
1	L1	3718	A2M	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	COA	Nd	301	-	44,50,50	2.89	14 (31%)	65,75,75	2.53	15 (23%)
89	GTP	L2	201	48	30,34,34	0.50	0	46,54,54	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	COA	Nd	301	-	-	13/48/64/64	0/3/3/3
89	GTP	L2	201	48	-	2/22/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	Nd	301	COA	O4B-C1B	7.68	1.60	1.42
88	Nd	301	COA	C5P-N4P	6.92	1.49	1.33
88	Nd	301	COA	C2B-C1B	-6.21	1.33	1.53
88	Nd	301	COA	C6A-N6A	5.98	1.49	1.34
88	Nd	301	COA	C3B-C4B	-5.89	1.37	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	Nd	301	COA	N6A-C6A-N1A	-10.32	95.75	118.35
88	Nd	301	COA	C5A-C6A-N6A	9.21	143.47	123.43
88	Nd	301	COA	C1B-N9A-C8A	-5.71	114.23	127.14
88	Nd	301	COA	N3A-C2A-N1A	-5.54	119.93	128.60
88	Nd	301	COA	C4A-N9A-C1B	4.63	137.62	126.59

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	Nd	301	COA	C5B-O5B-P1A-O1A
88	Nd	301	COA	C5B-O5B-P1A-O2A
88	Nd	301	COA	CAP-CBP-CCP-O6A
88	Nd	301	COA	N8P-C9P-CAP-OAP
89	L2	201	GTP	O4'-C4'-C5'-O5'

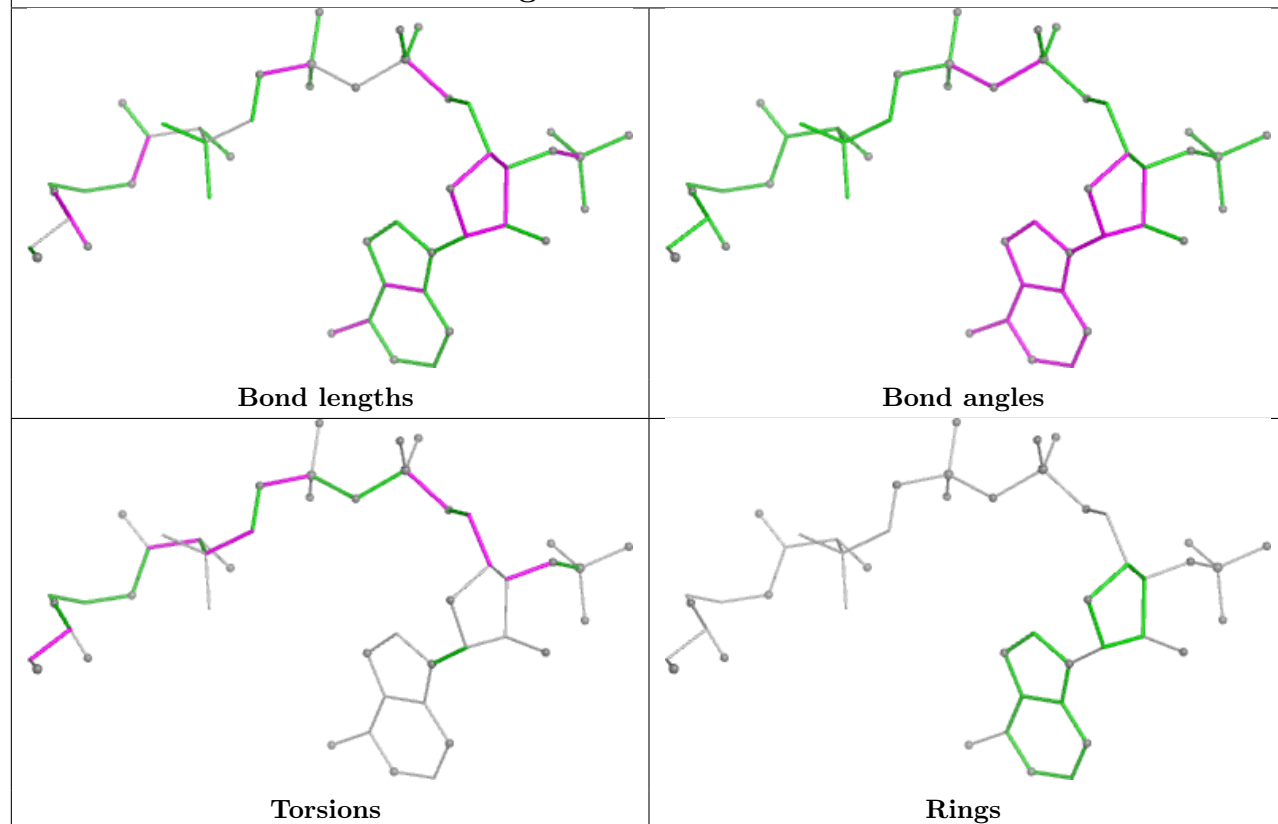
There are no ring outliers.

2 monomers are involved in 6 short contacts:

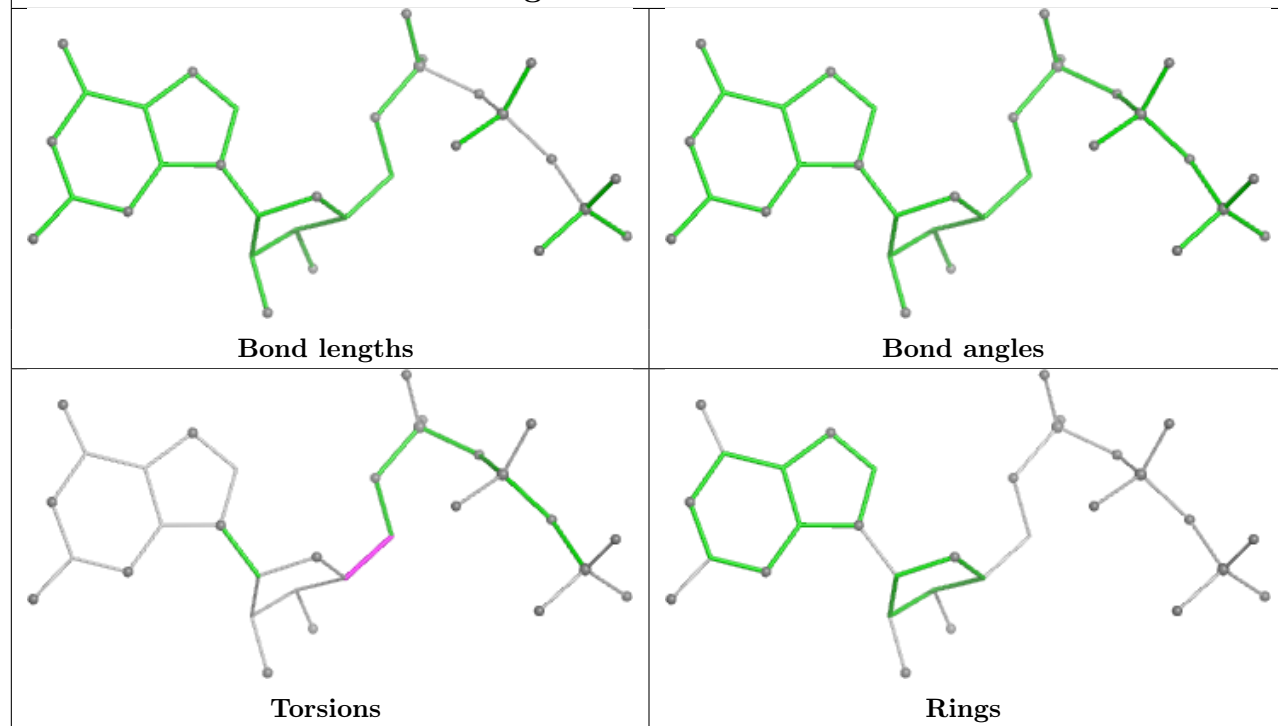
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	Nd	301	COA	5	0
89	L2	201	GTP	1	0

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

Ligand COA Nd 301



Ligand GTP L2 201



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

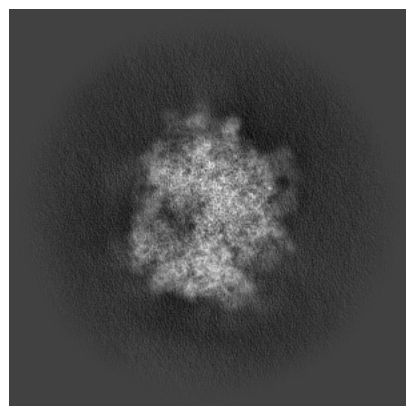
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55351. These allow visual inspection of the internal detail of the map and identification of artifacts.

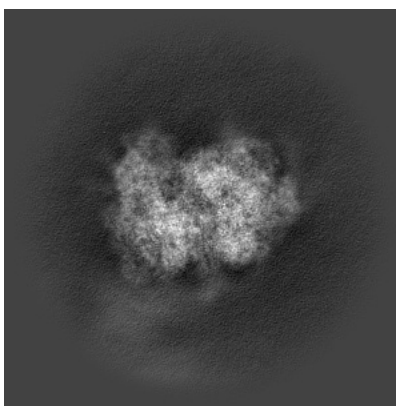
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

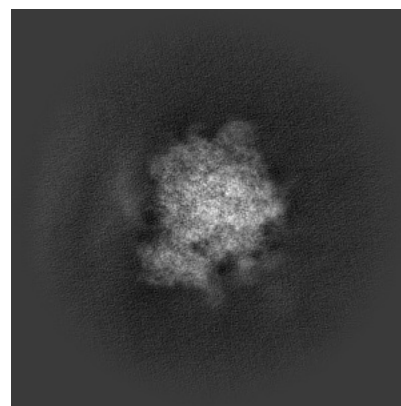
6.1.1 Primary map



X

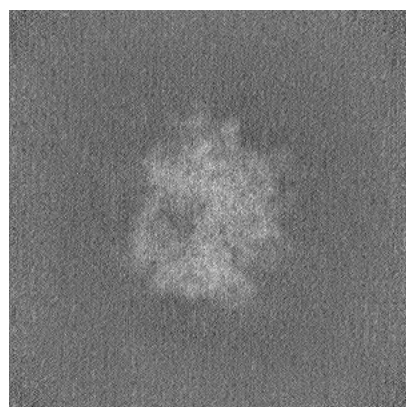


Y

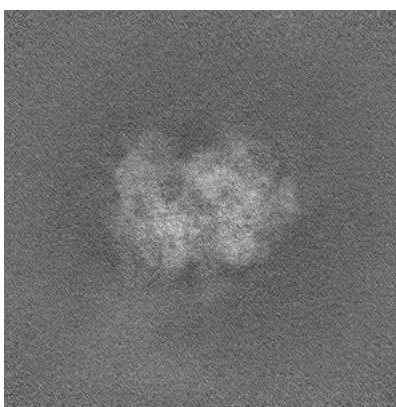


Z

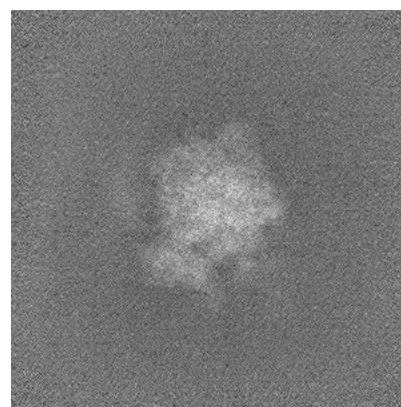
6.1.2 Raw map



X



Y

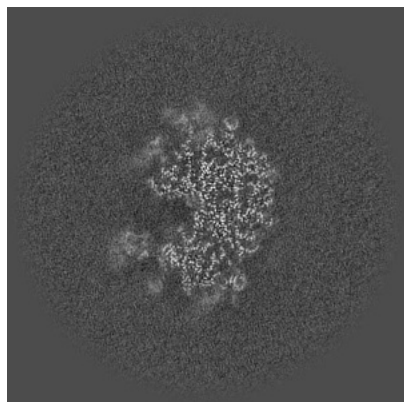


Z

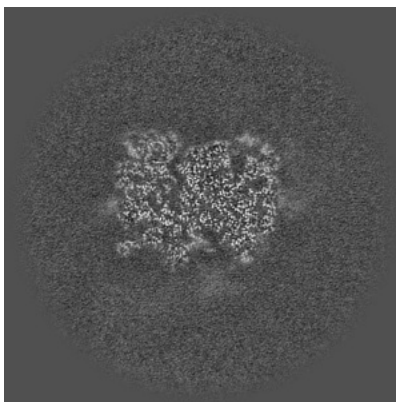
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

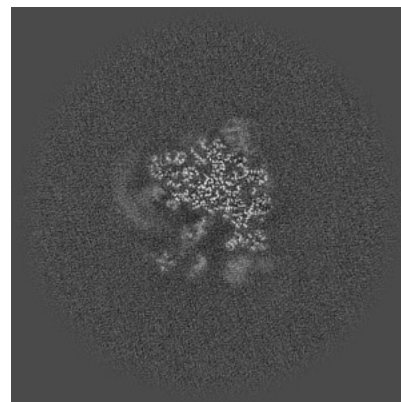
6.2.1 Primary map



X Index: 280

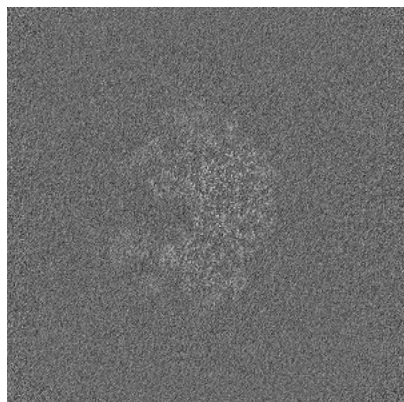


Y Index: 280

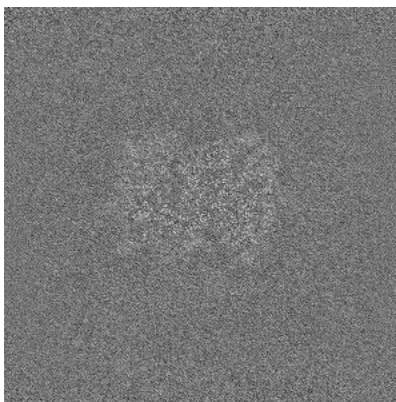


Z Index: 280

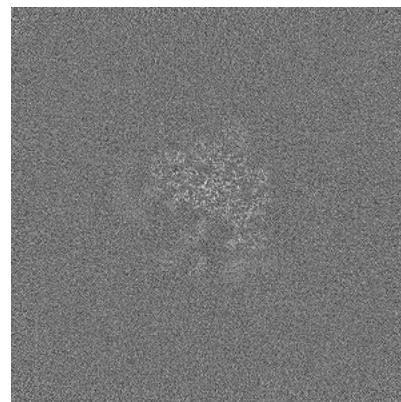
6.2.2 Raw map



X Index: 280



Y Index: 280

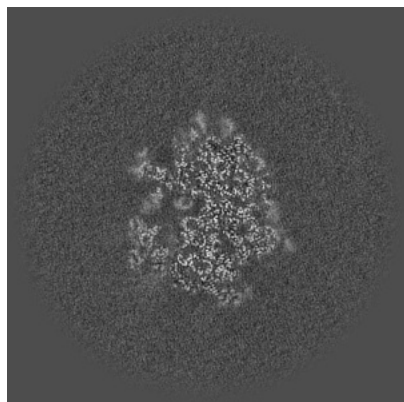


Z Index: 280

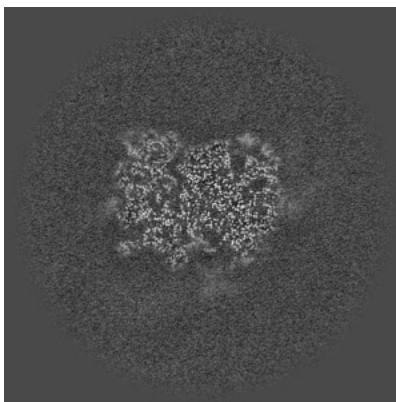
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

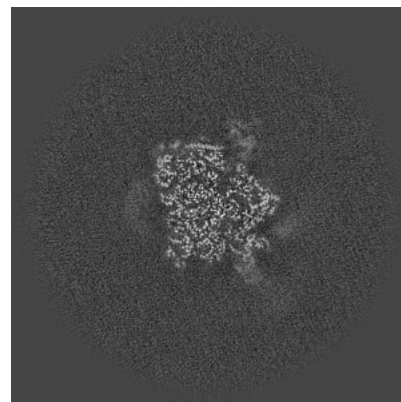
6.3.1 Primary map



X Index: 263

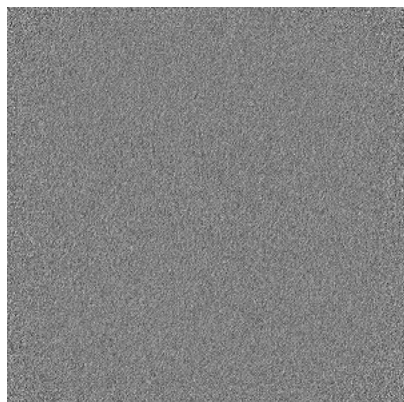


Y Index: 281

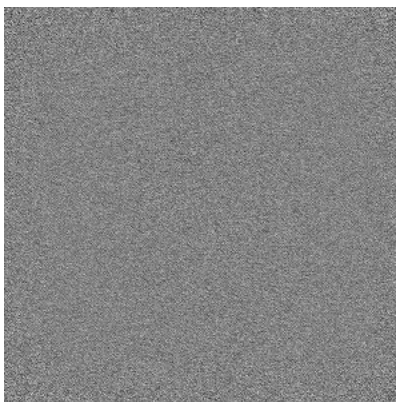


Z Index: 309

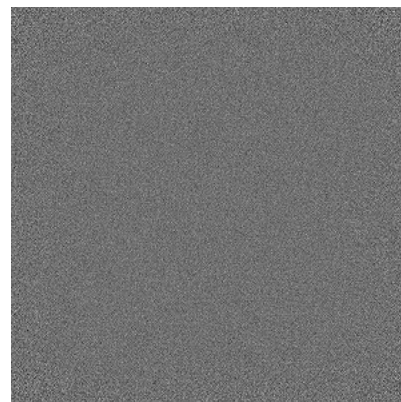
6.3.2 Raw map



X Index: 0



Y Index: 0

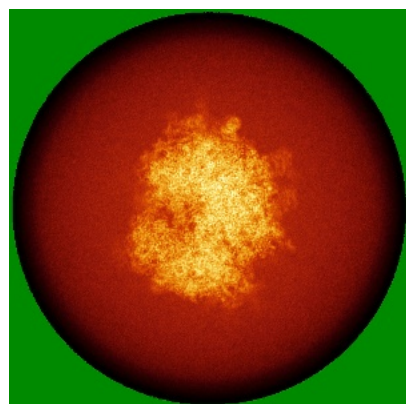


Z Index: 0

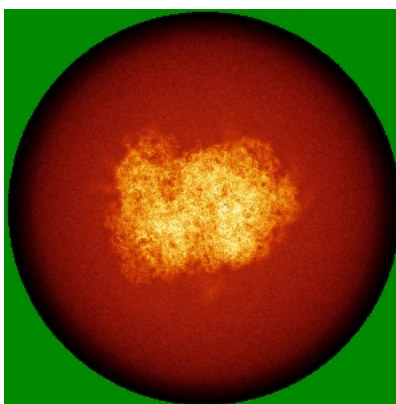
The images above show the largest variance slices of the map in three orthogonal directions.

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

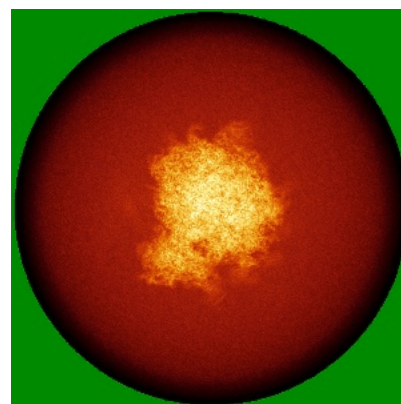
6.4.1 Primary map



X

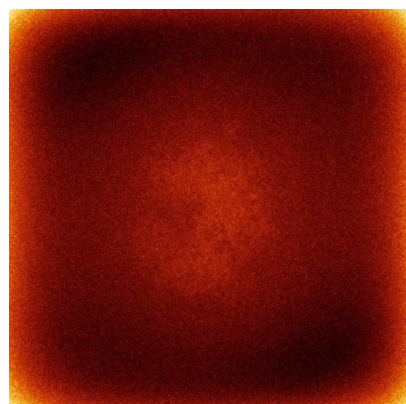


Y

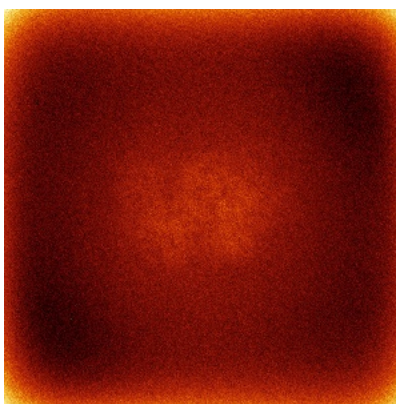


Z

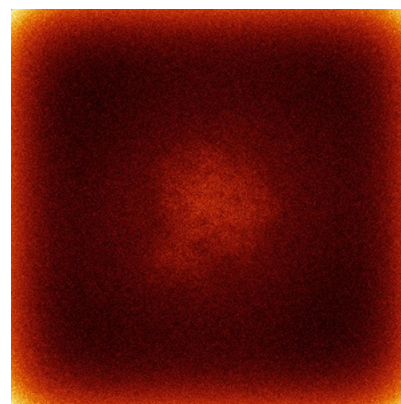
6.4.2 Raw map



X



Y

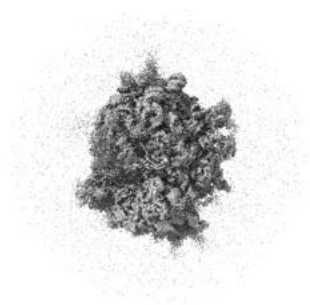


Z

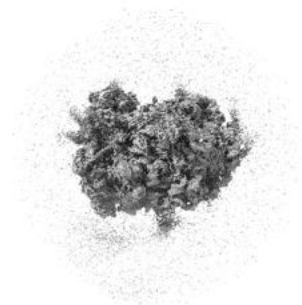
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

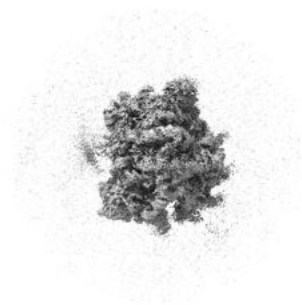
6.5.1 Primary map



X



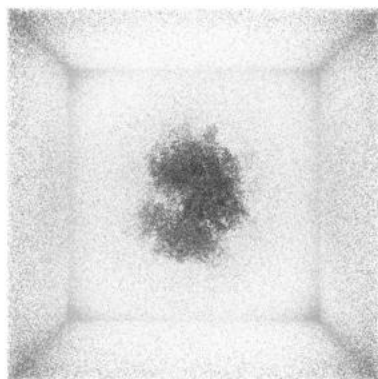
Y



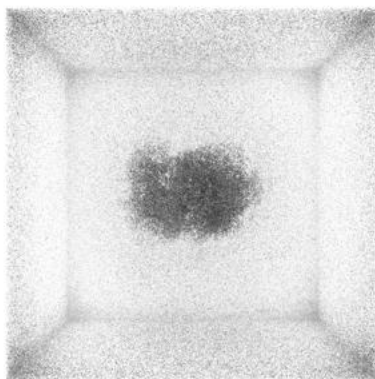
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

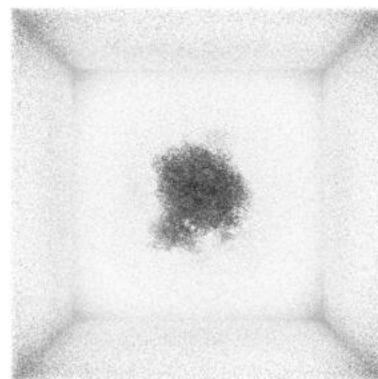
6.5.2 Raw map



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.

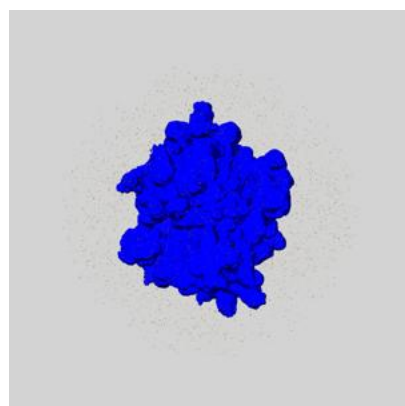
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

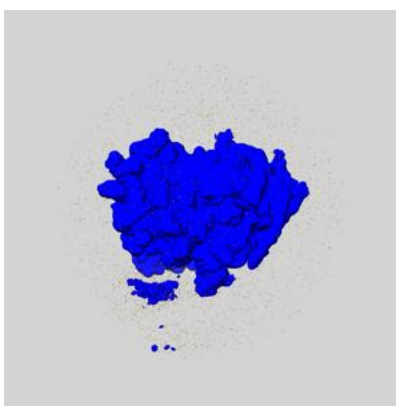
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

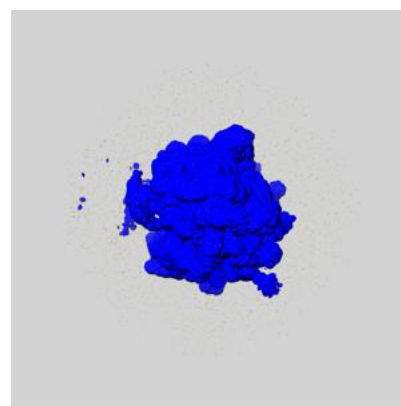
6.6.1 emd_55351_msk_1.map [i](#)



X



Y

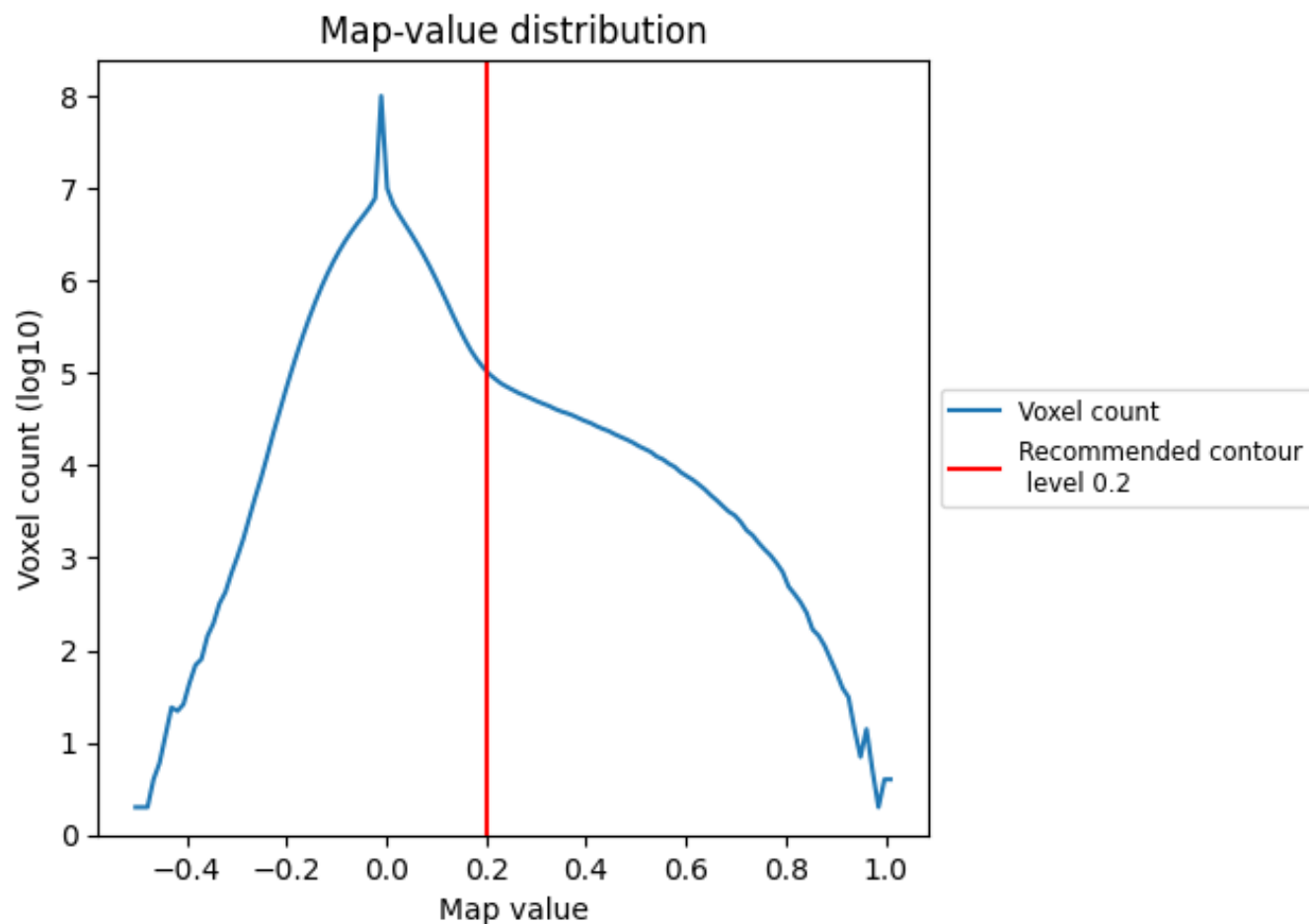


Z

7 Map analysis [i](#)

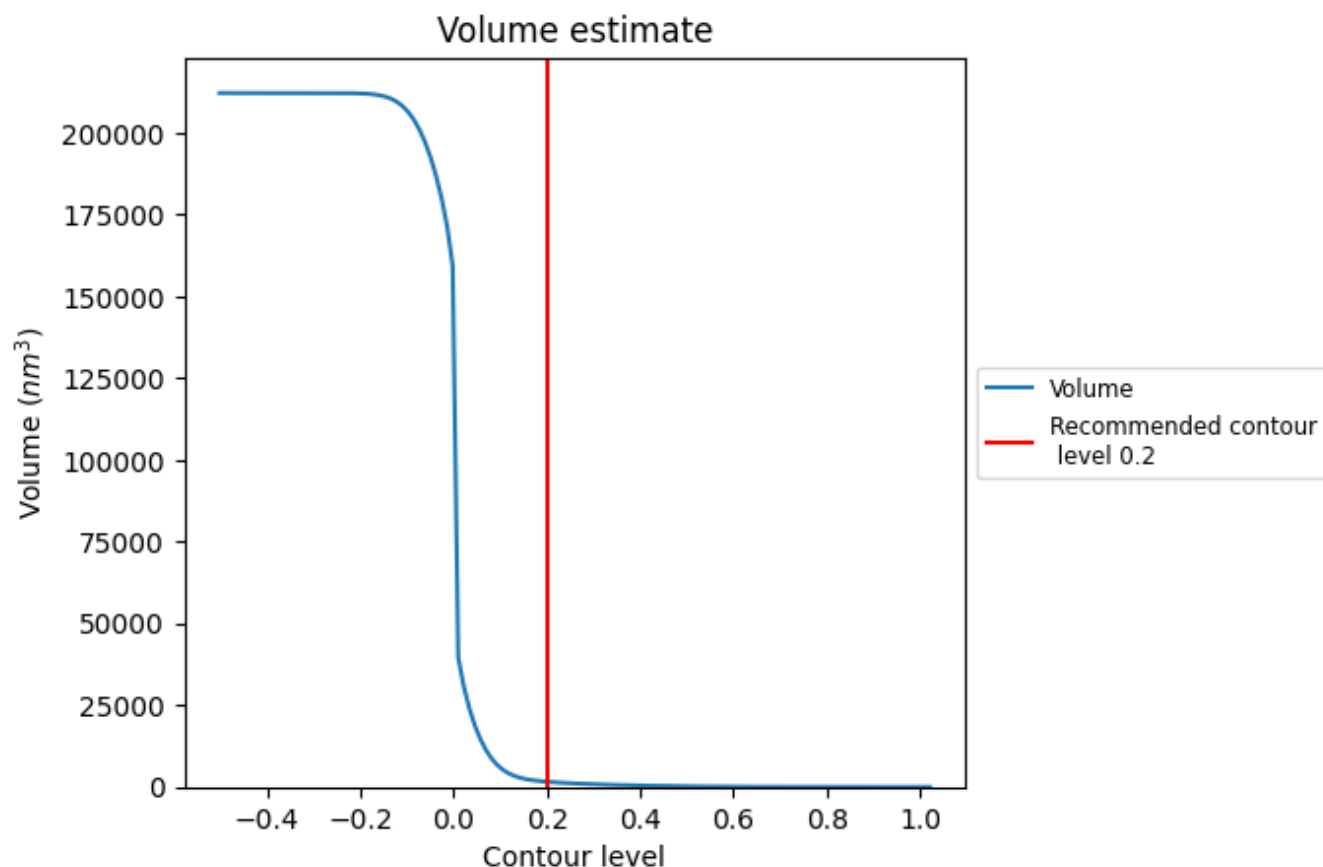
This section contains the results of statistical analysis of the map.

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.

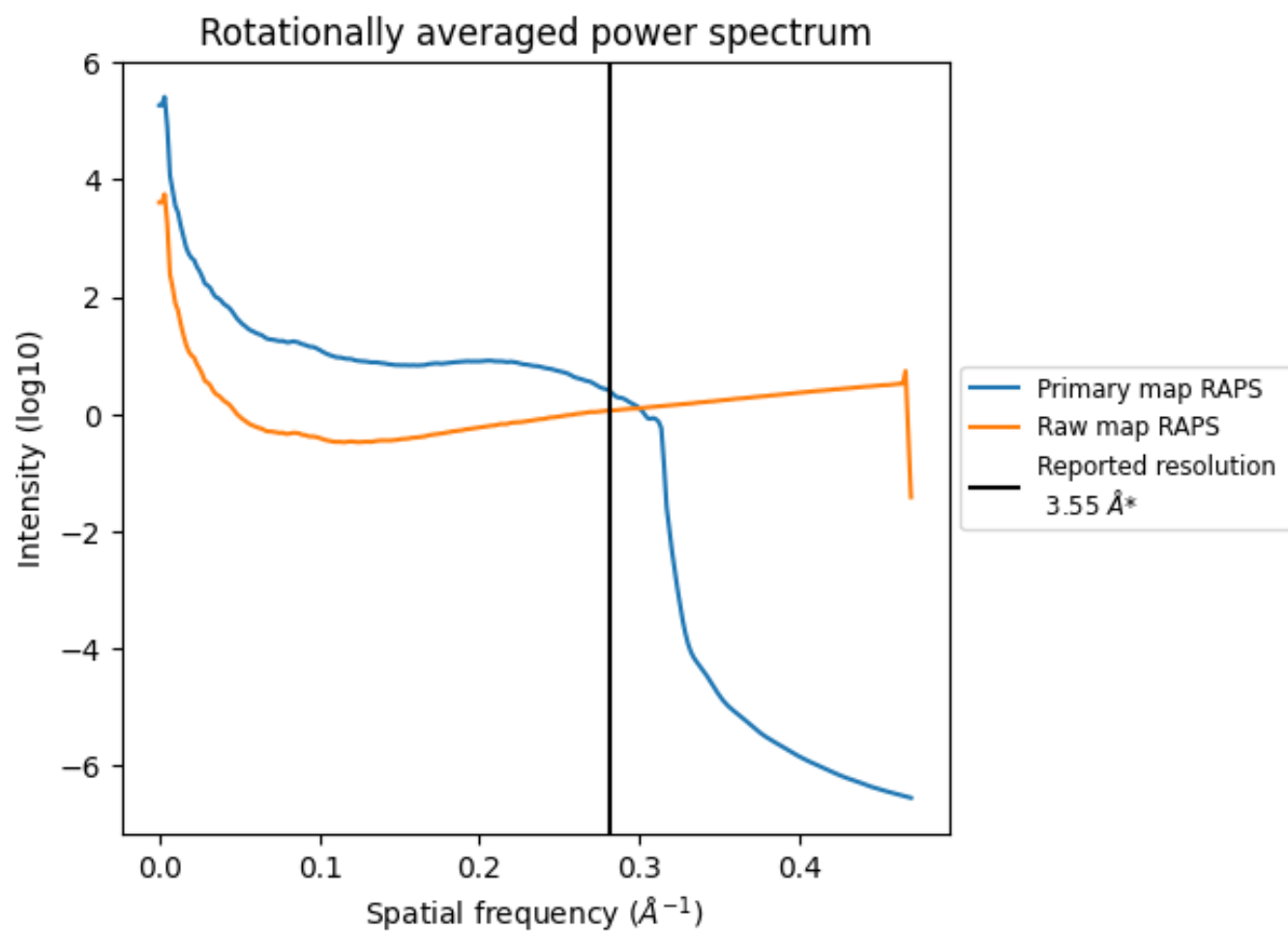
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1583 nm^3 ; this corresponds to an approximate mass of 1430 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 ⓘ

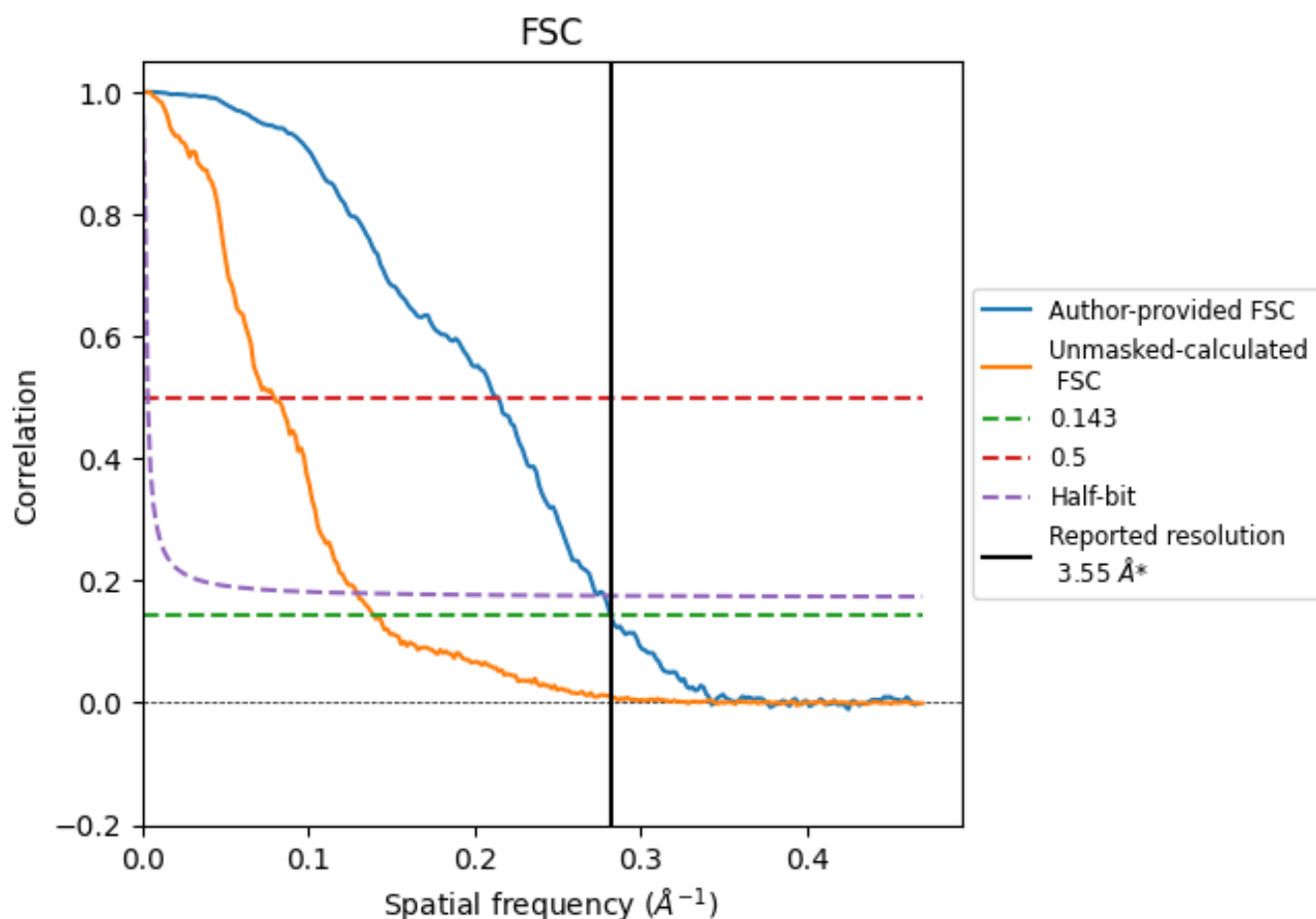


*Reported resolution corresponds to spatial frequency of 0.282 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.282 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

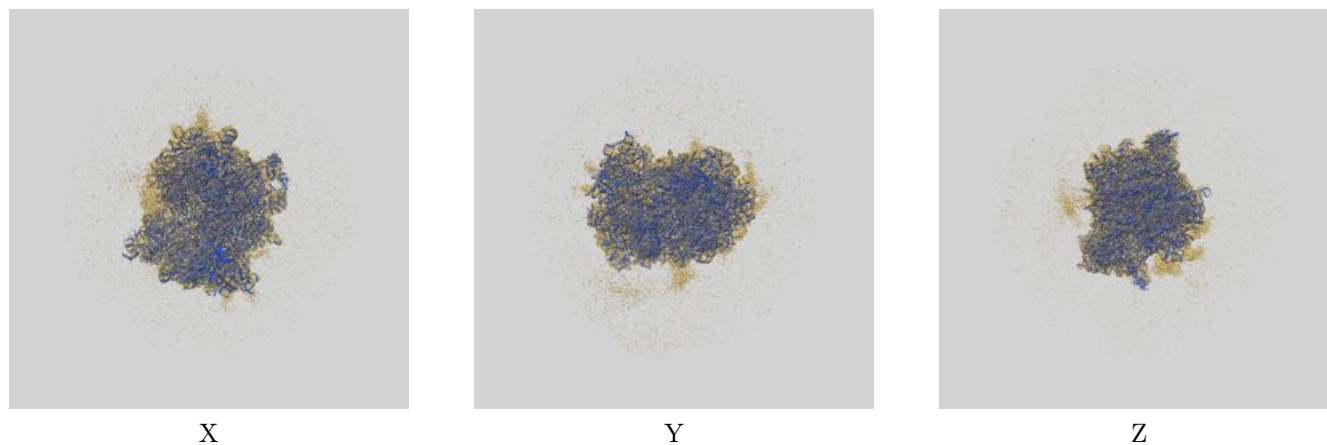
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	3.55	4.68	3.60
Unmasked-calculated*	7.17	12.59	7.72

*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 7.17 differs from the reported value 3.55 by more than 10 %

9 Map-model fit [i](#)

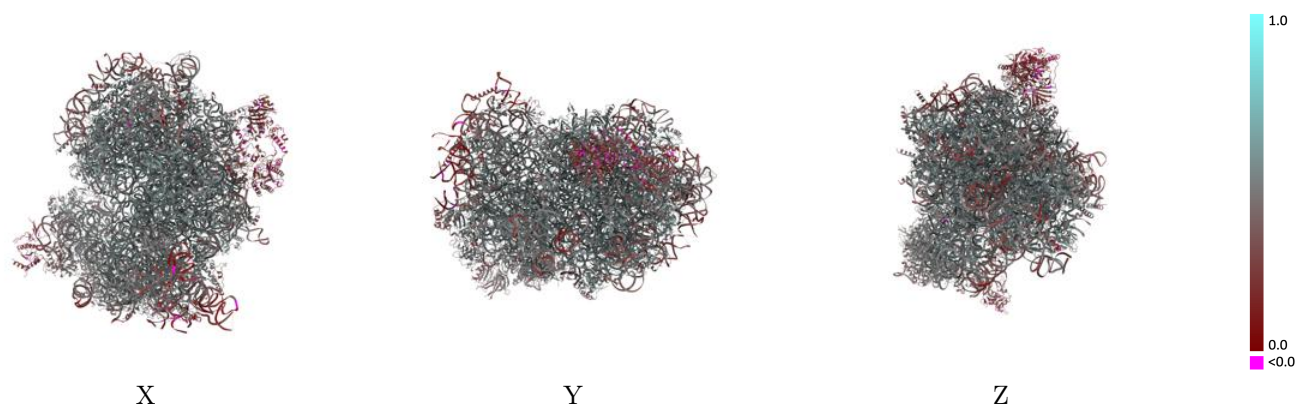
This section contains information regarding the fit between EMDB map EMD-55351 and PDB model 9SYR. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



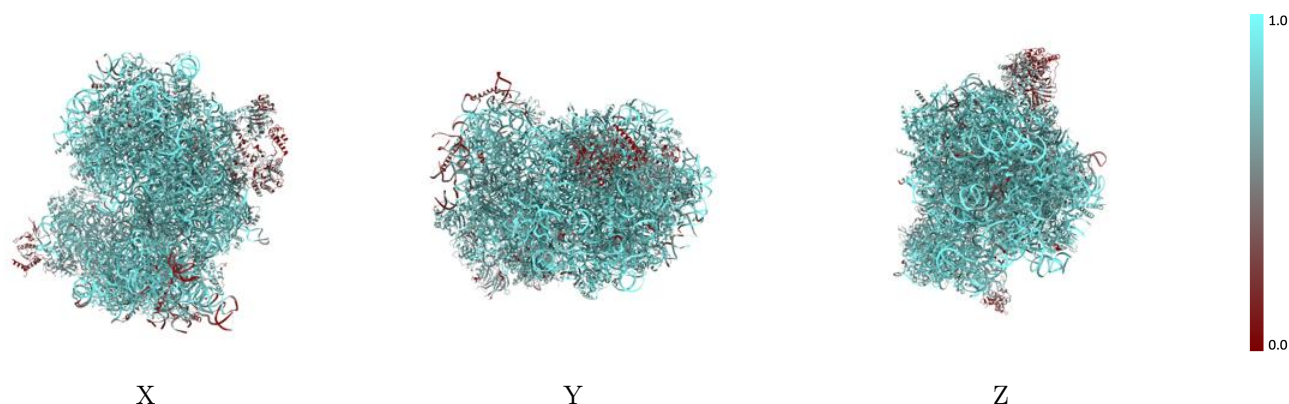
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



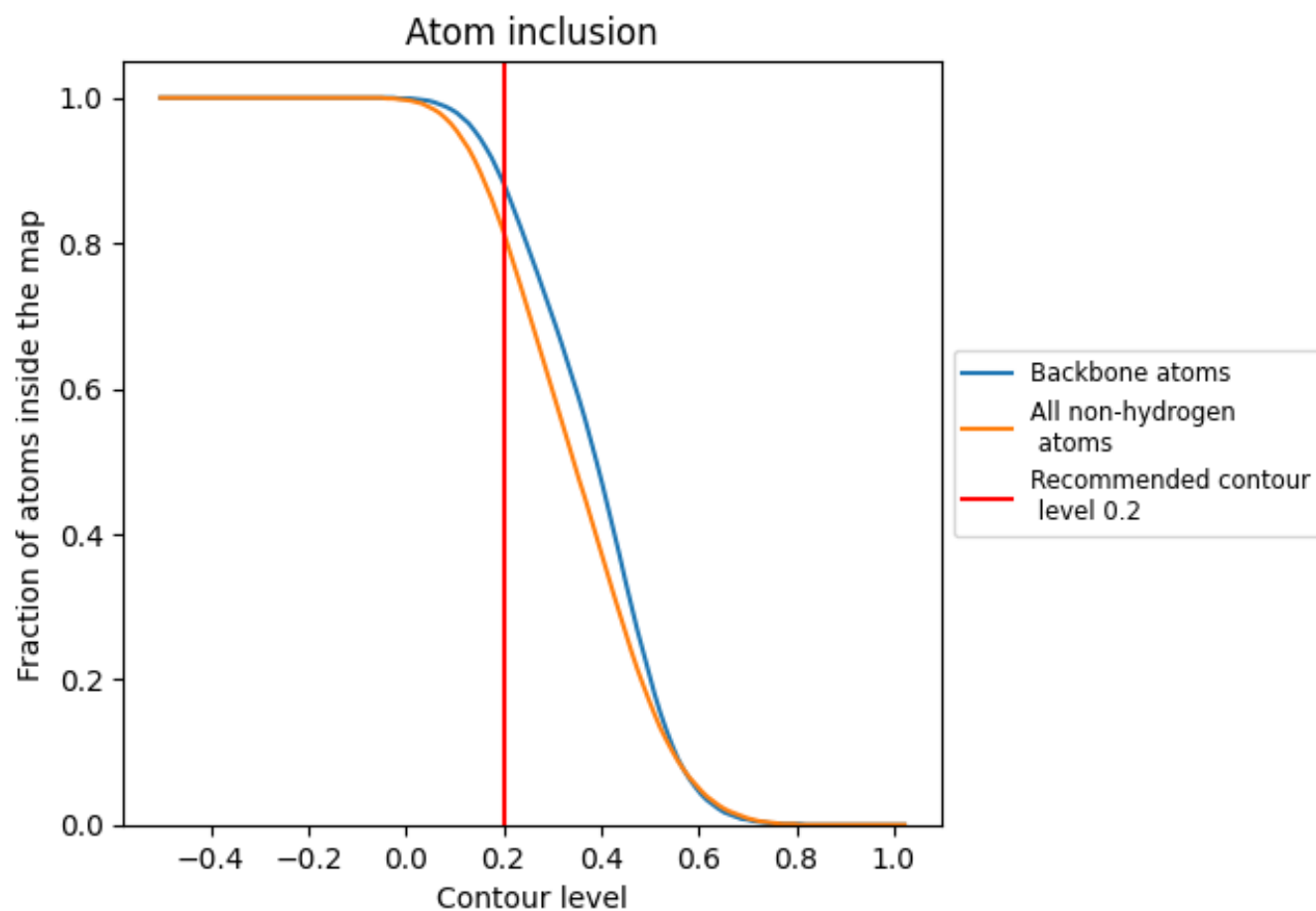
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8160	 0.4720
L1	 0.9060	 0.4830
L2	 0.9670	 0.5050
L3	 0.9360	 0.5010
LA	 0.8500	 0.5430
LB	 0.6910	 0.4550
LC	 0.7940	 0.5330
LD	 0.7430	 0.5020
LE	 0.7850	 0.5190
LF	 0.7660	 0.5290
LG	 0.8310	 0.5190
LH	 0.8310	 0.5440
LI	 0.7960	 0.5150
LJ	 0.7770	 0.4900
LK	 0.7810	 0.4970
LM	 0.7720	 0.5060
LN	 0.5020	 0.4660
LO	 0.7750	 0.4880
LP	 0.7820	 0.5020
LQ	 0.7940	 0.4970
La	 0.8120	 0.5470
Lb	 0.8190	 0.5300
Lc	 0.8090	 0.5200
Ld	 0.8180	 0.4890
Le	 0.7870	 0.4910
Lf	 0.7960	 0.5190
Lg	 0.8090	 0.5370
Lh	 0.8030	 0.5340
Li	 0.7860	 0.5010
Lj	 0.8200	 0.5230
Lk	 0.7930	 0.5210
Ll	 0.7770	 0.4660
Lm	 0.7870	 0.5330
Ln	 0.5520	 0.4130
Lo	 0.7430	 0.5010



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Chain	Atom inclusion	Q-score
Lp	 0.7810	 0.4970
Lq	 0.8190	 0.5060
Lr	 0.8320	 0.5330
Ls	 0.7280	 0.4590
Lt	 0.7750	 0.5050
Lu	 0.8040	 0.5150
Lv	 0.8230	 0.5360
Lw	 0.8430	 0.5450
Lx	 0.7780	 0.5070
Ly	 0.7610	 0.4870
Lz	 0.7420	 0.4850
Na	 0.3420	 0.2330
Nb	 0.4100	 0.3030
Nd	 0.5310	 0.2690
Nm	 0.2760	 0.2020
S1	 0.8600	 0.4510
S2	 0.7970	 0.4790
S3	 0.8440	 0.4410
SA	 0.7440	 0.4820
SB	 0.7920	 0.4890
SC	 0.6920	 0.4730
SD	 0.7330	 0.4960
SE	 0.6510	 0.4190
SF	 0.7620	 0.5000
SG	 0.7250	 0.4980
SH	 0.1900	 0.2180
Sa	 0.7070	 0.4560
Sb	 0.6960	 0.4570
Sc	 0.7120	 0.4790
Sd	 0.7570	 0.4630
Se	 0.7550	 0.5010
Sf	 0.7880	 0.5250
Sg	 0.7970	 0.5230
Sh	 0.7520	 0.4540
Si	 0.7230	 0.4580
Sj	 0.7670	 0.5020
Sk	 0.6940	 0.4560
Sl	 0.6730	 0.4370
Sm	 0.6380	 0.4370
Sn	 0.6330	 0.4490
So	 0.6670	 0.4770
Sp	 0.7260	 0.4670

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Sq	 0.6420	 0.5000
Sr	 0.0660	 0.2120
Ss	 0.6010	 0.3930
St	 0.7550	 0.4800
Su	 0.7020	 0.4870
Sv	 0.7560	 0.5060
Sw	 0.7570	 0.4950
Sx	 0.6520	 0.4520
Sy	 0.6760	 0.4170
Sz	 0.6610	 0.4250