



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 02:50 am BST

PDB ID : 9RHU / pdb_00009rhu
EMDB ID : EMD-53976
Title : Rabbit 80S ribosome in complex with eRF1-AAQ, stalled at the Stop codon in mutated F2A sequence
Authors : Li, X.; Zuber, P.K.; Loughran, G.; Bhatt, P.R.; Alquraish, F.; Ramakrishnan, V.; Firth, A.E.; Atkins, J.F.
Deposited on : 2025-06-10
Resolution : 2.65 Å (reported)
Based on initial model : 7O80

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:

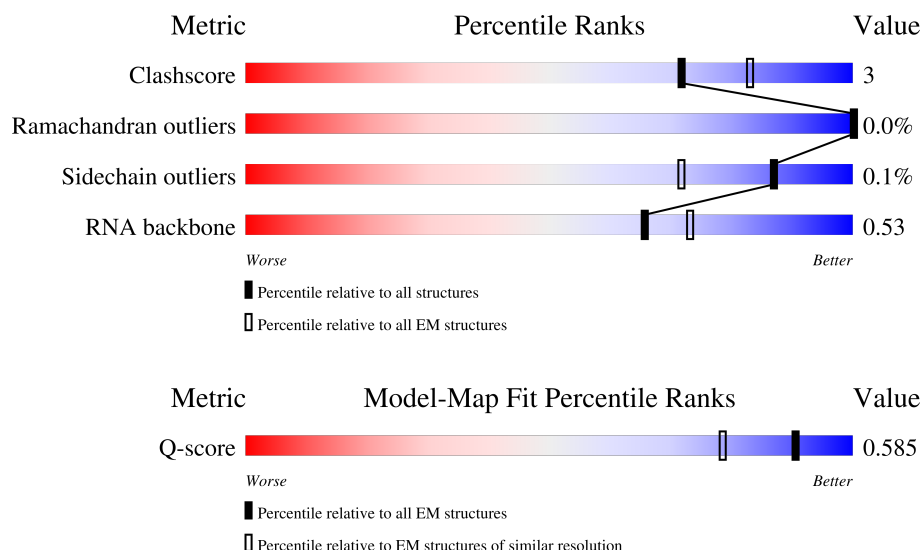
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.65 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	9050 (2.15 - 3.15)

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	MB	117	
2	A1	1870	

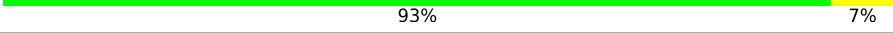
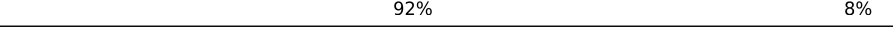
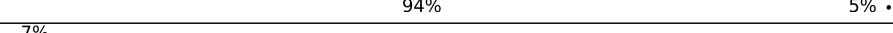
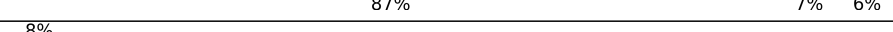
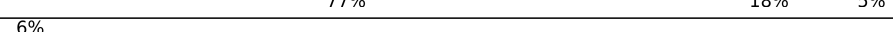
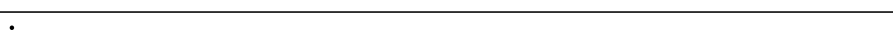
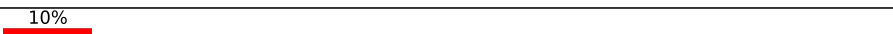
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	A2	291	
4	A3	4808	
5	B1	84	
6	B2	249	
7	B3	119	
8	C1	69	
9	C2	319	
10	C3	158	
11	D1	80	
12	D2	192	
13	D3	257	
14	E1	59	
15	E2	214	
16	E3	403	
17	F1	115	
18	F2	178	
19	F3	413	
20	G1	317	
21	G2	184	
22	G3	296	
23	H1	56	
24	H2	211	
25	I1	659	
26	I2	218	
27	J1	75	

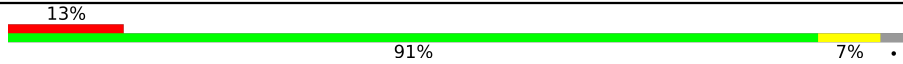
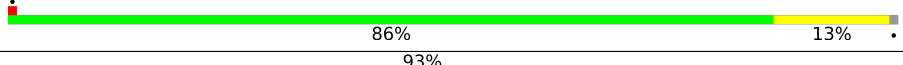
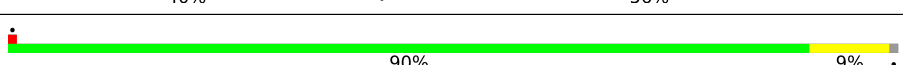
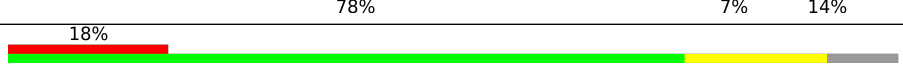
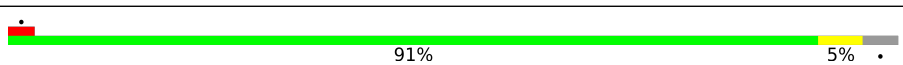
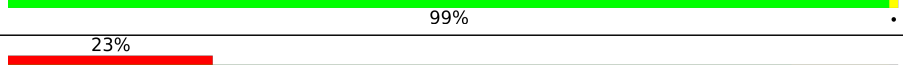
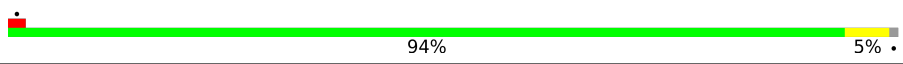
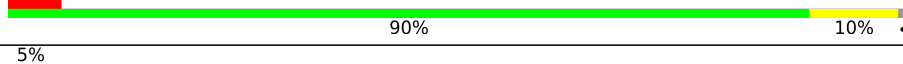
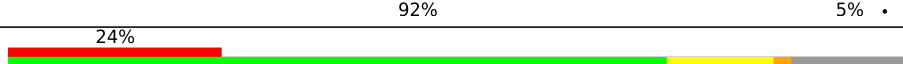
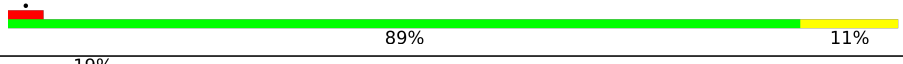
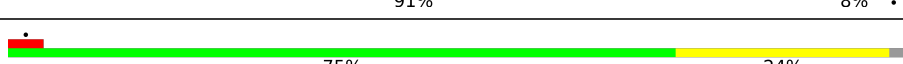
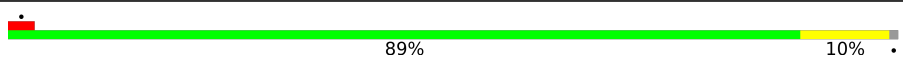
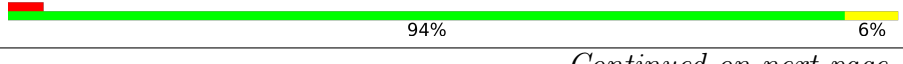
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	J2	204	
29	K1	74	
30	K2	203	
31	L1	295	
32	L2	184	
33	M1	264	
34	M2	188	
35	N1	293	
36	N2	196	
37	O1	243	
38	O2	176	
39	P1	263	
40	P2	160	
41	Q1	204	
42	Q2	128	
43	R1	249	
44	R2	140	
45	S1	194	
46	S2	157	
47	T1	208	
48	T2	156	
49	U1	194	
50	U2	145	
51	V1	165	
52	V2	136	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	W1	158	
54	W2	148	
55	X1	132	
56	X2	245	
57	Y1	151	
58	Y2	115	
59	Z1	151	
60	Z2	125	
61	a1	145	
62	a2	135	
63	b1	146	
64	b2	110	
65	c1	135	
66	d1	152	
67	d2	123	
68	e1	144	
69	e2	105	
70	f1	119	
71	f2	97	
72	g1	84	
73	g2	70	
74	h1	130	
75	h2	51	
76	i1	143	
77	i2	52	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
78	j1	133	
79	j2	141	
80	k1	124	
81	k2	92	
82	l1	25	
83	l2	137	
84	m2	318	
85	n2	165	
86	o2	217	
87	p2	438	
88	q2	599	

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 233632 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L34.

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

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	1770	Total	C	N	O	P	0	0
			37833	16911	6781	12371	1770		

- Molecule 3 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A3	3764	Total	C	N	O	P	0	0
			80772	36003	14762	26243	3764		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 5 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B1	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 6 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B2	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

- Molecule 7 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B3	119	Total	C	N	O	P	0	0
			2538	1131	451	837	119		

- Molecule 8 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C1	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 9 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C2	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	86	ALA	VAL	conflict	UNP G1STW0
C2	191	GLY	CYS	conflict	UNP G1STW0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C3	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 11 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D1	68	Total	C	N	O	S	0	0
			554	349	103	95	7		

- Molecule 12 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D2	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 13 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D3	253	Total	C	N	O	S	0	0
			1940	1214	396	324	6		

- Molecule 14 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E1	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 15 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E2	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 16 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E3	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

- Molecule 17 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F1	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 18 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F2	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 19 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F3	363	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	2	ACE	-	acetylation	UNP G1SVW5

- Molecule 20 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G1	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 21 is a protein called Choriogonadotropin subunit beta variant 1,Genome polyprotein,Genome polyprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	G2	24	Total	C	N	O	0	0
			176	113	29	34		

- Molecule 22 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G3	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G3	2	MET	-	initiating methionine	UNP P19949

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	H1	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 24 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	H2	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H2	74	ARG	HIS	conflict	UNP G1TKB3
H2	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 25 is a RNA chain called mRNA containing F2A sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	I1	18	Total	C	N	O	P	0	0
			374	167	56	133	18		

- Molecule 26 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	I2	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 27 is a RNA chain called E-site tRNA-Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	J1	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 28 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	J2	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 29 is a RNA chain called P-site tRNA-Gly.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	K1	74	Total	C	N	O	P	0	0
			1582	711	273	524	74		

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K2	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 31 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L1	222	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L1	1	ACE	-	acetylation	UNP G1TLT8

- Molecule 32 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L2	159	Total	C	N	O	S	0	0
			1289	809	249	222	9		

- Molecule 33 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	M1	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 34 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M2	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M2	134	ARG	CYS	conflict	UNP F6QK19

- Molecule 35 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N1	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N1	33	ILE	VAL	conflict	UNP O18789
N1	101	ALA	SER	conflict	UNP O18789

- Molecule 36 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	N2	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N2	38	ARG	HIS	conflict	UNP G1TYL6
N2	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 37 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	O1	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 38 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O2	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

- Molecule 39 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P1	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P1	25	GLY	SER	conflict	UNP G1TK17
P1	51	ARG	LYS	conflict	UNP G1TK17
P1	78	THR	ALA	conflict	UNP G1TK17
P1	156	VAL	MET	conflict	UNP G1TK17

- Molecule 40 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	P2	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 41 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Q1	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 42 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Q2	98	Total	C	N	O	S	0	0
			797	511	139	145	2		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q2	32	GLY	ARG	conflict	UNP G1TSG1
Q2	36	ALA	GLU	conflict	UNP G1TSG1
Q2	39	PHE	SER	conflict	UNP G1TSG1
Q2	54	GLY	ARG	conflict	UNP G1TSG1
Q2	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 43 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R1	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 44 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	R2	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 45 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	S1	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 46 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S2	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 47 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	T1	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T1	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 48 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T2	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 49 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	U1	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 50 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	U2	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 51 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	V1	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 52 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	V2	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 53 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	W1	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 54 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W2	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 55 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	X1	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 56 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X2	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 57 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Y1	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 58 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Y2	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 59 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Z1	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Z2	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 61 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	a1	133	Total	C	N	O	S	0	0
			1091	694	205	185	7		

- Molecule 62 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	a2	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 63 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	b1	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 64 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	b2	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 65 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	c1	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 66 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	d1	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
d1	1	ACE	-	acetylation	UNP G1TPG3

- Molecule 67 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	d2	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 68 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	e1	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 69 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	e2	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e2	31	GLY	ARG	conflict	UNP G1TTQ5

- Molecule 70 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	f1	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 71 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	f2	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 72 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	g1	84	Total	C	N	O	S	0	0
			640	394	117	124	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g1	0	ACE	-	acetylation	UNP G1TM82

- Molecule 73 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	g2	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g2	24	LYS	ASN	conflict	UNP G1U001

- Molecule 74 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	h1	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 75 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	h2	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 76 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	i1	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 77 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	i2	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 78 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	j1	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 79 is a protein called Ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	j2	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 80 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	k1	74	Total	C	N	O	S	0	0
			587	376	107	103	1		

- Molecule 81 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	k2	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 82 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	l1	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 83 is a protein called [histone H4]-N-methyl-L-lysine20 N-methyltransferase KMT5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	l2	127	Total	C	N	O	S	0	0
			1014	629	209	170	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l2	1	ACE	-	acetylation	UNP A0A8C0DF35

- Molecule 84 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	m2	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 85 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	n2	156	Total	C	N	O	S	0	0
			1178	733	221	220	4		

- Molecule 86 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	o2	212	Total	C	N	O	S	0	0
			1707	1092	308	299	8		

- Molecule 87 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	p2	416	Total	C	N	O	S	0	0
			3280	2087	559	623	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p2	0	GLY	-	expression tag	UNP P62495
p2	1	PRO	-	expression tag	UNP P62495
p2	183	ALA	GLY	engineered mutation	UNP P62495
p2	184	ALA	GLY	engineered mutation	UNP P62495

- Molecule 88 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	q2	595	Total	C	N	O	S	0	0
			4668	2982	801	854	31		

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	MB	1	Total	Mg	0
			1	1	
89	A1	109	Total	Mg	0
			109	109	
89	A3	239	Total	Mg	0
			239	239	
89	B3	4	Total	Mg	0
			4	4	
89	C3	5	Total	Mg	0
			5	5	
89	E2	1	Total	Mg	0
			1	1	
89	E3	1	Total	Mg	0
			1	1	
89	I1	2	Total	Mg	0
			2	2	
89	J2	1	Total	Mg	0
			1	1	
89	L2	2	Total	Mg	0
			2	2	
89	R2	1	Total	Mg	0
			1	1	
89	i1	1	Total	Mg	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
90	MB	1	Total	Zn	0
			1	1	
90	D1	1	Total	Zn	0
			1	1	
90	F1	1	Total	Zn	0
			1	1	
90	H1	1	Total	Zn	0
			1	1	
90	f2	1	Total	Zn	0
			1	1	

Continued on next page...

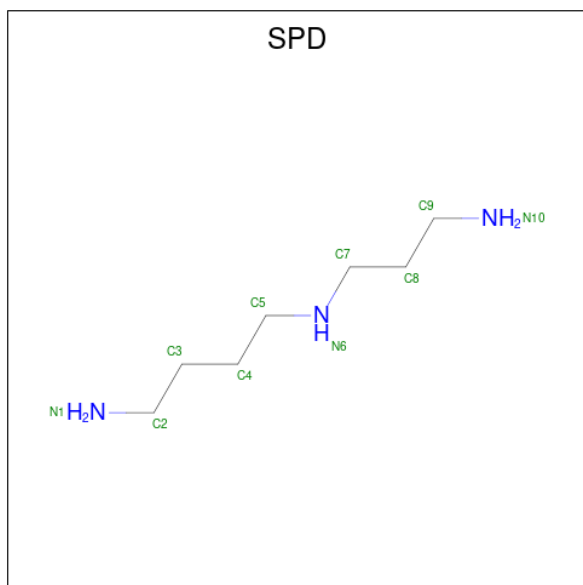
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
90	i2	1	Total 1	Zn 1	0
90	j2	1	Total 1	Zn 1	0
90	k2	1	Total 1	Zn 1	0

- Molecule 91 is POTASSIUM ION (CCD ID: K) (formula: K).

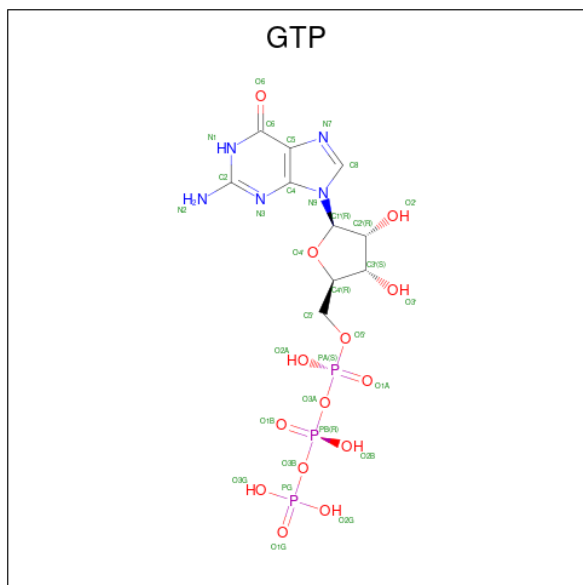
Mol	Chain	Residues	Atoms		AltConf
91	A1	9	Total 9	K 9	0
91	A3	22	Total 22	K 22	0
91	B3	2	Total 2	K 2	0
91	C3	1	Total 1	K 1	0
91	H1	1	Total 1	K 1	0
91	J2	1	Total 1	K 1	0
91	O2	1	Total 1	K 1	0

- Molecule 92 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



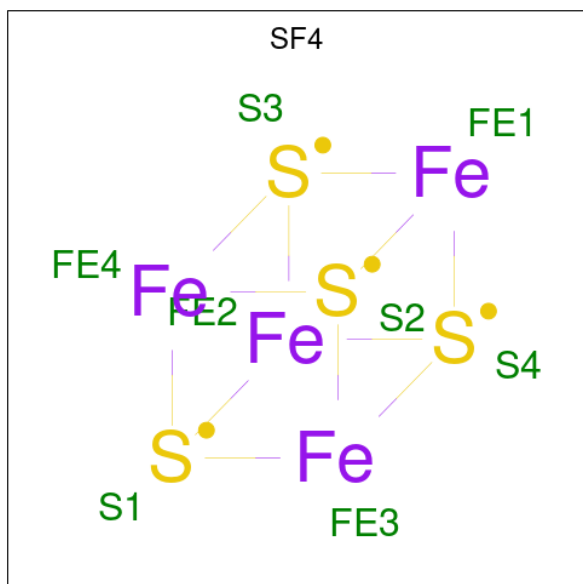
Mol	Chain	Residues	Atoms			AltConf
92	A3	1	Total	C	N	0
			10	7	3	
92	A3	1	Total	C	N	0
			10	7	3	

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
93	B3	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 94 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

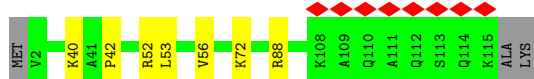


Mol	Chain	Residues	Atoms			AltConf
94	q2	1	Total 8	Fe 4	S 4	0
94	q2	1	Total 8	Fe 4	S 4	0

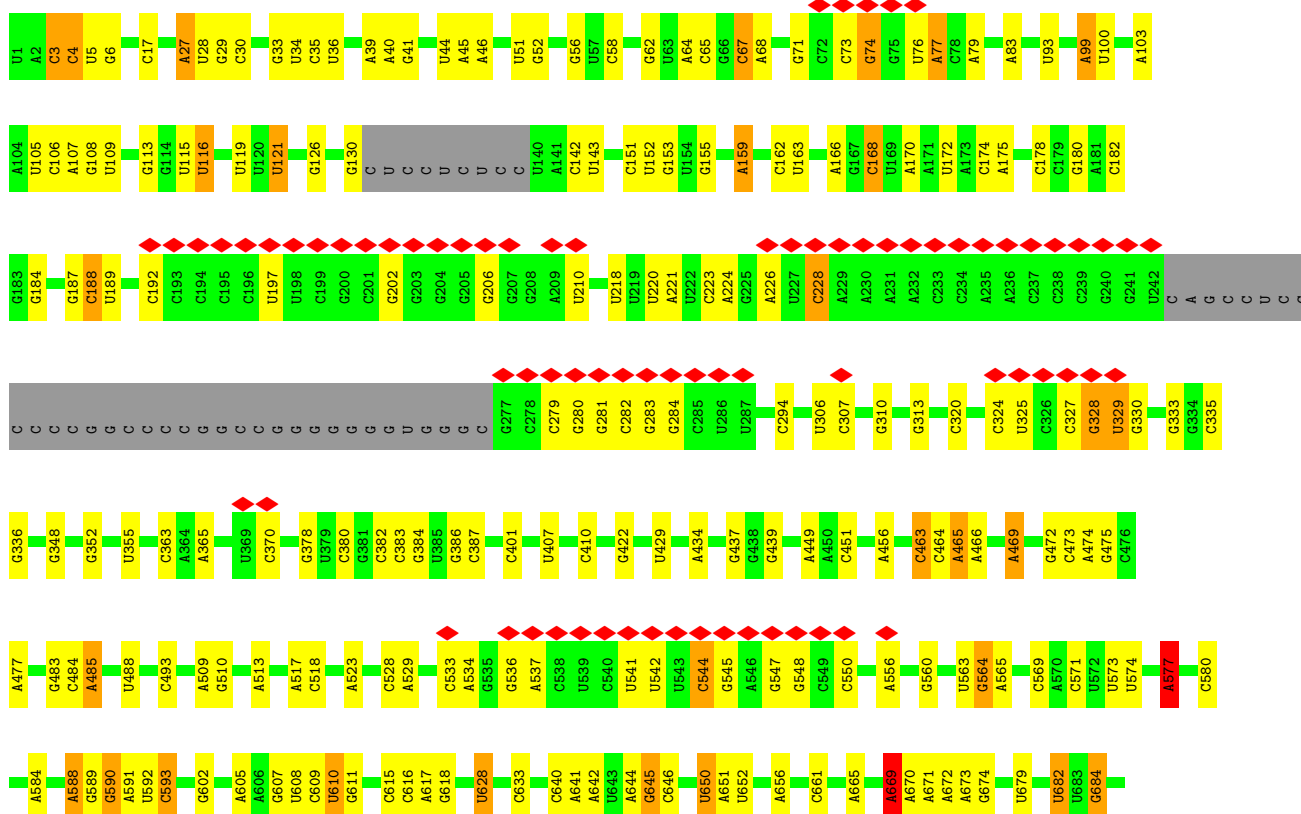
3 Residue-property plots

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.

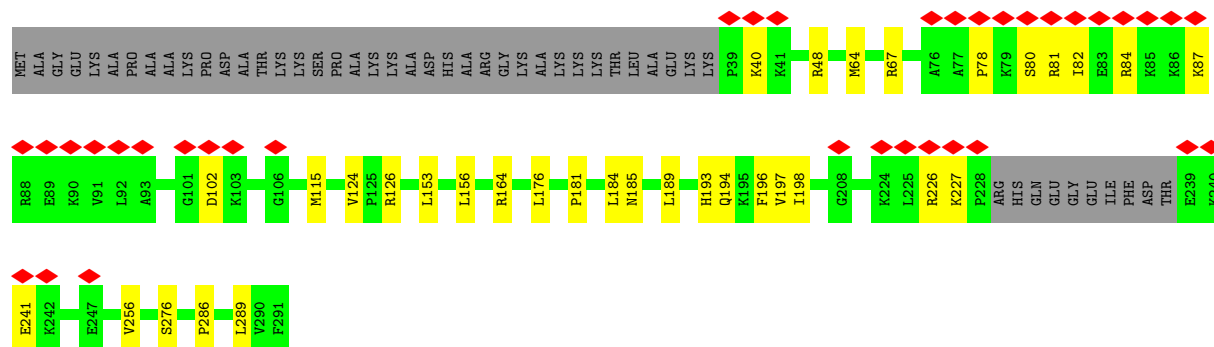
- Molecule 1: 60S ribosomal protein L34



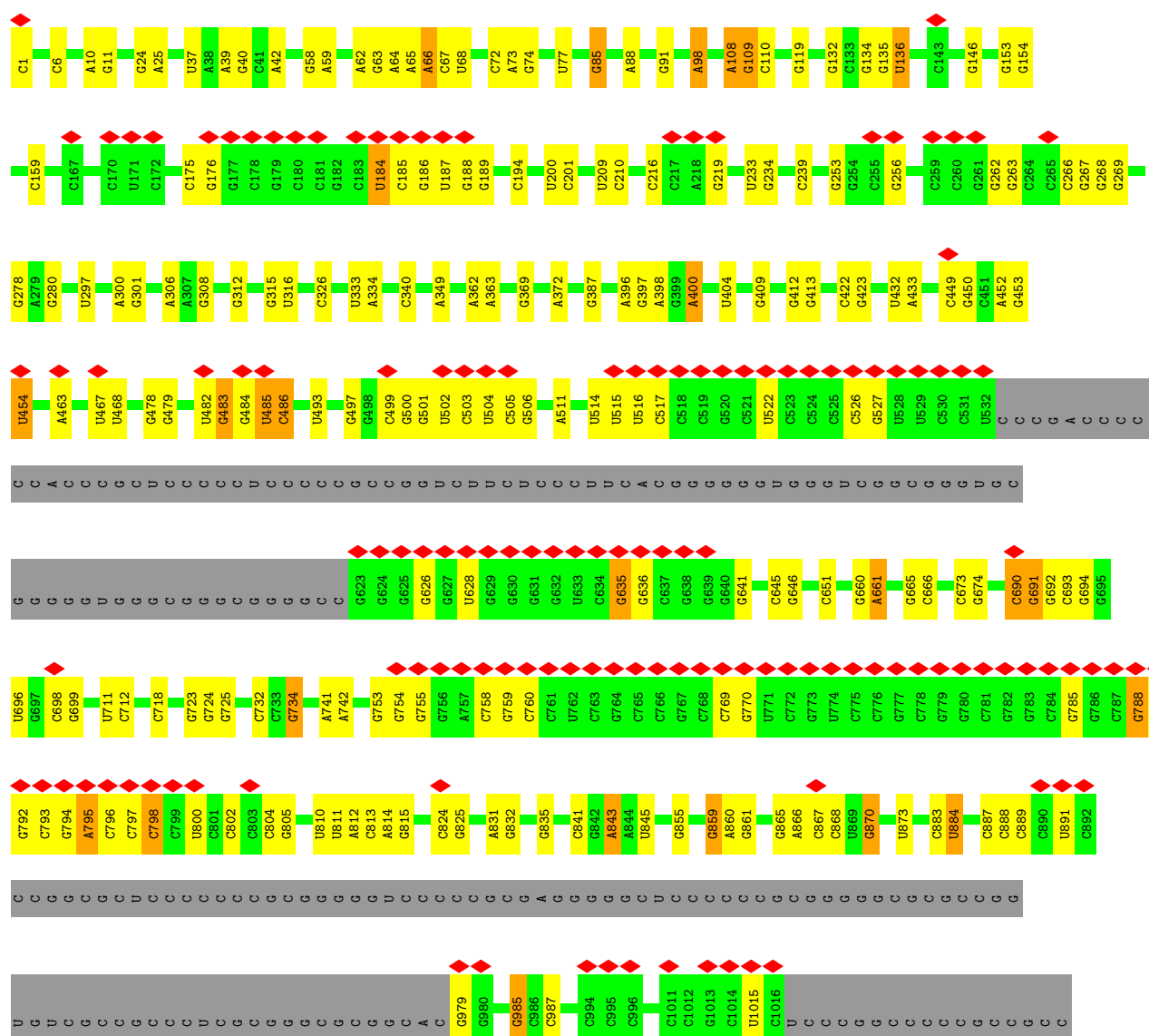
- Molecule 2: 18S rRNA

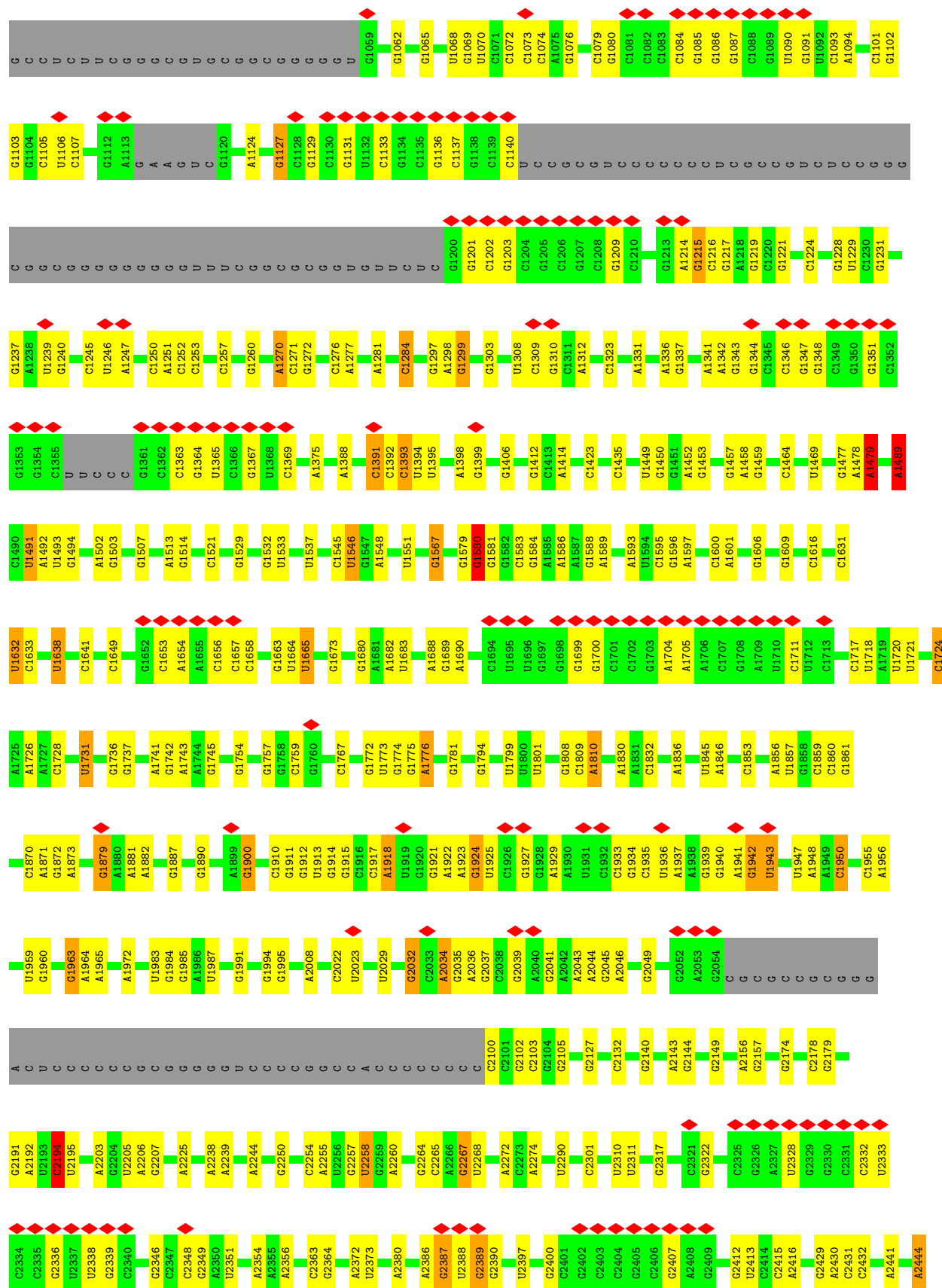




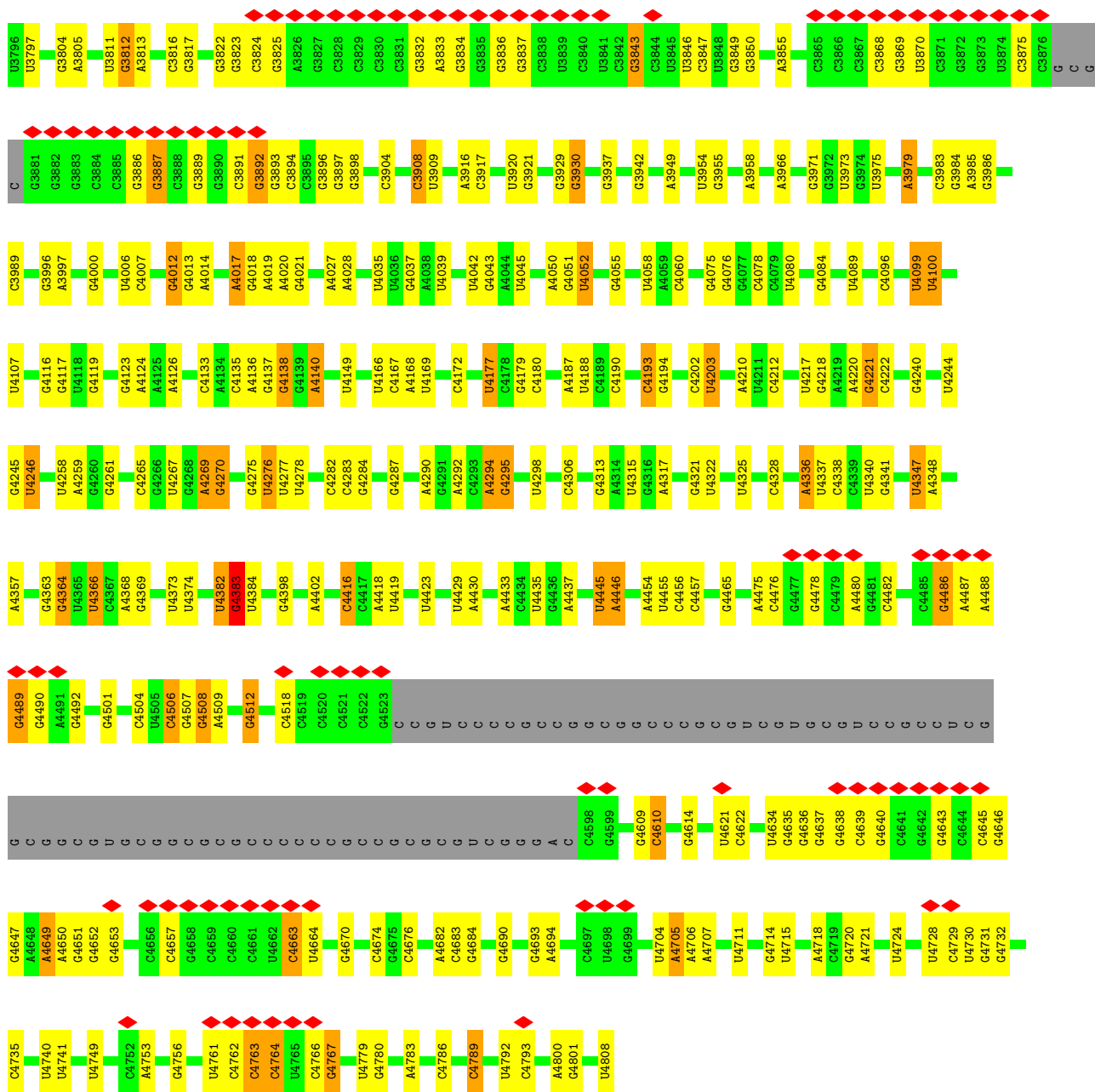


• Molecule 4: 28S rRNA

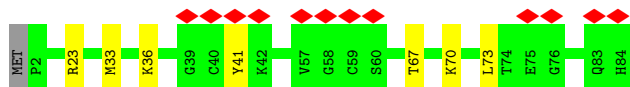
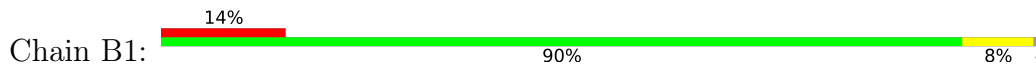




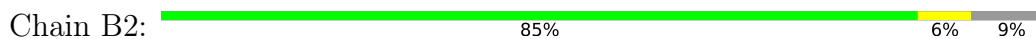


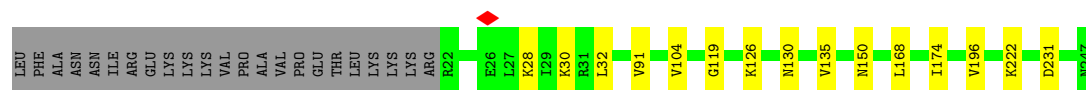


• Molecule 5: Small ribosomal subunit protein eS27

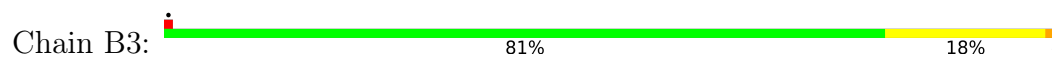


• Molecule 6: 60S ribosomal protein L7

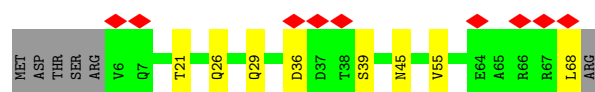
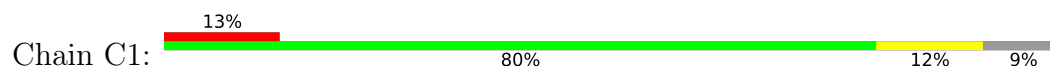




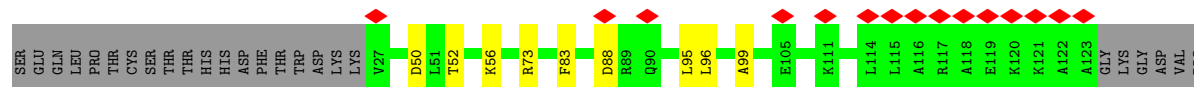
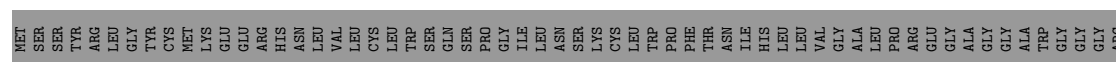
- Molecule 7: 5S rRNA



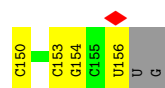
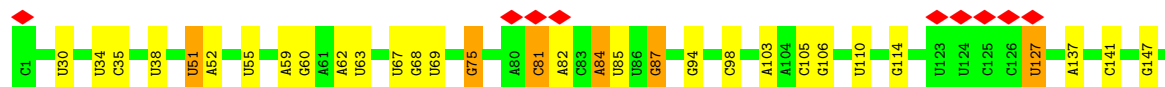
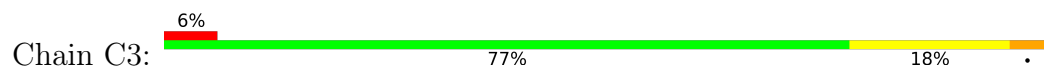
- Molecule 8: Small ribosomal subunit protein eS28



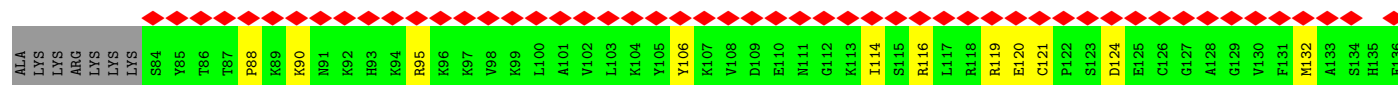
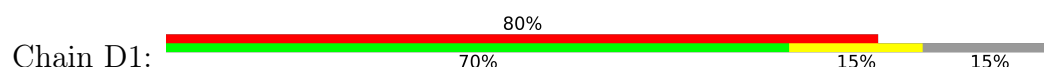
- Molecule 9: Large ribosomal subunit protein eL8

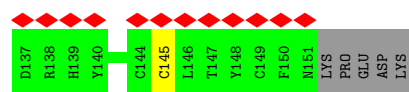


- Molecule 10: 5.8S rRNA



- Molecule 11: Ubiquitin-ribosomal protein eS31 fusion protein

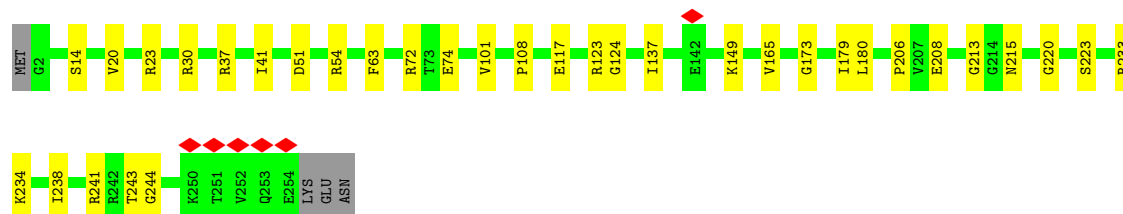




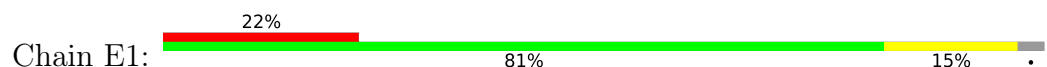
- Molecule 12: 60S ribosomal protein L9



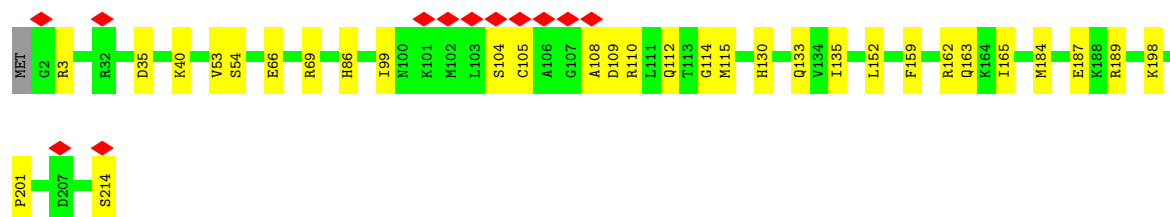
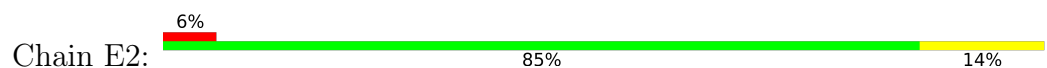
- Molecule 13: Large ribosomal subunit protein uL2



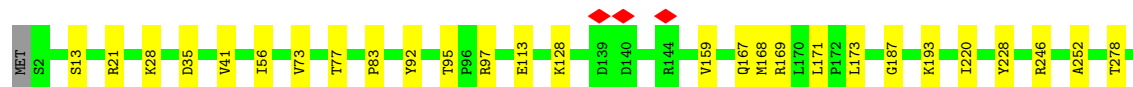
- Molecule 14: 40S ribosomal protein eS30



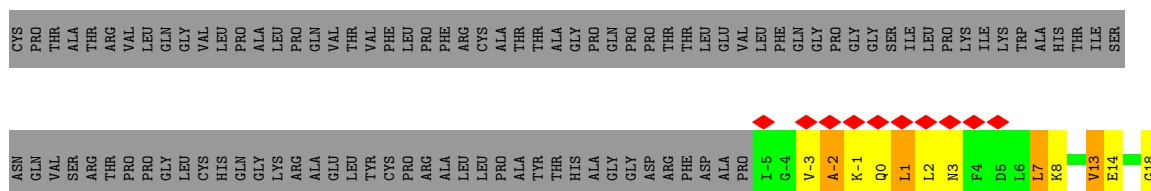
- Molecule 15: 60S ribosomal protein L10



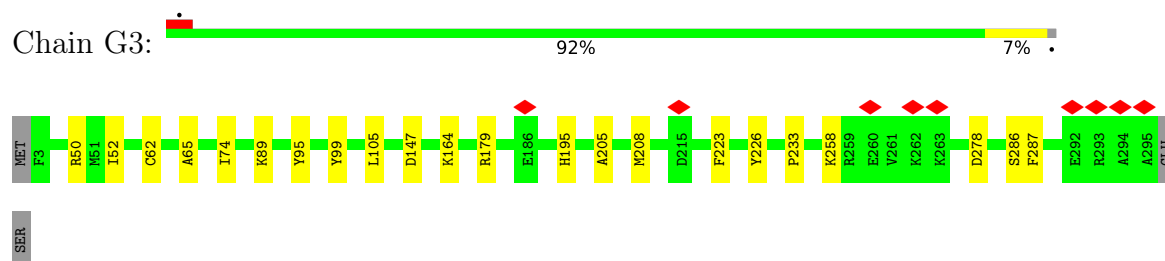
- Molecule 16: Ribosomal protein L3



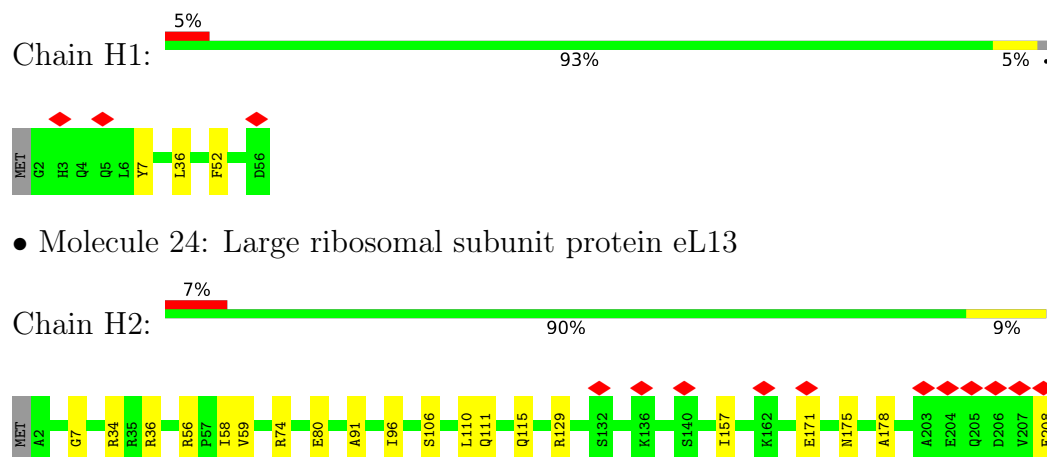




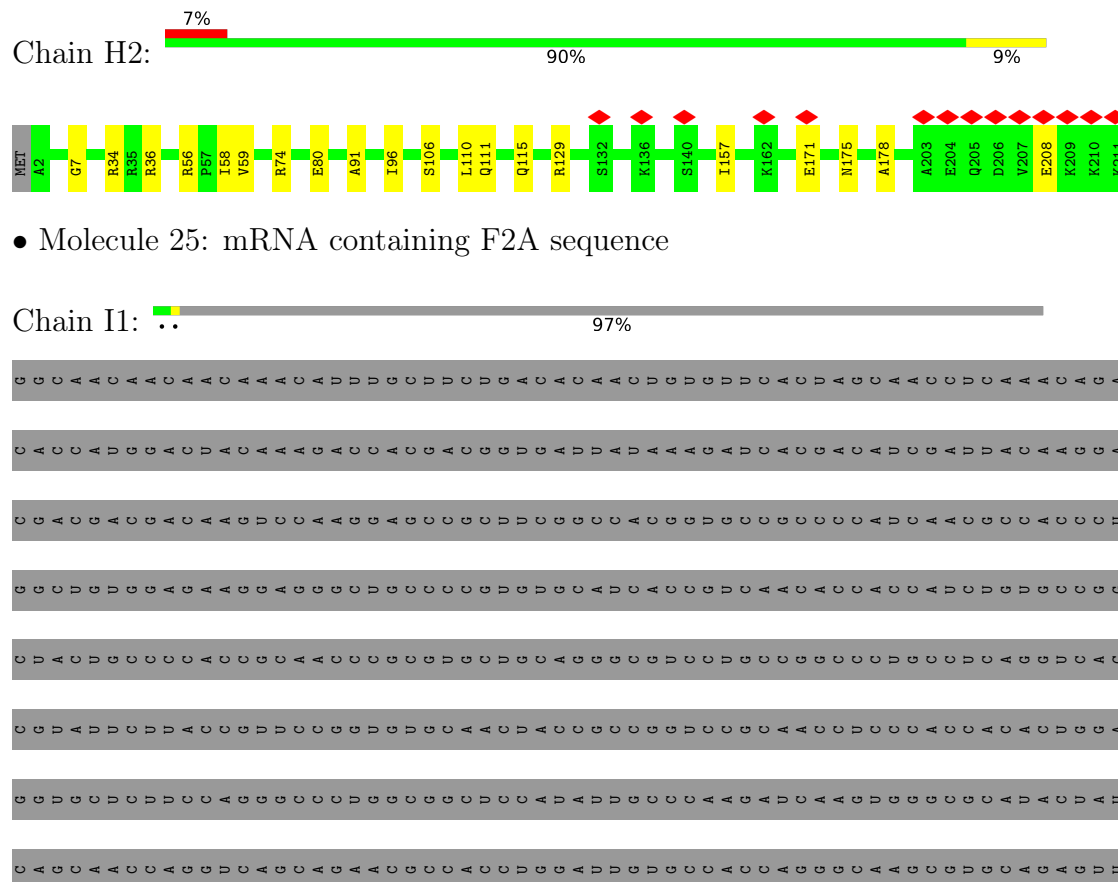
- Molecule 22: Large ribosomal subunit protein uL18



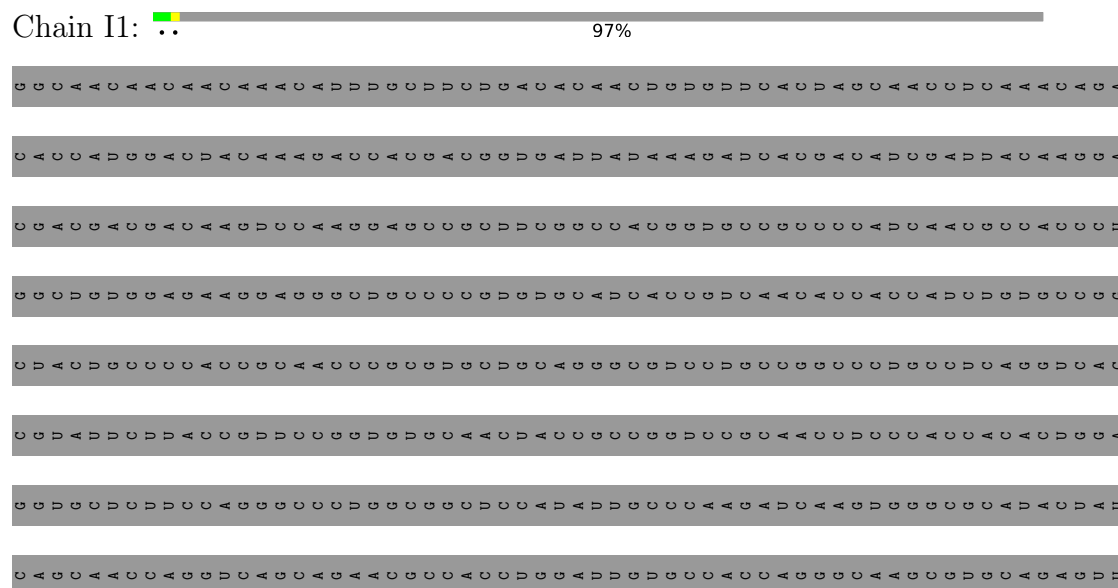
- Molecule 23: Small ribosomal subunit protein uS14

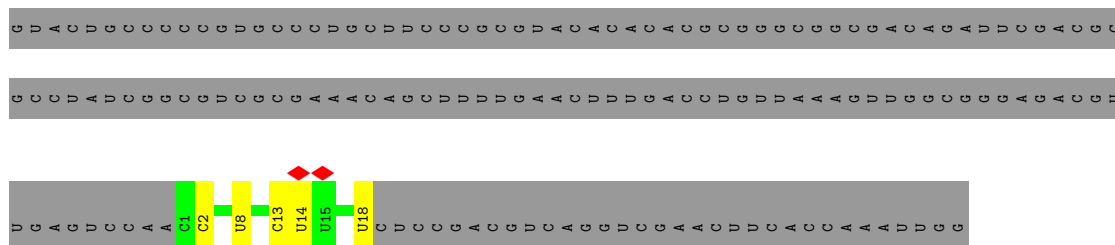


- Molecule 24: Large ribosomal subunit protein eL13

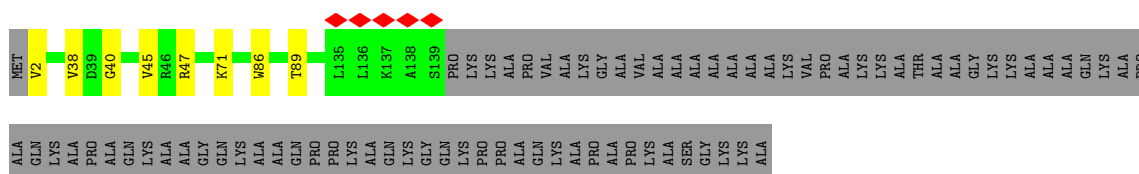


- Molecule 25: mRNA containing F2A sequence

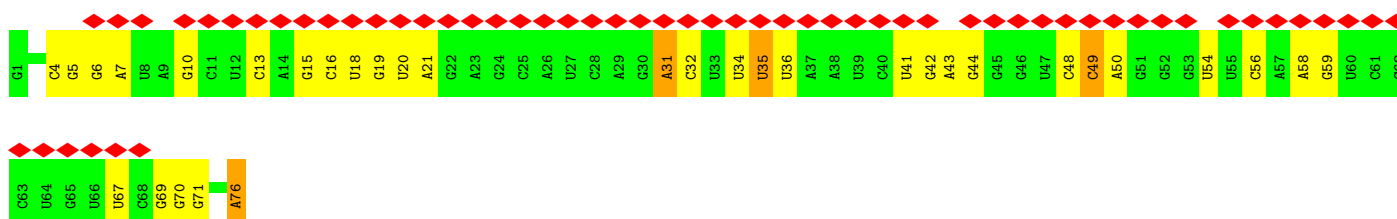
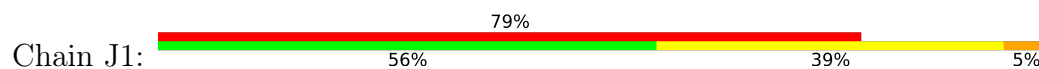




• Molecule 26: 60S ribosomal protein L14



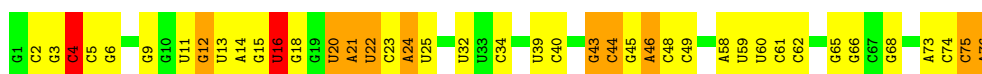
• Molecule 27: E-site tRNA-Pro



• Molecule 28: Ribosomal protein L15



• Molecule 29: P-site tRNA-Gly

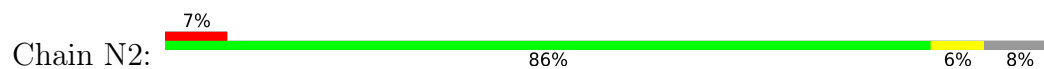


• Molecule 30: Large ribosomal subunit protein uL13

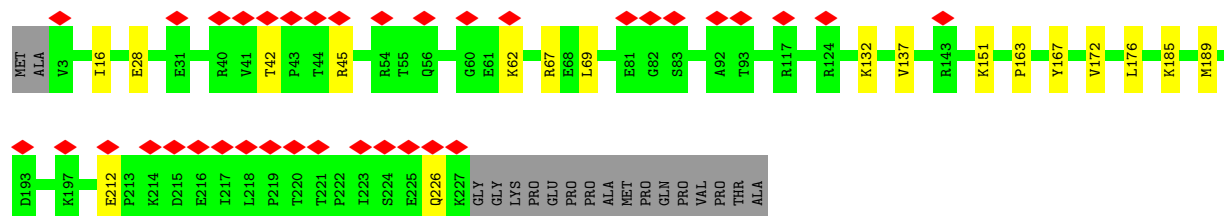
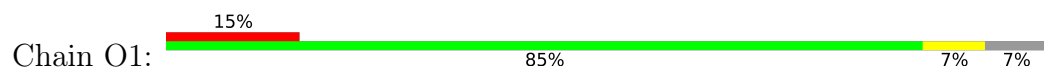




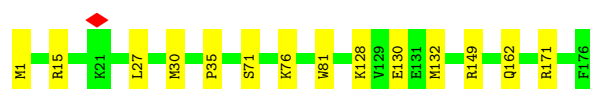
- Molecule 36: Ribosomal protein L19



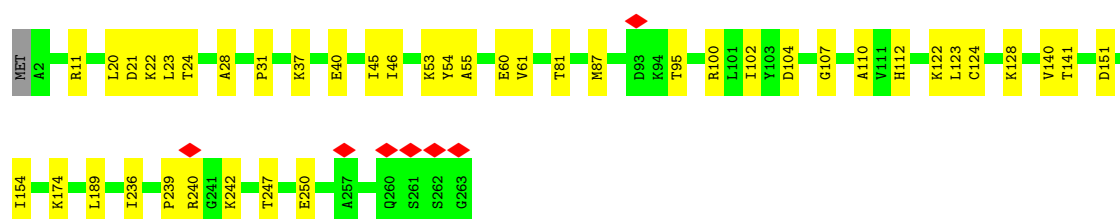
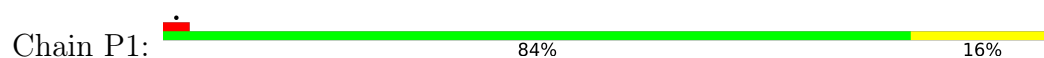
- Molecule 37: Small ribosomal subunit protein uS3



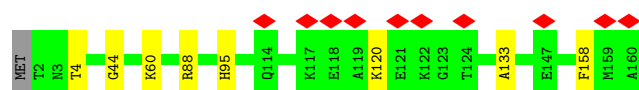
- Molecule 38: Large ribosomal subunit protein eL20



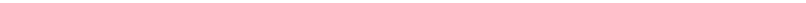
- Molecule 39: 40S ribosomal protein S4



- Molecule 40: 60S ribosomal protein L21

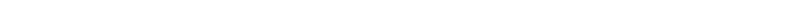


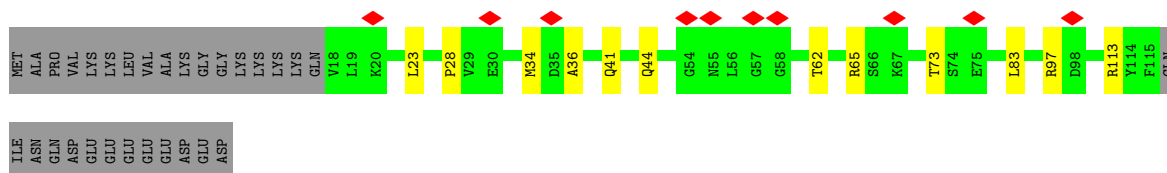
- Molecule 41: Small ribosomal subunit protein uS7

Chain Q1: 



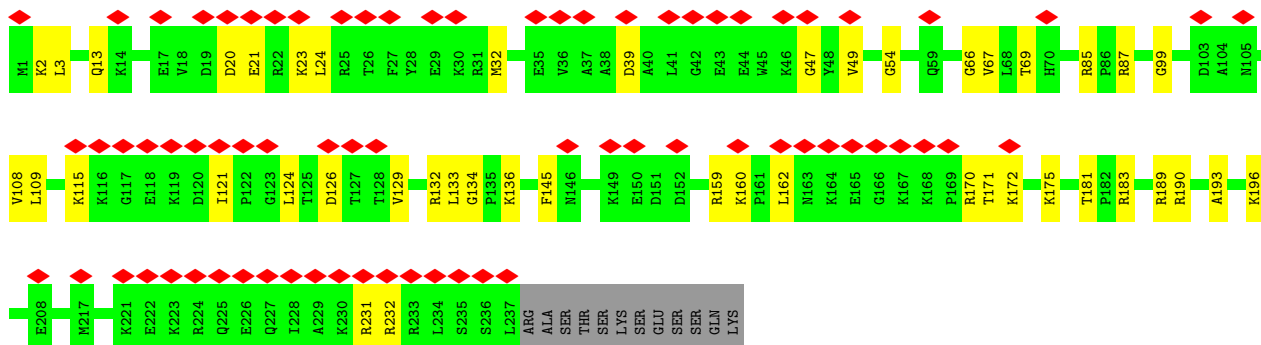
- Molecule 42: 60S ribosomal protein L22

Chain Q2: 



- Molecule 43: 40S ribosomal protein S6

Chain R1: 



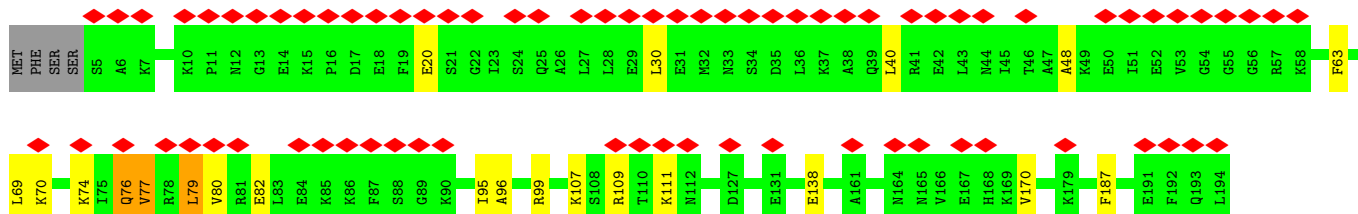
- Molecule 44: Ribosomal protein L23

Chain R2:

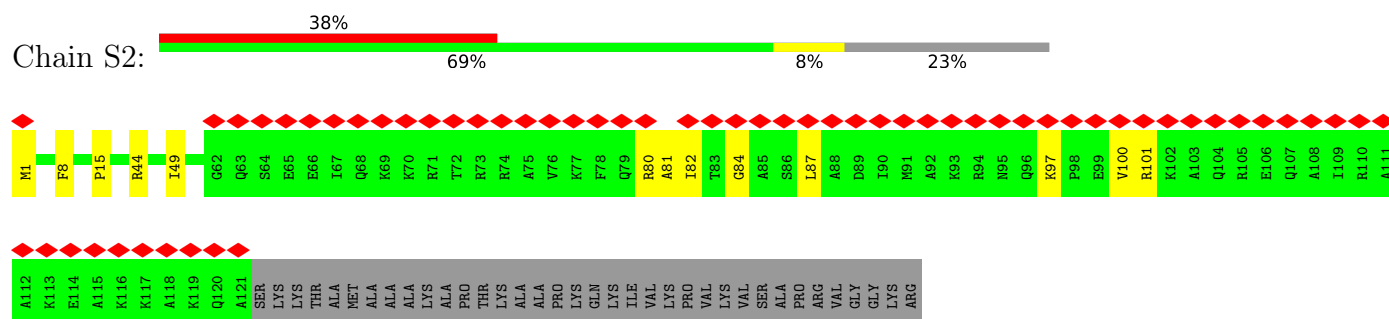


- Molecule 45: Small ribosomal subunit protein eS7

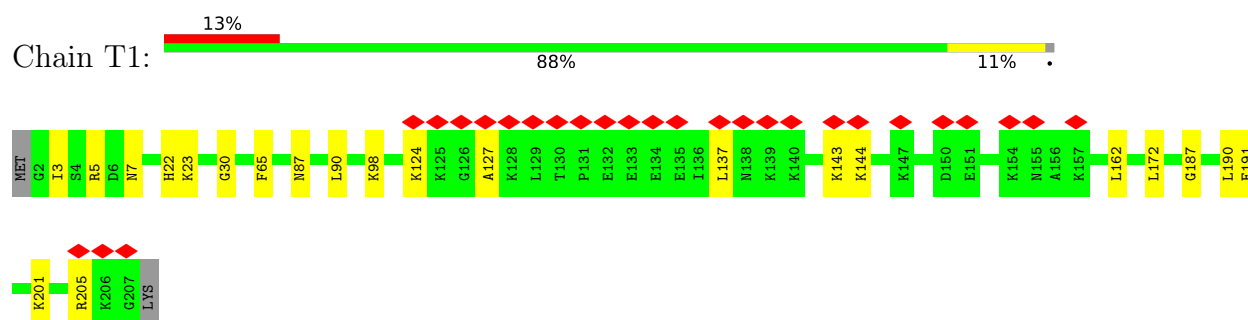
Chain S1:  39% 87% 10%



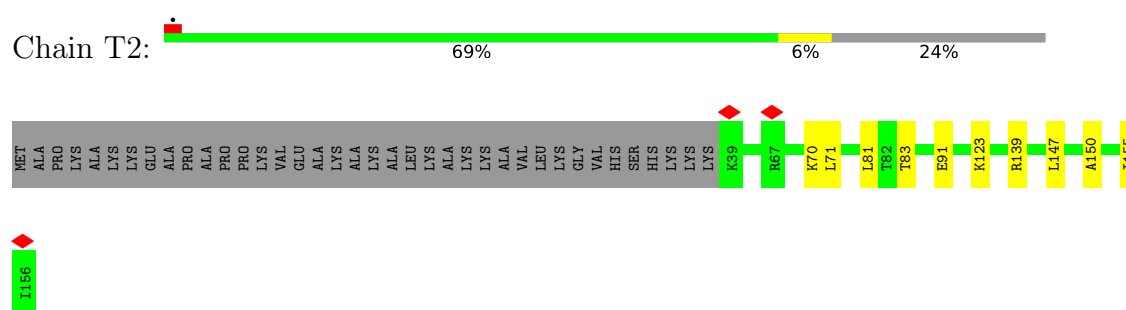
- Molecule 46: Ribosomal protein L24



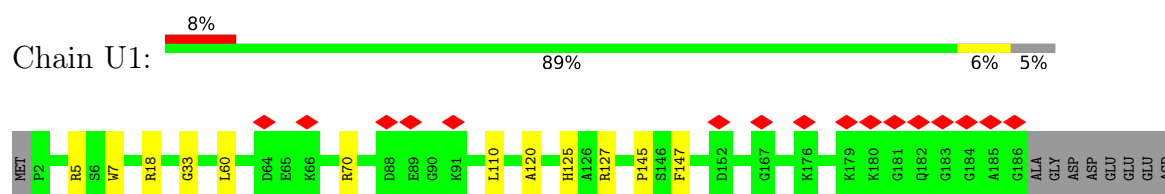
- Molecule 47: 40S ribosomal protein S8



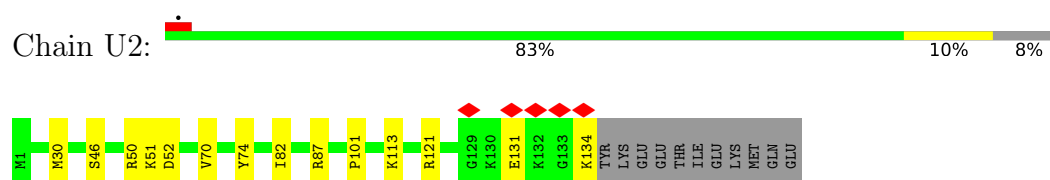
- Molecule 48: Large ribosomal subunit protein uL23



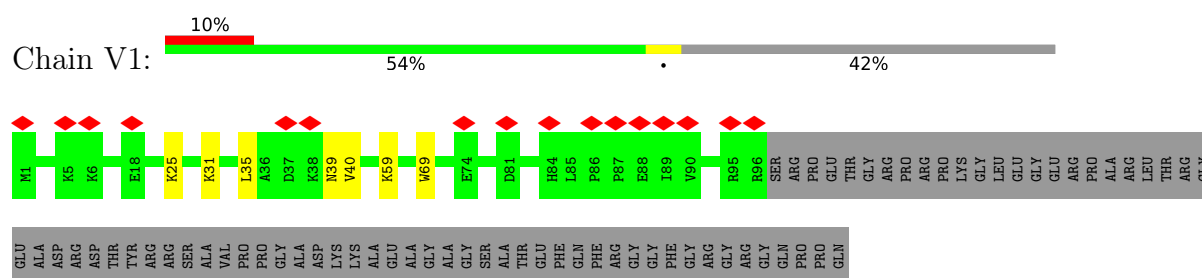
- Molecule 49: Small ribosomal subunit protein uS4



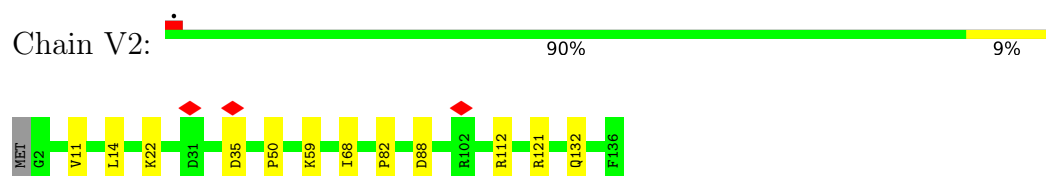
- Molecule 50: Ribosomal protein L26



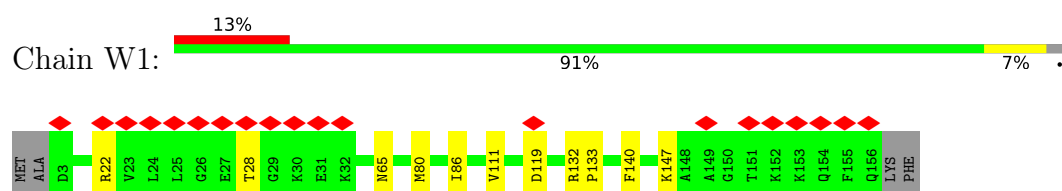
- Molecule 51: eS10



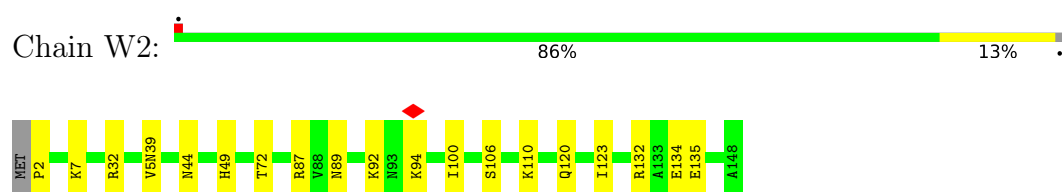
- Molecule 52: 60S ribosomal protein L27



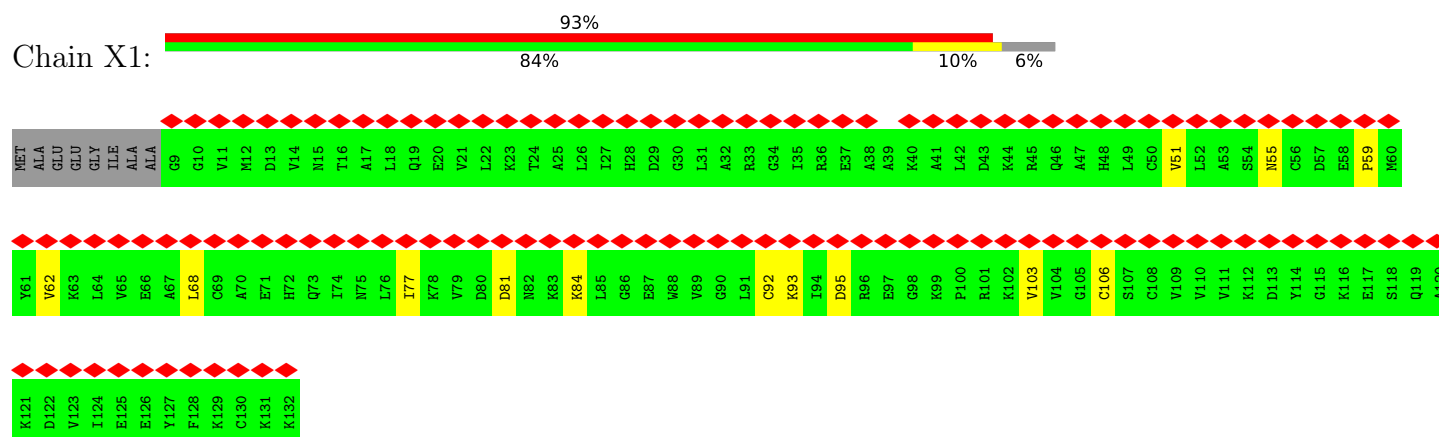
- Molecule 53: Small ribosomal subunit protein uS17



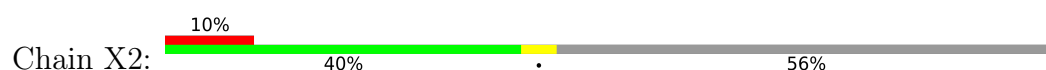
- Molecule 54: 60S ribosomal protein L27a

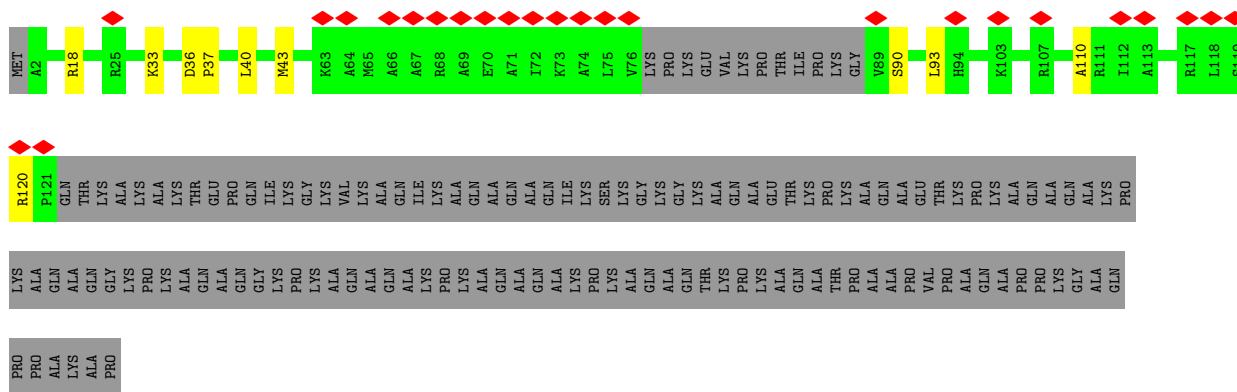


- Molecule 55: Small ribosomal subunit protein eS12



- Molecule 56: 60S ribosomal protein L29

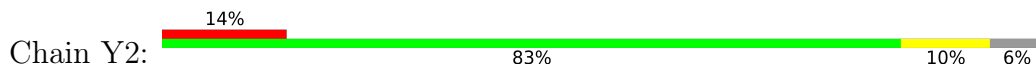




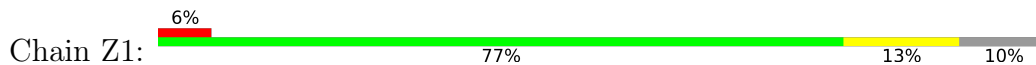
- Molecule 57: Small ribosomal subunit protein uS15



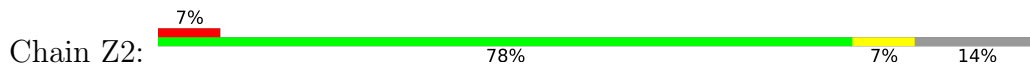
- Molecule 58: 60S ribosomal protein L30



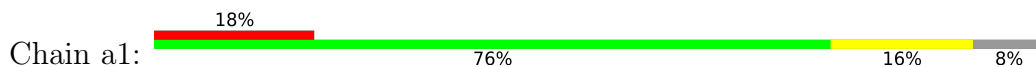
- Molecule 59: Small ribosomal subunit protein uS11

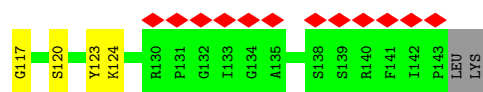


- Molecule 60: 60S ribosomal protein L31

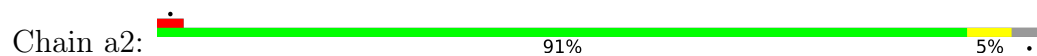


- Molecule 61: Small ribosomal subunit protein uS19

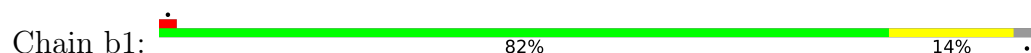




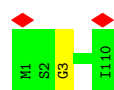
- Molecule 62: Ribosomal protein L32



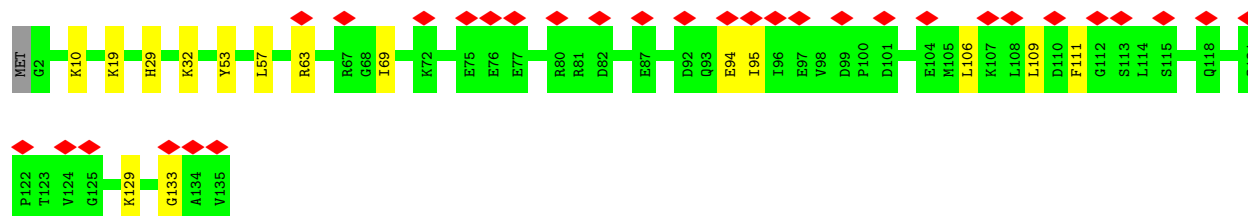
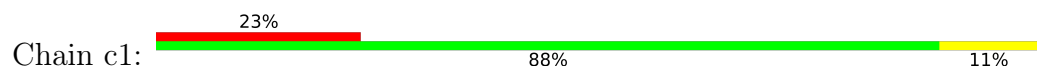
- Molecule 63: Small ribosomal subunit protein uS9



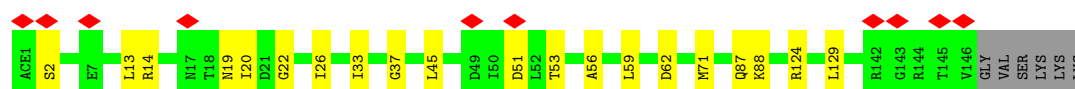
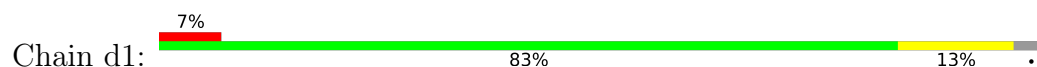
- Molecule 64: 60S ribosomal protein L35a



- Molecule 65: Small ribosomal subunit protein eS17



- Molecule 66: Small ribosomal subunit protein uS13

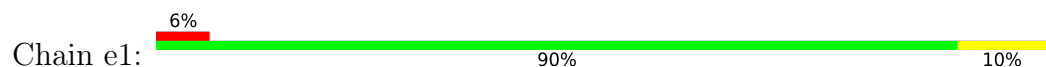


- Molecule 67: 60S ribosomal protein L35





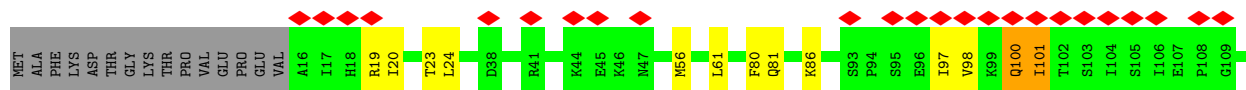
- Molecule 68: 40S ribosomal protein eS19



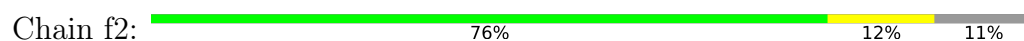
- Molecule 69: Large ribosomal subunit protein eL36



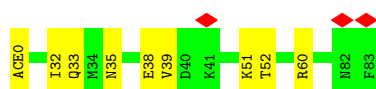
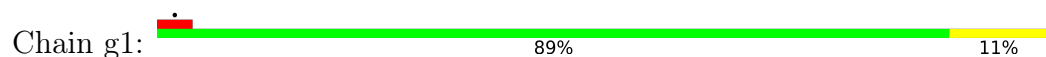
- Molecule 70: Small ribosomal subunit protein uS10



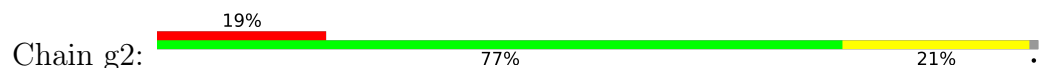
- Molecule 71: Ribosomal protein L37

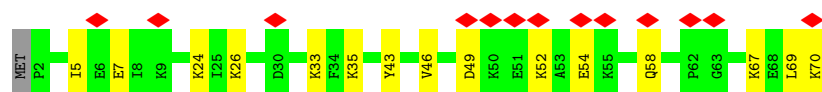


- Molecule 72: Small ribosomal subunit protein eS21



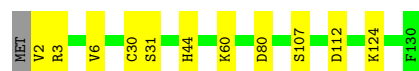
- Molecule 73: 60S ribosomal protein L38





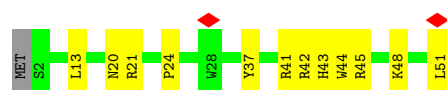
- Molecule 74: Small ribosomal subunit protein uS8

Chain h1: 91% 8%



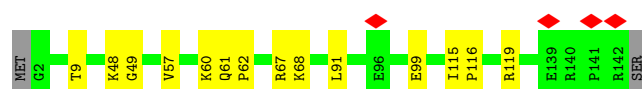
- Molecule 75: 60S ribosomal protein L39-like

Chain h2: 75% 24%



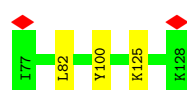
- Molecule 76: 40S ribosomal protein S23

Chain i1: 89% 10%



- Molecule 77: Ubiquitin-ribosomal protein eL40 fusion protein

Chain i2: 94% 6%



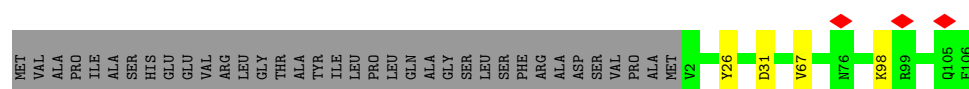
- Molecule 78: 40S ribosomal protein S24

Chain j1: 9% 80% 14% 6%

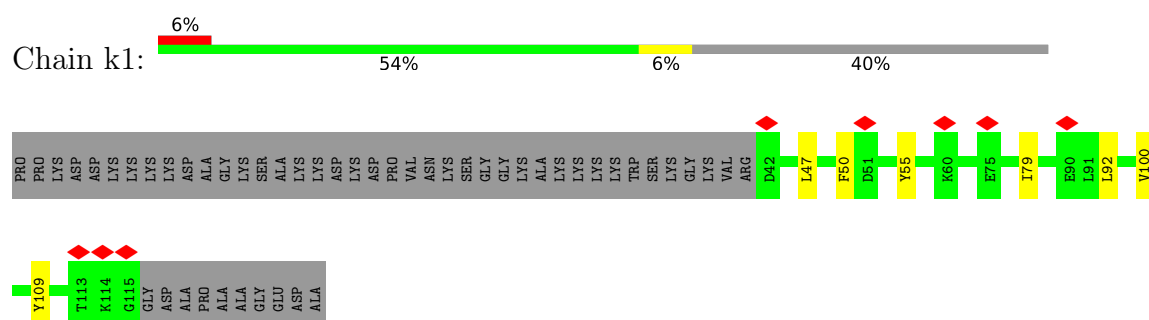


- Molecule 79: Ribosomal protein L36a

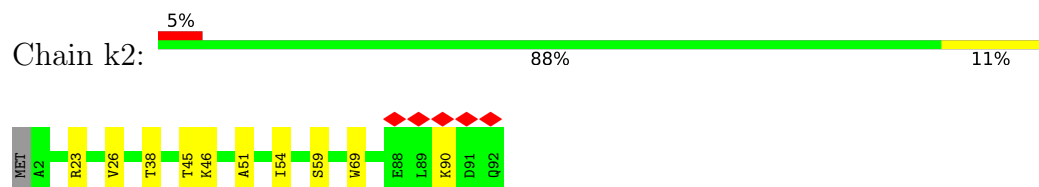
Chain j2: 72% 26%



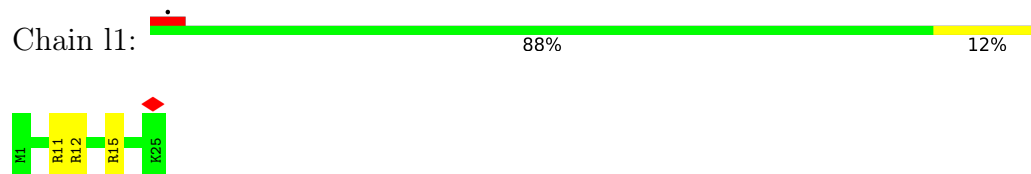
- Molecule 80: Small ribosomal subunit protein eS25



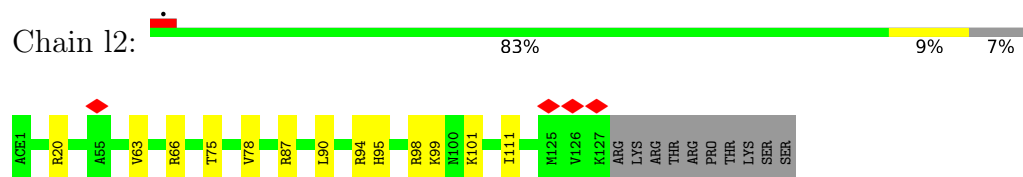
- Molecule 81: 60S ribosomal protein L37a



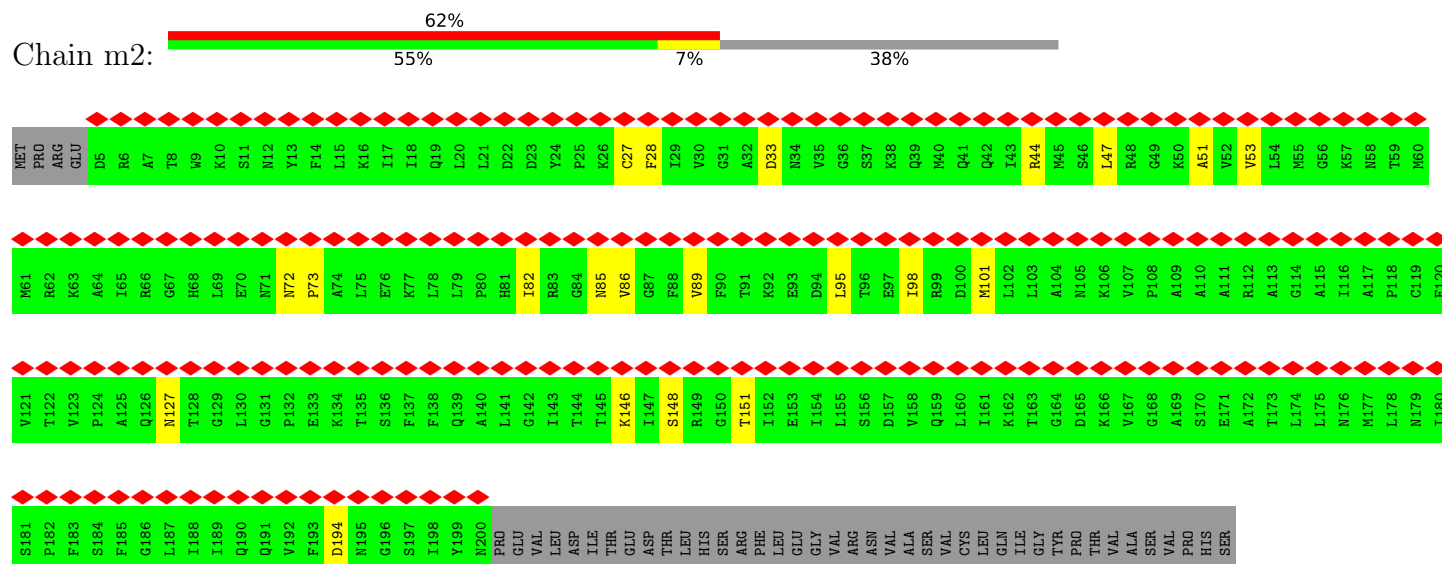
- Molecule 82: Small ribosomal subunit protein eS32



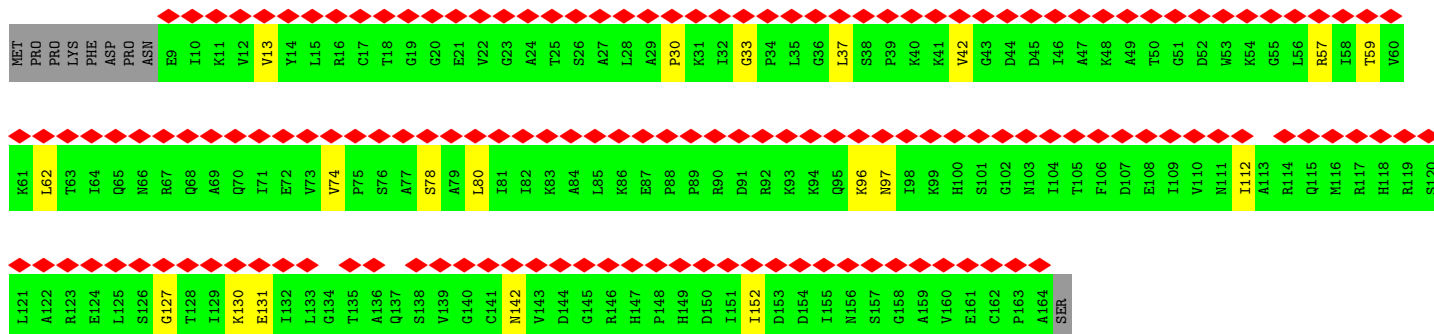
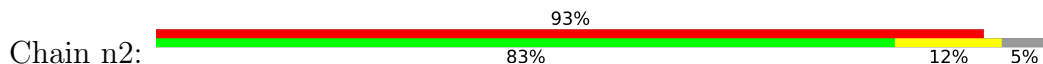
- Molecule 83: [histone H4]-N-methyl-L-lysine20 N-methyltransferase KMT5B



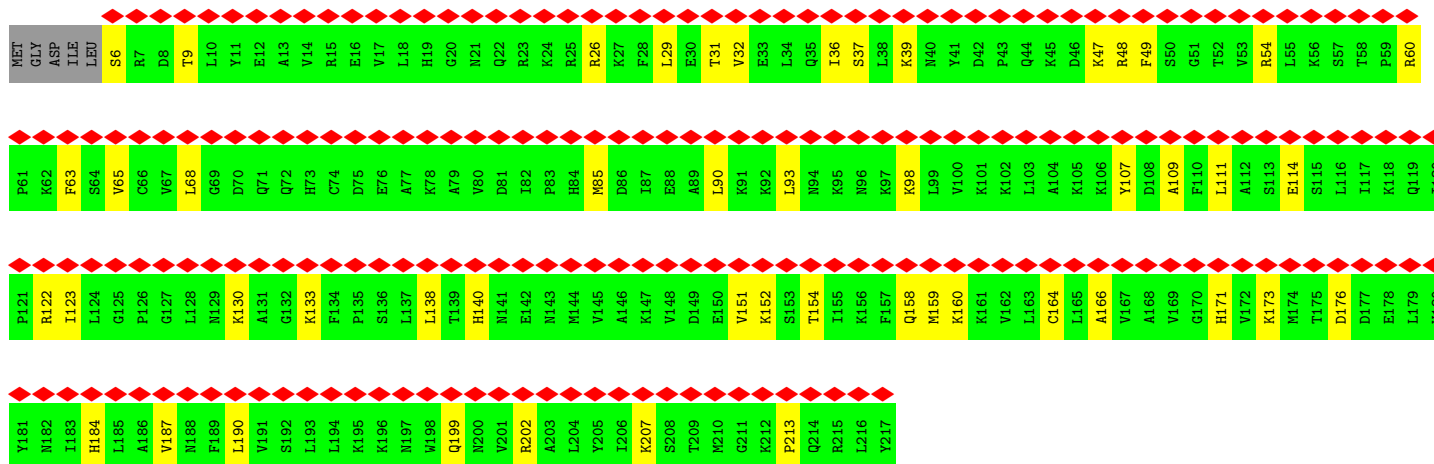
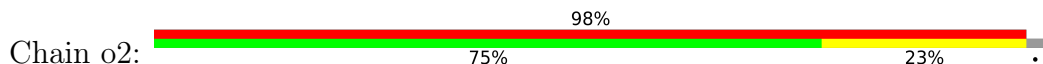
- Molecule 84: Large ribosomal subunit protein uL10



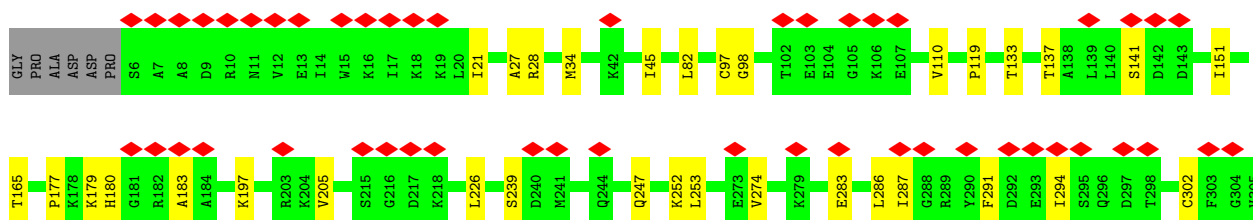
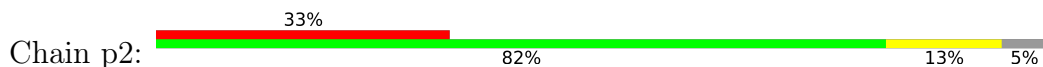
- Molecule 85: 60S ribosomal protein L12

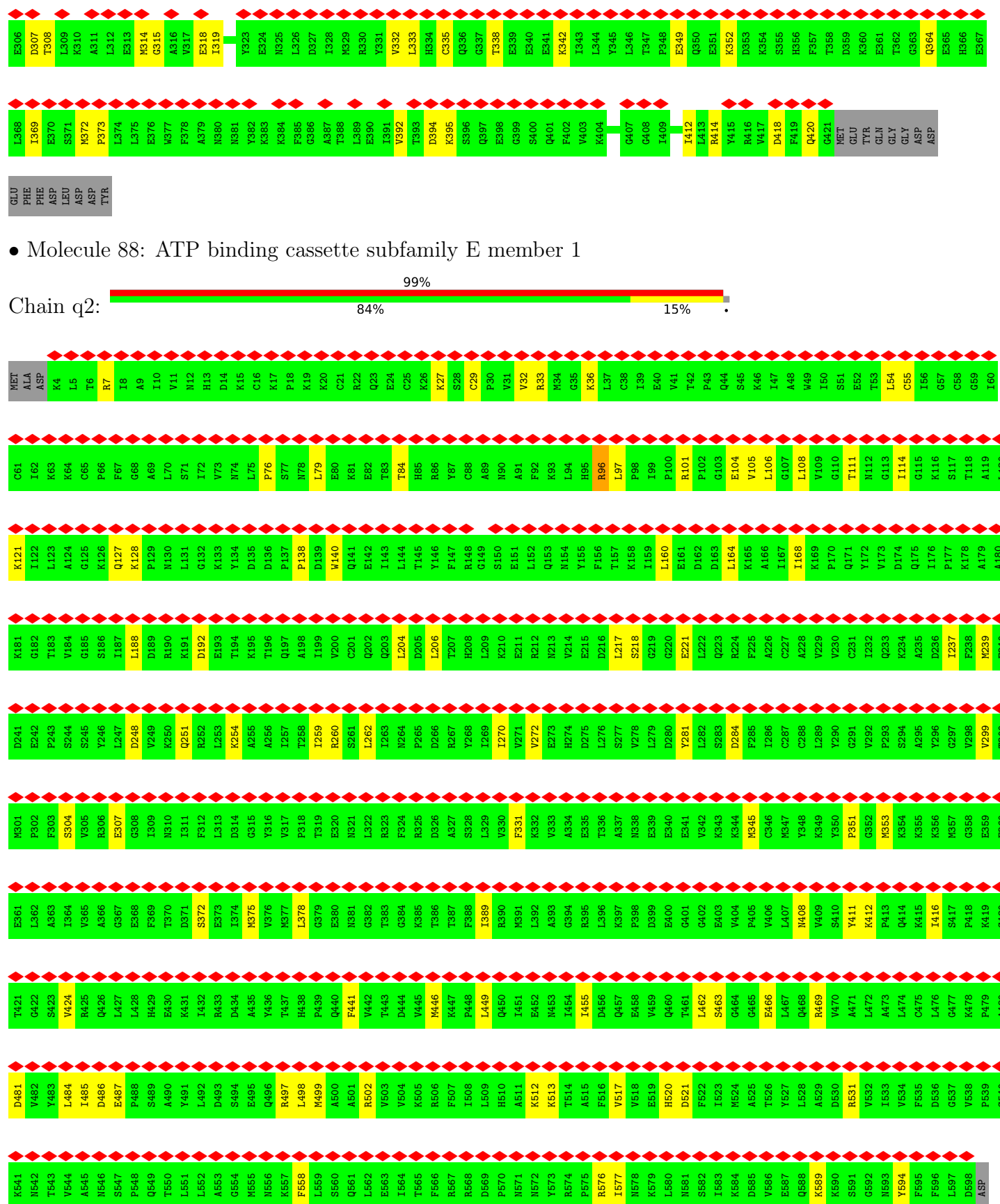


- Molecule 86: Ribosomal protein uL1



- Molecule 87: Eukaryotic peptide chain release factor subunit 1





- Molecule 88: ATP binding cassette subfamily E member 1

99%

Chain q2:

84%

15%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49964	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	421.2, 421.2, 421.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.702, 0.702, 0.702	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 5MU, HY3, 4AC, HIC, SPD, SF4, K, OMG, MLZ, PSU, UR3, ACE, M3L, ZN, V5N, MG, B8N, UY1, MA6, NMM, OMC, 6MZ, H2U, 5MC, GTP, 1MA, A2M, G7M, 1MG

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	MB	0.17	0/916	0.39	0/1220
2	A1	0.25	0/40342	0.38	1/62877 (0.0%)
3	A2	0.16	0/1998	0.37	0/2673
4	A3	0.23	0/87403	0.38	0/136359
5	B1	0.16	0/665	0.43	0/891
6	B2	0.21	0/1922	0.44	0/2563
7	B3	0.22	0/2835	0.36	0/4418
8	C1	0.14	0/497	0.35	0/666
9	C2	0.19	0/1908	0.47	0/2566
10	C3	0.22	0/3635	0.36	0/5661
11	D1	0.17	0/566	0.44	0/753
12	D2	0.17	0/1535	0.43	0/2063
13	D3	0.18	0/1965	0.39	0/2633
14	E1	0.13	0/462	0.39	0/607
15	E2	0.18	0/1756	0.40	0/2346
16	E3	0.17	0/3261	0.40	0/4364
17	F1	0.20	0/828	0.48	0/1109
18	F2	0.17	0/1385	0.41	0/1852
19	F3	0.24	0/2938	0.41	0/3948
20	G1	0.22	0/2493	0.53	0/3394
21	G2	1.02	0/177	1.17	0/238
22	G3	0.15	0/2437	0.38	0/3264
23	H1	0.16	0/470	0.38	0/623
24	H2	0.17	0/1733	0.39	0/2316
25	I1	0.29	0/414	0.44	0/641
26	I2	0.19	0/1158	0.43	0/1547
27	J1	0.17	0/1779	0.39	0/2771
28	J2	0.17	0/1746	0.40	0/2338
29	K1	1.10	2/1456 (0.1%)	0.99	5/2269 (0.2%)
30	K2	0.21	0/1662	0.42	0/2222
31	L1	0.19	0/1778	0.45	0/2416

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	L2	0.18	0/1317	0.42	0/1768
33	M1	0.19	0/1841	0.45	0/2459
34	M2	0.18	0/1539	0.44	0/2054
35	N1	0.19	0/1742	0.44	0/2354
36	N2	0.18	0/1524	0.41	0/2013
37	O1	0.17	0/1779	0.43	0/2395
38	O2	0.21	0/1497	0.40	0/2008
39	P1	0.16	0/2118	0.42	0/2849
40	P2	0.16	0/1326	0.38	0/1770
41	Q1	0.20	0/1531	0.48	0/2059
42	Q2	0.18	0/811	0.46	0/1088
43	R1	0.17	0/1946	0.43	0/2590
44	R2	0.16	0/1048	0.42	0/1402
45	S1	0.27	0/1552	0.50	0/2079
46	S2	0.16	0/1006	0.39	0/1334
47	T1	0.23	0/1715	0.47	0/2287
48	T2	0.17	0/984	0.39	0/1323
49	U1	0.17	0/1550	0.42	0/2069
50	U2	0.27	0/1132	0.52	0/1504
51	V1	0.20	0/834	0.49	0/1125
52	V2	0.15	0/1130	0.33	0/1507
53	W1	0.16	0/1284	0.38	0/1717
54	W2	0.16	0/1179	0.38	0/1572
55	X1	0.23	0/968	0.57	0/1296
56	X2	0.16	0/884	0.39	0/1169
57	Y1	0.18	0/1232	0.39	0/1656
58	Y2	0.19	0/847	0.43	0/1134
59	Z1	0.18	0/1029	0.41	0/1380
60	Z2	0.19	0/903	0.43	0/1216
61	a1	0.21	0/1114	0.46	0/1490
62	a2	0.17	0/1088	0.43	0/1451
63	b1	0.22	0/1142	0.46	0/1528
64	b2	0.17	0/903	0.36	0/1208
65	c1	0.19	0/1094	0.44	0/1469
66	d1	0.19	0/1216	0.44	0/1630
67	d2	0.16	0/1021	0.37	0/1348
68	e1	0.16	0/1119	0.39	0/1498
69	e2	0.19	0/841	0.44	0/1112
70	f1	0.33	0/832	0.62	0/1117
71	f2	0.17	0/720	0.42	0/952
72	g1	0.30	1/645 (0.2%)	0.47	0/864
73	g2	0.18	0/575	0.40	0/761
74	h1	0.17	0/1051	0.40	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	h2	0.17	0/459	0.38	0/608
76	i1	0.21	0/1107	0.42	0/1475
77	i2	0.17	0/426	0.43	0/564
78	j1	0.17	0/1032	0.41	0/1371
79	j2	0.15	0/866	0.35	0/1141
80	k1	0.19	0/593	0.45	0/796
81	k2	0.20	0/718	0.49	0/953
82	l1	0.20	0/240	0.42	0/305
83	l2	0.19	0/1027	0.44	0/1376
84	m2	0.19	0/1530	0.49	0/2064
85	n2	0.20	0/1193	0.51	0/1609
86	o2	0.21	0/1735	0.51	0/2328
87	p2	0.27	0/3333	0.52	0/4483
88	q2	0.20	0/4755	0.50	0/6421
All	All	0.23	3/244743 (0.0%)	0.41	6/358113 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
19	F3	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K1	46	A	O3'-P	22.69	1.95	1.61
29	K1	16	H2U	O3'-P	22.66	1.95	1.61
72	g1	0	ACE	C-N	6.16	1.45	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K1	16	H2U	O3'-P-O5'	-10.44	88.34	104.00
29	K1	46	A	OP2-P-O3'	9.41	136.25	108.00
29	K1	46	A	P-O3'-C3'	9.10	133.85	120.20
29	K1	16	H2U	OP2-P-O3'	8.32	132.96	108.00
29	K1	16	H2U	P-O3'-C3'	7.53	131.50	120.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	F3	248	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	MB	906	0	998	5	0
2	A1	37833	0	19168	222	0
3	A2	1960	0	2153	24	0
4	A3	80772	0	40889	411	0
5	B1	651	0	672	4	0
6	B2	1886	0	2008	9	0
7	B3	2538	0	1284	10	0
8	C1	495	0	523	6	0
9	C2	1877	0	2023	13	0
10	C3	3319	0	1684	17	0
11	D1	554	0	556	9	0
12	D2	1516	0	1597	10	0
13	D3	1940	0	2029	25	0
14	E1	457	0	502	8	0
15	E2	1717	0	1764	24	0
16	E3	3206	0	3353	28	0
17	F1	814	0	863	12	0
18	F2	1362	0	1399	7	0
19	F3	2886	0	3057	18	0
20	G1	2436	0	2389	29	0
21	G2	176	0	186	18	0
22	G3	2391	0	2424	15	0
23	H1	459	0	448	3	0
24	H2	1702	0	1820	16	0
25	I1	374	0	191	0	0
26	I2	1137	0	1211	5	0
27	J1	1593	0	809	15	0
28	J2	1701	0	1749	13	0
29	K1	1582	0	819	18	0
30	K2	1630	0	1778	8	0
31	L1	1743	0	1748	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L2	1289	0	1329	4	0
33	M1	1815	0	1908	23	0
34	M2	1515	0	1634	10	0
35	N1	1706	0	1796	13	0
36	N2	1508	0	1664	12	0
37	O1	1751	0	1846	11	0
38	O2	1457	0	1492	9	0
39	P1	2076	0	2177	24	0
40	P2	1298	0	1366	7	0
41	Q1	1509	0	1563	11	0
42	Q2	797	0	819	7	0
43	R1	1923	0	2089	34	0
44	R2	1034	0	1097	9	0
45	S1	1529	0	1627	15	0
46	S2	991	0	1048	9	0
47	T1	1686	0	1772	16	0
48	T2	967	0	1040	6	0
49	U1	1525	0	1640	11	0
50	U2	1115	0	1205	10	0
51	V1	810	0	836	4	0
52	V2	1107	0	1182	9	0
53	W1	1262	0	1335	6	0
54	W2	1163	0	1202	14	0
55	X1	958	0	993	10	0
56	X2	881	0	957	7	0
57	Y1	1208	0	1294	10	0
58	Y2	836	0	888	7	0
59	Z1	1016	0	1039	14	0
60	Z2	888	0	930	6	0
61	a1	1091	0	1138	16	0
62	a2	1070	0	1165	5	0
63	b1	1124	0	1193	12	0
64	b2	884	0	924	1	0
65	c1	1080	0	1135	10	0
66	d1	1200	0	1262	16	0
67	d2	1013	0	1147	6	0
68	e1	1113	0	1145	10	0
69	e2	830	0	916	4	0
70	f1	822	0	887	9	0
71	f2	705	0	737	10	0
72	g1	640	0	633	5	0
73	g2	569	0	637	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	h1	1034	0	1080	8	0
75	h2	447	0	480	10	0
76	i1	1099	0	1162	9	0
77	i2	432	0	470	4	0
78	j1	1015	0	1086	12	0
79	j2	863	0	929	3	0
80	k1	587	0	643	4	0
81	k2	708	0	756	7	0
82	l1	239	0	289	2	0
83	l2	1014	0	1083	9	0
84	m2	1507	0	1564	13	0
85	n2	1178	0	1235	13	0
86	o2	1707	0	1815	36	0
87	p2	3280	0	3326	39	0
88	q2	4668	0	4784	53	0
89	A1	109	0	0	0	0
89	A3	239	0	0	0	0
89	B3	4	0	0	0	0
89	C3	5	0	0	0	0
89	E2	1	0	0	0	0
89	E3	1	0	0	0	0
89	I1	2	0	0	0	0
89	J2	1	0	0	0	0
89	L2	2	0	0	0	0
89	MB	1	0	0	0	0
89	R2	1	0	0	0	0
89	i1	1	0	0	0	0
90	D1	1	0	0	0	0
90	F1	1	0	0	0	0
90	H1	1	0	0	0	0
90	MB	1	0	0	0	0
90	f2	1	0	0	0	0
90	i2	1	0	0	0	0
90	j2	1	0	0	0	0
90	k2	1	0	0	0	0
91	A1	9	0	0	0	0
91	A3	22	0	0	0	0
91	B3	2	0	0	0	0
91	C3	1	0	0	0	0
91	H1	1	0	0	0	0
91	J2	1	0	0	0	0
91	O2	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	A3	20	0	38	1	0
93	B3	32	0	11	0	0
94	q2	16	0	0	0	0
All	All	233632	0	175532	1370	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 3.

The worst 5 of 1370 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)
20:G1:153:CYS:HB3	20:G1:168:CYS:O	1.60	1.00
4:A3:3703:G:H21	4:A3:3778:A:N6	1.60	0.99
2:A1:541:U:H3	2:A1:544:C:N4	1.60	0.97
4:A3:755:G:H1	4:A3:800:U:H3	1.03	0.95
19:F3:71:ARG:HH22	21:G2:1:LEU:HD11	1.33	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MB	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
3	A2	239/291 (82%)	233 (98%)	6 (2%)	0	100	100
5	B1	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
6	B2	224/249 (90%)	216 (96%)	7 (3%)	1 (0%)	30	45
8	C1	61/69 (88%)	60 (98%)	1 (2%)	0	100	100
9	C2	229/319 (72%)	224 (98%)	5 (2%)	0	100	100
11	D1	66/80 (82%)	62 (94%)	4 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	D2	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
13	D3	250/257 (97%)	247 (99%)	3 (1%)	0	100	100
14	E1	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
15	E2	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
16	E3	395/403 (98%)	390 (99%)	5 (1%)	0	100	100
17	F1	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
18	F2	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
19	F3	361/413 (87%)	354 (98%)	7 (2%)	0	100	100
20	G1	311/317 (98%)	294 (94%)	17 (6%)	0	100	100
21	G2	22/184 (12%)	19 (86%)	1 (4%)	2 (9%)	0	0
22	G3	291/296 (98%)	287 (99%)	4 (1%)	0	100	100
23	H1	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
24	H2	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
26	I2	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
28	J2	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
30	K2	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
31	L1	220/295 (75%)	215 (98%)	5 (2%)	0	100	100
32	L2	157/184 (85%)	154 (98%)	3 (2%)	0	100	100
33	M1	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
34	M2	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
35	N1	218/293 (74%)	216 (99%)	2 (1%)	0	100	100
36	N2	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
37	O1	223/243 (92%)	222 (100%)	1 (0%)	0	100	100
38	O2	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
39	P1	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
40	P2	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
41	Q1	189/204 (93%)	183 (97%)	6 (3%)	0	100	100
42	Q2	96/128 (75%)	92 (96%)	4 (4%)	0	100	100
43	R1	235/249 (94%)	229 (97%)	6 (3%)	0	100	100
44	R2	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
45	S1	188/194 (97%)	178 (95%)	10 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	S2	119/157 (76%)	117 (98%)	2 (2%)	0	100	100
47	T1	204/208 (98%)	203 (100%)	1 (0%)	0	100	100
48	T2	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
49	U1	183/194 (94%)	178 (97%)	5 (3%)	0	100	100
50	U2	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
51	V1	94/165 (57%)	93 (99%)	1 (1%)	0	100	100
52	V2	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
53	W1	152/158 (96%)	145 (95%)	7 (5%)	0	100	100
54	W2	144/148 (97%)	140 (97%)	4 (3%)	0	100	100
55	X1	122/132 (92%)	115 (94%)	7 (6%)	0	100	100
56	X2	103/245 (42%)	100 (97%)	3 (3%)	0	100	100
57	Y1	148/151 (98%)	148 (100%)	0	0	100	100
58	Y2	106/115 (92%)	104 (98%)	2 (2%)	0	100	100
59	Z1	134/151 (89%)	127 (95%)	7 (5%)	0	100	100
60	Z2	105/125 (84%)	105 (100%)	0	0	100	100
61	a1	131/145 (90%)	129 (98%)	2 (2%)	0	100	100
62	a2	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
63	b1	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
64	b2	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
65	c1	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
66	d1	144/152 (95%)	137 (95%)	7 (5%)	0	100	100
67	d2	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
68	e1	140/144 (97%)	139 (99%)	1 (1%)	0	100	100
69	e2	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
70	f1	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
71	f2	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
72	g1	82/84 (98%)	82 (100%)	0	0	100	100
73	g2	67/70 (96%)	67 (100%)	0	0	100	100
74	h1	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
75	h2	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
76	i1	138/143 (96%)	133 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	i2	49/52 (94%)	49 (100%)	0	0	100	100
78	j1	123/133 (92%)	121 (98%)	2 (2%)	0	100	100
79	j2	102/141 (72%)	100 (98%)	2 (2%)	0	100	100
80	k1	72/124 (58%)	71 (99%)	1 (1%)	0	100	100
81	k2	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
82	l1	23/25 (92%)	23 (100%)	0	0	100	100
83	l2	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
84	m2	194/318 (61%)	181 (93%)	13 (7%)	0	100	100
85	n2	154/165 (93%)	146 (95%)	8 (5%)	0	100	100
86	o2	210/217 (97%)	202 (96%)	8 (4%)	0	100	100
87	p2	414/438 (94%)	397 (96%)	16 (4%)	1 (0%)	43	60
88	q2	593/599 (99%)	574 (97%)	18 (3%)	1 (0%)	43	60
All	All	12928/14622 (88%)	12619 (98%)	304 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
88	q2	96	ARG
21	G2	-1	LYS
87	p2	180	HIS
21	G2	-2	ALA
6	B2	196	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	MB	98/100 (98%)	98 (100%)	0	100	100
3	A2	216/251 (86%)	216 (100%)	0	100	100
5	B1	75/76 (99%)	75 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B2	197/218 (90%)	197 (100%)	0	100	100
8	C1	56/62 (90%)	56 (100%)	0	100	100
9	C2	199/271 (73%)	199 (100%)	0	100	100
11	D1	61/72 (85%)	61 (100%)	0	100	100
12	D2	169/171 (99%)	169 (100%)	0	100	100
13	D3	194/198 (98%)	194 (100%)	0	100	100
14	E1	47/49 (96%)	47 (100%)	0	100	100
15	E2	180/181 (99%)	180 (100%)	0	100	100
16	E3	344/347 (99%)	344 (100%)	0	100	100
17	F1	88/98 (90%)	88 (100%)	0	100	100
18	F2	143/149 (96%)	143 (100%)	0	100	100
19	F3	302/336 (90%)	302 (100%)	0	100	100
20	G1	272/275 (99%)	272 (100%)	0	100	100
21	G2	19/154 (12%)	14 (74%)	5 (26%)	0	0
22	G3	247/250 (99%)	247 (100%)	0	100	100
23	H1	48/49 (98%)	48 (100%)	0	100	100
24	H2	175/176 (99%)	175 (100%)	0	100	100
26	I2	117/161 (73%)	117 (100%)	0	100	100
28	J2	171/172 (99%)	171 (100%)	0	100	100
30	K2	171/173 (99%)	171 (100%)	0	100	100
31	L1	183/243 (75%)	183 (100%)	0	100	100
32	L2	140/163 (86%)	140 (100%)	0	100	100
33	M1	203/231 (88%)	203 (100%)	0	100	100
34	M2	164/165 (99%)	164 (100%)	0	100	100
35	N1	185/223 (83%)	185 (100%)	0	100	100
36	N2	159/175 (91%)	159 (100%)	0	100	100
37	O1	189/202 (94%)	189 (100%)	0	100	100
38	O2	154/154 (100%)	154 (100%)	0	100	100
39	P1	224/225 (100%)	224 (100%)	0	100	100
40	P2	139/140 (99%)	139 (100%)	0	100	100
41	Q1	161/170 (95%)	161 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	Q2	87/113 (77%)	87 (100%)	0	100	100
43	R1	207/218 (95%)	207 (100%)	0	100	100
44	R2	106/107 (99%)	106 (100%)	0	100	100
45	S1	170/174 (98%)	167 (98%)	3 (2%)	51	72
46	S2	100/126 (79%)	100 (100%)	0	100	100
47	T1	178/180 (99%)	177 (99%)	1 (1%)	78	88
48	T2	106/134 (79%)	106 (100%)	0	100	100
49	U1	161/168 (96%)	161 (100%)	0	100	100
50	U2	124/135 (92%)	124 (100%)	0	100	100
51	V1	87/136 (64%)	87 (100%)	0	100	100
52	V2	117/118 (99%)	117 (100%)	0	100	100
53	W1	139/142 (98%)	139 (100%)	0	100	100
54	W2	118/119 (99%)	118 (100%)	0	100	100
55	X1	104/108 (96%)	104 (100%)	0	100	100
56	X2	87/183 (48%)	87 (100%)	0	100	100
57	Y1	130/131 (99%)	130 (100%)	0	100	100
58	Y2	92/98 (94%)	92 (100%)	0	100	100
59	Z1	106/119 (89%)	106 (100%)	0	100	100
60	Z2	98/110 (89%)	98 (100%)	0	100	100
61	a1	119/130 (92%)	119 (100%)	0	100	100
62	a2	116/121 (96%)	116 (100%)	0	100	100
63	b1	117/121 (97%)	117 (100%)	0	100	100
64	b2	89/89 (100%)	89 (100%)	0	100	100
65	c1	120/121 (99%)	120 (100%)	0	100	100
66	d1	126/131 (96%)	125 (99%)	1 (1%)	73	85
67	d2	109/110 (99%)	109 (100%)	0	100	100
68	e1	112/113 (99%)	112 (100%)	0	100	100
69	e2	86/89 (97%)	86 (100%)	0	100	100
70	f1	94/107 (88%)	92 (98%)	2 (2%)	47	69
71	f2	73/80 (91%)	73 (100%)	0	100	100
72	g1	68/68 (100%)	68 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	g2	64/65 (98%)	64 (100%)	0	100	100
74	h1	112/113 (99%)	112 (100%)	0	100	100
75	h2	47/48 (98%)	47 (100%)	0	100	100
76	i1	112/114 (98%)	111 (99%)	1 (1%)	70	82
77	i2	47/47 (100%)	47 (100%)	0	100	100
78	j1	107/115 (93%)	107 (100%)	0	100	100
79	j2	92/120 (77%)	92 (100%)	0	100	100
80	k1	65/102 (64%)	65 (100%)	0	100	100
81	k2	74/75 (99%)	74 (100%)	0	100	100
82	l1	24/24 (100%)	24 (100%)	0	100	100
83	l2	110/120 (92%)	110 (100%)	0	100	100
84	m2	164/258 (64%)	164 (100%)	0	100	100
85	n2	128/137 (93%)	128 (100%)	0	100	100
86	o2	191/195 (98%)	191 (100%)	0	100	100
87	p2	358/376 (95%)	358 (100%)	0	100	100
88	q2	516/526 (98%)	516 (100%)	0	100	100
All	All	11247/12414 (91%)	11234 (100%)	13 (0%)	87	95

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	S1	79	LEU
47	T1	137	LEU
76	i1	61	GLN
70	f1	100	GLN
70	f1	101	ILE

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

Mol	Chain	Res	Type
53	W1	19	ASN
62	a2	52	GLN
53	W1	100	ASN
56	X2	60	ASN
75	h2	17	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	C3	155/158 (98%)	19 (12%)	0
2	A1	1764/1870 (94%)	285 (16%)	4 (0%)
25	I1	17/659 (2%)	5 (29%)	0
27	J1	74/75 (98%)	18 (24%)	1 (1%)
29	K1	73/74 (98%)	21 (28%)	4 (5%)
4	A3	3752/4808 (78%)	599 (15%)	8 (0%)
7	B3	118/119 (99%)	11 (9%)	0
All	All	5953/7763 (76%)	958 (16%)	17 (0%)

5 of 958 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A1	3	C
2	A1	4	C
2	A1	17	C
2	A1	33	G
2	A1	41	G

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	K1	16	H2U
29	K1	75	C
4	A3	2431	C
4	A3	4012	G
4	A3	4124	A

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

230 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
4	PSU	A3	3494	4	18,21,22	1.07	1 (5%)	22,30,33	1.62	4 (18%)
2	PSU	A1	823	2	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
4	A2M	A3	398	4	22,25,26	1.25	1 (4%)	31,36,39	1.54	7 (22%)
2	PSU	A1	218	2	18,21,22	1.05	1 (5%)	22,30,33	1.65	4 (18%)
2	A2M	A1	485	2	22,25,26	1.27	1 (4%)	31,36,39	1.43	6 (19%)
2	OMC	A1	1704	2	19,22,23	2.99	8 (42%)	26,31,34	0.83	1 (3%)
4	A2M	A3	4317	4	22,25,26	1.36	2 (9%)	31,36,39	1.59	9 (29%)
29	1MA	K1	14	29	21,25,26	0.36	0	31,37,40	0.77	0
56	MLZ	X2	5	56	8,9,10	0.76	0	4,9,11	0.61	0
4	PSU	A3	3466	4	18,21,22	1.01	1 (5%)	22,30,33	1.66	5 (22%)
2	G7M	A1	1640	2,29	23,26,27	2.60	8 (34%)	35,39,42	2.45	10 (28%)
29	1MG	K1	9	29	22,26,27	0.61	0	33,39,42	0.67	0
54	V5N	W2	39	54	9,11,12	0.77	0	9,14,16	1.14	1 (11%)
2	PSU	A1	1245	2	18,21,22	1.08	1 (5%)	22,30,33	1.67	4 (18%)
4	PSU	A3	1731	4	18,21,22	1.02	1 (5%)	22,30,33	1.63	4 (18%)
2	OMC	A1	1392	2	19,22,23	3.03	8 (42%)	26,31,34	1.03	2 (7%)
2	A2M	A1	669	89,2	22,25,26	1.42	2 (9%)	31,36,39	1.58	9 (29%)
2	OMU	A1	628	2	19,22,23	3.05	8 (42%)	26,31,34	1.68	5 (19%)
2	PSU	A1	967	2	18,21,22	0.89	1 (5%)	22,30,33	0.60	0
2	OMG	A1	1448	2	23,26,27	2.32	6 (26%)	33,38,41	2.34	10 (30%)
2	PSU	A1	1644	89,2	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)
4	PSU	A3	4382	4	18,21,22	1.04	1 (5%)	22,30,33	1.67	5 (22%)
2	4AC	A1	1338	2	21,24,25	3.34	10 (47%)	29,34,37	1.81	6 (20%)
4	PSU	A3	2351	4	18,21,22	1.05	1 (5%)	22,30,33	1.66	4 (18%)
4	PSU	A3	4203	4	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
2	6MZ	A1	1833	89,2	22,25,26	2.67	4 (18%)	30,36,39	2.28	7 (23%)
4	PSU	A3	3462	4	18,21,22	1.05	1 (5%)	22,30,33	1.65	4 (18%)
2	OMU	A1	1327	89,2	19,22,23	3.04	8 (42%)	26,31,34	1.72	5 (19%)
4	PSU	A3	1638	4	18,21,22	1.10	1 (5%)	22,30,33	1.66	4 (18%)
2	OMU	A1	1805	2	19,22,23	3.07	8 (42%)	26,31,34	1.71	4 (15%)
77	M3L	i2	98	77	10,11,12	0.39	0	9,14,16	0.29	0
4	PSU	A3	3616	4	18,21,22	1.07	1 (5%)	22,30,33	1.69	4 (18%)
2	PSU	A1	682	2	18,21,22	1.07	1 (5%)	22,30,33	1.65	4 (18%)
2	OMU	A1	1289	2	19,22,23	3.05	8 (42%)	26,31,34	1.67	4 (15%)
4	A2M	A3	3517	4	22,25,26	3.18	11 (50%)	31,36,39	3.72	13 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMC	A3	2265	89,4	19,22,23	3.03	8 (42%)	26,31,34	0.80	1 (3%)
2	OMG	A1	437	2	23,26,27	2.30	6 (26%)	33,38,41	2.29	12 (36%)
4	OMC	A3	2647	4	19,22,23	2.98	8 (42%)	26,31,34	0.67	0
4	PSU	A3	3576	4	18,21,22	1.09	1 (5%)	22,30,33	1.61	4 (18%)
4	OMG	A3	3631	89,4	23,26,27	2.27	6 (26%)	33,38,41	2.25	11 (33%)
2	PSU	A1	573	2	18,21,22	1.04	1 (5%)	22,30,33	1.60	4 (18%)
2	PSU	A1	109	2	18,21,22	1.08	1 (5%)	22,30,33	1.75	5 (22%)
4	OMC	A3	3433	4,91	19,22,23	2.92	8 (42%)	26,31,34	0.75	0
2	PSU	A1	1693	2	18,21,22	1.08	1 (5%)	22,30,33	1.65	4 (18%)
4	OMG	A3	4364	4	23,26,27	2.26	7 (30%)	33,38,41	2.25	12 (36%)
4	OMG	A3	2267	4	23,26,27	2.32	6 (26%)	33,38,41	2.41	9 (27%)
2	PSU	A1	864	2	18,21,22	1.00	1 (5%)	22,30,33	1.60	4 (18%)
4	A2M	A3	4336	4	22,25,26	1.22	1 (4%)	31,36,39	1.54	7 (22%)
10	OMG	C3	75	10	23,26,27	2.28	7 (30%)	33,38,41	2.29	12 (36%)
4	OMU	A3	3973	4	19,22,23	3.04	8 (42%)	26,31,34	1.75	5 (19%)
29	5MU	K1	54	29	19,22,23	0.23	0	28,32,35	0.31	0
4	OMG	A3	2719	4	23,26,27	2.30	6 (26%)	33,38,41	2.45	10 (30%)
2	A2M	A1	469	2	22,25,26	1.42	1 (4%)	31,36,39	1.55	8 (25%)
4	OMG	A3	4245	4	23,26,27	2.28	6 (26%)	33,38,41	2.35	10 (30%)
2	A2M	A1	27	89,2	22,25,26	1.32	1 (4%)	31,36,39	1.51	7 (22%)
2	OMG	A1	684	2	23,26,27	2.31	6 (26%)	33,38,41	2.26	10 (30%)
4	OMC	A3	2208	4	19,22,23	0.27	0	26,31,34	0.40	0
4	PSU	A3	4149	4	18,21,22	1.00	1 (5%)	22,30,33	1.72	5 (22%)
2	A2M	A1	1384	2	22,25,26	1.33	1 (4%)	31,36,39	1.62	8 (25%)
2	PSU	A1	1348	2	18,21,22	1.07	1 (5%)	22,30,33	1.68	4 (18%)
2	PSU	A1	1046	2	18,21,22	1.02	1 (5%)	22,30,33	1.64	4 (18%)
4	PSU	A3	4039	4	18,21,22	1.12	1 (5%)	22,30,33	1.73	4 (18%)
2	OMU	A1	121	2	19,22,23	3.00	8 (42%)	26,31,34	1.61	5 (19%)
4	PSU	A3	3502	4	18,21,22	1.10	1 (5%)	22,30,33	1.61	4 (18%)
4	A2M	A3	1810	4	22,25,26	1.32	1 (4%)	31,36,39	1.66	8 (25%)
4	A2M	A3	2658	4	22,25,26	1.29	1 (4%)	31,36,39	1.51	8 (25%)
4	PSU	A3	4042	4	18,21,22	1.03	1 (5%)	22,30,33	1.66	4 (18%)
2	A2M	A1	159	2	22,25,26	1.37	1 (4%)	31,36,39	1.56	8 (25%)
4	A2M	A3	3557	4	22,25,26	1.28	1 (4%)	31,36,39	1.57	7 (22%)
4	A2M	A3	3492	4	22,25,26	1.33	1 (4%)	31,36,39	1.51	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	HIC	E3	245	16	10,11,12	0.52	0	8,14,16	0.48	0
4	PSU	A3	4217	4	18,21,22	1.07	1 (5%)	22,30,33	1.57	4 (18%)
4	OMG	A3	3524	4	23,26,27	2.28	6 (26%)	33,38,41	2.24	11 (33%)
2	OMG	A1	510	89,2	23,26,27	2.23	6 (26%)	33,38,41	2.29	10 (30%)
2	PSU	A1	105	2	18,21,22	1.06	1 (5%)	22,30,33	1.67	4 (18%)
4	PSU	A3	3369	89,4	18,21,22	0.89	1 (5%)	22,30,33	0.79	0
2	PSU	A1	93	2	18,21,22	1.08	1 (5%)	22,30,33	1.58	4 (18%)
79	MLZ	j2	53	79	8,9,10	0.71	0	4,9,11	0.57	0
2	PSU	A1	1233	2	18,21,22	1.14	1 (5%)	22,30,33	1.65	4 (18%)
2	MA6	A1	1851	2	23,26,27	1.29	4 (17%)	34,38,41	2.68	13 (38%)
2	PSU	A1	650	2	18,21,22	1.10	1 (5%)	22,30,33	1.67	4 (18%)
2	MA6	A1	1852	2	23,26,27	1.25	4 (17%)	34,38,41	2.71	13 (38%)
29	5MC	K1	50	29	18,22,23	0.31	0	26,32,35	0.51	0
4	OMC	A3	3601	4	19,22,23	2.98	8 (42%)	26,31,34	0.77	0
4	OMC	A3	2667	4	19,22,23	3.02	8 (42%)	26,31,34	0.74	0
4	OMG	A3	1580	4	23,26,27	2.32	6 (26%)	33,38,41	2.36	9 (27%)
2	OMG	A1	602	2	23,26,27	2.29	6 (26%)	33,38,41	2.34	12 (36%)
4	A2M	A3	2244	4	22,25,26	1.34	1 (4%)	31,36,39	1.55	7 (22%)
2	A2M	A1	99	89,2	22,25,26	1.26	1 (4%)	31,36,39	1.46	6 (19%)
4	PSU	A3	4435	4	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
4	PSU	A3	4246	4	18,21,22	1.00	1 (5%)	22,30,33	1.79	4 (18%)
2	PSU	A1	1446	2	18,21,22	1.07	1 (5%)	22,30,33	1.81	4 (18%)
2	OMC	A1	518	2	19,22,23	3.05	8 (42%)	26,31,34	0.88	1 (3%)
29	H2U	K1	16	29	18,21,22	0.71	1 (5%)	21,30,33	0.77	0
4	A2M	A3	3450	4	22,25,26	1.28	1 (4%)	31,36,39	1.58	6 (19%)
4	OMG	A3	1260	4	23,26,27	2.29	6 (26%)	33,38,41	2.31	11 (33%)
2	PSU	A1	36	2	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
4	A2M	A3	3456	4	22,25,26	1.31	1 (4%)	31,36,39	1.52	7 (22%)
4	PSU	A3	4099	4	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
4	PSU	A3	3585	89,4	18,21,22	1.05	1 (5%)	22,30,33	1.60	4 (18%)
4	PSU	A3	1632	4	18,21,22	1.07	1 (5%)	22,30,33	1.78	5 (22%)
2	OMU	A1	172	2	19,22,23	3.02	8 (42%)	26,31,34	1.74	5 (19%)
2	OMU	A1	355	2	19,22,23	3.02	8 (42%)	26,31,34	1.75	5 (19%)
2	OMG	A1	1491	89,2	23,26,27	2.32	6 (26%)	33,38,41	2.35	9 (27%)
2	PSU	A1	816	2	18,21,22	1.08	1 (5%)	22,30,33	1.67	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	A3	3500	4	18,21,22	0.88	1 (5%)	22,30,33	0.60	0
4	OMC	A3	3540	4	19,22,23	2.96	8 (42%)	26,31,34	0.79	1 (3%)
4	A2M	A3	1489	89,4	22,25,26	1.39	3 (13%)	31,36,39	1.55	9 (29%)
4	OMC	A3	3619	4	19,22,23	3.02	8 (42%)	26,31,34	0.88	1 (3%)
4	OMG	A3	4383	4,91	23,26,27	2.27	6 (26%)	33,38,41	2.32	11 (33%)
29	PSU	K1	13	29	18,21,22	0.85	1 (5%)	22,30,33	0.72	0
4	PSU	A3	4107	4	18,21,22	1.05	1 (5%)	22,30,33	1.59	4 (18%)
2	OMG	A1	1329	91,2	23,26,27	2.29	6 (26%)	33,38,41	2.32	11 (33%)
2	OMG	A1	645	2	23,26,27	2.26	6 (26%)	33,38,41	2.30	11 (33%)
29	OMC	K1	34	25,29	19,22,23	4.09	13 (68%)	26,31,34	0.89	1 (3%)
4	UR3	A3	4276	4	19,22,23	2.85	7 (36%)	26,32,35	1.35	3 (11%)
4	PSU	A3	1683	4	18,21,22	1.07	1 (5%)	22,30,33	1.66	4 (18%)
4	PSU	A3	4045	4	18,21,22	1.04	1 (5%)	22,30,33	1.65	4 (18%)
4	PSU	A3	4374	4	18,21,22	1.09	1 (5%)	22,30,33	1.82	4 (18%)
29	OMU	K1	32	29	19,22,23	0.21	0	26,31,34	0.40	0
29	1MA	K1	58	29	21,25,26	1.41	2 (9%)	31,37,40	1.33	5 (16%)
4	5MC	A3	4193	4,91	18,22,23	3.52	7 (38%)	26,32,35	1.23	2 (7%)
29	OMU	K1	39	29	19,22,23	0.20	0	26,31,34	0.43	0
4	PSU	A3	3496	4	18,21,22	1.05	1 (5%)	22,30,33	1.67	4 (18%)
4	OMG	A3	4138	4	23,26,27	2.27	6 (26%)	33,38,41	2.30	12 (36%)
4	OMG	A3	4369	4	23,26,27	2.27	6 (26%)	33,38,41	2.27	11 (33%)
4	A2M	A3	3599	4	22,25,26	1.33	1 (4%)	31,36,39	1.50	8 (25%)
4	OMC	A3	2194	89,4	19,22,23	2.97	8 (42%)	26,31,34	1.40	4 (15%)
4	A2M	A3	4269	89,4	22,25,26	1.33	1 (4%)	31,36,39	1.58	7 (22%)
4	OMU	A3	2680	4	19,22,23	3.04	8 (42%)	26,31,34	1.77	5 (19%)
4	PSU	A3	1537	4	18,21,22	1.08	1 (5%)	22,30,33	1.57	5 (22%)
4	OMG	A3	1477	4	23,26,27	2.25	6 (26%)	33,38,41	2.26	11 (33%)
4	PSU	A3	4278	4	18,21,22	1.10	1 (5%)	22,30,33	1.63	4 (18%)
2	PSU	A1	1057	2	18,21,22	1.05	1 (5%)	22,30,33	1.70	4 (18%)
4	OMC	A3	2704	4	19,22,23	3.03	8 (42%)	26,31,34	0.82	1 (3%)
4	OMG	A3	3942	89,4,29	23,26,27	2.30	6 (26%)	33,38,41	2.32	10 (30%)
2	PSU	A1	687	2	18,21,22	1.06	1 (5%)	22,30,33	1.68	4 (18%)
4	PSU	A3	4325	4	18,21,22	1.00	1 (5%)	22,30,33	1.62	4 (18%)
4	PSU	A3	1721	4	18,21,22	1.08	1 (5%)	22,30,33	1.62	4 (18%)
4	PSU	A3	4298	4	18,21,22	1.09	1 (5%)	22,30,33	1.70	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	A1	463	2	19,22,23	3.03	8 (42%)	26,31,34	0.91	1 (3%)
2	PSU	A1	1178	2	18,21,22	1.11	1 (5%)	22,30,33	1.67	4 (18%)
29	5MC	K1	49	29	18,22,23	0.32	0	26,32,35	0.46	0
4	A2M	A3	1479	4	22,25,26	1.38	2 (9%)	31,36,39	1.49	8 (25%)
4	PSU	A3	1801	4	18,21,22	1.06	1 (5%)	22,30,33	1.67	4 (18%)
2	PSU	A1	1005	2	18,21,22	1.12	1 (5%)	22,30,33	1.64	4 (18%)
2	PSU	A1	210	2	18,21,22	1.08	1 (5%)	22,30,33	1.71	4 (18%)
4	A2M	A3	400	4	22,25,26	1.34	1 (4%)	31,36,39	1.54	9 (29%)
4	5MC	A3	3514	89,4	18,22,23	3.53	7 (38%)	26,32,35	1.12	3 (11%)
2	PSU	A1	1175	91,2	18,21,22	1.10	1 (5%)	22,30,33	1.67	4 (18%)
4	OMC	A3	4202	4	19,22,23	2.97	8 (42%)	26,31,34	0.92	2 (7%)
4	OMG	A3	3974	4	23,26,27	0.31	0	33,38,41	0.45	0
29	5MC	K1	72	29	18,22,23	0.32	0	26,32,35	0.43	0
4	PSU	A3	4711	4	18,21,22	1.04	1 (5%)	22,30,33	1.66	4 (18%)
4	A2M	A3	2630	89,4	22,25,26	1.27	1 (4%)	31,36,39	1.55	8 (25%)
2	A2M	A1	166	2	22,25,26	1.35	1 (4%)	31,36,39	1.56	8 (25%)
4	OMC	A3	1820	89,4	19,22,23	0.29	0	26,31,34	0.73	0
2	PSU	A1	407	2	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)
4	PSU	A3	2475	4	18,21,22	1.07	1 (5%)	22,30,33	1.58	4 (18%)
4	OMC	A3	3573	4	19,22,23	3.00	8 (42%)	26,31,34	0.74	0
4	PSU	A3	3554	4	18,21,22	1.07	1 (5%)	22,30,33	1.70	4 (18%)
4	PSU	A3	4169	4	18,21,22	1.10	1 (5%)	22,30,33	1.66	4 (18%)
2	A2M	A1	1032	2	22,25,26	1.30	1 (4%)	31,36,39	1.50	7 (22%)
2	PSU	A1	119	2	18,21,22	1.04	1 (5%)	22,30,33	1.55	4 (18%)
4	OMC	A3	4282	4	19,22,23	3.01	8 (42%)	26,31,34	0.88	1 (3%)
2	PSU	A1	34	2	18,21,22	1.04	1 (5%)	22,30,33	1.65	4 (18%)
4	PSU	A3	3490	4	18,21,22	0.88	1 (5%)	22,30,33	0.61	0
4	OMG	A3	4240	4	23,26,27	2.28	6 (26%)	33,38,41	2.31	10 (30%)
4	A2M	A3	2206	89,4	22,25,26	0.18	0	31,36,39	0.32	0
2	A2M	A1	513	2	22,25,26	1.46	1 (4%)	31,36,39	1.61	6 (19%)
2	4AC	A1	1843	2	21,24,25	3.24	10 (47%)	29,34,37	1.16	3 (10%)
2	A2M	A1	591	2	22,25,26	1.40	1 (4%)	31,36,39	1.48	7 (22%)
4	UY1	A3	3550	89,4	19,22,23	0.85	1 (5%)	22,31,34	0.65	0
76	HY3	i1	62	76	6,8,9	1.84	1 (16%)	5,10,12	1.00	0
4	OMC	A3	1284	4	19,22,23	2.90	8 (42%)	26,31,34	0.81	0
2	OMC	A1	174	89,2	19,22,23	3.05	8 (42%)	26,31,34	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMU	A3	4244	89,4	19,22,23	3.04	8 (42%)	26,31,34	1.73	5 (19%)
10	PSU	C3	55	10	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)
2	PSU	A1	802	2	18,21,22	1.10	1 (5%)	22,30,33	1.64	4 (18%)
4	PSU	A3	4188	4	18,21,22	1.05	1 (5%)	22,30,33	1.69	5 (22%)
29	OMC	K1	4	29	19,22,23	4.10	13 (68%)	26,31,34	1.33	3 (11%)
2	PSU	A1	1047	2	18,21,22	1.08	1 (5%)	22,30,33	1.63	4 (18%)
2	A2M	A1	1679	2	22,25,26	1.33	2 (9%)	31,36,39	1.53	9 (29%)
10	PSU	C3	69	10	18,21,22	1.06	1 (5%)	22,30,33	1.66	5 (22%)
4	OMG	A3	2207	4	23,26,27	0.29	0	33,38,41	0.37	0
2	OMG	A1	868	2	23,26,27	2.36	6 (26%)	33,38,41	2.41	10 (30%)
2	B8N	A1	1249	2	24,29,30	2.89	5 (20%)	29,42,45	1.76	6 (20%)
4	6MZ	A3	3966	4	22,25,26	2.59	4 (18%)	30,36,39	2.23	8 (26%)
4	PSU	A3	4177	4	18,21,22	1.10	1 (5%)	22,30,33	1.65	4 (18%)
4	OMG	A3	3359	4	23,26,27	2.26	7 (30%)	33,38,41	2.23	13 (39%)
4	PSU	A3	3652	89,4	18,21,22	1.03	1 (5%)	22,30,33	1.64	4 (18%)
2	PSU	A1	1626	2	18,21,22	1.08	1 (5%)	22,30,33	1.60	4 (18%)
4	PSU	A3	4419	4	18,21,22	1.10	1 (5%)	22,30,33	1.65	4 (18%)
2	PSU	A1	1239	2	18,21,22	1.08	1 (5%)	22,30,33	1.67	4 (18%)
4	PSU	A3	1718	4	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)
2	OMU	A1	1443	89,2	19,22,23	3.05	8 (42%)	26,31,34	1.68	4 (15%)
4	OMU	A3	4366	4	19,22,23	2.95	8 (42%)	26,31,34	1.63	4 (15%)
4	PSU	A3	4740	4	18,21,22	1.10	1 (5%)	22,30,33	1.62	4 (18%)
4	1MA	A3	1266	89,4	21,25,26	0.45	0	31,37,40	0.59	0
4	OMG	A3	4116	4	23,26,27	2.29	6 (26%)	33,38,41	2.30	10 (30%)
4	OMU	A3	2258	4	19,22,23	3.05	8 (42%)	26,31,34	1.69	4 (15%)
4	OMU	A3	3657	4	19,22,23	3.01	8 (42%)	26,31,34	1.77	5 (19%)
4	PSU	A3	4166	4	18,21,22	1.04	1 (5%)	22,30,33	1.56	5 (22%)
4	OMU	A3	4052	4	19,22,23	3.01	8 (42%)	26,31,34	1.72	5 (19%)
2	PSU	A1	610	2	18,21,22	1.08	1 (5%)	22,30,33	1.66	4 (18%)
2	PSU	A1	815	2	18,21,22	1.02	1 (5%)	22,30,33	1.59	4 (18%)
2	A2M	A1	577	2	22,25,26	1.33	1 (4%)	31,36,39	1.52	7 (22%)
4	OMG	A3	3476	4	23,26,27	2.29	6 (26%)	33,38,41	2.31	11 (33%)
4	PSU	A3	4749	4	18,21,22	1.12	1 (5%)	22,30,33	1.66	4 (18%)
4	PSU	A3	1799	4	18,21,22	1.06	1 (5%)	22,30,33	1.65	4 (18%)
4	PSU	A3	1720	4	18,21,22	1.08	1 (5%)	22,30,33	1.59	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	A3	1491	4	18,21,22	1.11	1 (5%)	22,30,33	1.76	4 (18%)
4	A2M	A3	3562	4	22,25,26	1.31	1 (4%)	31,36,39	1.58	6 (19%)
4	PSU	A3	3583	4	18,21,22	1.07	1 (5%)	22,30,33	1.62	4 (18%)
2	OMU	A1	429	2	19,22,23	0.22	0	26,31,34	0.44	0
2	PSU	A1	1082	2	18,21,22	1.06	1 (5%)	22,30,33	1.67	4 (18%)
2	PSU	A1	1368	2	18,21,22	1.04	1 (5%)	22,30,33	1.66	4 (18%)
4	PSU	A3	3427	4	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
2	OMU	A1	116	2	19,22,23	3.01	8 (42%)	26,31,34	1.57	4 (15%)
4	PSU	A3	4267	89,4,91	18,21,22	1.13	1 (5%)	22,30,33	1.77	4 (18%)
4	A2M	A3	1270	4	22,25,26	1.29	1 (4%)	31,36,39	1.53	9 (29%)
4	PSU	A3	3371	4	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
2	PSU	A1	652	2	18,21,22	1.12	1 (5%)	22,30,33	1.68	4 (18%)
4	PSU	A3	4322	4	18,21,22	1.08	1 (5%)	22,30,33	1.66	4 (18%)
68	NMM	e1	67	68	9,11,12	0.65	0	6,12,14	2.31	2 (33%)
2	PSU	A1	867	2	18,21,22	1.13	1 (5%)	22,30,33	1.66	4 (18%)
4	OMG	A3	3676	4	23,26,27	2.32	6 (26%)	33,38,41	2.25	10 (30%)
4	PSU	A3	3447	4	18,21,22	1.09	1 (5%)	22,30,33	1.67	4 (18%)
13	V5N	D3	216	13	9,11,12	0.80	0	9,14,16	0.99	0
4	PSU	A3	4058	4	18,21,22	1.07	1 (5%)	22,30,33	1.66	4 (18%)

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
4	PSU	A3	3494	4	-	2/7/25/26	0/2/2/2
2	PSU	A1	823	2	-	0/7/25/26	0/2/2/2
4	A2M	A3	398	4	-	1/9/27/28	0/3/3/3
2	PSU	A1	218	2	-	0/7/25/26	0/2/2/2
2	A2M	A1	485	2	-	0/9/27/28	0/3/3/3
2	OMC	A1	1704	2	-	0/9/27/28	0/2/2/2
4	A2M	A3	4317	4	-	0/9/27/28	0/3/3/3
29	1MA	K1	14	29	-	1/7/25/26	0/3/3/3
56	MLZ	X2	5	56	-	4/7/8/10	-
4	PSU	A3	3466	4	-	1/7/25/26	0/2/2/2
2	G7M	A1	1640	2,29	-	2/7/25/26	0/3/3/3
29	1MG	K1	9	29	-	1/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	V5N	W2	39	54	-	2/9/10/12	0/1/1/1
2	PSU	A1	1245	2	-	2/7/25/26	0/2/2/2
4	PSU	A3	1731	4	-	2/7/25/26	0/2/2/2
2	OMC	A1	1392	2	-	2/9/27/28	0/2/2/2
2	A2M	A1	669	89,2	-	4/9/27/28	0/3/3/3
2	OMU	A1	628	2	-	1/9/27/28	0/2/2/2
2	PSU	A1	967	2	-	0/7/25/26	0/2/2/2
2	OMG	A1	1448	2	-	2/9/27/28	0/3/3/3
2	PSU	A1	1644	89,2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4382	4	-	3/7/25/26	0/2/2/2
2	4AC	A1	1338	2	-	1/11/29/30	0/2/2/2
4	PSU	A3	2351	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4203	4	-	0/7/25/26	0/2/2/2
2	6MZ	A1	1833	89,2	-	0/9/27/28	0/3/3/3
4	PSU	A3	3462	4	-	0/7/25/26	0/2/2/2
2	OMU	A1	1327	89,2	-	0/9/27/28	0/2/2/2
4	PSU	A3	1638	4	-	0/7/25/26	0/2/2/2
2	OMU	A1	1805	2	-	0/9/27/28	0/2/2/2
77	M3L	i2	98	77	-	0/9/10/12	-
4	PSU	A3	3616	4	-	0/7/25/26	0/2/2/2
2	PSU	A1	682	2	-	0/7/25/26	0/2/2/2
2	OMU	A1	1289	2	-	0/9/27/28	0/2/2/2
4	A2M	A3	3517	4	-	3/9/27/28	0/3/3/3
4	OMC	A3	2265	89,4	-	2/9/27/28	0/2/2/2
2	OMG	A1	437	2	-	2/9/27/28	0/3/3/3
4	OMC	A3	2647	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	3576	4	-	1/7/25/26	0/2/2/2
4	OMG	A3	3631	89,4	-	2/9/27/28	0/3/3/3
2	PSU	A1	573	2	-	0/7/25/26	0/2/2/2
2	PSU	A1	109	2	-	0/7/25/26	0/2/2/2
4	OMC	A3	3433	4,91	-	4/9/27/28	0/2/2/2
2	PSU	A1	1693	2	-	0/7/25/26	0/2/2/2
4	OMG	A3	4364	4	-	2/9/27/28	0/3/3/3
4	OMG	A3	2267	4	-	1/9/27/28	0/3/3/3
2	PSU	A1	864	2	-	0/7/25/26	0/2/2/2
4	A2M	A3	4336	4	-	1/9/27/28	0/3/3/3
10	OMG	C3	75	10	-	1/9/27/28	0/3/3/3
4	OMU	A3	3973	4	-	0/9/27/28	0/2/2/2
29	5MU	K1	54	29	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	A3	2719	4	-	0/9/27/28	0/3/3/3
2	A2M	A1	469	2	-	2/9/27/28	0/3/3/3
4	OMG	A3	4245	4	-	0/9/27/28	0/3/3/3
2	A2M	A1	27	89,2	-	1/9/27/28	0/3/3/3
2	OMG	A1	684	2	-	2/9/27/28	0/3/3/3
4	OMC	A3	2208	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	4149	4	-	0/7/25/26	0/2/2/2
2	A2M	A1	1384	2	-	1/9/27/28	0/3/3/3
2	PSU	A1	1348	2	-	0/7/25/26	0/2/2/2
2	PSU	A1	1046	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4039	4	-	0/7/25/26	0/2/2/2
2	OMU	A1	121	2	-	1/9/27/28	0/2/2/2
4	PSU	A3	3502	4	-	0/7/25/26	0/2/2/2
4	A2M	A3	1810	4	-	0/9/27/28	0/3/3/3
4	A2M	A3	2658	4	-	1/9/27/28	0/3/3/3
4	PSU	A3	4042	4	-	0/7/25/26	0/2/2/2
2	A2M	A1	159	2	-	1/9/27/28	0/3/3/3
4	A2M	A3	3557	4	-	0/9/27/28	0/3/3/3
4	A2M	A3	3492	4	-	0/9/27/28	0/3/3/3
16	HIC	E3	245	16	-	0/5/6/8	0/1/1/1
4	PSU	A3	4217	4	-	1/7/25/26	0/2/2/2
4	OMG	A3	3524	4	-	0/9/27/28	0/3/3/3
2	OMG	A1	510	89,2	-	1/9/27/28	0/3/3/3
2	PSU	A1	105	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	3369	89,4	-	0/7/25/26	0/2/2/2
2	PSU	A1	93	2	-	0/7/25/26	0/2/2/2
79	MLZ	j2	53	79	-	1/7/8/10	-
2	PSU	A1	1233	2	-	0/7/25/26	0/2/2/2
2	MA6	A1	1851	2	-	0/11/29/30	0/3/3/3
2	PSU	A1	650	2	-	0/7/25/26	0/2/2/2
2	MA6	A1	1852	2	-	1/11/29/30	0/3/3/3
29	5MC	K1	50	29	-	0/7/25/26	0/2/2/2
4	OMC	A3	3601	4	-	2/9/27/28	0/2/2/2
4	OMC	A3	2667	4	-	0/9/27/28	0/2/2/2
4	OMG	A3	1580	4	-	0/9/27/28	0/3/3/3
2	OMG	A1	602	2	-	0/9/27/28	0/3/3/3
4	A2M	A3	2244	4	-	0/9/27/28	0/3/3/3
2	A2M	A1	99	89,2	-	0/9/27/28	0/3/3/3
4	PSU	A3	4435	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4246	4	-	1/7/25/26	0/2/2/2
2	PSU	A1	1446	2	-	0/7/25/26	0/2/2/2
2	OMC	A1	518	2	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	H2U	K1	16	29	-	0/7/38/39	0/2/2/2
4	A2M	A3	3450	4	-	1/9/27/28	0/3/3/3
4	OMG	A3	1260	4	-	0/9/27/28	0/3/3/3
2	PSU	A1	36	2	-	0/7/25/26	0/2/2/2
4	A2M	A3	3456	4	-	0/9/27/28	0/3/3/3
4	PSU	A3	4099	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	3585	89,4	-	0/7/25/26	0/2/2/2
4	PSU	A3	1632	4	-	3/7/25/26	0/2/2/2
2	OMU	A1	172	2	-	0/9/27/28	0/2/2/2
2	OMU	A1	355	2	-	0/9/27/28	0/2/2/2
2	OMG	A1	1491	89,2	-	1/9/27/28	0/3/3/3
2	PSU	A1	816	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	3500	4	-	0/7/25/26	0/2/2/2
4	OMC	A3	3540	4	-	0/9/27/28	0/2/2/2
4	A2M	A3	1489	89,4	-	2/9/27/28	0/3/3/3
4	OMC	A3	3619	4	-	1/9/27/28	0/2/2/2
4	OMG	A3	4383	4,91	-	1/9/27/28	0/3/3/3
29	PSU	K1	13	29	-	2/7/25/26	0/2/2/2
4	PSU	A3	4107	4	-	1/7/25/26	0/2/2/2
2	OMG	A1	1329	91,2	-	0/9/27/28	0/3/3/3
2	OMG	A1	645	2	-	3/9/27/28	0/3/3/3
29	OMC	K1	34	25,29	-	0/9/27/28	0/2/2/2
4	UR3	A3	4276	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	1683	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4045	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4374	4	-	0/7/25/26	0/2/2/2
29	OMU	K1	32	29	-	1/9/27/28	0/2/2/2
29	1MA	K1	58	29	-	0/7/25/26	0/3/3/3
4	5MC	A3	4193	4,91	-	4/7/25/26	0/2/2/2
29	OMU	K1	39	29	-	1/9/27/28	0/2/2/2
4	PSU	A3	3496	4	-	0/7/25/26	0/2/2/2
4	OMG	A3	4138	4	-	0/9/27/28	0/3/3/3
4	OMG	A3	4369	4	-	0/9/27/28	0/3/3/3
4	A2M	A3	3599	4	-	2/9/27/28	0/3/3/3
4	OMC	A3	2194	89,4	-	3/9/27/28	0/2/2/2
4	A2M	A3	4269	89,4	-	1/9/27/28	0/3/3/3
4	OMU	A3	2680	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	1537	4	-	0/7/25/26	0/2/2/2
4	OMG	A3	1477	4	-	0/9/27/28	0/3/3/3
4	PSU	A3	4278	4	-	0/7/25/26	0/2/2/2
2	PSU	A1	1057	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMC	A3	2704	4	-	0/9/27/28	0/2/2/2
4	OMG	A3	3942	89,4,29	-	0/9/27/28	0/3/3/3
2	PSU	A1	687	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4325	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	1721	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4298	4	-	0/7/25/26	0/2/2/2
2	OMC	A1	463	2	-	1/9/27/28	0/2/2/2
2	PSU	A1	1178	2	-	0/7/25/26	0/2/2/2
29	5MC	K1	49	29	-	2/7/25/26	0/2/2/2
4	A2M	A3	1479	4	-	1/9/27/28	0/3/3/3
4	PSU	A3	1801	4	-	0/7/25/26	0/2/2/2
2	PSU	A1	1005	2	-	0/7/25/26	0/2/2/2
2	PSU	A1	210	2	-	2/7/25/26	0/2/2/2
4	A2M	A3	400	4	-	0/9/27/28	0/3/3/3
4	5MC	A3	3514	89,4	-	0/7/25/26	0/2/2/2
2	PSU	A1	1175	91,2	-	0/7/25/26	0/2/2/2
4	OMC	A3	4202	4	-	0/9/27/28	0/2/2/2
4	OMG	A3	3974	4	-	0/9/27/28	0/3/3/3
29	5MC	K1	72	29	-	0/7/25/26	0/2/2/2
4	PSU	A3	4711	4	-	0/7/25/26	0/2/2/2
4	A2M	A3	2630	89,4	-	3/9/27/28	0/3/3/3
2	A2M	A1	166	2	-	0/9/27/28	0/3/3/3
4	OMC	A3	1820	89,4	-	0/9/27/28	0/2/2/2
2	PSU	A1	407	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	2475	4	-	0/7/25/26	0/2/2/2
4	OMC	A3	3573	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	3554	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	4169	4	-	0/7/25/26	0/2/2/2
2	A2M	A1	1032	2	-	0/9/27/28	0/3/3/3
2	PSU	A1	119	2	-	0/7/25/26	0/2/2/2
4	OMC	A3	4282	4	-	0/9/27/28	0/2/2/2
2	PSU	A1	34	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	3490	4	-	0/7/25/26	0/2/2/2
4	OMG	A3	4240	4	-	0/9/27/28	0/3/3/3
4	A2M	A3	2206	89,4	-	0/9/27/28	0/3/3/3
2	A2M	A1	513	2	-	2/9/27/28	0/3/3/3
2	4AC	A1	1843	2	-	0/11/29/30	0/2/2/2
2	A2M	A1	591	2	-	1/9/27/28	0/3/3/3
4	UY1	A3	3550	89,4	-	3/9/27/28	0/2/2/2
76	HY3	i1	62	76	-	1/1/12/14	0/1/1/1
4	OMC	A3	1284	4	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	A1	174	89,2	-	2/9/27/28	0/2/2/2
4	OMU	A3	4244	89,4	-	1/9/27/28	0/2/2/2
10	PSU	C3	55	10	-	0/7/25/26	0/2/2/2
2	PSU	A1	802	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4188	4	-	0/7/25/26	0/2/2/2
29	OMC	K1	4	29	-	1/9/27/28	0/2/2/2
2	PSU	A1	1047	2	-	0/7/25/26	0/2/2/2
2	A2M	A1	1679	2	-	1/9/27/28	0/3/3/3
10	PSU	C3	69	10	-	0/7/25/26	0/2/2/2
4	OMG	A3	2207	4	-	1/9/27/28	0/3/3/3
2	OMG	A1	868	2	-	2/9/27/28	0/3/3/3
2	B8N	A1	1249	2	-	3/16/34/35	0/2/2/2
4	6MZ	A3	3966	4	-	0/9/27/28	0/3/3/3
4	PSU	A3	4177	4	-	0/7/25/26	0/2/2/2
4	OMG	A3	3359	4	-	1/9/27/28	0/3/3/3
4	PSU	A3	3652	89,4	-	0/7/25/26	0/2/2/2
2	PSU	A1	1626	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4419	4	-	0/7/25/26	0/2/2/2
2	PSU	A1	1239	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	1718	4	-	0/7/25/26	0/2/2/2
2	OMU	A1	1443	89,2	-	1/9/27/28	0/2/2/2
4	OMU	A3	4366	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	4740	4	-	0/7/25/26	0/2/2/2
4	1MA	A3	1266	89,4	-	0/7/25/26	0/3/3/3
4	OMG	A3	4116	4	-	1/9/27/28	0/3/3/3
4	OMU	A3	2258	4	-	0/9/27/28	0/2/2/2
4	OMU	A3	3657	4	-	0/9/27/28	0/2/2/2
4	PSU	A3	4166	4	-	4/7/25/26	0/2/2/2
4	OMU	A3	4052	4	-	0/9/27/28	0/2/2/2
2	PSU	A1	610	2	-	0/7/25/26	0/2/2/2
2	PSU	A1	815	2	-	0/7/25/26	0/2/2/2
2	A2M	A1	577	2	-	3/9/27/28	0/3/3/3
4	OMG	A3	3476	4	-	0/9/27/28	0/3/3/3
4	PSU	A3	4749	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	1799	4	-	0/7/25/26	0/2/2/2
4	PSU	A3	1720	4	-	2/7/25/26	0/2/2/2
4	PSU	A3	1491	4	-	0/7/25/26	0/2/2/2
4	A2M	A3	3562	4	-	0/9/27/28	0/3/3/3
4	PSU	A3	3583	4	-	2/7/25/26	0/2/2/2
2	OMU	A1	429	2	-	4/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A1	1082	2	-	0/7/25/26	0/2/2/2
2	PSU	A1	1368	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	3427	4	-	0/7/25/26	0/2/2/2
2	OMU	A1	116	2	-	1/9/27/28	0/2/2/2
4	PSU	A3	4267	89,4,91	-	0/7/25/26	0/2/2/2
4	A2M	A3	1270	4	-	3/9/27/28	0/3/3/3
4	PSU	A3	3371	4	-	0/7/25/26	0/2/2/2
2	PSU	A1	652	2	-	0/7/25/26	0/2/2/2
4	PSU	A3	4322	4	-	0/7/25/26	0/2/2/2
68	NMM	e1	67	68	-	1/9/11/13	-
2	PSU	A1	867	2	-	0/7/25/26	0/2/2/2
4	OMG	A3	3676	4	-	2/9/27/28	0/3/3/3
4	PSU	A3	3447	4	-	0/7/25/26	0/2/2/2
13	V5N	D3	216	13	-	1/9/10/12	0/1/1/1
4	PSU	A3	4058	4	-	0/7/25/26	0/2/2/2

The worst 5 of 689 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A1	1833	6MZ	C6-N6	11.13	1.46	1.34
4	A3	3966	6MZ	C6-N6	10.73	1.45	1.34
4	A3	4193	5MC	C6-C5	9.53	1.50	1.34
4	A3	3514	5MC	C6-C5	9.09	1.49	1.34
4	A3	3517	A2M	C3'-C4'	-8.36	1.31	1.53

The worst 5 of 1098 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	3517	A2M	C1'-N9-C8	-9.64	105.36	127.14
2	A1	1852	MA6	N1-C6-N6	-7.55	108.83	117.08
2	A1	1851	MA6	N1-C6-N6	-7.39	109.00	117.08
4	A3	2719	OMG	C1'-N9-C8	-7.26	106.02	126.70
4	A3	2267	OMG	C1'-N9-C8	-6.97	106.84	126.70

There are no chirality outliers.

5 of 146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A3	398	A2M	C1'-C2'-O2'-CM'
4	A3	2207	OMG	C1'-C2'-O2'-CM2
4	A3	2658	A2M	C1'-C2'-O2'-CM'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A3	3433	OMC	C2'-C1'-N1-C6
4	A3	3450	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

61 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A1	485	A2M	1	0
2	A1	1640	G7M	1	0
2	A1	1392	OMC	1	0
2	A1	669	A2M	1	0
2	A1	1338	4AC	2	0
4	A3	4203	PSU	1	0
2	A1	1833	6MZ	1	0
4	A3	1638	PSU	1	0
2	A1	682	PSU	1	0
2	A1	1289	OMU	1	0
4	A3	4364	OMG	1	0
4	A3	2267	OMG	1	0
10	C3	75	OMG	1	0
2	A1	469	A2M	1	0
2	A1	27	A2M	2	0
2	A1	1384	A2M	1	0
2	A1	121	OMU	1	0
4	A3	1810	A2M	1	0
4	A3	2658	A2M	2	0
2	A1	159	A2M	2	0
2	A1	1233	PSU	2	0
2	A1	650	PSU	1	0
4	A3	1580	OMG	1	0
2	A1	99	A2M	3	0
2	A1	1446	PSU	1	0
29	K1	16	H2U	2	0
4	A3	3450	A2M	3	0
4	A3	3456	A2M	2	0
4	A3	4099	PSU	1	0
4	A3	3540	OMC	1	0
4	A3	1489	A2M	2	0
4	A3	4383	OMG	2	0
4	A3	4276	UR3	1	0
29	K1	32	OMU	1	0
4	A3	4193	5MC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	K1	39	OMU	1	0
4	A3	4138	OMG	2	0
4	A3	3599	A2M	4	0
4	A3	2194	OMC	1	0
4	A3	4269	A2M	2	0
2	A1	463	OMC	1	0
4	A3	1479	A2M	2	0
4	A3	400	A2M	1	0
2	A1	1032	A2M	1	0
4	A3	3490	PSU	1	0
4	A3	2206	A2M	2	0
2	A1	1843	4AC	1	0
4	A3	1284	OMC	1	0
29	K1	4	OMC	1	0
2	A1	1679	A2M	1	0
4	A3	2207	OMG	1	0
4	A3	4177	PSU	1	0
4	A3	4366	OMU	1	0
4	A3	2258	OMU	1	0
4	A3	3657	OMU	1	0
2	A1	610	PSU	1	0
2	A1	577	A2M	2	0
4	A3	1491	PSU	1	0
2	A1	429	OMU	1	0
2	A1	116	OMU	1	0
4	A3	3676	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 417 ligands modelled in this entry, 412 are monoatomic - leaving 5 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
94	SF4	q2	601	88	0,12,12	-	-	-		
92	SPD	A3	5161	-	9,9,9	0.32	0	8,8,8	0.83	0
92	SPD	A3	5160	-	9,9,9	0.34	0	8,8,8	0.80	0
93	GTP	B3	201	7	30,34,34	1.53	5 (16%)	46,54,54	1.43	6 (13%)
94	SF4	q2	602	88	0,12,12	-	-	-		

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
94	SF4	q2	601	88	-	-	0/6/5/5
92	SPD	A3	5161	-	-	4/7/7/7	-
92	SPD	A3	5160	-	-	2/7/7/7	-
93	GTP	B3	201	7	-	2/22/38/38	0/3/3/3
94	SF4	q2	602	88	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
93	B3	201	GTP	PA-O5'	5.63	1.82	1.59
93	B3	201	GTP	O5'-C5'	-2.55	1.35	1.44
93	B3	201	GTP	C4-N3	2.21	1.39	1.34
93	B3	201	GTP	C8-N9	2.08	1.42	1.37
93	B3	201	GTP	C2-N2	2.04	1.39	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	B3	201	GTP	O5'-PA-O1A	-3.78	94.30	109.07
93	B3	201	GTP	C3'-C2'-C1'	-2.46	96.75	101.43
93	B3	201	GTP	C2-N1-C6	-2.45	120.63	125.10
93	B3	201	GTP	O6-C6-N1	-2.44	115.44	120.12
93	B3	201	GTP	N1-C2-N3	2.32	127.66	123.32

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
93	B3	201	GTP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

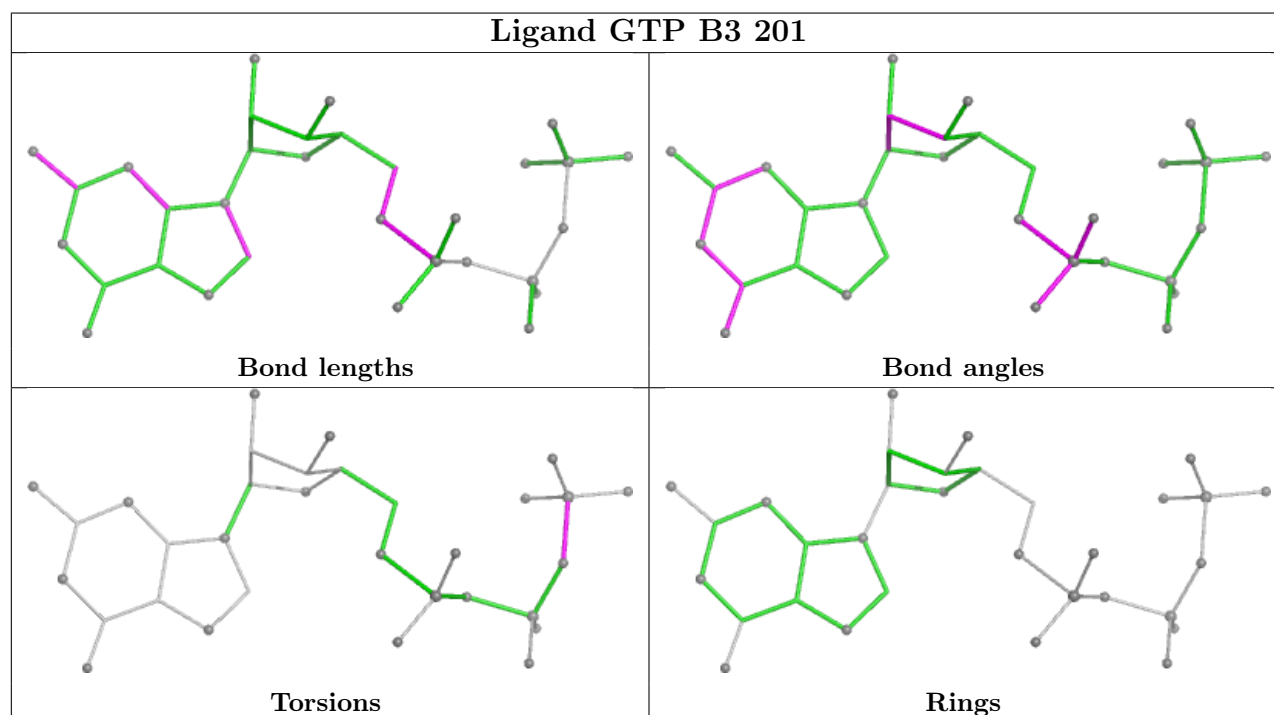
Mol	Chain	Res	Type	Atoms
92	A3	5160	SPD	N6-C7-C8-C9
92	A3	5161	SPD	N6-C7-C8-C9
92	A3	5161	SPD	C7-C8-C9-N10
92	A3	5160	SPD	C3-C4-C5-N6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	A3	5161	SPD	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
29	K1	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K1	16:H2U	O3'	18:G	P	1.95
1	K1	46:A	O3'	48:C	P	1.95

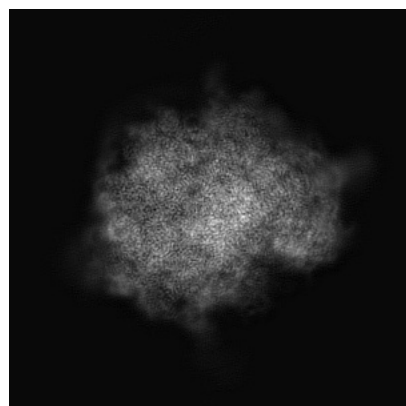
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53976. These allow visual inspection of the internal detail of the map and identification of artifacts.

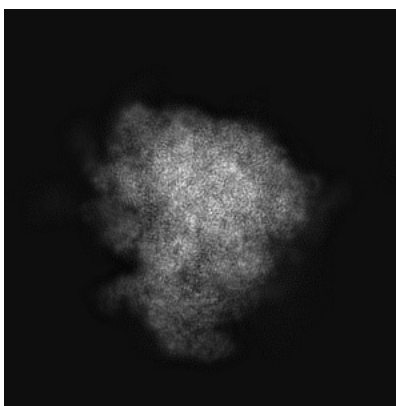
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

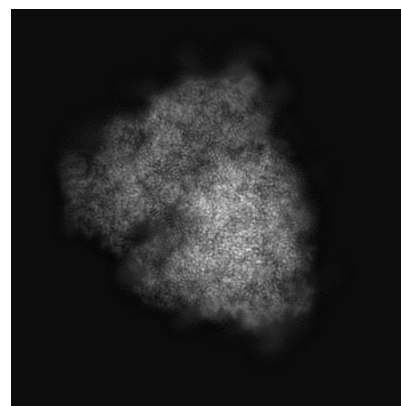
6.1.1 Primary map



X

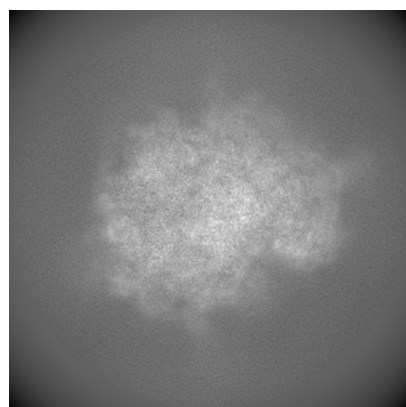


Y

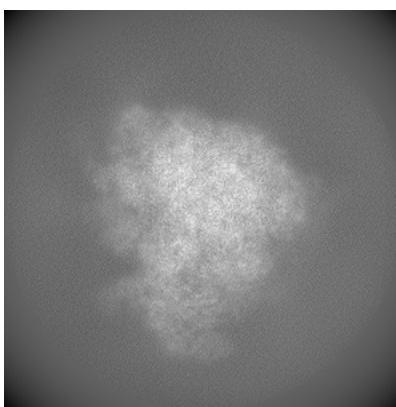


Z

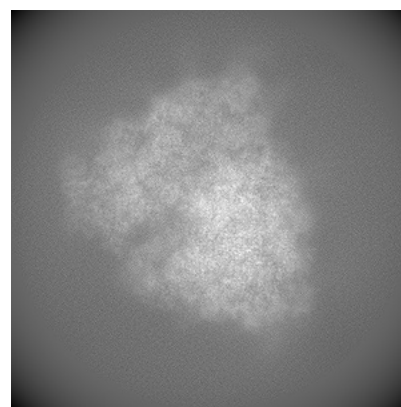
6.1.2 Raw map



X



Y

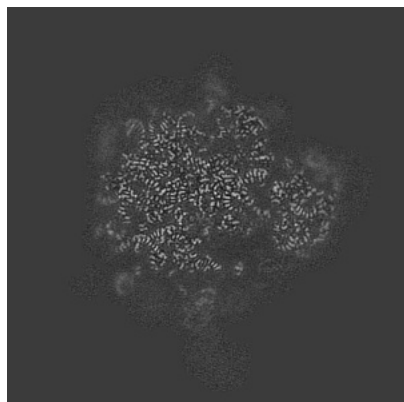


Z

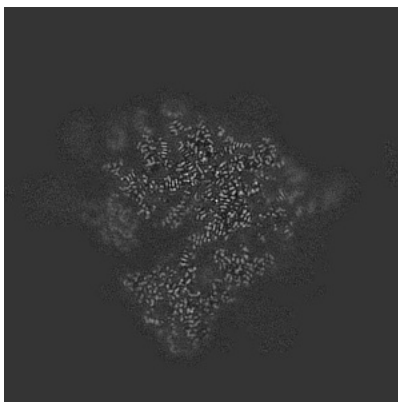
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

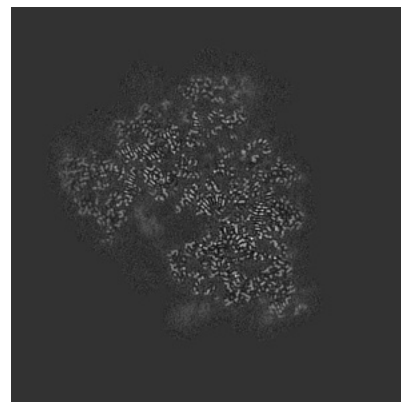
6.2.1 Primary map



X Index: 300

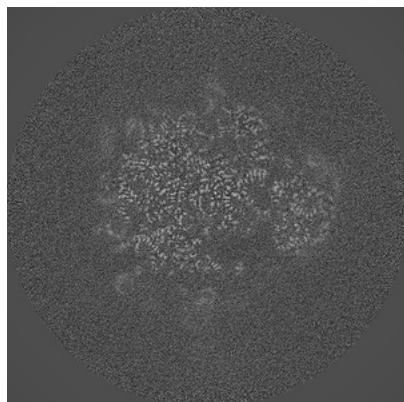


Y Index: 300

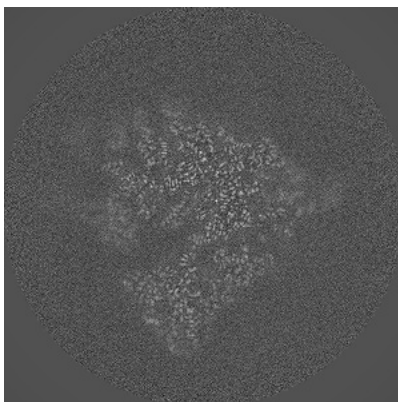


Z Index: 300

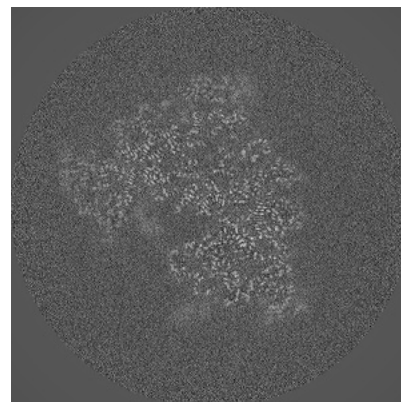
6.2.2 Raw map



X Index: 300



Y Index: 300

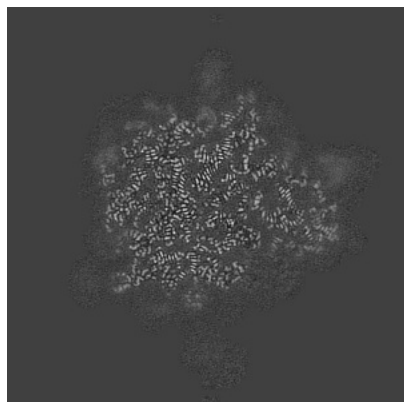


Z Index: 300

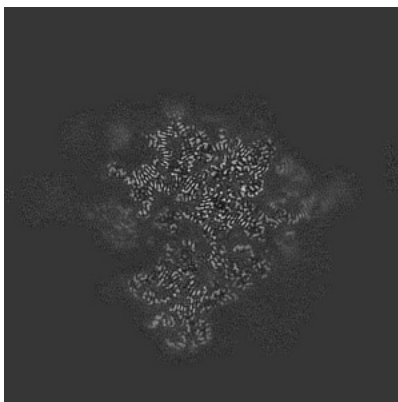
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

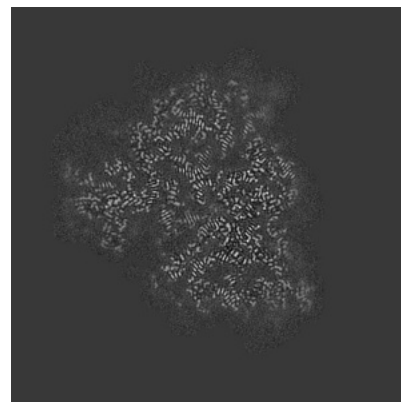
6.3.1 Primary map



X Index: 322

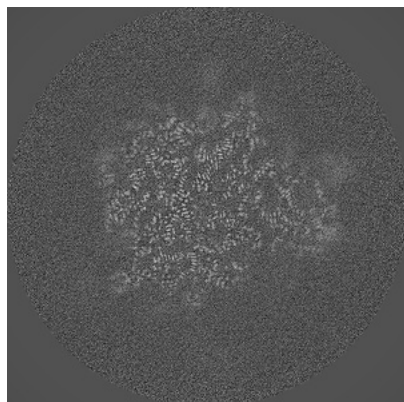


Y Index: 309

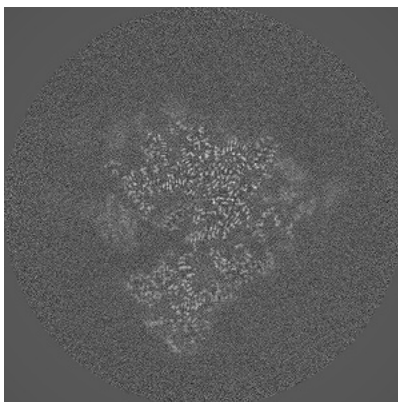


Z Index: 281

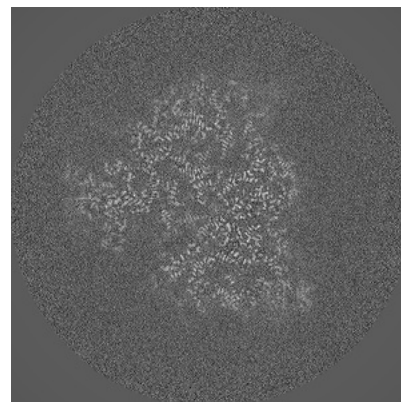
6.3.2 Raw map



X Index: 323



Y Index: 303

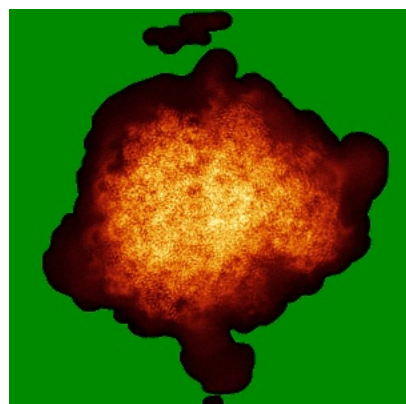


Z Index: 281

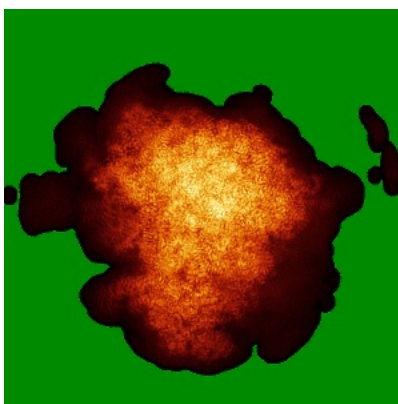
The images above show the largest variance slices of the map in three orthogonal directions.

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

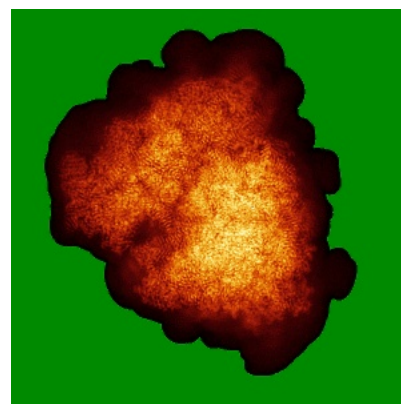
6.4.1 Primary map



X

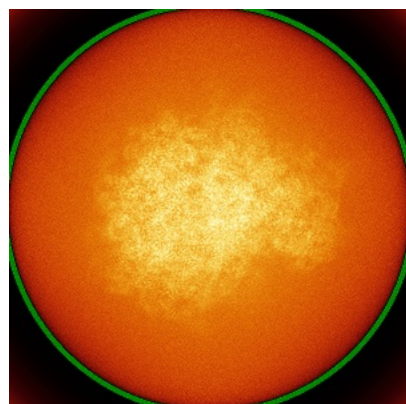


Y

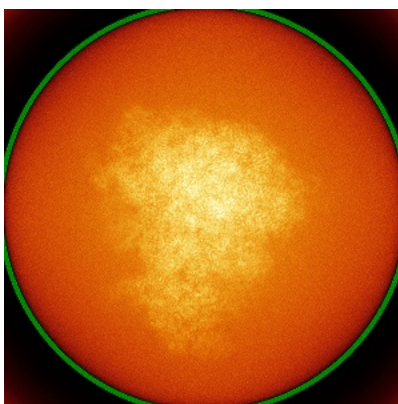


Z

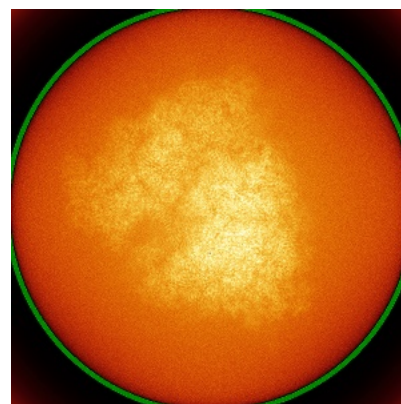
6.4.2 Raw map



X



Y

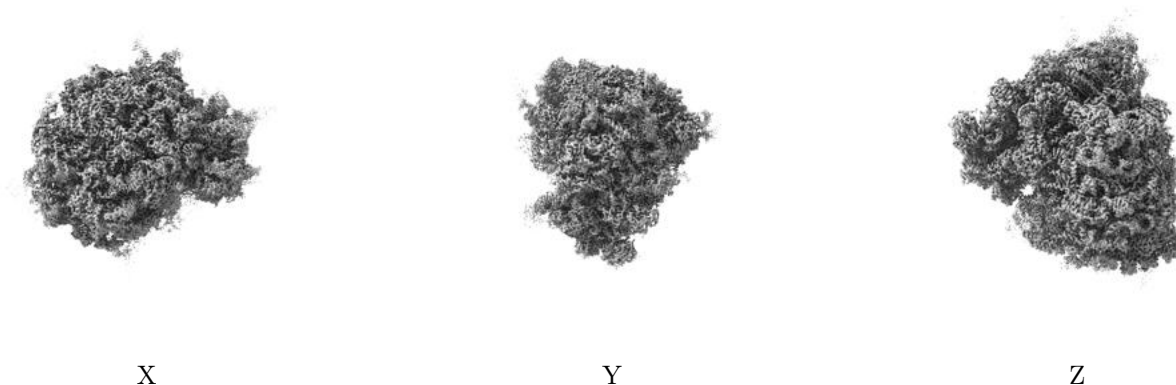


Z

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.

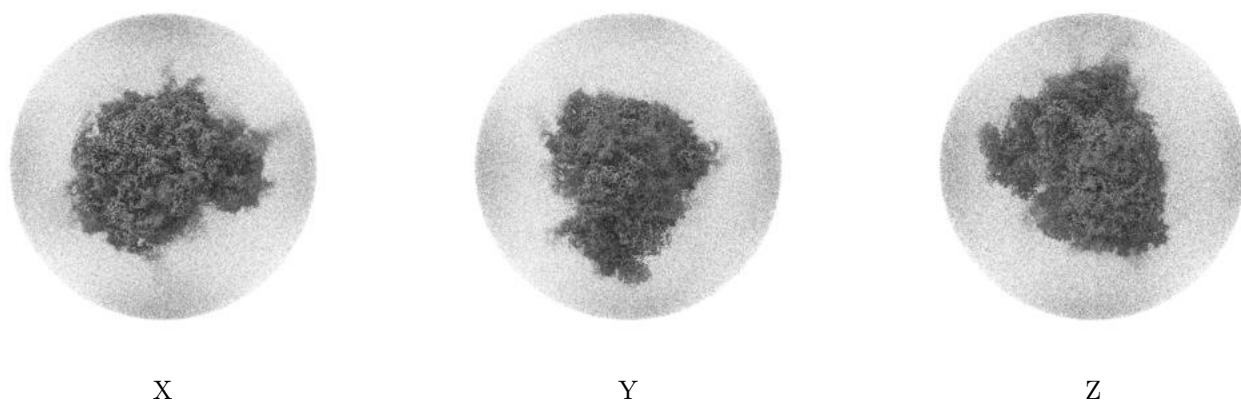
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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



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.

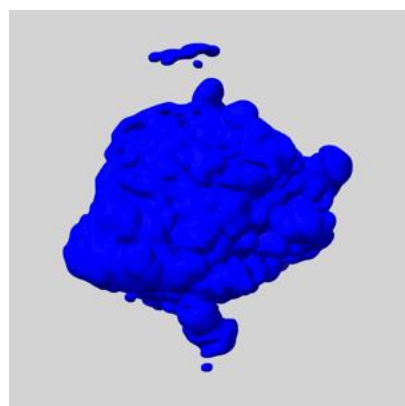
6.6 Mask visualisation [i](#)

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

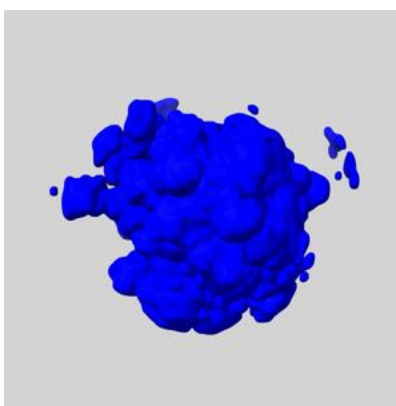
A mask typically either:

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

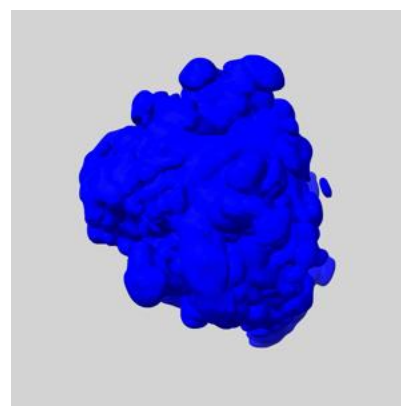
6.6.1 emd_53976_msk_1.map [i](#)



X



Y

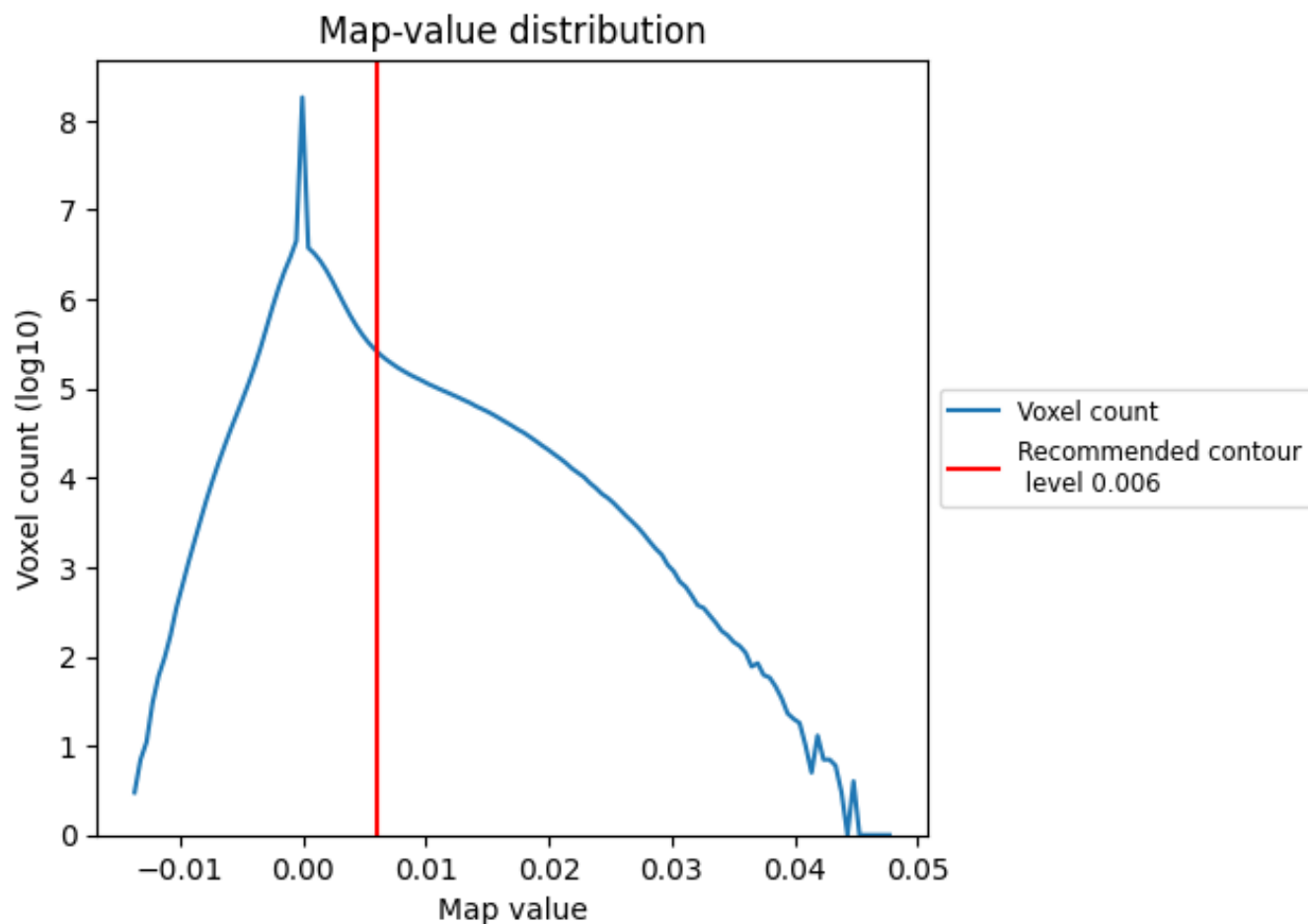


Z

7 Map analysis [i](#)

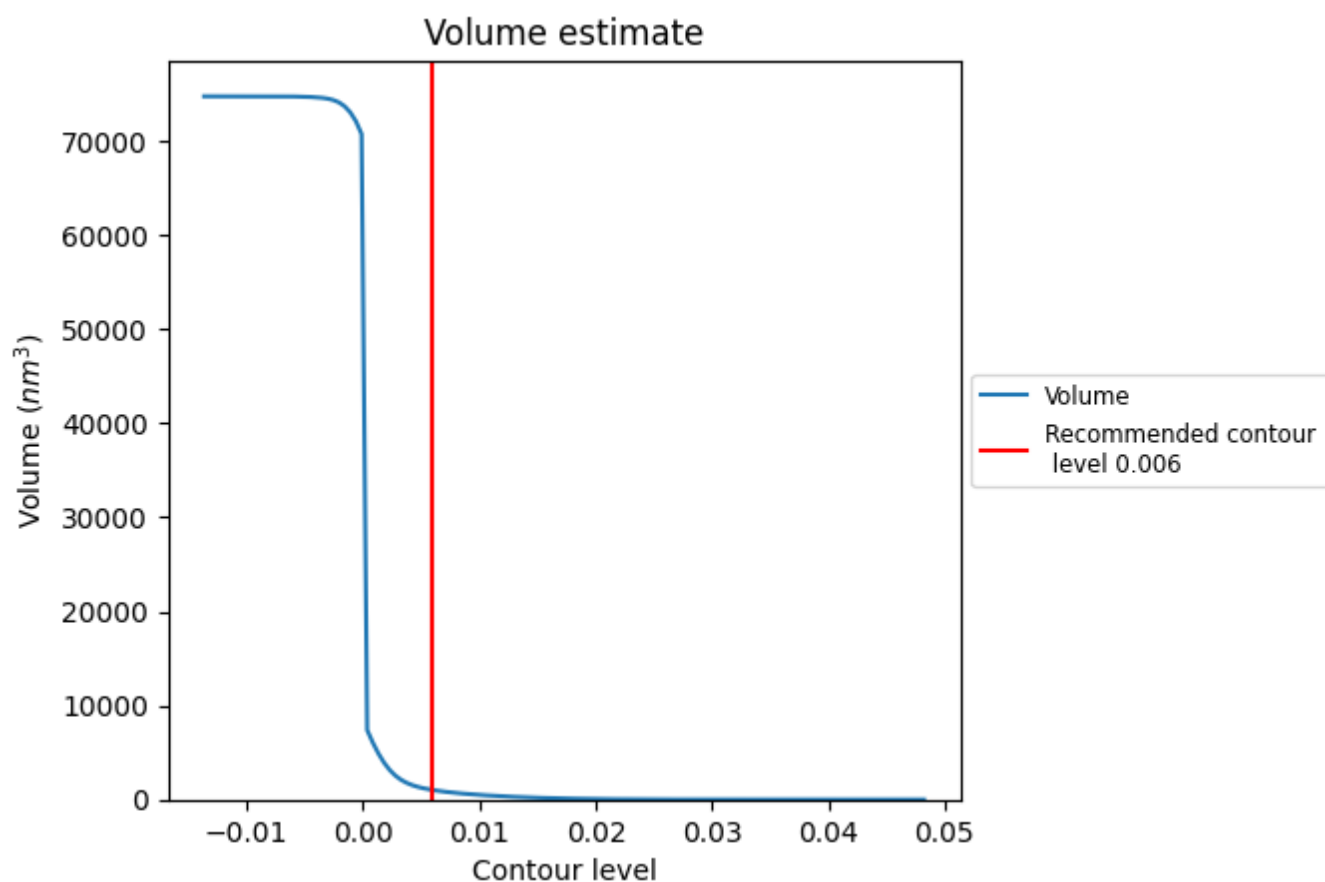
This section contains the results of statistical analysis of the map.

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.

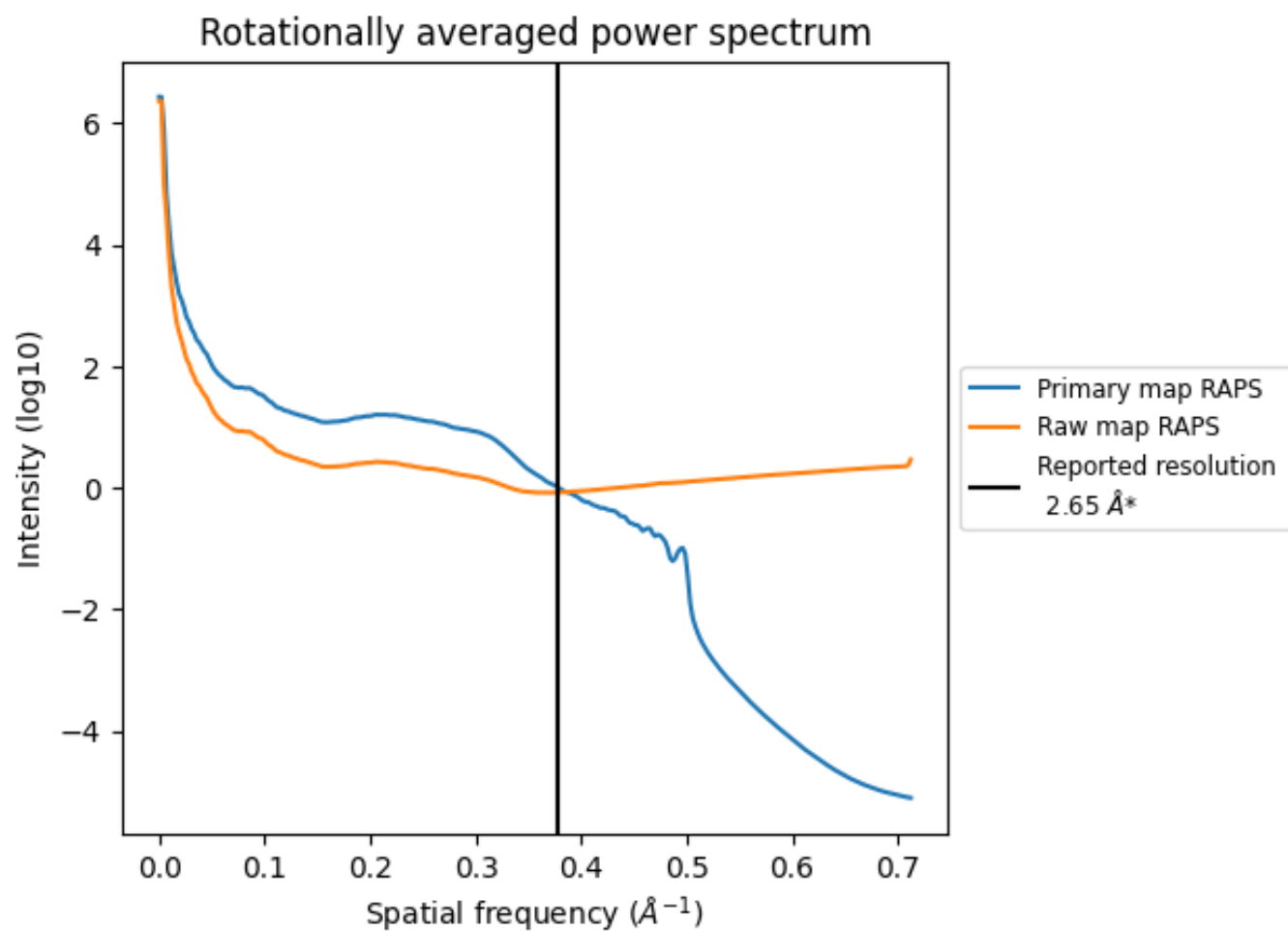
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1010 nm³; this corresponds to an approximate mass of 913 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 ⓘ

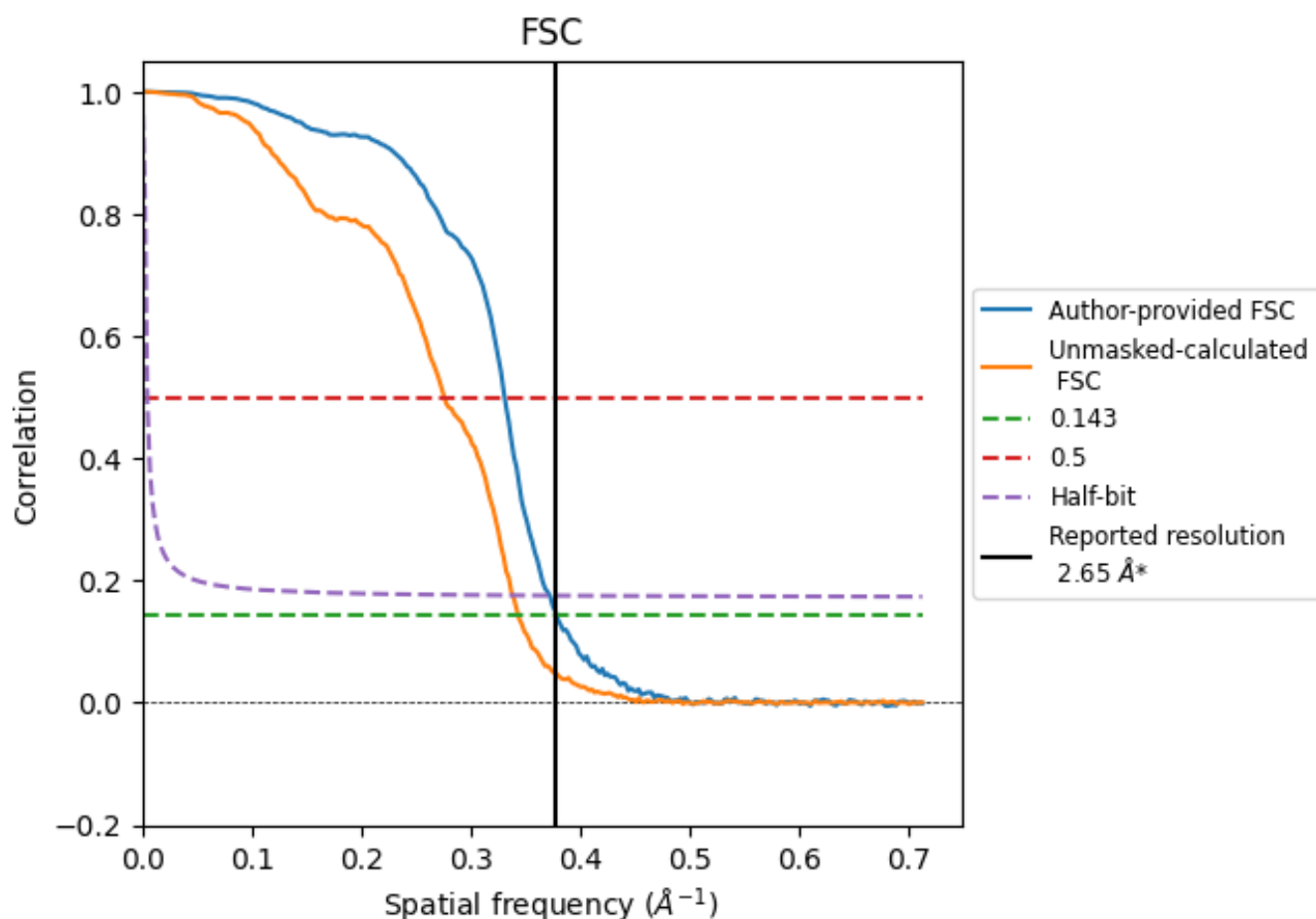


*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

8.2 Resolution estimates [i](#)

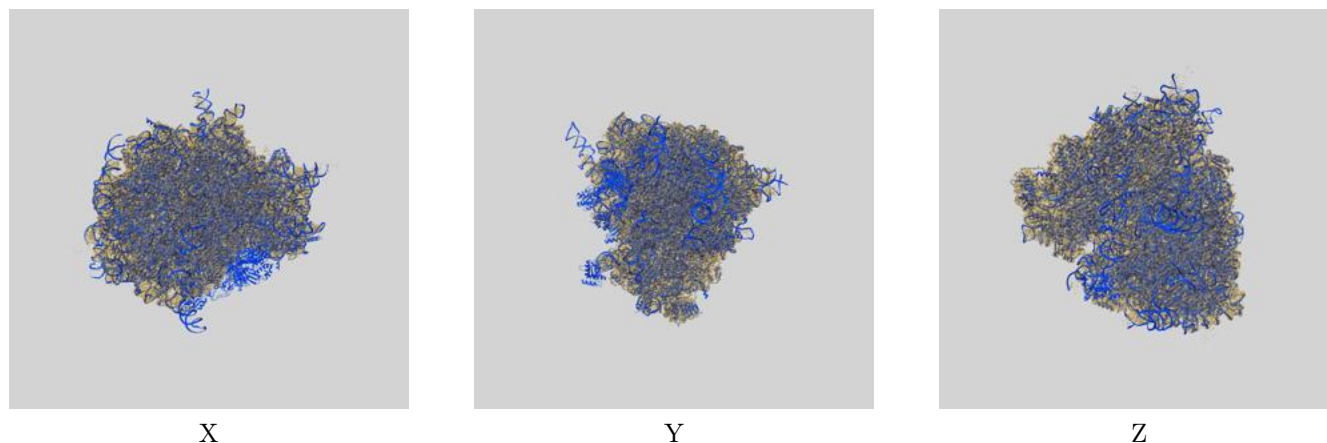
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.64	3.02	2.69
Unmasked-calculated*	2.91	3.62	2.96

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

9 Map-model fit [i](#)

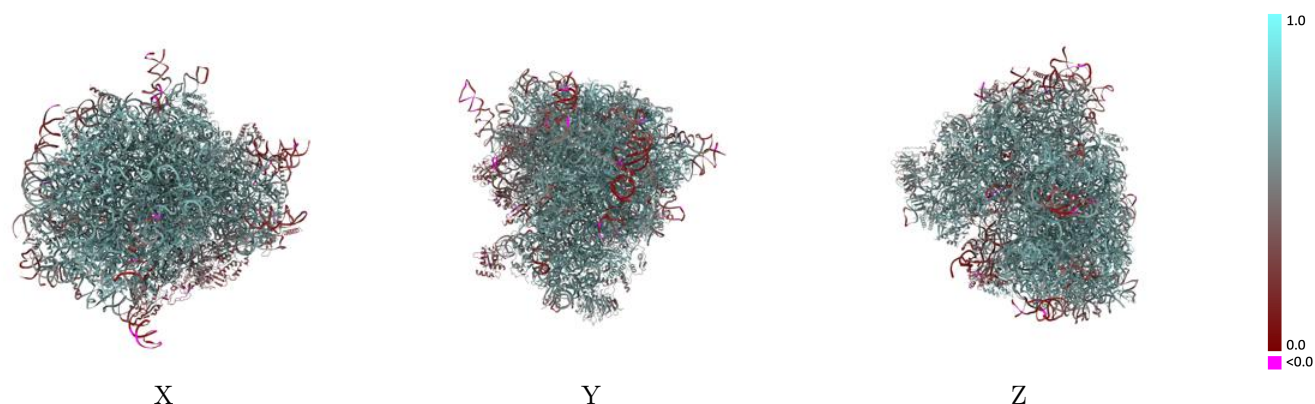
This section contains information regarding the fit between EMDB map EMD-53976 and PDB model 9RHU. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



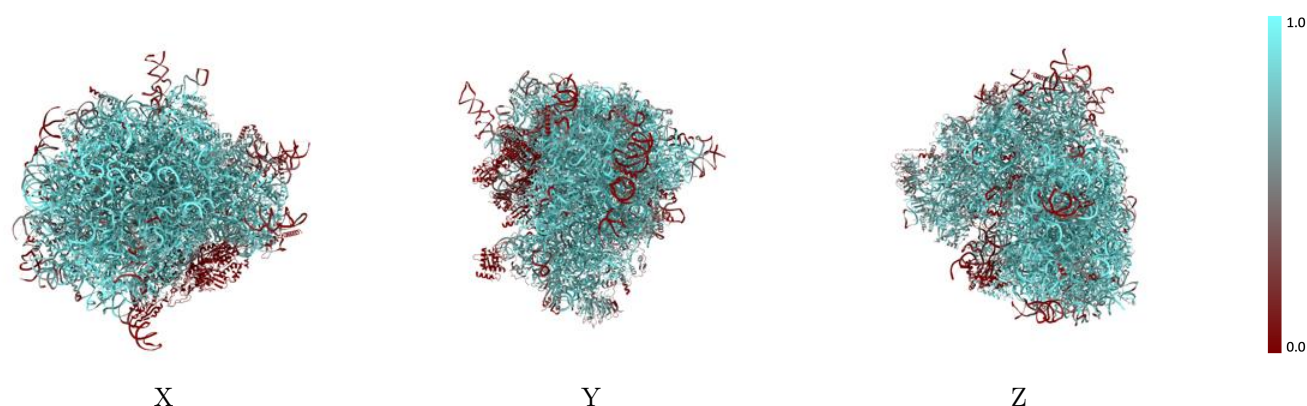
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



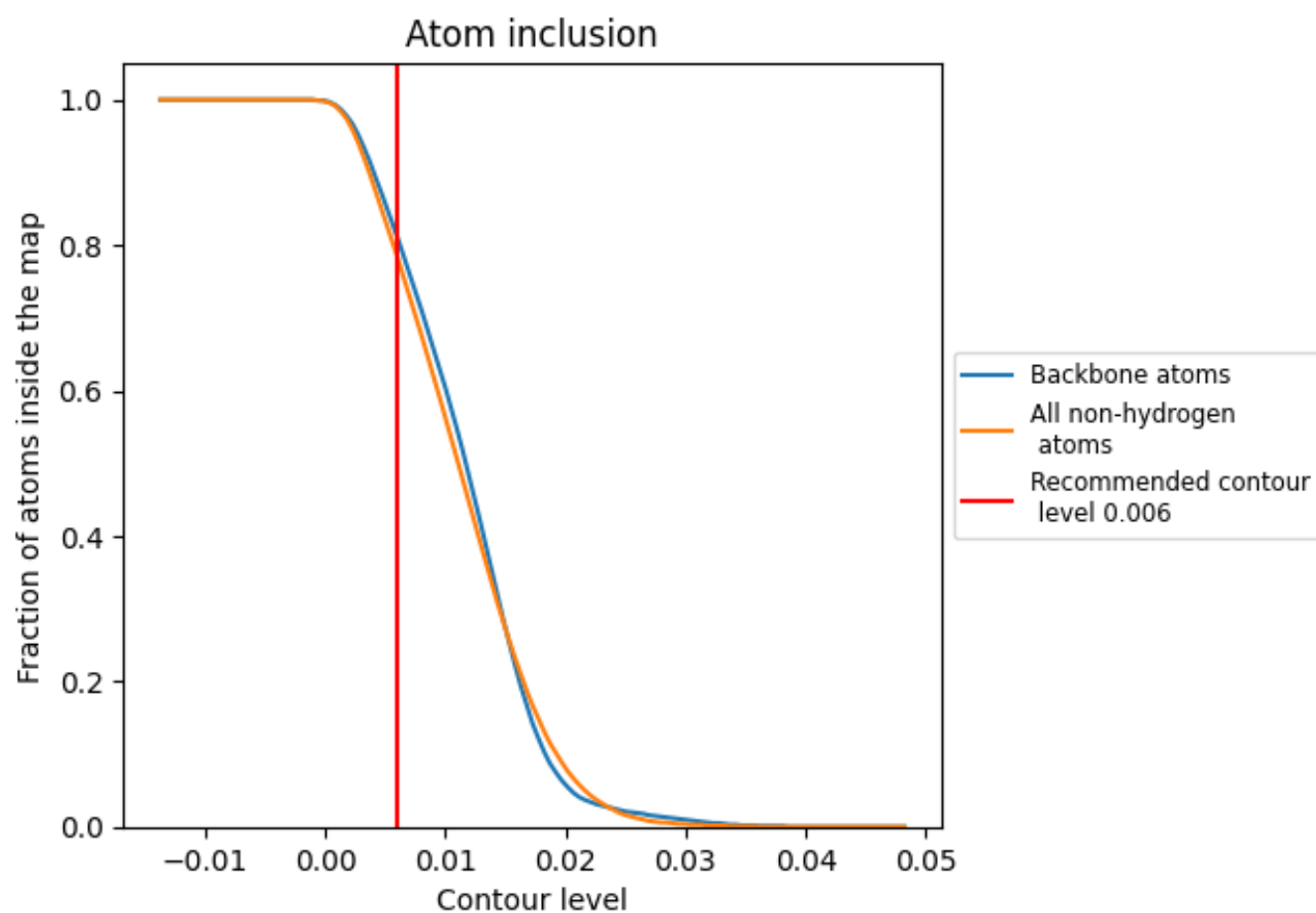
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.5850
A1	 0.8370	 0.5770
A2	 0.7420	 0.5900
A3	 0.8460	 0.5900
B1	 0.6980	 0.5850
B2	 0.9230	 0.6750
B3	 0.9770	 0.6570
C1	 0.7070	 0.5880
C2	 0.7550	 0.5970
C3	 0.9100	 0.6260
D1	 0.0850	 0.3660
D2	 0.8290	 0.6310
D3	 0.9240	 0.6770
E1	 0.6290	 0.5670
E2	 0.8510	 0.6420
E3	 0.8940	 0.6600
F1	 0.8240	 0.6230
F2	 0.8030	 0.6210
F3	 0.9160	 0.6610
G1	 0.5450	 0.5060
G2	 0.4430	 0.4950
G3	 0.8560	 0.6320
H1	 0.8740	 0.6320
H2	 0.8480	 0.6340
I1	 0.7370	 0.5550
I2	 0.8780	 0.6400
J1	 0.3300	 0.3500
J2	 0.9700	 0.6840
K1	 0.9240	 0.6170
K2	 0.9190	 0.6680
L1	 0.7640	 0.5960
L2	 0.8800	 0.6600
M1	 0.7620	 0.6100
M2	 0.9340	 0.6750
MB	 0.8590	 0.6410



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
N1	 0.8240	 0.6240
N2	 0.8190	 0.6210
O1	 0.6550	 0.5650
O2	 0.9230	 0.6670
P1	 0.8290	 0.6100
P2	 0.8560	 0.6430
Q1	 0.7740	 0.6040
Q2	 0.6730	 0.5580
R1	 0.5380	 0.4720
R2	 0.8580	 0.6570
S1	 0.4980	 0.5040
S2	 0.5020	 0.4870
T1	 0.7840	 0.6050
T2	 0.8530	 0.6330
U1	 0.7770	 0.5950
U2	 0.8630	 0.6300
V1	 0.6430	 0.5490
V2	 0.8520	 0.6390
W1	 0.7850	 0.6070
W2	 0.9420	 0.6770
X1	 0.0240	 0.2890
X2	 0.6900	 0.5760
Y1	 0.8370	 0.6300
Y2	 0.7590	 0.5850
Z1	 0.8230	 0.6250
Z2	 0.8450	 0.6380
a1	 0.6610	 0.5690
a2	 0.9130	 0.6720
b1	 0.7910	 0.6070
b2	 0.9470	 0.6800
c1	 0.6220	 0.5450
d1	 0.7500	 0.5950
d2	 0.8410	 0.6350
e1	 0.7860	 0.6030
e2	 0.8130	 0.6170
f1	 0.6090	 0.5330
f2	 0.9500	 0.6760
g1	 0.7420	 0.6040
g2	 0.6590	 0.5720
h1	 0.8870	 0.6450
h2	 0.9020	 0.6450
i1	 0.8670	 0.6440

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i2	 0.8740	 0.6440
j1	 0.7010	 0.5710
j2	 0.8680	 0.6630
k1	 0.6880	 0.5850
k2	 0.8720	 0.6560
l1	 0.8760	 0.6510
l2	 0.9110	 0.6560
m2	 0.0220	 0.2620
n2	 0.0820	 0.3120
o2	 0.0180	 0.2240
p2	 0.5290	 0.5010
q2	 0.0150	 0.4050