



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 02:21 pm BST

PDB ID : 8Q87 / pdb_00008q87
EMDB ID : EMD-18169
Title : Structure of the G. gallus 80S rotated ribosome in complex with eEF2 and SERBP1
Authors : Nurullina, L.; Jenner, L.; Yusupov, M.
Deposited on : 2023-08-18
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

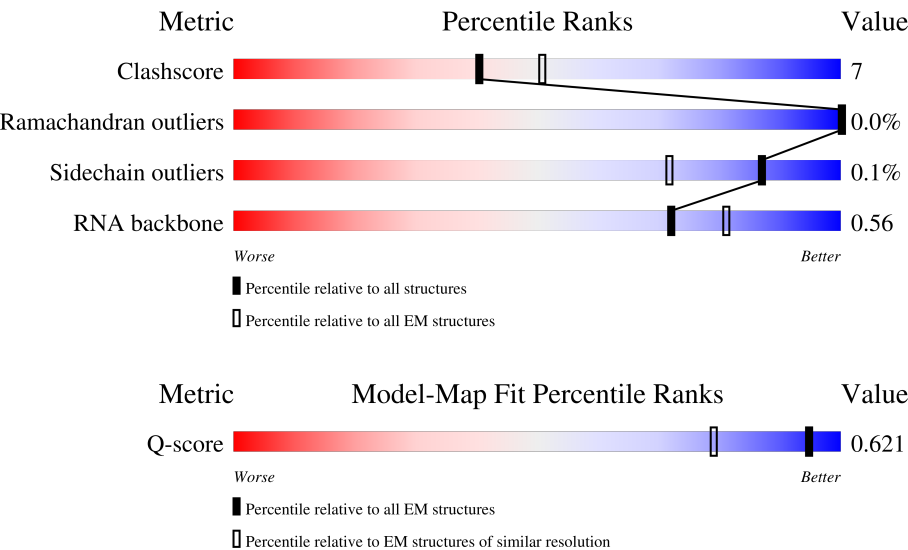
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 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	5628 (1.90 - 2.90)

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	B5	4441	9% 47% 30% 5% 18%
2	B8	157	6% 64% 32% .
3	B7	119	73% 24% .

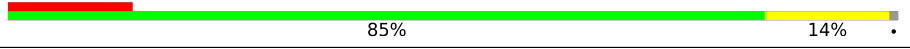
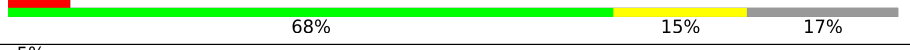
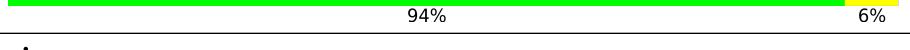
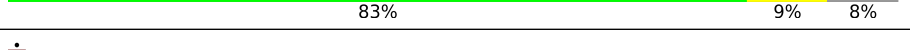
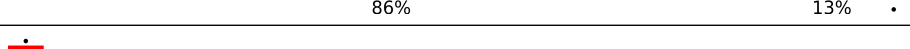
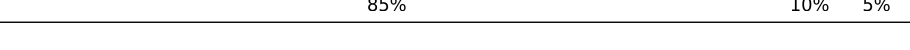
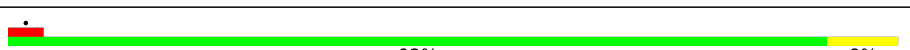
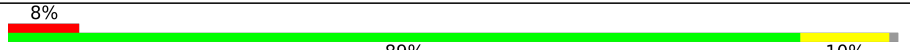
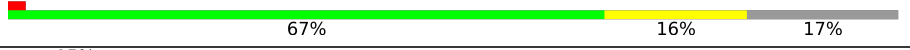
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Mol	Chain	Length	Quality of chain
4	Az	25	
5	BA	257	
6	BB	403	
7	BC	421	
8	BD	297	
9	BE	298	
10	BF	246	
11	BG	266	
12	BH	192	
13	BI	214	
14	BJ	178	
15	BL	211	
16	BM	131	
17	BN	204	
18	BO	203	
19	BP	184	
20	BQ	187	
21	BR	196	
22	BS	176	
23	BT	160	
24	BU	128	
25	BV	140	
26	BW	157	
27	BX	155	
28	BY	145	

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Mol	Chain	Length	Quality of chain
29	BZ	136	
30	Ba	148	
31	Bb	71	
32	Bc	115	
33	Bd	176	
34	Be	135	
35	Bf	110	
36	Bg	117	
37	Bh	123	
38	Bi	105	
39	Bj	97	
40	Bk	70	
41	Bl	51	
42	Bm	128	
43	Bo	105	
44	Bp	92	
45	Br	138	
46	A2	1823	
47	Aa	264	
48	AA	84	
49	AB	69	
50	Ab	264	
51	AC	156	
52	Ac	243	
53	Ad	263	

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Mol	Chain	Length	Quality of chain
54	AD	133	
55	AE	115	
56	Ae	204	
57	Af	249	
58	AF	317	
59	Ag	194	
60	AG	171	
61	Ah	207	
62	Ai	194	
63	Aj	165	
64	Ak	158	
65	Al	132	
66	Am	151	
67	An	151	
68	Ao	145	
69	Aq	135	
70	Ar	152	
71	As	145	
72	At	119	
73	Au	84	
74	Av	130	
75	Aw	143	
76	Ax	131	
77	Ay	125	
78	AZ	296	

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Mol	Chain	Length	Quality of chain
79	Ap	146	
80	V	76	
81	S	404	
82	A	858	
83	Bs	316	
84	Bt	165	
85	Bv	217	

2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 228127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B5	3638	Total	C	N	O	P	0	0
			78070	34789	14272	25371	3638		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3295	UY1	U	modified residue	GB KT445934.2

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B8	157	Total	C	N	O	P	0	0
			3338	1490	588	1103	157		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B7	119	Total	C	N	O	P	0	0
			2536	1130	449	838	119		

- Molecule 4 is a protein called 60S ribosomal protein L41.

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

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	246	Total	C	N	O	S	0	0
			1887	1185	385	311	6		

- Molecule 6 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	398	Total	C	N	O	S	0	0
			3209	2042	603	550	14		

- Molecule 7 is a protein called 60S ribosomal protein L4 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BC	361	Total	C	N	O	S	0	0
			2888	1816	574	484	14		

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BD	296	Total	C	N	O	S	0	0
			2388	1506	437	433	12		

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BE	225	Total	C	N	O	S	0	0
			1820	1167	355	296	2		

- Molecule 10 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BF	234	Total	C	N	O	S	0	0
			1939	1245	377	309	8		

- Molecule 11 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BG	210	Total	C	N	O	S	0	0
			1704	1089	326	284	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BH	192	Total	C	N	O	S	0	0
			1533	962	288	277	6		

- Molecule 13 is a protein called Ribosomal protein uL16, Large ribosomal subunit protein uL16, Large ribosomal subunit protein uL16, Large ribosomal subunit protein uL16, Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BI	213	Total	C	N	O	S	0	0
			1710	1082	334	279	15		

- Molecule 14 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	170	Total	C	N	O	S	0	0
			1362	861	255	241	5		

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BL	208	Total	C	N	O	S	0	0
			1691	1060	350	276	5		

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BM	130	Total	C	N	O	S	0	0
			1077	688	209	172	8		

- Molecule 17 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BN	203	Total	C	N	O	S	0	0
			1700	1071	359	266	4		

- Molecule 18 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BO	201	Total	C	N	O	S	0	0
			1642	1058	321	258	5		

- Molecule 19 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BP	155	Total	C	N	O	S	0	0
			1259	788	244	218	9		

- Molecule 20 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BQ	187	Total	C	N	O	S	0	0
			1502	939	314	244	5		

- Molecule 21 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BR	166	Total	C	N	O	S	0	0
			1378	856	295	217	10		

- Molecule 22 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	176	Total	C	N	O	S	0	0
			1463	931	286	235	11		

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BT	159	Total	C	N	O	S	0	0
			1299	825	252	216	6		

- Molecule 24 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BU	100	Total	C	N	O	S	0	0
			817	523	143	149	2		

- Molecule 25 is a protein called Ribosomal protei uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BV	139	Total	C	N	O	S	0	0
			1033	648	199	181	5		

- Molecule 26 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BW	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 27 is a protein called Ribosomal protein uL23.

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

- Molecule 28 is a protein called Ribosomal protein L26 like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BY	133	Total	C	N	O	S	0	0
			1106	694	224	185	3		

- Molecule 29 is a protein called Large ribosomal subunit protein eL27.

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

- Molecule 30 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ba	147	Total	C	N	O	S	0	0
			1179	748	240	187	4		

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bb	70	Total	C	N	O	S	0	0
			582	360	126	94	2		

- Molecule 32 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bc	95	Total	C	N	O	S	0	0
			738	468	131	133	6		

- Molecule 33 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bd	105	Total	C	N	O	S	0	0
			867	549	168	148	2		

- Molecule 34 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Be	130	Total	C	N	O	S	0	0
			1074	681	219	169	5		

- Molecule 35 is a protein called Ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bf	110	Total	C	N	O	S	0	0
			886	559	178	144	5		

- Molecule 36 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bg	108	Total	C	N	O	S	0	0
			860	540	178	137	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bh	122	Total	C	N	O	S	1	0
			1023	646	208	168	1		

- Molecule 38 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bi	100	Total	C	N	O	S	0	0
			821	515	173	127	6		

- Molecule 39 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bj	86	Total	C	N	O	S	0	0
			704	432	155	112	5		

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

- Molecule 41 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bl	50	Total	C	N	O	S	0	0
			442	281	96	64	1		

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 43 is a protein called Ribosomal protein L36a like.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bo	105	Total	C	N	O	S	0	0
			861	540	177	138	6		

- Molecule 44 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bp	91	Total	C	N	O	S	0	0
			706	445	134	120	7		

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Br	124	Total	C	N	O	S	0	0
			1007	624	213	167	3		

- Molecule 46 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	A2	1697	Total	C	N	O	P	0	0
			36242	16199	6484	11862	1697		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1206	B8N	U	modified residue	GB KT445934.2
A2	1295	4AC	C	modified residue	GB KT445934.2
A2	1796	4AC	C	modified residue	GB KT445934.2

- Molecule 47 is a protein called Ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Aa	213	Total	C	N	O	S	0	0
			1730	1098	309	309	14		

- Molecule 48 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	83	Total	C	N	O	S	0	0
			657	410	125	115	7		

- Molecule 49 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AB	61	Total	C	N	O	S	0	0
			476	290	93	91	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ab	219	Total	C	N	O	S	0	0
			1698	1099	291	299	9		

- Molecule 51 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AC	63	Total	C	N	O	S	0	0
			516	325	98	86	7		

- Molecule 52 is a protein called DNA-(apurinic or apyrimidinic site) lyase.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Ad	262	Total	C	N	O	S	0	0
			2076	1324	387	357	8		

- Molecule 54 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AD	57	Total	C	N	O	S	0	0
			452	279	99	73	1		

- Molecule 55 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AE	99	Total	C	N	O	S	0	0
			793	492	165	131	5		

- Molecule 56 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Ae	191	Total	C	N	O	S	0	0
			1508	943	286	272	7		

- Molecule 57 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Af	227	Total	C	N	O	S	0	0
			1838	1144	367	320	7		

- Molecule 58 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AF	311	Total	C	N	O	S	0	0
			2420	1526	422	460	12		

- Molecule 59 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ag	187	Total	C	N	O	S	0	0
			1500	956	276	267	1		

- Molecule 60 is a protein called 40S ribosomal protein S29.

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

- Molecule 61 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Ah	203	Total	C	N	O	S	1	0
			1669	1050	328	286	5		

- Molecule 62 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Ai	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 63 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Aj	96	Total	C	N	O	S	0	0
			812	532	143	131	6		

- Molecule 64 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Ak	150	Total	C	N	O	S	0	0
			1218	773	229	210	6		

- Molecule 65 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Al	111	Total	C	N	O	S	0	0
			860	540	151	161	8		

- Molecule 66 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 67 is a protein called Ribosomal protein S14.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	IAS	ASP	modified residue	UNP Q5ZHW8

- Molecule 68 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Ao	128	Total	C	N	O	S	0	0
			1050	666	198	179	7		

- Molecule 69 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Aq	133	Total	C	N	O	S	0	0
			1073	673	200	196	4		

- Molecule 70 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ar	144	Total	C	N	O	S	0	0
			1191	748	241	201	1		

- Molecule 71 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	As	143	Total	C	N	O	S	0	0
			1115	698	216	199	2		

- Molecule 72 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	At	103	Total	C	N	O	S	0	0
			815	511	154	146	4		

- Molecule 73 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Au	84	Total	C	N	O	S	0	0
			640	394	118	124	4		

- Molecule 74 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Av	129	Total	C	N	O	S	0	0
			1035	659	193	177	6		

- Molecule 75 is a protein called Ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Aw	142	Total	C	N	O	S	0	0
			1104	696	220	185	3		

- Molecule 76 is a protein called 40S ribosomal protein S24.

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

- Molecule 77 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ay	70	Total	C	N	O	S	0	0
			555	357	101	96	1		

- Molecule 78 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AZ	207	Total	C	N	O	S	0	0
			1626	1036	287	295	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	2	ACE	-	acetylation	UNP P50890

- Molecule 79 is a protein called Ribosomal protein S16.

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

- Molecule 80 is a RNA chain called Phe tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	V	76	Total	C	N	O	P	0	0
			1628	727	302	524	75		

- Molecule 81 is a protein called SERPINE1 mRNA binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	S	42	Total	C	N	O	0	0
			325	190	69	66		

- Molecule 82 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	A	857	Total	C	N	O	S	0	0
			6690	4244	1151	1249	46		

- Molecule 83 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Bs	199	Total	C	N	O	S	0	0
			1527	972	266	279	10		

- Molecule 84 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bt	152	Total	C	N	O	S	0	0
			1135	704	210	217	4		

- Molecule 85 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Bv	215	Total	C	N	O	S	0	0
			1722	1107	303	305	7		

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	B5	337	Total	Mg	0
			337	337	
86	B8	8	Total	Mg	0
			8	8	
86	B7	6	Total	Mg	0
			6	6	

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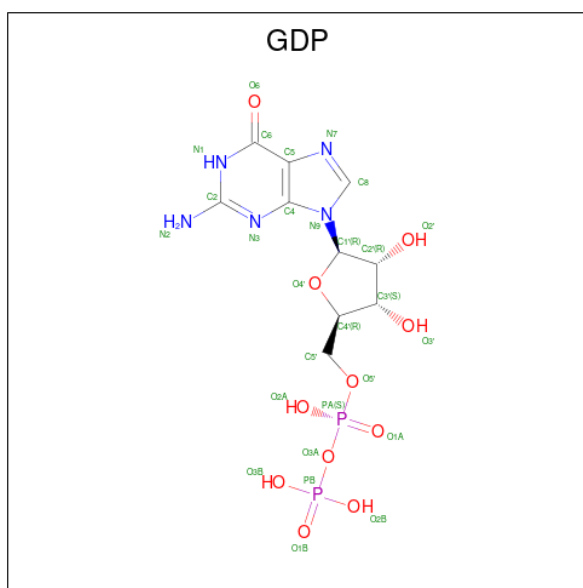
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Mol	Chain	Residues	Atoms		AltConf
86	BA	3	Total 3	Mg 3	0
86	BB	1	Total 1	Mg 1	0
86	BH	1	Total 1	Mg 1	0
86	BI	1	Total 1	Mg 1	0
86	BN	2	Total 2	Mg 2	0
86	BP	2	Total 2	Mg 2	0
86	BV	1	Total 1	Mg 1	0
86	Ba	1	Total 1	Mg 1	0
86	Bb	2	Total 2	Mg 2	0
86	Be	2	Total 2	Mg 2	0
86	Bf	1	Total 1	Mg 1	0
86	Bg	1	Total 1	Mg 1	0
86	Bo	1	Total 1	Mg 1	0
86	A2	116	Total 116	Mg 116	0
86	AG	1	Total 1	Mg 1	0
86	Ak	1	Total 1	Mg 1	0
86	An	1	Total 1	Mg 1	0
86	As	1	Total 1	Mg 1	0
86	At	1	Total 1	Mg 1	0
86	A	1	Total 1	Mg 1	0

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

Mol	Chain	Residues	Atoms		AltConf
87	Bg	1	Total 1	Zn 1	0
87	Bj	1	Total 1	Zn 1	0
87	Bm	1	Total 1	Zn 1	0
87	Bo	1	Total 1	Zn 1	0
87	Bp	1	Total 1	Zn 1	0
87	AC	1	Total 1	Zn 1	0
87	AE	1	Total 1	Zn 1	0
87	AG	1	Total 1	Zn 1	0

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



Mol	Chain	Residues	Atoms					AltConf
88	A	1	Total 28	C 10	N 5	O 11	P 2	0

- Molecule 89 is water.

Mol	Chain	Residues	Atoms	AltConf
89	B5	2982	Total O 2982 2982	0

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Mol	Chain	Residues	Atoms		AltConf
89	B8	81	Total 81	O 81	0
89	B7	69	Total 69	O 69	0
89	Az	1	Total 1	O 1	0
89	BA	18	Total 18	O 18	0
89	BB	21	Total 21	O 21	0
89	BC	30	Total 30	O 30	0
89	BD	25	Total 25	O 25	0
89	BE	10	Total 10	O 10	0
89	BF	9	Total 9	O 9	0
89	BG	1	Total 1	O 1	0
89	BH	11	Total 11	O 11	0
89	BI	21	Total 21	O 21	0
89	BL	24	Total 24	O 24	0
89	BM	10	Total 10	O 10	0
89	BN	32	Total 32	O 32	0
89	BO	24	Total 24	O 24	0
89	BP	22	Total 22	O 22	0
89	BQ	28	Total 28	O 28	0
89	BR	8	Total 8	O 8	0
89	BS	14	Total 14	O 14	0
89	BT	16	Total 16	O 16	0

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Mol	Chain	Residues	Atoms		AltConf
89	BV	7	Total 7	O 7	0
89	BW	3	Total 3	O 3	0
89	BX	6	Total 6	O 6	0
89	BY	10	Total 10	O 10	0
89	Ba	25	Total 25	O 25	0
89	Bb	7	Total 7	O 7	0
89	Bc	1	Total 1	O 1	0
89	Bd	5	Total 5	O 5	0
89	Be	29	Total 29	O 29	0
89	Bf	24	Total 24	O 24	0
89	Bg	14	Total 14	O 14	0
89	Bh	7	Total 7	O 7	0
89	Bi	12	Total 12	O 12	0
89	Bj	9	Total 9	O 9	0
89	Bl	4	Total 4	O 4	0
89	Bm	12	Total 12	O 12	0
89	Bo	15	Total 15	O 15	0
89	Bp	9	Total 9	O 9	0
89	Br	7	Total 7	O 7	0
89	A2	197	Total 197	O 197	0
89	Ab	8	Total 8	O 8	0

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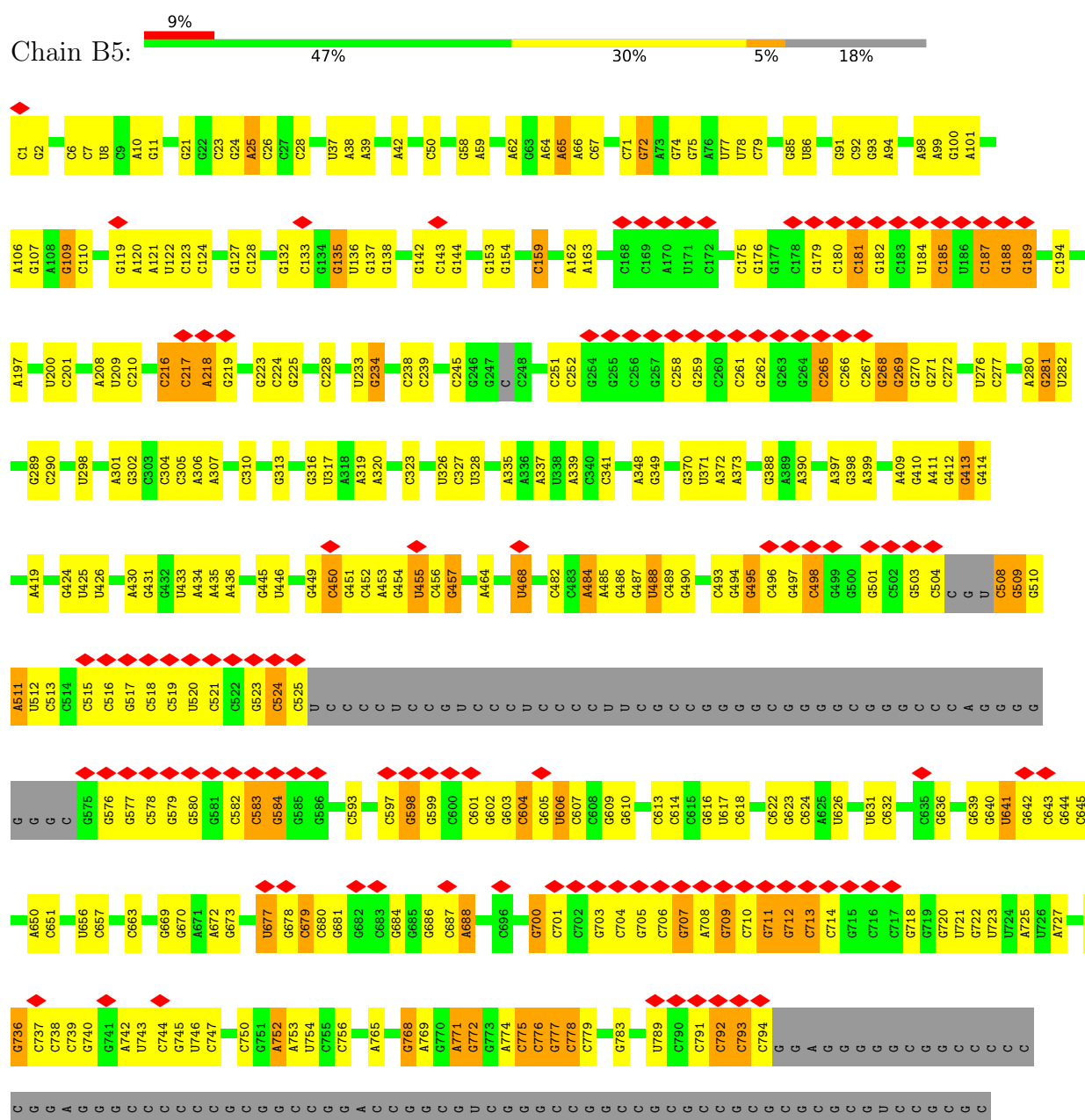
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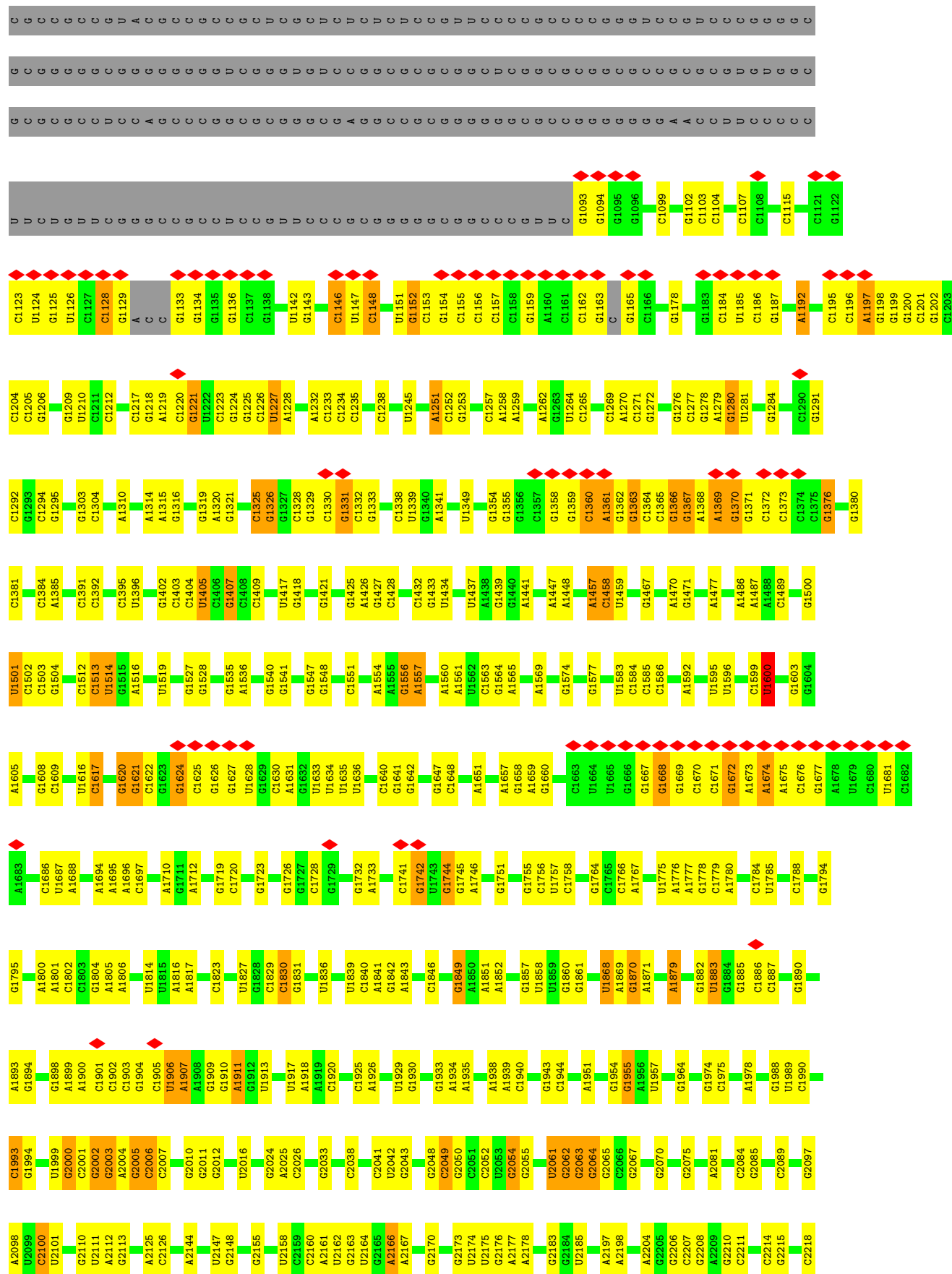
Mol	Chain	Residues	Atoms		AltConf
89	Ad	1	Total 1	O 1	0
89	AE	2	Total 2	O 2	0
89	Ae	1	Total 1	O 1	0
89	AG	1	Total 1	O 1	0
89	Ak	1	Total 1	O 1	0
89	Am	1	Total 1	O 1	0
89	An	1	Total 1	O 1	0
89	Ar	2	Total 2	O 2	0
89	As	1	Total 1	O 1	0
89	Au	1	Total 1	O 1	0
89	Av	2	Total 2	O 2	0
89	Ax	1	Total 1	O 1	0
89	AZ	1	Total 1	O 1	0
89	V	9	Total 9	O 9	0
89	A	2	Total 2	O 2	0

3 Residue-property plots

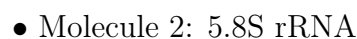
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 28S rRNA

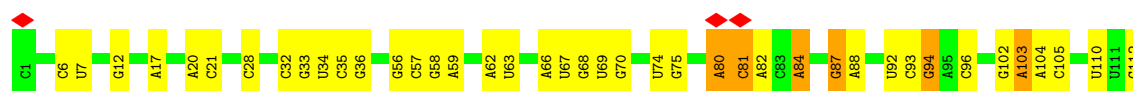






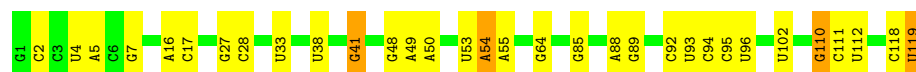


Frequency	Percentage
Very often	6%
Often	64%
Sometimes	32%
Never	0%

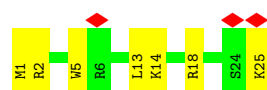
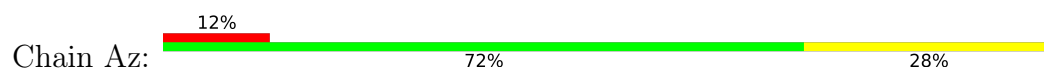




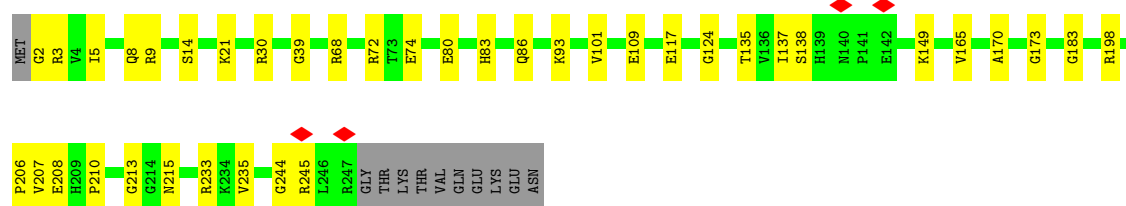
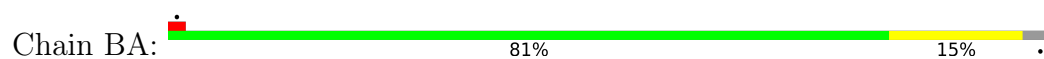
- Molecule 3: 5S rRNA



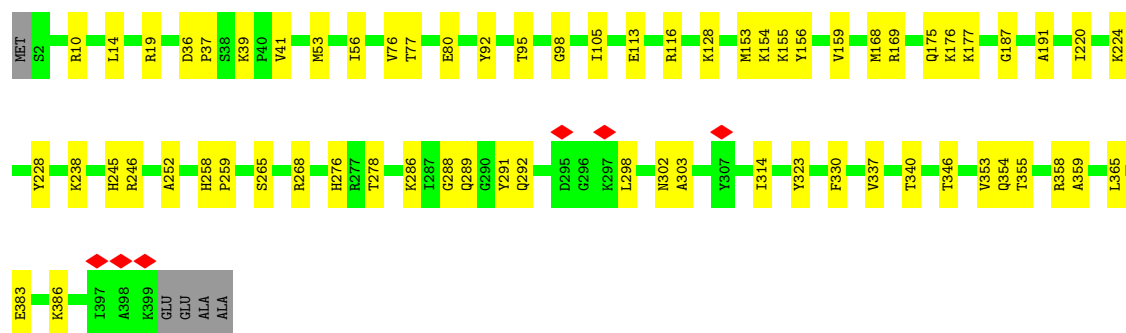
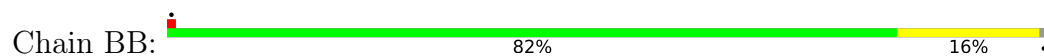
- Molecule 4: 60S ribosomal protein L41



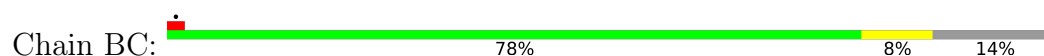
- Molecule 5: 60S ribosomal protein L8



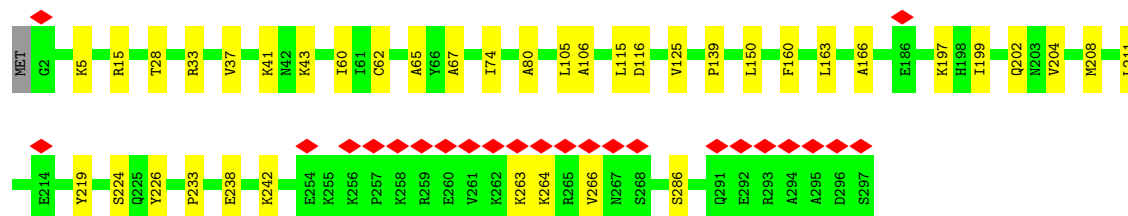
- Molecule 6: Ribosomal protein uL3



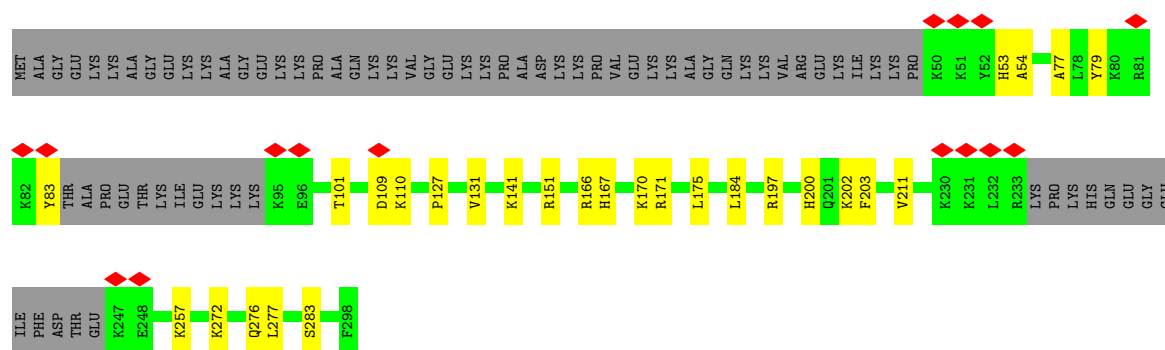
- Molecule 7: 60S ribosomal protein L4 C-terminal domain-containing protein



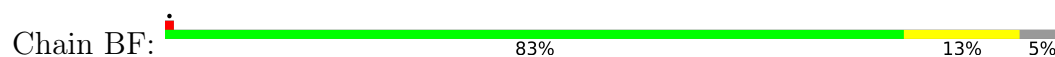
- Molecule 8: Large ribosomal subunit protein uL18



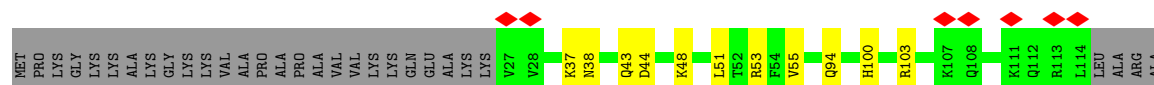
- Molecule 9: 60S ribosomal protein L6



- Molecule 10: Large ribosomal subunit protein uL30

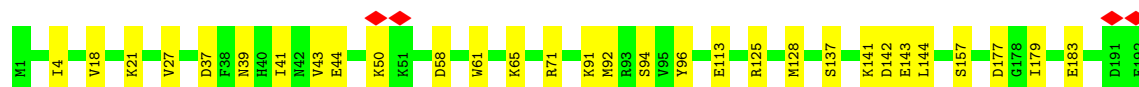
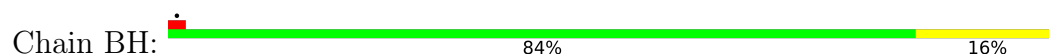


- Molecule 11: Large ribosomal subunit protein eL8

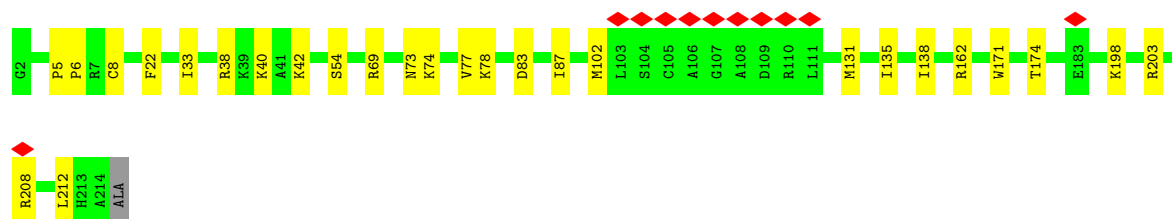
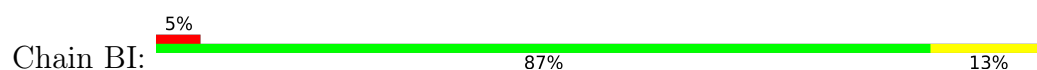




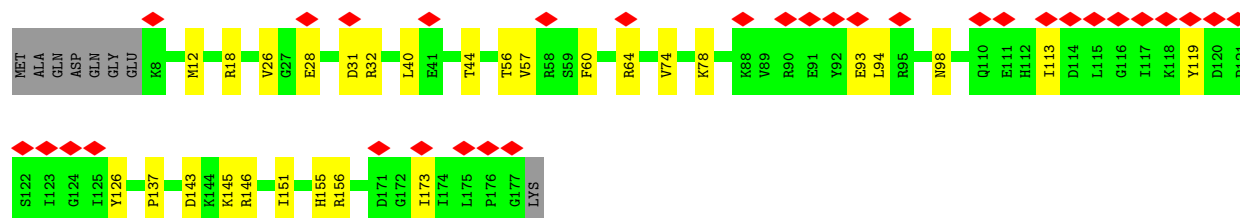
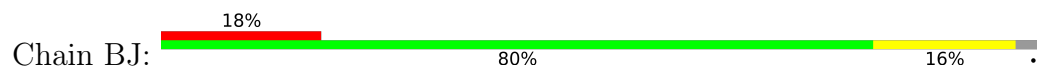
- Molecule 12: 60S ribosomal protein L9



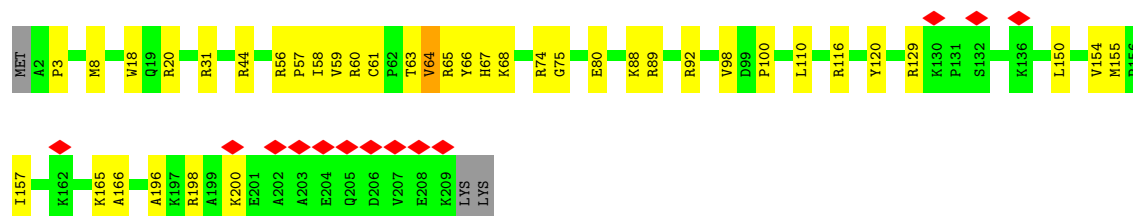
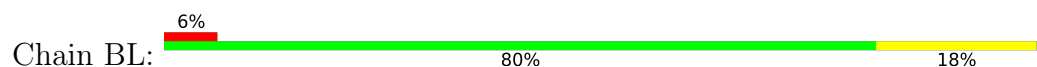
- Molecule 13: Ribosomal protein uL16, Large ribosomal subunit protein uL16, Large ribosomal subunit protein uL16, Large ribosomal subunit protein uL16, Large ribosomal subunit protein uL16



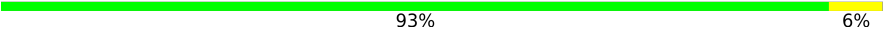
- Molecule 14: 60S ribosomal protein L11



- Molecule 15: Large ribosomal subunit protein eL13



- Molecule 16: 60S ribosomal protein L14

Chain BM:  93% 6%



- Molecule 17: Ribosomal protein L15

Chain BN:  86% 13%



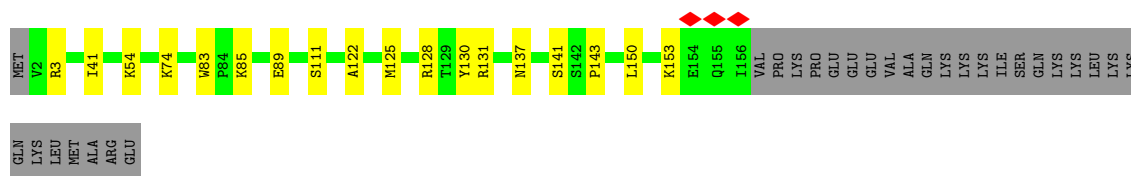
- Molecule 18: Ribosomal protein uL13

Chain BO:  89% 10%



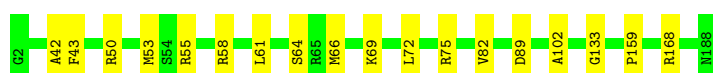
- Molecule 19: Large ribosomal subunit protein uL22

Chain BP:  74% 10% 16%



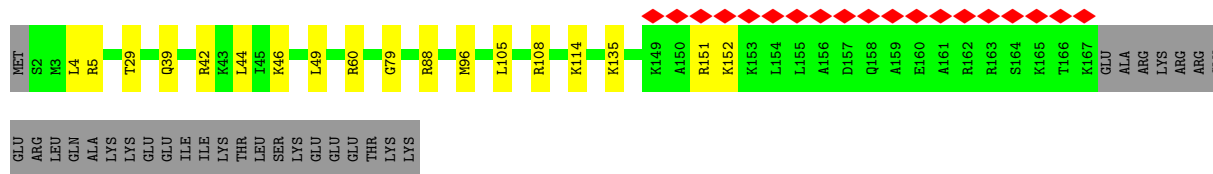
- Molecule 20: Ribosomal protein eL18

Chain BQ:  90% 10%



- Molecule 21: Ribosomal protein L19

Chain BR:  10% 76% 9% 15%



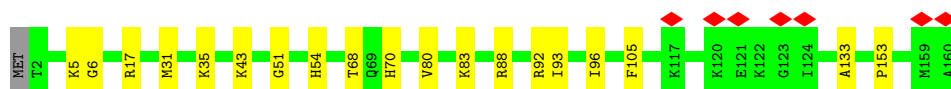
- Molecule 22: Ribosomal protein eL20

Chain BS:  89% 11%



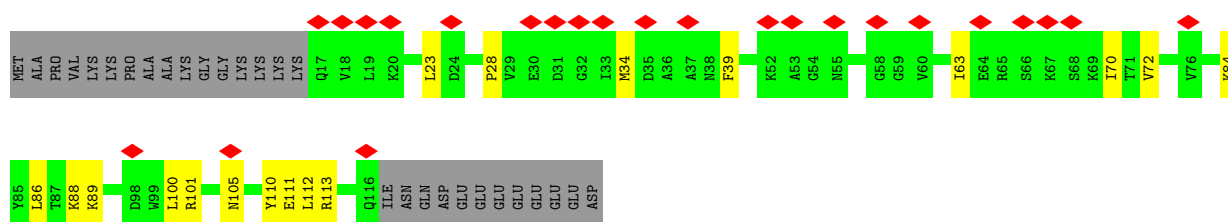
- Molecule 23: 60S ribosomal protein L21

Chain BT: 88% 12%



- Molecule 24: Large ribosomal subunit protein eL22

Chain BU: 19% 64% 14% 22%



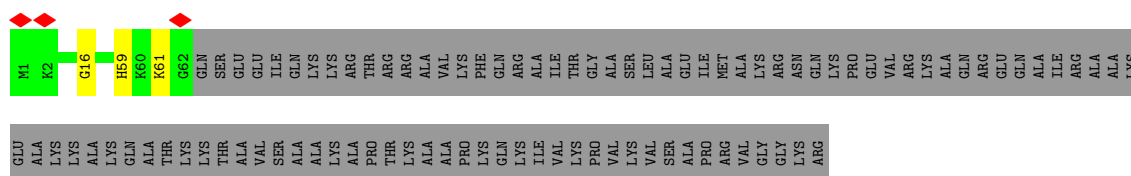
- Molecule 25: Ribosomal protein uL14

Chain BV: 89% 11%



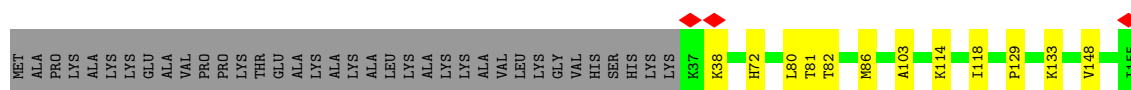
- Molecule 26: Ribosomal protein L24

Chain BW: 38% 61%



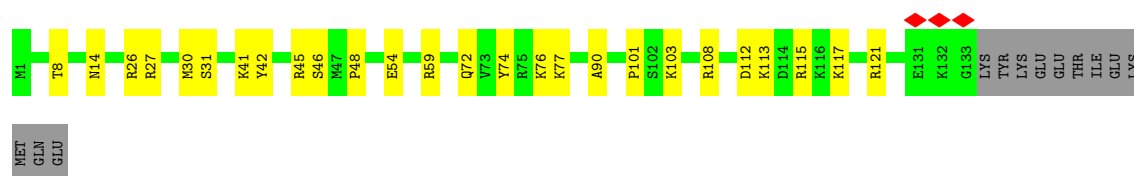
- Molecule 27: Ribosomal protein uL23

Chain BX: 69% 8% 23%

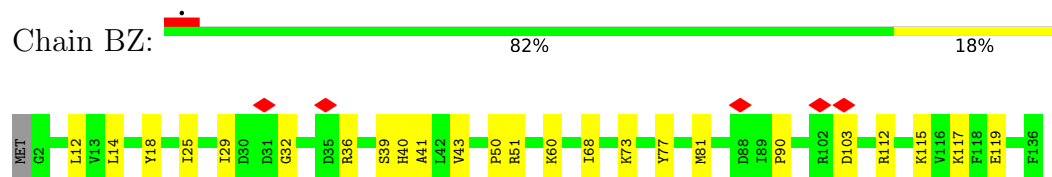


- Molecule 28: Ribosomal protein L26 like 1

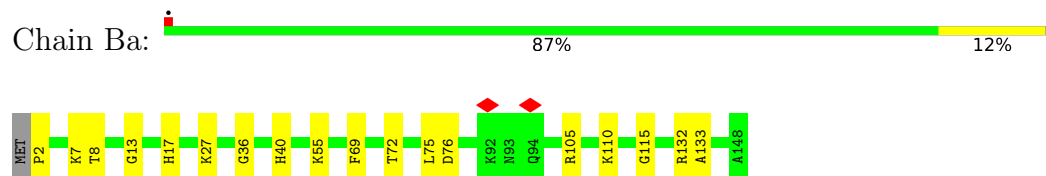
Chain BY: 74% 18% 8%



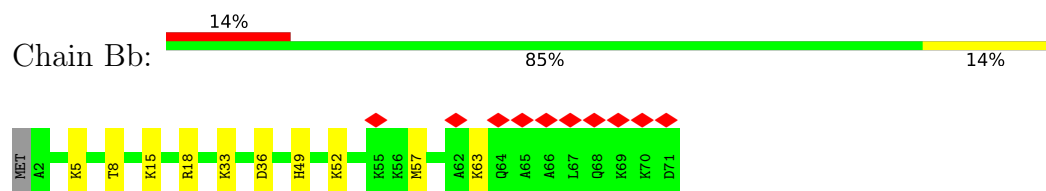
- Molecule 29: Large ribosomal subunit protein eL27



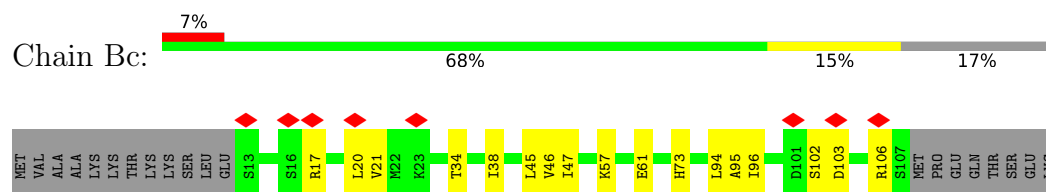
- Molecule 30: Ribosomal protein uL15



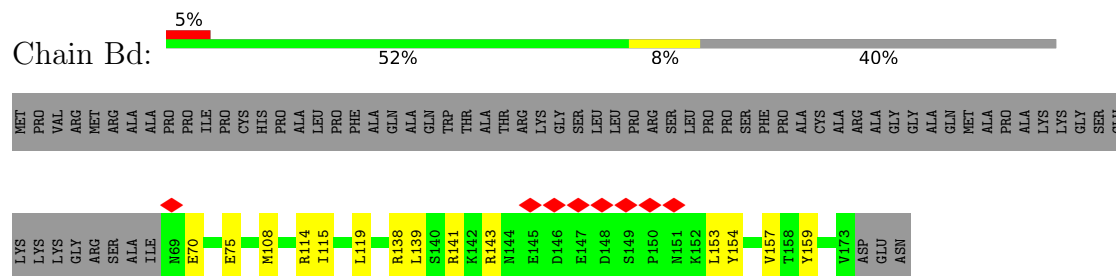
- Molecule 31: 60S ribosomal protein L29



- Molecule 32: Large ribosomal subunit protein eL30



- Molecule 33: 60S ribosomal protein L31



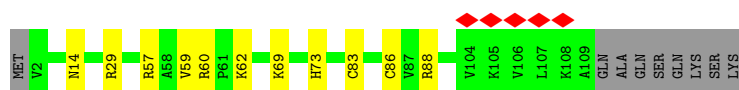
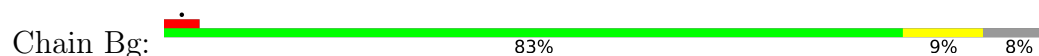
- Molecule 34: Ribosomal protein L32



- Molecule 35: Ribosomal protein eL33



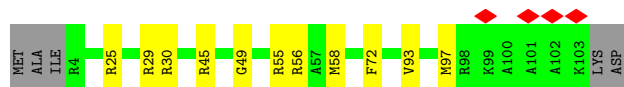
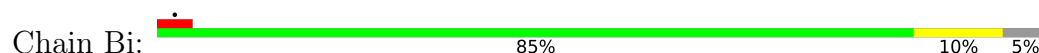
- Molecule 36: 60S ribosomal protein L34



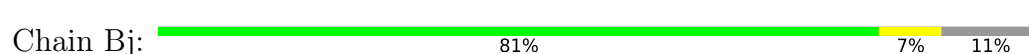
- Molecule 37: Large ribosomal subunit protein uL29



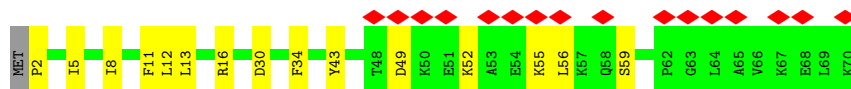
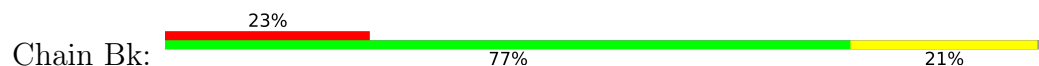
- Molecule 38: Large ribosomal subunit protein eL36



- Molecule 39: Ribosomal protein L37



- Molecule 40: 60S ribosomal protein L38



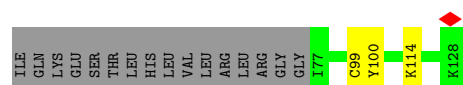
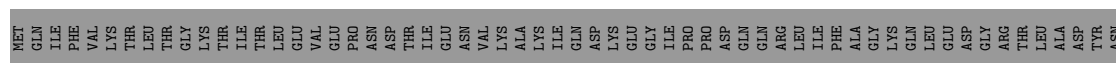
- Molecule 41: Large ribosomal subunit protein eL39

Chain Bl:  80% 18%

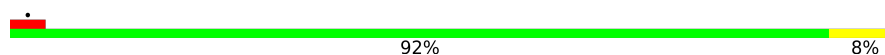


- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain Bm:  38% 59%

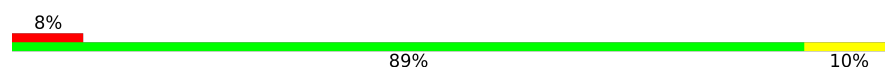


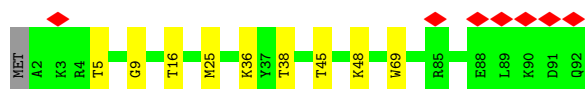
- Molecule 43: Ribosomal protein L36a like

Chain Bo:  92% 8%



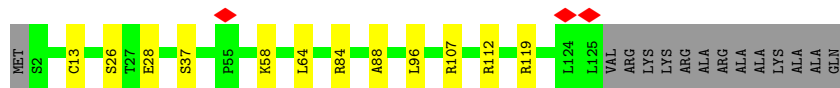
- Molecule 44: Large ribosomal subunit protein eL43

Chain Bp:  89% 10%



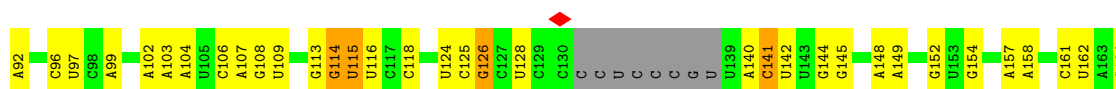
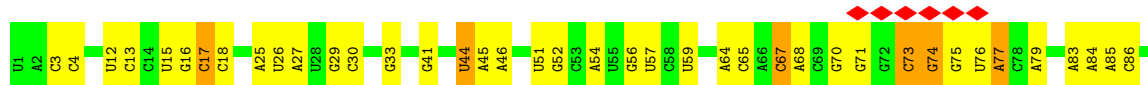
- Molecule 45: 60S ribosomal protein L28

Chain Br:  81% 9% 10%

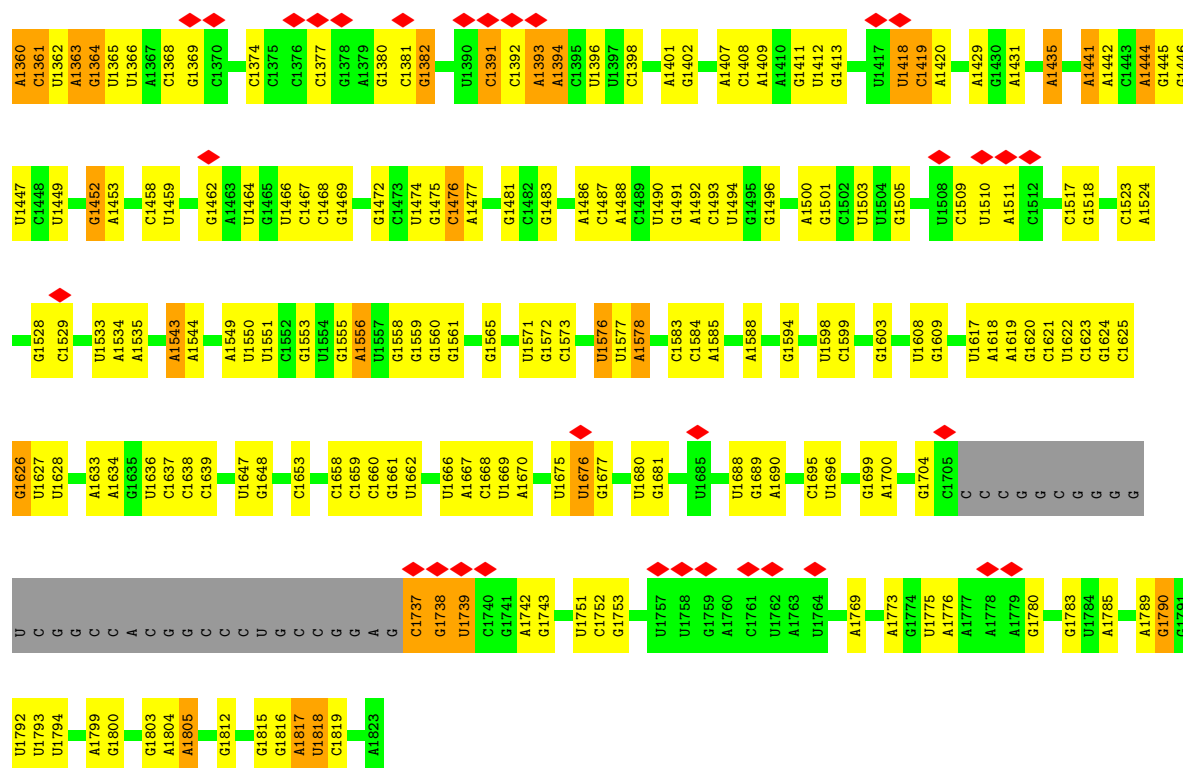


- Molecule 46: 18S rRNA

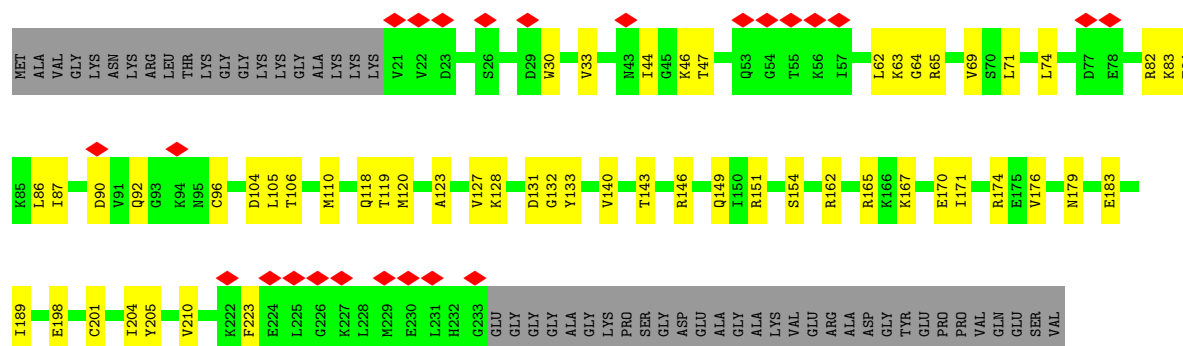
Chain A2:  53% 34% 6% 7%



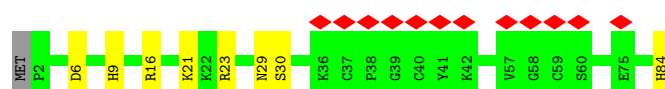
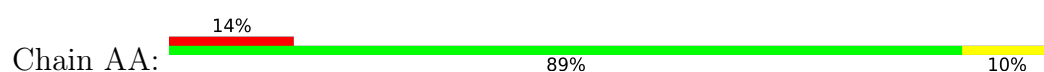




• Molecule 47: Ribosomal protein eS1



• Molecule 48: 40S ribosomal protein S27

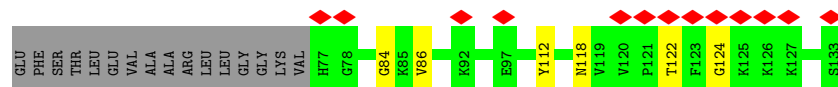
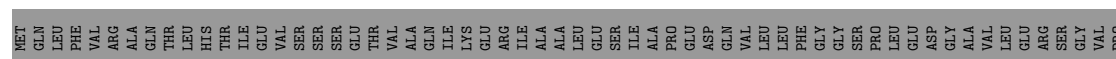
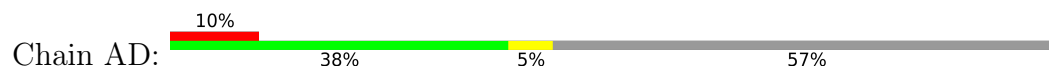


• Molecule 49: 40S ribosomal protein S28

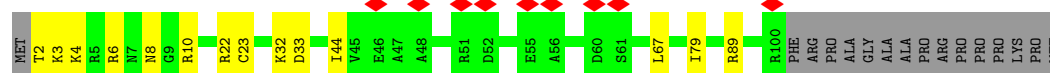
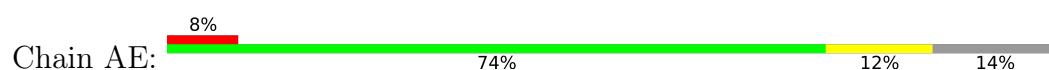




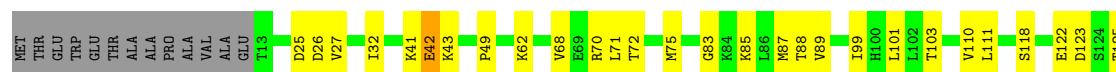
- Molecule 54: Ribosomal protein eS30



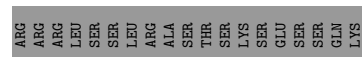
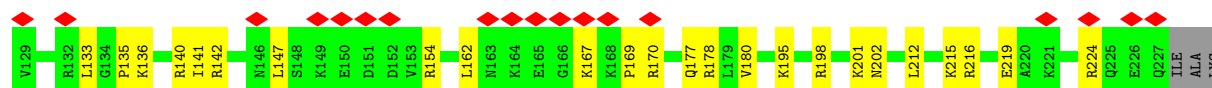
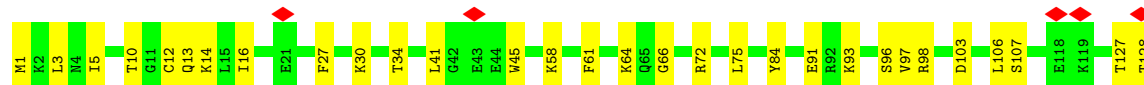
- Molecule 55: 40S ribosomal protein S26



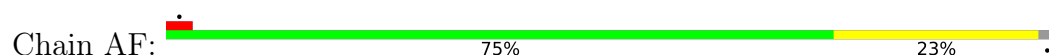
- Molecule 56: Ribosomal protein S5

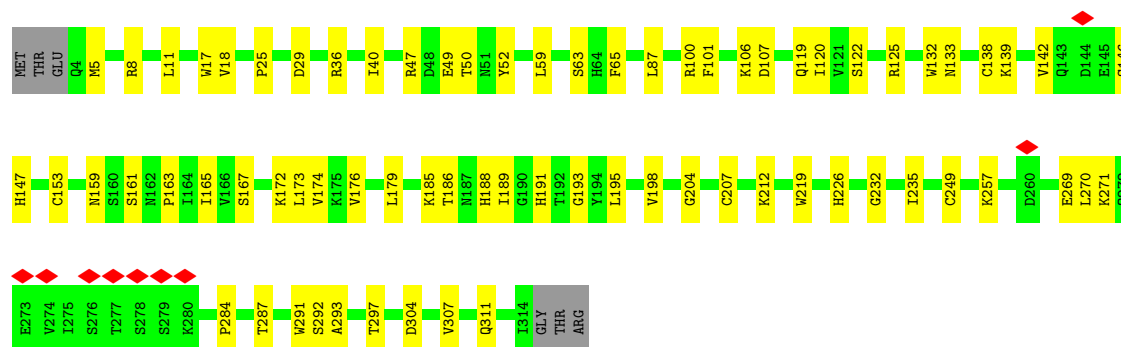


- Molecule 57: Small ribosomal subunit protein eS6

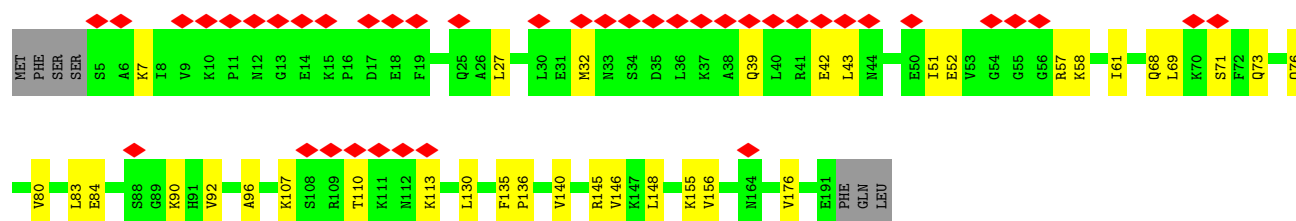
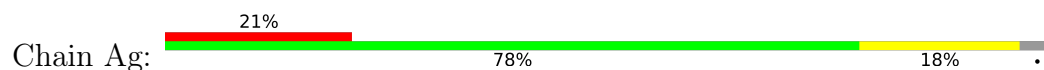


- Molecule 58: Small ribosomal subunit protein RACK1

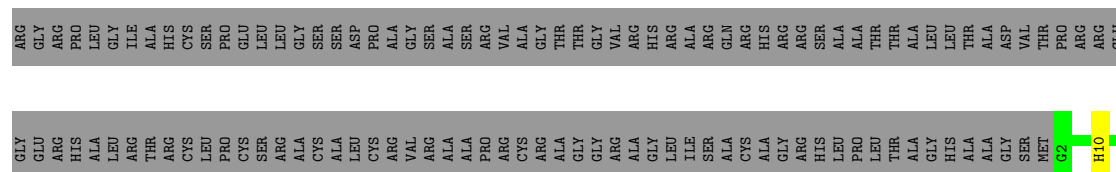




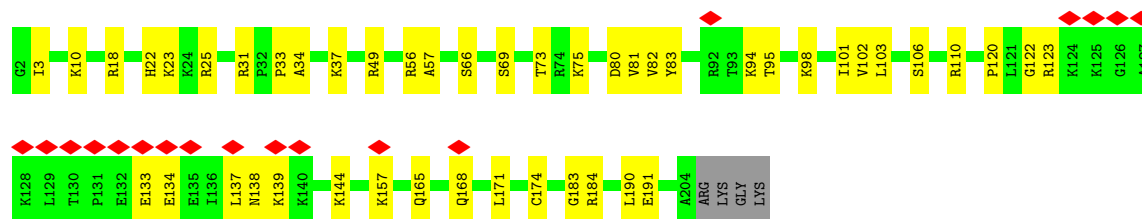
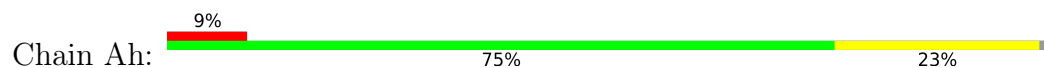
• Molecule 59: 40S ribosomal protein S7



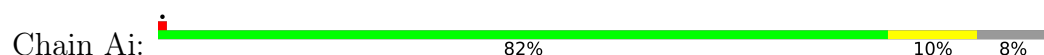
• Molecule 60: 40S ribosomal protein S29



• Molecule 61: 40S ribosomal protein S8

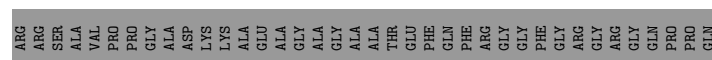
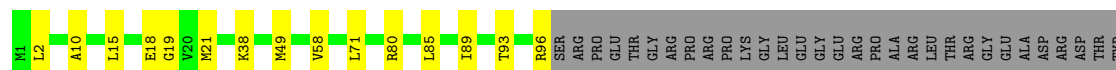


• Molecule 62: 40S ribosomal protein S9

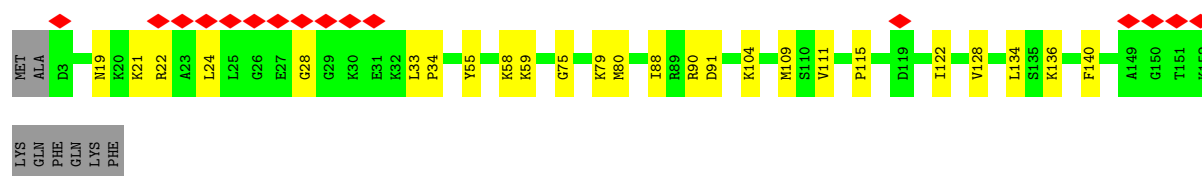
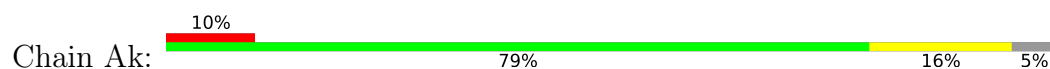




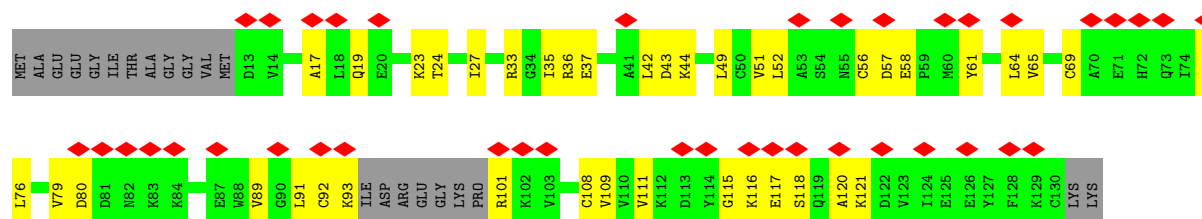
• Molecule 63: Ribosomal protein S10



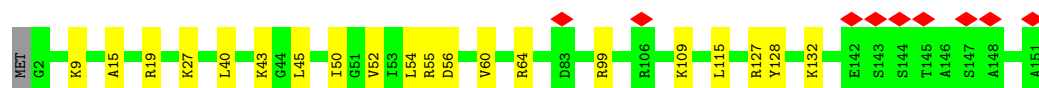
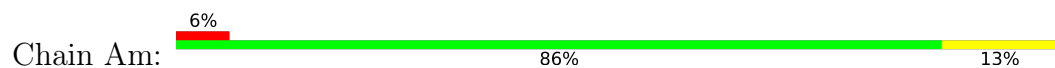
• Molecule 64: 40S ribosomal protein S11



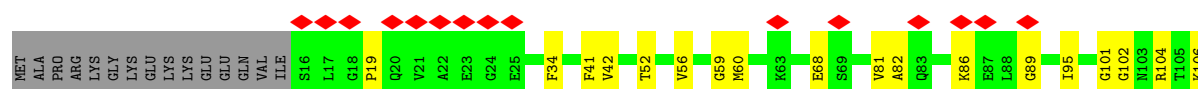
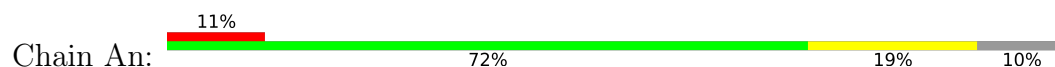
• Molecule 65: Small ribosomal subunit protein eS12

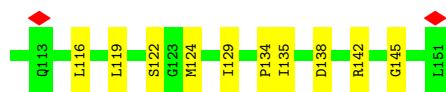


• Molecule 66: Small ribosomal subunit protein uS15

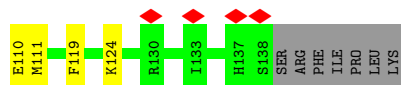
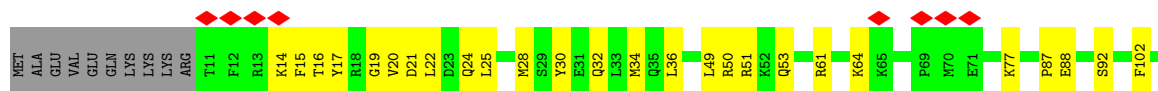


• Molecule 67: Ribosomal protein S14

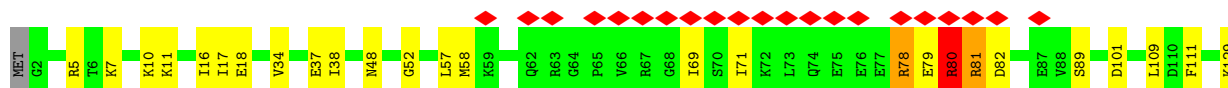
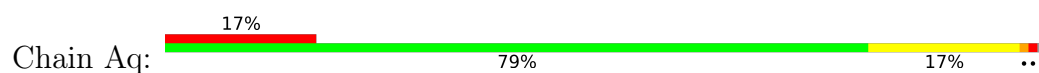




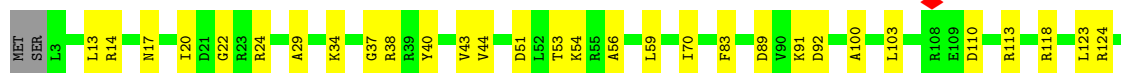
- Molecule 68: Small ribosomal subunit protein uS19



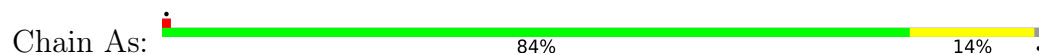
- Molecule 69: Small ribosomal subunit protein eS17



- Molecule 70: 40S ribosomal protein S18



- Molecule 71: Ribosomal protein eS19



- Molecule 72: 40S ribosomal protein S20





- Molecule 73: Small ribosomal subunit protein eS21

Chain Au: 87% 13%



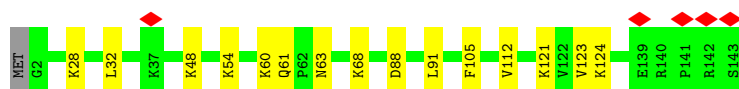
- Molecule 74: 40S ribosomal protein S15a

Chain Av: 84% 15%



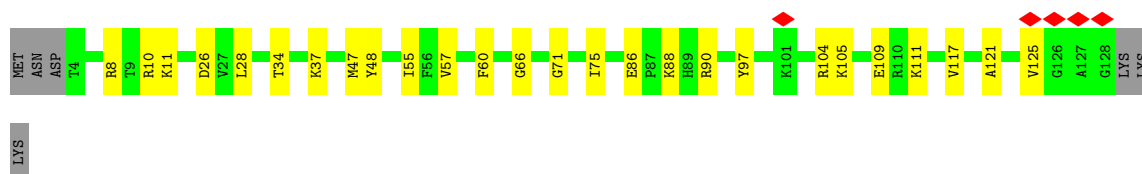
- Molecule 75: Ribosomal protein uS12

Chain Aw: 89% 10%



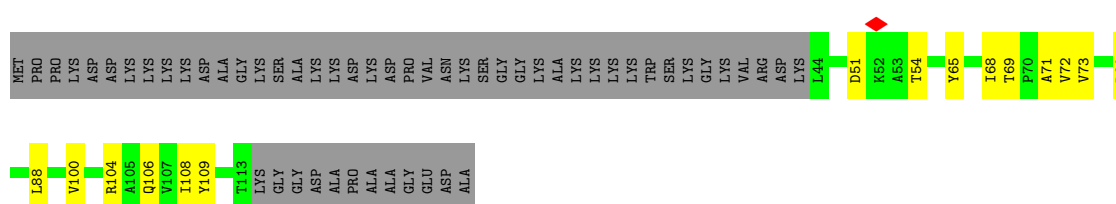
- Molecule 76: 40S ribosomal protein S24

Chain Ax: 76% 20% 5%



- Molecule 77: 40S ribosomal protein S25

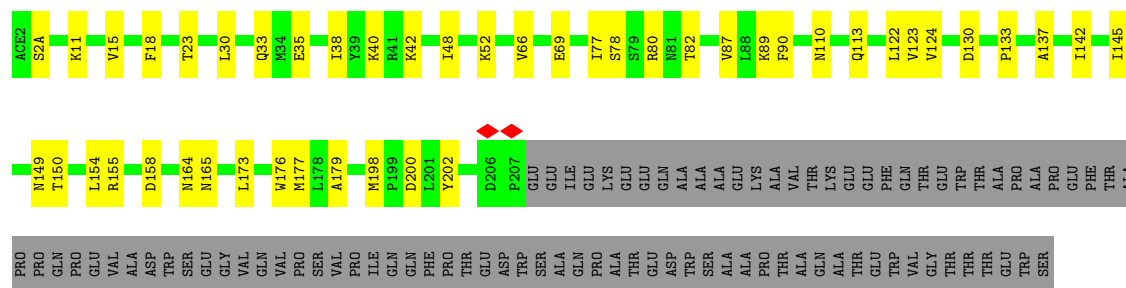
Chain Ay: 44% 12% 44%



- Molecule 78: Small ribosomal subunit protein uS2

Chain AZ: 54% 16% 30%





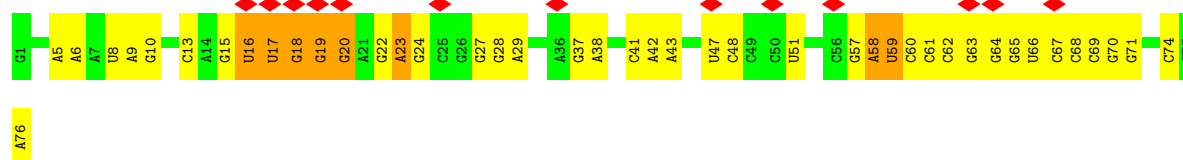
• Molecule 79: Ribosomal protein S16

Chain Ap: 80% 16%



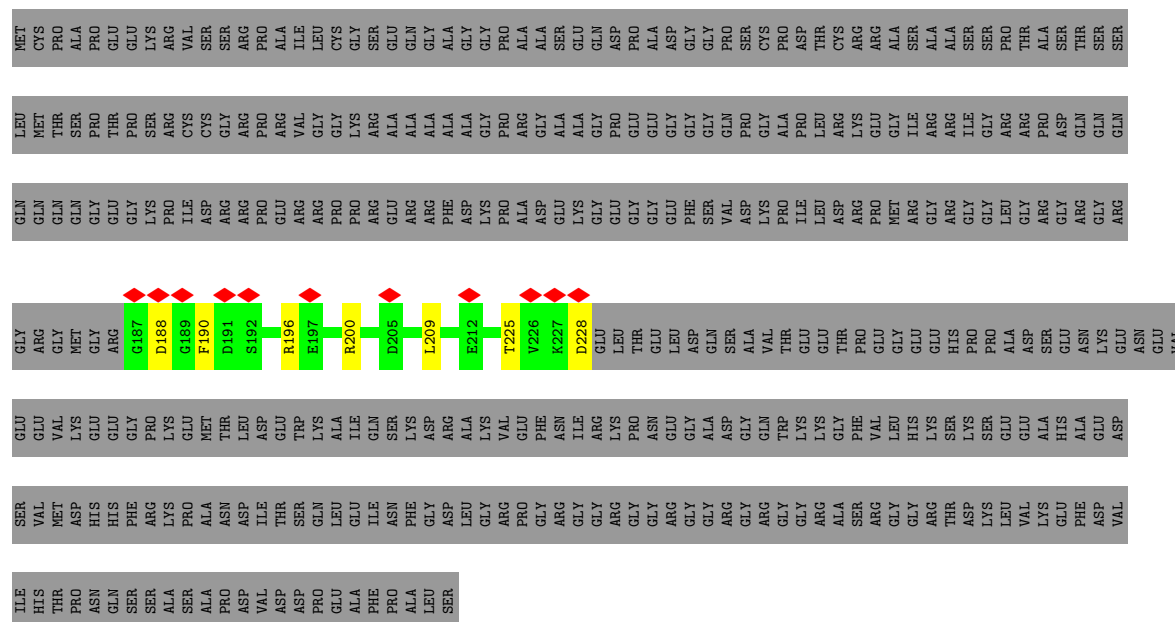
• Molecule 80: Phe tRNA

Chain V: 17% 43% 46% 11%

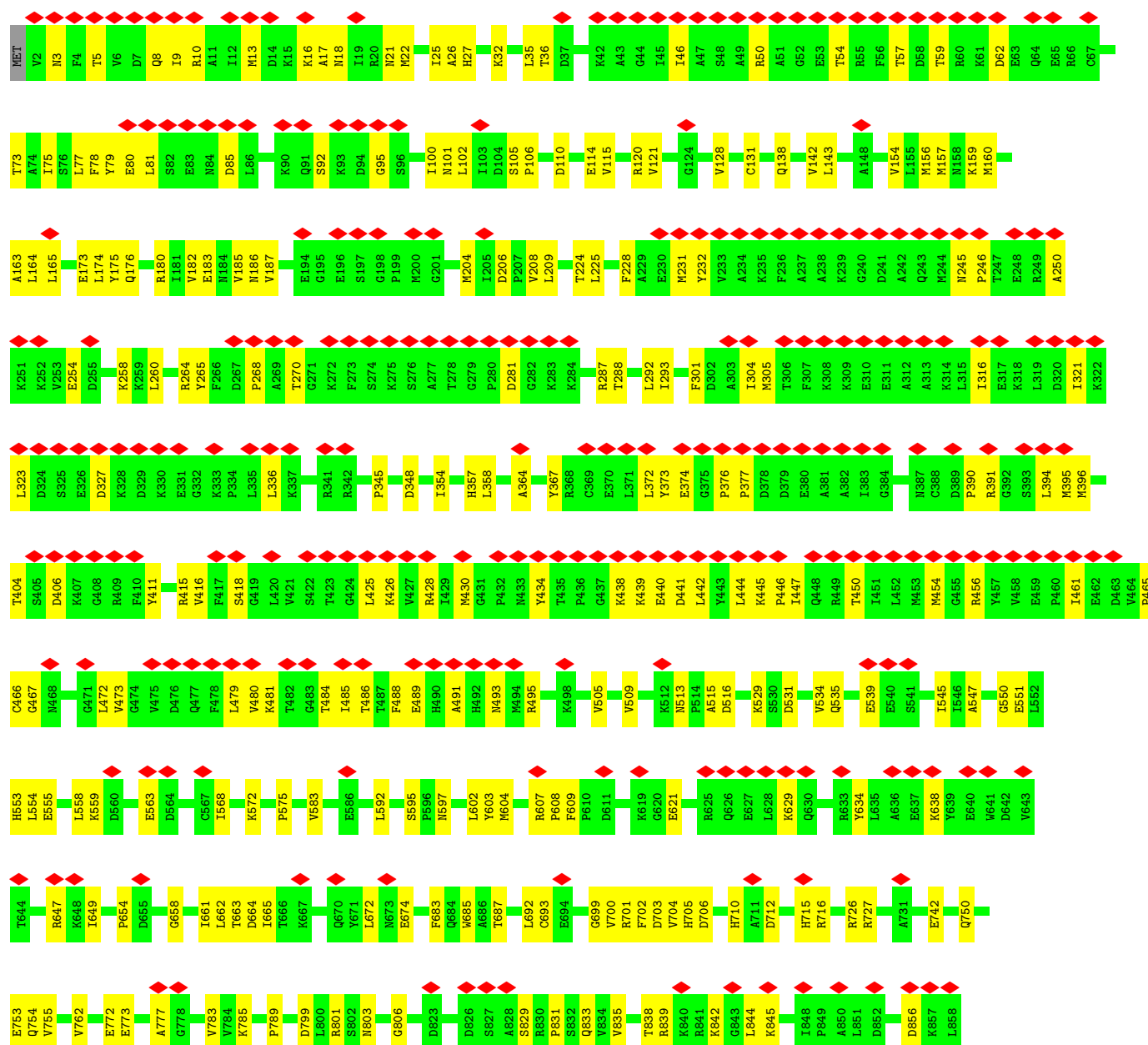
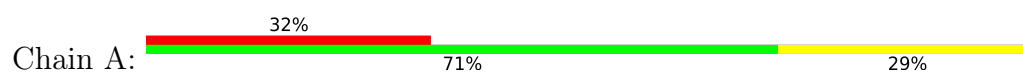


• Molecule 81: SERPINE1 mRNA binding protein 1

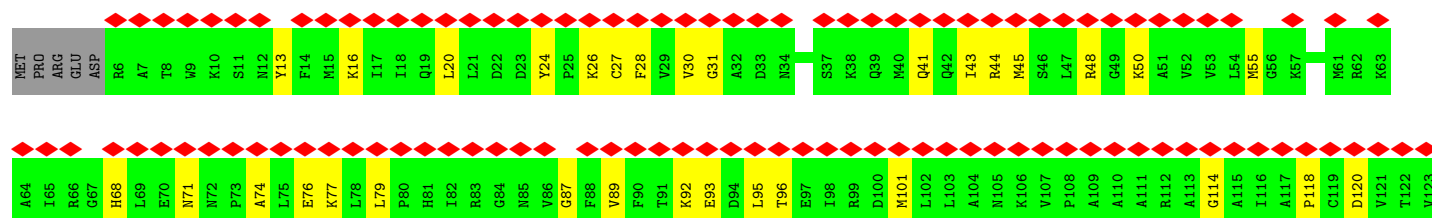
Chain S: 9% 90%

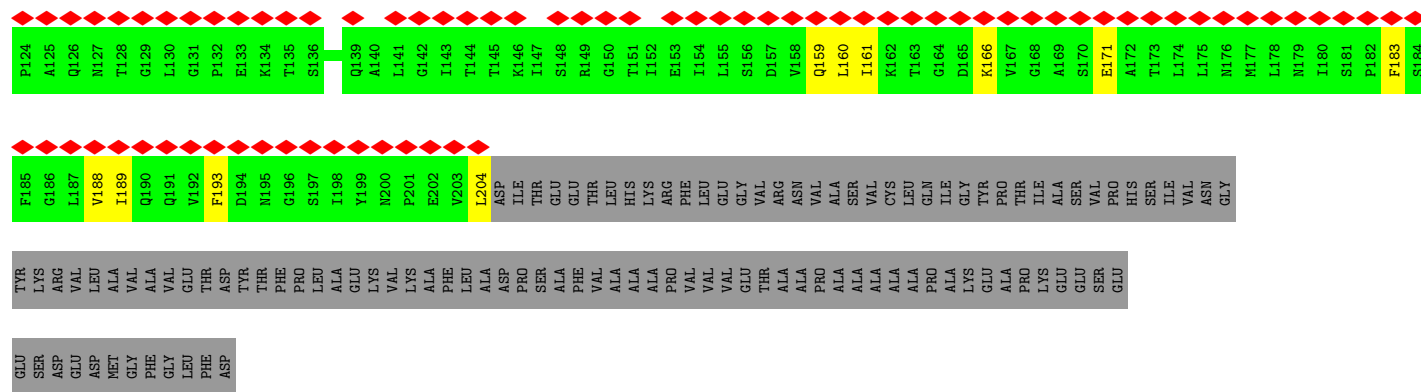


• Molecule 82: Elongation factor 2

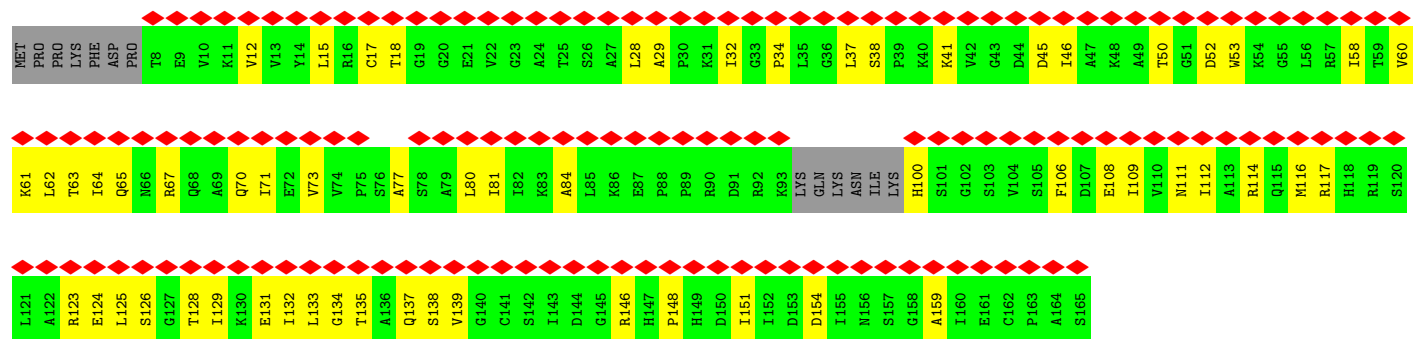
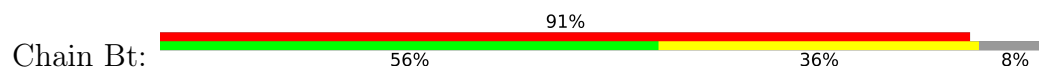


• Molecule 83: Large ribosomal subunit protein uL10

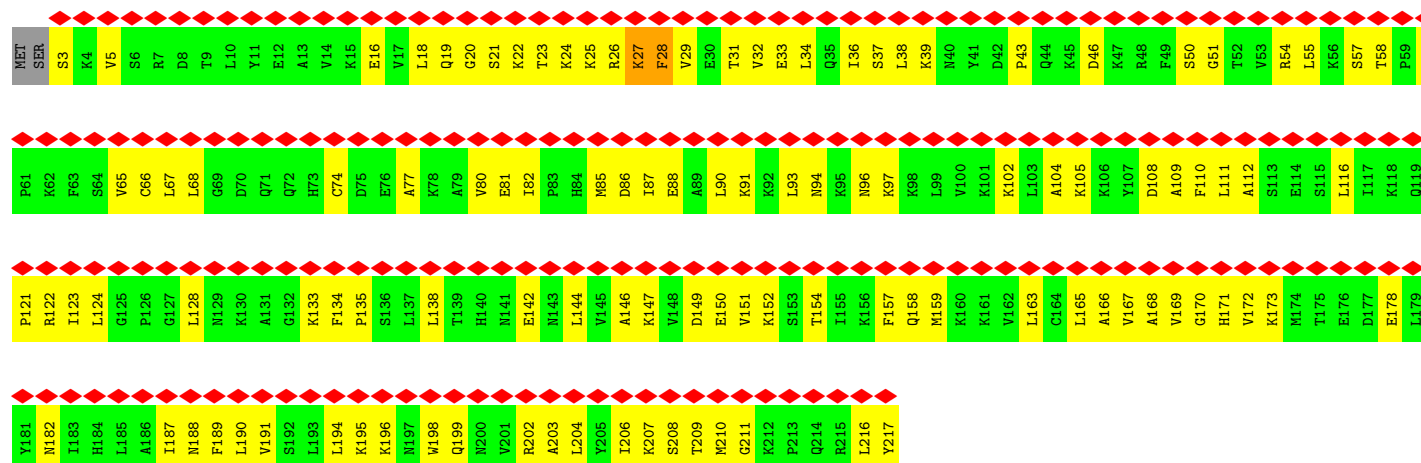




• Molecule 84: 60S ribosomal protein L12



• Molecule 85: Ribosomal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100204	Depositor
Resolution determination method	FSC 3 SIGMA CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	35.598	Depositor
Minimum map value	-17.913	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	1.080	Depositor
Recommended contour level	3	Depositor
Map size (Å)	465.74, 465.74, 465.74	wwPDB
Map dimensions	580, 580, 580	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.803, 0.803, 0.803	Depositor

5 Model quality

5.1 Standard geometry

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

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	B5	0.20	0/85039	0.30	0/132680
2	B8	0.17	0/3656	0.25	0/5693
3	B7	0.17	0/2832	0.25	0/4413
4	Az	0.12	0/240	0.29	0/305
5	BA	0.17	0/1926	0.32	0/2582
6	BB	0.21	0/3264	0.33	0/4363
7	BC	0.16	0/2942	0.28	0/3950
8	BD	0.18	0/2431	0.29	1/3255 (0.0%)
9	BE	0.12	0/1854	0.25	0/2477
10	BF	0.15	0/1975	0.28	0/2634
11	BG	0.14	0/1736	0.28	0/2342
12	BH	0.14	0/1552	0.24	0/2086
13	BI	0.14	0/1751	0.29	0/2342
14	BJ	0.13	0/1385	0.29	0/1852
15	BL	0.14	0/1723	0.28	0/2302
16	BM	0.13	0/1097	0.22	0/1460
17	BN	0.16	0/1745	0.26	0/2337
18	BO	0.16	0/1674	0.29	0/2239
19	BP	0.15	0/1285	0.28	0/1723
20	BQ	0.16	0/1526	0.30	0/2038
21	BR	0.13	0/1394	0.24	0/1845
22	BS	0.16	0/1502	0.28	0/2016
23	BT	0.15	0/1327	0.25	0/1771
24	BU	0.11	0/831	0.26	0/1115
25	BV	0.15	0/1047	0.29	0/1402
26	BW	0.13	0/532	0.25	0/708
27	BX	0.14	0/993	0.27	0/1334
28	BY	0.15	0/1123	0.28	0/1493
29	BZ	0.12	0/1130	0.22	0/1507
30	Ba	0.16	0/1209	0.30	0/1615
31	Bb	0.15	0/593	0.29	0/782

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Bc	0.12	0/748	0.25	0/1004
33	Bd	0.14	0/882	0.25	0/1187
34	Be	0.16	0/1093	0.27	0/1457
35	Bf	0.16	0/905	0.27	0/1211
36	Bg	0.13	0/870	0.28	0/1159
37	Bh	0.22	0/1034	0.26	0/1365
38	Bi	0.13	0/832	0.26	0/1100
39	Bj	0.17	0/718	0.29	0/948
40	Bk	0.11	0/575	0.24	0/761
41	Bl	0.15	0/452	0.27	0/596
42	Bm	0.14	0/435	0.27	0/575
43	Bo	0.14	0/864	0.26	0/1139
44	Bp	0.14	0/716	0.28	0/950
45	Br	0.15	0/1024	0.26	0/1374
46	A2	0.20	0/39536	0.28	0/61603
47	Aa	0.16	0/1757	0.30	0/2352
48	AA	0.17	0/670	0.29	0/897
49	AB	0.16	0/478	0.34	0/641
50	Ab	0.16	0/1734	0.27	0/2342
51	AC	0.13	0/526	0.33	0/696
52	Ac	0.15	0/1780	0.28	0/2396
53	Ad	0.26	0/2118	0.31	0/2848
54	AD	0.13	0/458	0.25	0/602
55	AE	0.13	0/806	0.26	0/1080
56	Ae	0.19	0/1530	0.34	0/2059
57	Af	0.15	0/1861	0.27	0/2481
58	AF	0.17	0/2477	0.32	0/3372
59	Ag	0.14	0/1522	0.30	0/2039
60	AG	0.18	0/470	0.29	0/623
61	Ah	0.17	0/1702	0.30	0/2273
62	Ai	0.31	0/1520	0.35	0/2030
63	Aj	0.17	0/836	0.30	0/1128
64	Ak	0.18	0/1239	0.28	0/1657
65	Al	0.13	0/868	0.34	0/1165
66	Am	0.14	0/1232	0.27	0/1656
67	An	0.14	0/1020	0.29	0/1366
68	Ao	0.17	0/1071	0.29	0/1432
69	Aq	0.21	0/1087	0.43	1/1459 (0.1%)
70	Ar	0.18	0/1209	0.35	0/1620
71	As	0.18	0/1120	0.25	0/1499
72	At	0.17	0/825	0.33	0/1108
73	Au	0.16	0/644	0.26	0/863
74	Av	0.22	0/1052	0.33	0/1408

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Aw	0.24	0/1122	0.35	0/1498
76	Ax	0.20	0/1032	0.31	0/1371
77	Ay	0.18	0/561	0.30	0/755
78	AZ	0.19	0/1661	0.30	0/2259
79	Ap	0.19	0/1141	0.37	0/1527
80	V	0.13	0/1822	0.25	0/2841
81	S	0.10	0/331	0.22	0/436
82	A	0.13	0/6798	0.35	0/9181
83	Bs	0.12	0/1551	0.30	0/2094
84	Bt	0.11	0/1149	0.36	0/1549
85	Bv	0.14	0/1749	0.40	0/2344
All	All	0.18	0/236527	0.29	2/346037 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	Aq	79	GLU	N-CA-C	-6.80	105.53	114.31
8	BD	43	LYS	N-CA-C	-5.79	105.40	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B5	78070	0	39518	993	0
2	B8	3338	0	1695	33	0
3	B7	2536	0	1284	22	0
4	Az	239	0	289	6	0
5	BA	1887	0	1985	28	0
6	BB	3209	0	3351	49	0
7	BC	2888	0	3057	32	0
8	BD	2388	0	2424	25	0
9	BE	1820	0	1986	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	BF	1939	0	2084	25	0
11	BG	1704	0	1821	27	0
12	BH	1533	0	1608	20	0
13	BI	1710	0	1758	22	0
14	BJ	1362	0	1398	23	0
15	BL	1691	0	1803	32	0
16	BM	1077	0	1140	7	0
17	BN	1700	0	1747	22	0
18	BO	1642	0	1787	15	0
19	BP	1259	0	1293	11	0
20	BQ	1502	0	1624	15	0
21	BR	1378	0	1518	15	0
22	BS	1463	0	1512	16	0
23	BT	1299	0	1370	16	0
24	BU	817	0	839	13	0
25	BV	1033	0	1097	9	0
26	BW	519	0	533	2	0
27	BX	976	0	1053	8	0
28	BY	1106	0	1192	23	0
29	BZ	1107	0	1182	16	0
30	Ba	1179	0	1225	13	0
31	Bb	582	0	614	8	0
32	Bc	738	0	774	9	0
33	Bd	867	0	917	9	0
34	Be	1074	0	1174	9	0
35	Bf	886	0	924	6	0
36	Bg	860	0	955	8	0
37	Bh	1023	0	1161	15	0
38	Bi	821	0	903	8	0
39	Bj	704	0	738	7	0
40	Bk	569	0	637	10	0
41	Bl	442	0	483	9	0
42	Bm	429	0	465	2	0
43	Bo	861	0	930	6	0
44	Bp	706	0	756	8	0
45	Br	1007	0	1065	9	0
46	A2	36242	0	18334	446	0
47	Aa	1730	0	1803	37	0
48	AA	657	0	678	7	0
49	AB	476	0	499	12	0
50	Ab	1698	0	1788	32	0
51	AC	516	0	523	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	Ac	1752	0	1848	28	0
53	Ad	2076	0	2176	28	0
54	AD	452	0	494	5	0
55	AE	793	0	841	13	0
56	Ae	1508	0	1563	36	0
57	Af	1838	0	1973	40	0
58	AF	2420	0	2380	47	0
59	Ag	1500	0	1602	25	0
60	AG	459	0	448	10	0
61	Ah	1669	0	1756	37	0
62	Ai	1495	0	1615	12	0
63	Aj	812	0	840	11	0
64	Ak	1218	0	1285	16	0
65	Al	860	0	885	33	0
66	Am	1208	0	1294	18	0
67	An	1016	0	1038	18	0
68	Ao	1050	0	1094	21	0
69	Aq	1073	0	1126	23	0
70	Ar	1191	0	1253	28	0
71	As	1115	0	1147	13	0
72	At	815	0	878	16	0
73	Au	640	0	643	9	0
74	Av	1035	0	1080	16	0
75	Aw	1104	0	1172	12	0
76	Ax	1015	0	1086	20	0
77	Ay	555	0	608	12	0
78	AZ	1626	0	1636	33	0
79	Ap	1123	0	1193	18	0
80	V	1628	0	826	40	0
81	S	325	0	291	6	0
82	A	6690	0	6773	161	0
83	Bs	1527	0	1585	29	0
84	Bt	1135	0	1178	44	0
85	Bv	1722	0	1849	95	0
86	A	1	0	0	0	0
86	A2	116	0	0	0	0
86	AG	1	0	0	0	0
86	Ak	1	0	0	0	0
86	An	1	0	0	0	0
86	As	1	0	0	0	0
86	At	1	0	0	0	0
86	B5	337	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	B7	6	0	0	0	0
86	B8	8	0	0	0	0
86	BA	3	0	0	0	0
86	BB	1	0	0	0	0
86	BH	1	0	0	0	0
86	BI	1	0	0	0	0
86	BN	2	0	0	0	0
86	BP	2	0	0	0	0
86	BV	1	0	0	0	0
86	Ba	1	0	0	0	0
86	Bb	2	0	0	0	0
86	Be	2	0	0	0	0
86	Bf	1	0	0	0	0
86	Bg	1	0	0	0	0
86	Bo	1	0	0	0	0
87	AC	1	0	0	0	0
87	AE	1	0	0	0	0
87	AG	1	0	0	0	0
87	Bg	1	0	0	0	0
87	Bj	1	0	0	0	0
87	Bm	1	0	0	0	0
87	Bo	1	0	0	0	0
87	Bp	1	0	0	0	0
88	A	28	0	12	1	0
89	A	2	0	0	0	0
89	A2	197	0	0	2	0
89	AE	2	0	0	0	0
89	AG	1	0	0	0	0
89	AZ	1	0	0	0	0
89	Ab	8	0	0	1	0
89	Ad	1	0	0	0	0
89	Ae	1	0	0	1	0
89	Ak	1	0	0	0	0
89	Am	1	0	0	0	0
89	An	1	0	0	0	0
89	Ar	2	0	0	0	0
89	As	1	0	0	0	0
89	Au	1	0	0	0	0
89	Av	2	0	0	0	0
89	Ax	1	0	0	0	0
89	Az	1	0	0	0	0
89	B5	2982	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	B7	69	0	0	0	0
89	B8	81	0	0	0	0
89	BA	18	0	0	0	0
89	BB	21	0	0	0	0
89	BC	30	0	0	0	0
89	BD	25	0	0	0	0
89	BE	10	0	0	0	0
89	BF	9	0	0	0	0
89	BG	1	0	0	0	0
89	BH	11	0	0	0	0
89	BI	21	0	0	0	0
89	BL	24	0	0	0	0
89	BM	10	0	0	0	0
89	BN	32	0	0	0	0
89	BO	24	0	0	1	0
89	BP	22	0	0	0	0
89	BQ	28	0	0	0	0
89	BR	8	0	0	0	0
89	BS	14	0	0	0	0
89	BT	16	0	0	0	0
89	BV	7	0	0	0	0
89	BW	3	0	0	0	0
89	BX	6	0	0	0	0
89	BY	10	0	0	0	0
89	Ba	25	0	0	0	0
89	Bb	7	0	0	0	0
89	Bc	1	0	0	0	0
89	Bd	5	0	0	0	0
89	Be	29	0	0	0	0
89	Bf	24	0	0	1	0
89	Bg	14	0	0	0	0
89	Bh	7	0	0	0	0
89	Bi	12	0	0	0	0
89	Bj	9	0	0	0	0
89	Bl	4	0	0	0	0
89	Bm	12	0	0	0	0
89	Bo	15	0	0	1	0
89	Bp	9	0	0	0	0
89	Br	7	0	0	1	0
89	V	9	0	0	0	0
All	All	228127	0	168762	2717	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 7.

The worst 5 of 2717 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:3442:A:N6	1:B5:3493:G:H21	1.45	1.15
1:B5:3442:A:H61	1:B5:3493:G:N2	1.46	1.12
80:V:28:G:H1	80:V:42:A:H2	0.99	0.99
1:B5:3543:G:H1	1:B5:3561:U:H3	1.07	0.95
46:A2:661:U:H3	46:A2:687:C:H42	0.95	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Az	23/25 (92%)	23 (100%)	0	0	100	100
5	BA	244/257 (95%)	235 (96%)	9 (4%)	0	100	100
6	BB	395/403 (98%)	387 (98%)	8 (2%)	0	100	100
7	BC	359/421 (85%)	354 (99%)	5 (1%)	0	100	100
8	BD	294/297 (99%)	282 (96%)	12 (4%)	0	100	100
9	BE	219/298 (74%)	211 (96%)	8 (4%)	0	100	100
10	BF	232/246 (94%)	225 (97%)	7 (3%)	0	100	100
11	BG	206/266 (77%)	198 (96%)	8 (4%)	0	100	100
12	BH	190/192 (99%)	188 (99%)	2 (1%)	0	100	100
13	BI	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
14	BJ	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
15	BL	206/211 (98%)	200 (97%)	5 (2%)	1 (0%)	24	37
16	BM	128/131 (98%)	126 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	BN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
18	BO	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
19	BP	153/184 (83%)	150 (98%)	3 (2%)	0	100	100
20	BQ	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
21	BR	164/196 (84%)	164 (100%)	0	0	100	100
22	BS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
23	BT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
24	BU	98/128 (77%)	97 (99%)	1 (1%)	0	100	100
25	BV	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
26	BW	60/157 (38%)	59 (98%)	1 (2%)	0	100	100
27	BX	117/155 (76%)	114 (97%)	3 (3%)	0	100	100
28	BY	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
29	BZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
30	Ba	145/148 (98%)	140 (97%)	5 (3%)	0	100	100
31	Bb	68/71 (96%)	68 (100%)	0	0	100	100
32	Bc	93/115 (81%)	93 (100%)	0	0	100	100
33	Bd	103/176 (58%)	101 (98%)	2 (2%)	0	100	100
34	Be	128/135 (95%)	128 (100%)	0	0	100	100
35	Bf	108/110 (98%)	108 (100%)	0	0	100	100
36	Bg	106/117 (91%)	105 (99%)	1 (1%)	0	100	100
37	Bh	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
38	Bi	98/105 (93%)	98 (100%)	0	0	100	100
39	Bj	84/97 (87%)	84 (100%)	0	0	100	100
40	Bk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
41	Bl	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
42	Bm	50/128 (39%)	50 (100%)	0	0	100	100
43	Bo	102/105 (97%)	99 (97%)	3 (3%)	0	100	100
44	Bp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
45	Br	122/138 (88%)	119 (98%)	3 (2%)	0	100	100
47	Aa	211/264 (80%)	204 (97%)	7 (3%)	0	100	100
48	AA	81/84 (96%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	AB	59/69 (86%)	58 (98%)	1 (2%)	0	100	100
50	Ab	217/264 (82%)	216 (100%)	1 (0%)	0	100	100
51	AC	61/156 (39%)	58 (95%)	3 (5%)	0	100	100
52	Ac	223/243 (92%)	216 (97%)	7 (3%)	0	100	100
53	Ad	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
54	AD	55/133 (41%)	55 (100%)	0	0	100	100
55	AE	97/115 (84%)	97 (100%)	0	0	100	100
56	Ae	189/204 (93%)	180 (95%)	8 (4%)	1 (0%)	24	37
57	Af	225/249 (90%)	221 (98%)	4 (2%)	0	100	100
58	AF	309/317 (98%)	290 (94%)	19 (6%)	0	100	100
59	Ag	185/194 (95%)	173 (94%)	12 (6%)	0	100	100
60	AG	53/171 (31%)	53 (100%)	0	0	100	100
61	Ah	202/207 (98%)	194 (96%)	8 (4%)	0	100	100
62	Ai	177/194 (91%)	175 (99%)	2 (1%)	0	100	100
63	Aj	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
64	Ak	148/158 (94%)	141 (95%)	7 (5%)	0	100	100
65	Al	107/132 (81%)	96 (90%)	11 (10%)	0	100	100
66	Am	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
67	An	132/151 (87%)	128 (97%)	4 (3%)	0	100	100
68	Ao	126/145 (87%)	121 (96%)	5 (4%)	0	100	100
69	Aq	131/135 (97%)	122 (93%)	7 (5%)	2 (2%)	8	12
70	Ar	142/152 (93%)	132 (93%)	10 (7%)	0	100	100
71	As	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
72	At	101/119 (85%)	94 (93%)	7 (7%)	0	100	100
73	Au	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
74	Av	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
75	Aw	140/143 (98%)	137 (98%)	3 (2%)	0	100	100
76	Ax	123/131 (94%)	123 (100%)	0	0	100	100
77	Ay	68/125 (54%)	66 (97%)	2 (3%)	0	100	100
78	AZ	205/296 (69%)	202 (98%)	3 (2%)	0	100	100
79	Ap	139/146 (95%)	134 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
81	S	40/404 (10%)	37 (92%)	3 (8%)	0	100	100
82	A	854/858 (100%)	813 (95%)	41 (5%)	0	100	100
83	Bs	197/316 (62%)	194 (98%)	3 (2%)	0	100	100
84	Bt	148/165 (90%)	132 (89%)	16 (11%)	0	100	100
85	Bv	213/217 (98%)	192 (90%)	20 (9%)	1 (0%)	24	37
All	All	12525/14686 (85%)	12158 (97%)	362 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	BL	64	VAL
56	Ae	42	GLU
69	Aq	80	ARG
85	Bv	28	PHE
69	Aq	81	ARG

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	
4	Az	24/24 (100%)	24 (100%)	0	100	100
5	BA	189/199 (95%)	189 (100%)	0	100	100
6	BB	346/349 (99%)	346 (100%)	0	100	100
7	BC	305/338 (90%)	305 (100%)	0	100	100
8	BD	248/249 (100%)	248 (100%)	0	100	100
9	BE	196/256 (77%)	196 (100%)	0	100	100
10	BF	201/211 (95%)	201 (100%)	0	100	100
11	BG	186/225 (83%)	186 (100%)	0	100	100
12	BH	171/171 (100%)	171 (100%)	0	100	100
13	BI	178/178 (100%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	BJ	142/148 (96%)	142 (100%)	0	100	100
15	BL	175/178 (98%)	175 (100%)	0	100	100
16	BM	112/113 (99%)	112 (100%)	0	100	100
17	BN	171/172 (99%)	171 (100%)	0	100	100
18	BO	172/173 (99%)	172 (100%)	0	100	100
19	BP	136/163 (83%)	136 (100%)	0	100	100
20	BQ	159/159 (100%)	159 (100%)	0	100	100
21	BR	147/175 (84%)	147 (100%)	0	100	100
22	BS	157/157 (100%)	157 (100%)	0	100	100
23	BT	139/140 (99%)	139 (100%)	0	100	100
24	BU	90/113 (80%)	90 (100%)	0	100	100
25	BV	106/107 (99%)	106 (100%)	0	100	100
26	BW	54/127 (42%)	54 (100%)	0	100	100
27	BX	107/134 (80%)	107 (100%)	0	100	100
28	BY	123/135 (91%)	123 (100%)	0	100	100
29	BZ	117/118 (99%)	117 (100%)	0	100	100
30	Ba	121/122 (99%)	121 (100%)	0	100	100
31	Bb	61/62 (98%)	61 (100%)	0	100	100
32	Bc	80/98 (82%)	80 (100%)	0	100	100
33	Bd	95/148 (64%)	95 (100%)	0	100	100
34	Be	118/123 (96%)	118 (100%)	0	100	100
35	Bf	89/89 (100%)	89 (100%)	0	100	100
36	Bg	93/101 (92%)	93 (100%)	0	100	100
37	Bh	110/110 (100%)	110 (100%)	0	100	100
38	Bi	85/89 (96%)	85 (100%)	0	100	100
39	Bj	73/80 (91%)	73 (100%)	0	100	100
40	Bk	64/65 (98%)	64 (100%)	0	100	100
41	Bl	47/48 (98%)	47 (100%)	0	100	100
42	Bm	48/115 (42%)	48 (100%)	0	100	100
43	Bo	92/92 (100%)	92 (100%)	0	100	100
44	Bp	74/75 (99%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	Br	109/118 (92%)	109 (100%)	0	100	100
47	Aa	194/228 (85%)	194 (100%)	0	100	100
48	AA	75/76 (99%)	75 (100%)	0	100	100
49	AB	54/62 (87%)	54 (100%)	0	100	100
50	Ab	185/214 (86%)	185 (100%)	0	100	100
51	AC	56/140 (40%)	56 (100%)	0	100	100
52	Ac	189/202 (94%)	189 (100%)	0	100	100
53	Ad	223/224 (100%)	222 (100%)	1 (0%)	84	92
54	AD	46/108 (43%)	46 (100%)	0	100	100
55	AE	87/99 (88%)	87 (100%)	0	100	100
56	Ae	161/170 (95%)	161 (100%)	0	100	100
57	Af	199/219 (91%)	199 (100%)	0	100	100
58	AF	270/275 (98%)	270 (100%)	0	100	100
59	Ag	167/174 (96%)	167 (100%)	0	100	100
60	AG	48/130 (37%)	48 (100%)	0	100	100
61	Ah	176/178 (99%)	176 (100%)	0	100	100
62	Ai	160/168 (95%)	159 (99%)	1 (1%)	78	89
63	Aj	88/136 (65%)	88 (100%)	0	100	100
64	Ak	133/140 (95%)	133 (100%)	0	100	100
65	Al	94/109 (86%)	94 (100%)	0	100	100
66	Am	130/131 (99%)	130 (100%)	0	100	100
67	An	105/118 (89%)	105 (100%)	0	100	100
68	Ao	114/130 (88%)	114 (100%)	0	100	100
69	Aq	119/121 (98%)	117 (98%)	2 (2%)	53	74
70	Ar	125/132 (95%)	125 (100%)	0	100	100
71	As	112/114 (98%)	112 (100%)	0	100	100
72	At	94/106 (89%)	94 (100%)	0	100	100
73	Au	69/69 (100%)	69 (100%)	0	100	100
74	Av	112/113 (99%)	112 (100%)	0	100	100
75	Aw	114/115 (99%)	113 (99%)	1 (1%)	70	85
76	Ax	107/113 (95%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	Ay	61/102 (60%)	61 (100%)	0	100	100
78	AZ	172/245 (70%)	171 (99%)	1 (1%)	78	89
79	Ap	116/119 (98%)	116 (100%)	0	100	100
81	S	33/312 (11%)	33 (100%)	0	100	100
82	A	729/730 (100%)	729 (100%)	0	100	100
83	Bs	167/259 (64%)	167 (100%)	0	100	100
84	Bt	124/137 (90%)	124 (100%)	0	100	100
85	Bv	194/196 (99%)	193 (100%)	1 (0%)	81	91
All	All	10912/12461 (88%)	10905 (100%)	7 (0%)	87	95

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	Aq	80	ARG
75	Aw	60	LYS
85	Bv	27	LYS
78	AZ	2(A)	SER
69	Aq	78	ARG

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

Mol	Chain	Res	Type
60	AG	26	ASN
71	As	117	GLN
62	Ai	27	GLN
66	Am	58	HIS
75	Aw	16	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B5	3632/4441 (81%)	564 (15%)	30 (0%)
2	B8	156/157 (99%)	19 (12%)	0
3	B7	118/119 (99%)	9 (7%)	0
46	A2	1691/1823 (92%)	279 (16%)	4 (0%)
80	V	75/76 (98%)	13 (17%)	2 (2%)
All	All	5672/6616 (85%)	884 (15%)	36 (0%)

5 of 884 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B5	2	G
1	B5	25	A
1	B5	39	A
1	B5	42	A
1	B5	58	G

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B5	4142	U
80	V	58	A
1	B5	4432	A
46	A2	1418	U
1	B5	1197	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	A2M	B5	2564	1	22,25,26	0.09	0	31,36,39	0.21	0
1	A2M	B5	3344	1	22,25,26	0.10	0	31,36,39	0.28	0
1	PSU	B5	2257	1	18,21,22	0.47	0	22,30,33	0.61	0
46	PSU	A2	258	46	18,21,22	0.53	0	22,30,33	0.61	0
46	B8N	A2	1206	46	24,29,30	0.57	0	29,42,45	0.64	0
46	PSU	A2	1132	86,46	18,21,22	0.50	0	22,30,33	0.59	0
46	OMU	A2	121	46	19,22,23	0.31	0	26,31,34	0.49	0
46	PSU	A2	109	86,46	18,21,22	0.54	0	22,30,33	0.56	0
46	OMG	A2	1445	86,46	23,26,27	0.29	0	33,38,41	0.35	0
1	PSU	B5	3172	1	18,21,22	0.48	0	22,30,33	0.63	0
1	A2M	B5	3302	1	22,25,26	0.09	0	31,36,39	0.31	0
1	A2M	B5	399	1	22,25,26	0.08	0	31,36,39	0.25	0
1	OMC	B5	3979	86,1	19,22,23	0.31	0	26,31,34	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	A2M	A2	629	86,46	22,25,26	0.12	0	31,36,39	0.31	0
46	PSU	A2	774	46	18,21,22	0.53	0	22,30,33	0.55	0
1	A2M	B5	401	1	22,25,26	0.09	0	31,36,39	0.20	0
46	OMU	A2	315	46	19,22,23	0.32	0	26,31,34	0.58	0
1	OMG	B5	1445	1	23,26,27	0.30	0	33,38,41	0.47	0
46	PSU	A2	821	46	18,21,22	0.54	0	22,30,33	0.54	0
1	5MC	B5	3890	86,1	18,22,23	0.36	0	26,32,35	0.65	0
46	A2M	A2	1341	46	22,25,26	0.09	0	31,36,39	0.38	0
1	UY1	B5	3295	86,1	19,22,23	0.49	0	22,31,34	0.56	0
46	4AC	A2	1295	46	21,24,25	0.34	0	29,34,37	0.41	0
46	MA6	A2	1805	46	23,26,27	0.31	0	34,38,41	0.67	1 (2%)
1	OMC	B5	3178	86,1	19,22,23	0.26	0	26,31,34	0.50	0
1	PSU	B5	3885	1	18,21,22	0.45	0	22,30,33	0.89	0
2	PSU	B8	55	2	18,21,22	0.49	0	22,30,33	0.60	0
1	OMU	B5	3402	1	19,22,23	0.33	0	26,31,34	0.53	0
43	MLZ	Bo	53	43	8,9,10	0.70	0	4,9,11	0.57	0
46	OMG	A2	1286	46	23,26,27	0.28	0	33,38,41	0.37	0
1	A2M	B5	4014	1	22,25,26	0.09	0	31,36,39	0.18	0
1	OMG	B5	4066	1	23,26,27	0.33	0	33,38,41	0.52	0
1	OMC	B5	2100	1	19,22,23	0.34	0	26,31,34	0.42	0
1	OMG	B5	2625	1	23,26,27	0.31	0	33,38,41	0.37	0
1	PSU	B5	3846	1	18,21,22	0.56	0	22,30,33	0.61	1 (4%)
46	4AC	A2	1796	46	21,24,25	0.30	0	29,34,37	0.30	0
46	A2M	A2	165	46	22,25,26	0.09	0	31,36,39	0.47	1 (3%)
1	OMG	B5	2173	1	23,26,27	0.29	0	33,38,41	0.35	0
1	OMU	B5	3941	86,1	19,22,23	0.30	0	26,31,34	0.44	0
1	PSU	B5	4372	86,1	18,21,22	0.50	0	22,30,33	0.57	0
1	OMG	B5	3269	1	23,26,27	0.29	0	33,38,41	0.33	0
1	OMC	B5	1265	1	19,22,23	0.29	0	26,31,34	0.45	0
46	OMU	A2	389	46	19,22,23	0.28	0	26,31,34	0.46	0
1	OMC	B5	3285	1	19,22,23	0.31	0	26,31,34	0.37	0
2	OMG	B8	75	2	23,26,27	0.31	0	33,38,41	0.41	0
46	OMC	A2	478	46	19,22,23	0.31	0	26,31,34	0.39	0
1	PSU	B5	3975	1	18,21,22	0.56	0	22,30,33	0.55	0
1	PSU	B5	1771	1	18,21,22	0.47	0	22,30,33	0.58	0
1	PSU	B5	3116	1	18,21,22	0.51	0	22,30,33	0.57	0
1	5MC	B5	3259	86,1	18,22,23	0.31	0	26,32,35	0.42	0
1	OMC	B5	2171	86,1	19,22,23	0.31	0	26,31,34	0.45	0
1	OMC	B5	3899	1	19,22,23	0.30	0	26,31,34	0.40	0
1	A2M	B5	1457	86,1	22,25,26	0.10	0	31,36,39	0.38	0
1	PSU	B5	3796	1	18,21,22	0.50	0	22,30,33	0.56	0
1	PSU	B5	3736	1	18,21,22	0.53	0	22,30,33	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	B5	1600	86,1	18,21,22	0.85	1 (5%)	22,30,33	0.62	0
1	OMG	B5	3639	1	23,26,27	0.31	0	33,38,41	0.34	0
46	A2M	A2	99	86,46	22,25,26	0.08	0	31,36,39	0.30	0
1	PSU	B5	4019	1	18,21,22	0.75	1 (5%)	22,30,33	0.55	0
46	OMG	A2	605	46	23,26,27	0.30	0	33,38,41	0.49	0
46	OMU	A2	171	46	19,22,23	0.27	0	26,31,34	0.63	0
1	PSU	B5	3874	1	18,21,22	0.50	0	22,30,33	0.61	0
1	OMU	B5	3670	1	19,22,23	0.33	0	26,31,34	0.46	0
46	OMG	A2	470	86,46	23,26,27	0.30	0	33,38,41	0.42	0
1	OMG	B5	1548	86,1	23,26,27	0.32	0	33,38,41	0.46	0
46	OMU	A2	1284	86,46	19,22,23	0.24	0	26,31,34	0.48	0
1	PSU	B5	3900	1	18,21,22	0.53	0	22,30,33	0.58	0
46	A2M	A2	551	46	22,25,26	0.12	0	31,36,39	0.37	0
1	PSU	B5	4022	1	18,21,22	0.53	0	22,30,33	0.59	0
1	PSU	B5	4116	1	18,21,22	0.52	0	22,30,33	0.57	0
1	A2M	B5	2536	1	22,25,26	0.11	0	31,36,39	0.50	0
1	OMU	B5	4063	1	19,22,23	0.33	0	26,31,34	0.67	0
1	OMG	B5	4061	1	23,26,27	0.31	0	33,38,41	0.46	0
2	PSU	B8	69	86,2	18,21,22	0.54	0	22,30,33	0.63	1 (4%)
1	A2M	B5	3195	1	22,25,26	0.09	0	31,36,39	0.25	0
1	UR3	B5	3973	1	19,22,23	0.31	0	26,32,35	0.30	0
1	OMG	B5	4080	1	23,26,27	0.34	0	33,38,41	0.38	0
1	OMC	B5	3318	1	19,22,23	0.30	0	26,31,34	0.40	0
1	6MZ	B5	3663	1	22,25,26	0.30	0	30,36,39	0.34	0
46	PSU	A2	775	46	18,21,22	0.54	0	22,30,33	0.61	0
46	6MZ	A2	1786	86,46	22,25,26	0.29	0	30,36,39	0.41	0
1	PSU	B5	1690	1	18,21,22	0.49	0	22,30,33	0.58	0
46	A2M	A2	27	86,46	22,25,26	0.09	0	31,36,39	0.24	0
1	OMC	B5	3364	1	19,22,23	0.34	0	26,31,34	0.46	0
1	A2M	B5	3201	1	22,25,26	0.08	0	31,36,39	0.21	0
46	OMC	A2	1658	46	19,22,23	0.27	0	26,31,34	0.43	0
1	OMG	B5	2113	86,1	23,26,27	0.30	0	33,38,41	0.39	0
71	NMM	As	67	71	9,11,12	1.56	1 (11%)	6,12,14	4.10	2 (33%)
46	PSU	A2	642	46	18,21,22	0.52	0	22,30,33	0.62	0
1	PSU	B5	3742	1	18,21,22	0.53	0	22,30,33	0.57	0
1	PSU	B5	3397	86,1	18,21,22	0.51	0	22,30,33	0.59	0
67	IAS	An	138	67	6,7,8	1.04	0	6,8,10	1.29	1 (16%)
6	HIC	BB	245	6	10,11,12	1.48	1 (10%)	8,14,16	0.97	0
1	OMU	B5	2586	1	19,22,23	0.33	0	26,31,34	0.55	0
1	A2M	B5	1251	1	22,25,26	0.09	0	31,36,39	0.26	0
1	A2M	B5	3307	1	22,25,26	0.09	0	31,36,39	0.32	0
1	PSU	B5	4071	1	18,21,22	0.53	0	22,30,33	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	B5	3813	1	23,26,27	0.30	0	33,38,41	0.38	0
1	OMG	B5	3835	1	23,26,27	0.28	0	33,38,41	0.36	0
46	A2M	A2	989	46	22,25,26	0.09	0	31,36,39	0.32	0
46	OMG	A2	562	46	23,26,27	0.31	0	33,38,41	0.35	0
1	OMC	B5	3346	1	19,22,23	0.30	0	26,31,34	0.41	0
1	OMG	B5	3937	1	23,26,27	0.33	0	33,38,41	0.40	0
1	A2M	B5	1780	86,1	22,25,26	0.09	0	31,36,39	0.47	0
1	OMC	B5	2553	1	19,22,23	0.30	0	26,31,34	0.39	0
1	PSU	B5	3739	1	18,21,22	0.47	0	22,30,33	0.62	0
1	A2M	B5	3262	1	22,25,26	0.13	0	31,36,39	0.49	0
1	PSU	B5	3114	86,1	18,21,22	0.47	0	22,30,33	0.59	0
46	PSU	A2	782	46	18,21,22	0.63	1 (5%)	22,30,33	0.67	1 (4%)
1	PSU	B5	3804	1	18,21,22	0.49	0	22,30,33	0.61	0
1	PSU	B5	3192	1	18,21,22	0.55	0	22,30,33	0.59	0
1	OMU	B5	3749	1	19,22,23	0.31	0	26,31,34	0.48	0
1	OMC	B5	2610	1	19,22,23	0.28	0	26,31,34	0.34	0
1	PSU	B5	1652	1	18,21,22	0.48	0	22,30,33	0.58	0
1	A2M	B5	1447	1	22,25,26	0.13	0	31,36,39	0.31	0
1	PSU	B5	3866	1	18,21,22	0.52	0	22,30,33	0.56	0
1	OMC	B5	1790	86,1	19,22,23	0.30	0	26,31,34	0.63	0
1	PSU	B5	3964	86,1	18,21,22	0.53	0	22,30,33	0.59	0
1	PSU	B5	1700	1	18,21,22	0.46	0	22,30,33	0.68	0
1	OMG	B5	1241	86,1	23,26,27	0.36	0	33,38,41	0.54	0
1	OMG	B5	3671	1	23,26,27	0.28	0	33,38,41	0.50	0
46	PSU	A2	93	46	18,21,22	0.52	0	22,30,33	0.56	0
1	A2M	B5	3966	86,1	22,25,26	0.10	0	31,36,39	0.45	0
46	PSU	A2	1039	46	18,21,22	0.66	1 (5%)	22,30,33	0.66	0
1	OMG	B5	3942	1	23,26,27	0.30	0	33,38,41	0.42	0
46	A2M	A2	445	46	22,25,26	0.09	0	31,36,39	0.23	0
82	DDE	A	715	82	17,20,21	0.36	0	20,28,30	0.24	0
46	OMU	A2	116	46	19,22,23	0.28	0	26,31,34	0.42	0
46	PSU	A2	610	46	18,21,22	0.49	0	22,30,33	0.61	0
1	PSU	B5	3755	1	18,21,22	0.49	0	22,30,33	0.58	0
1	PSU	B5	1606	86,1	18,21,22	0.52	0	22,30,33	0.61	0
1	PSU	B5	4132	1	18,21,22	0.52	0	22,30,33	0.62	0
1	PSU	B5	3995	1	18,21,22	0.50	0	22,30,33	0.64	0
1	A2M	B5	2112	86,1	22,25,26	0.09	0	31,36,39	0.21	0
46	PSU	A2	647	46	18,21,22	1.50	5 (27%)	22,30,33	2.11	5 (22%)
1	OMG	B5	3221	1	23,26,27	0.29	0	33,38,41	0.41	0
1	PSU	B5	4343	86,1	18,21,22	0.50	0	22,30,33	0.57	0
1	1MA	B5	1247	86,1	21,25,26	0.32	0	31,37,40	0.46	0
46	MA6	A2	1804	46	23,26,27	0.31	0	34,38,41	0.64	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	OMG	A2	644	46	23,26,27	0.31	0	33,38,41	0.47	0
1	PSU	B5	1769	1	18,21,22	0.50	0	22,30,33	0.59	0
1	OMG	B5	3104	1	23,26,27	0.31	0	33,38,41	0.51	0
1	OMG	B5	3376	86,1	23,26,27	0.33	0	33,38,41	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	B5	2564	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	3344	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	2257	1	-	0/7/25/26	0/2/2/2
46	PSU	A2	258	46	-	2/7/25/26	0/2/2/2
46	B8N	A2	1206	46	-	3/16/34/35	0/2/2/2
46	PSU	A2	1132	86,46	-	0/7/25/26	0/2/2/2
46	OMU	A2	121	46	-	0/9/27/28	0/2/2/2
46	PSU	A2	109	86,46	-	0/7/25/26	0/2/2/2
46	OMG	A2	1445	86,46	-	1/9/27/28	0/3/3/3
1	PSU	B5	3172	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3302	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	399	1	-	1/9/27/28	0/3/3/3
1	OMC	B5	3979	86,1	-	0/9/27/28	0/2/2/2
46	A2M	A2	629	86,46	-	4/9/27/28	0/3/3/3
46	PSU	A2	774	46	-	0/7/25/26	0/2/2/2
1	A2M	B5	401	1	-	0/9/27/28	0/3/3/3
46	OMU	A2	315	46	-	0/9/27/28	0/2/2/2
1	OMG	B5	1445	1	-	0/9/27/28	0/3/3/3
46	PSU	A2	821	46	-	0/7/25/26	0/2/2/2
1	5MC	B5	3890	86,1	-	3/7/25/26	0/2/2/2
46	A2M	A2	1341	46	-	0/9/27/28	0/3/3/3
1	UY1	B5	3295	86,1	-	2/9/27/28	0/2/2/2
46	4AC	A2	1295	46	-	2/11/29/30	0/2/2/2
46	MA6	A2	1805	46	-	1/11/29/30	0/3/3/3
1	OMC	B5	3178	86,1	-	4/9/27/28	0/2/2/2
1	PSU	B5	3885	1	-	0/7/25/26	0/2/2/2
2	PSU	B8	55	2	-	0/7/25/26	0/2/2/2
1	OMU	B5	3402	1	-	0/9/27/28	0/2/2/2
43	MLZ	Bo	53	43	-	1/7/8/10	-
46	OMG	A2	1286	46	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	B5	4014	1	-	0/9/27/28	0/3/3/3
1	OMG	B5	4066	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	2100	1	-	3/9/27/28	0/2/2/2
1	OMG	B5	2625	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3846	1	-	0/7/25/26	0/2/2/2
46	4AC	A2	1796	46	-	0/11/29/30	0/2/2/2
46	A2M	A2	165	46	-	0/9/27/28	0/3/3/3
1	OMG	B5	2173	1	-	0/9/27/28	0/3/3/3
1	OMU	B5	3941	86,1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4372	86,1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3269	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	1265	1	-	0/9/27/28	0/2/2/2
46	OMU	A2	389	46	-	4/9/27/28	0/2/2/2
1	OMC	B5	3285	1	-	0/9/27/28	0/2/2/2
2	OMG	B8	75	2	-	0/9/27/28	0/3/3/3
46	OMC	A2	478	46	-	0/9/27/28	0/2/2/2
1	PSU	B5	3975	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1771	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3116	1	-	0/7/25/26	0/2/2/2
1	5MC	B5	3259	86,1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2171	86,1	-	2/9/27/28	0/2/2/2
1	OMC	B5	3899	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	1457	86,1	-	2/9/27/28	0/3/3/3
1	PSU	B5	3796	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3736	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1600	86,1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3639	1	-	1/9/27/28	0/3/3/3
46	A2M	A2	99	86,46	-	0/9/27/28	0/3/3/3
1	PSU	B5	4019	1	-	2/7/25/26	0/2/2/2
46	OMG	A2	605	46	-	3/9/27/28	0/3/3/3
46	OMU	A2	171	46	-	0/9/27/28	0/2/2/2
1	PSU	B5	3874	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	3670	1	-	0/9/27/28	0/2/2/2
46	OMG	A2	470	86,46	-	1/9/27/28	0/3/3/3
1	OMG	B5	1548	86,1	-	1/9/27/28	0/3/3/3
46	OMU	A2	1284	86,46	-	0/9/27/28	0/2/2/2
1	PSU	B5	3900	1	-	0/7/25/26	0/2/2/2
46	A2M	A2	551	46	-	1/9/27/28	0/3/3/3
1	PSU	B5	4022	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4116	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	2536	1	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	B5	4063	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	4061	1	-	0/9/27/28	0/3/3/3
2	PSU	B8	69	86,2	-	0/7/25/26	0/2/2/2
1	A2M	B5	3195	1	-	0/9/27/28	0/3/3/3
1	UR3	B5	3973	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4080	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	3318	1	-	0/9/27/28	0/2/2/2
1	6MZ	B5	3663	1	-	0/9/27/28	0/3/3/3
46	PSU	A2	775	46	-	2/7/25/26	0/2/2/2
46	6MZ	A2	1786	86,46	-	0/9/27/28	0/3/3/3
1	PSU	B5	1690	1	-	0/7/25/26	0/2/2/2
46	A2M	A2	27	86,46	-	0/9/27/28	0/3/3/3
1	OMC	B5	3364	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	3201	1	-	1/9/27/28	0/3/3/3
46	OMC	A2	1658	46	-	0/9/27/28	0/2/2/2
1	OMG	B5	2113	86,1	-	2/9/27/28	0/3/3/3
71	NMM	As	67	71	-	4/9/11/13	-
46	PSU	A2	642	46	-	0/7/25/26	0/2/2/2
1	PSU	B5	3742	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3397	86,1	-	0/7/25/26	0/2/2/2
67	IAS	An	138	67	-	2/7/7/8	-
6	HIC	BB	245	6	-	0/5/6/8	0/1/1/1
1	OMU	B5	2586	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	1251	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	3307	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4071	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3813	1	-	2/9/27/28	0/3/3/3
1	OMG	B5	3835	1	-	0/9/27/28	0/3/3/3
46	A2M	A2	989	46	-	0/9/27/28	0/3/3/3
46	OMG	A2	562	46	-	0/9/27/28	0/3/3/3
1	OMC	B5	3346	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	3937	1	-	1/9/27/28	0/3/3/3
1	A2M	B5	1780	86,1	-	0/9/27/28	0/3/3/3
1	OMC	B5	2553	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	3739	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3262	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	3114	86,1	-	0/7/25/26	0/2/2/2
46	PSU	A2	782	46	-	0/7/25/26	0/2/2/2
1	PSU	B5	3804	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3192	1	-	2/7/25/26	0/2/2/2
1	OMU	B5	3749	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	B5	2610	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	1652	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	1447	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	3866	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	1790	86,1	-	0/9/27/28	0/2/2/2
1	PSU	B5	3964	86,1	-	2/7/25/26	0/2/2/2
1	PSU	B5	1700	1	-	1/7/25/26	0/2/2/2
1	OMG	B5	1241	86,1	-	0/9/27/28	0/3/3/3
1	OMG	B5	3671	1	-	1/9/27/28	0/3/3/3
46	PSU	A2	93	46	-	0/7/25/26	0/2/2/2
1	A2M	B5	3966	86,1	-	0/9/27/28	0/3/3/3
46	PSU	A2	1039	46	-	1/7/25/26	0/2/2/2
1	OMG	B5	3942	1	-	0/9/27/28	0/3/3/3
46	A2M	A2	445	46	-	0/9/27/28	0/3/3/3
82	DDE	A	715	82	-	5/20/21/23	0/1/1/1
46	OMU	A2	116	46	-	0/9/27/28	0/2/2/2
46	PSU	A2	610	46	-	0/7/25/26	0/2/2/2
1	PSU	B5	3755	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1606	86,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4132	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3995	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	2112	86,1	-	1/9/27/28	0/3/3/3
46	PSU	A2	647	46	-	0/7/25/26	0/2/2/2
1	OMG	B5	3221	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4343	86,1	-	0/7/25/26	0/2/2/2
1	1MA	B5	1247	86,1	-	2/7/25/26	0/3/3/3
46	MA6	A2	1804	46	-	0/11/29/30	0/3/3/3
46	OMG	A2	644	46	-	1/9/27/28	0/3/3/3
1	PSU	B5	1769	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3104	1	-	0/9/27/28	0/3/3/3
1	OMG	B5	3376	86,1	-	0/9/27/28	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	As	67	NMM	CZ-NH2	4.16	1.44	1.34
46	A2	647	PSU	C4-N3	-3.24	1.32	1.38
1	B5	1600	PSU	O4'-C1'	-3.21	1.39	1.43
6	BB	245	HIC	CD2-CG	2.91	1.41	1.36
1	B5	4019	PSU	O4'-C1'	-2.43	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	As	67	NMM	NE-CZ-NH2	-8.97	111.26	119.48
46	A2	647	PSU	N1-C2-N3	6.48	122.47	115.13
46	A2	647	PSU	C4-N3-C2	-4.44	119.95	126.34
71	As	67	NMM	NE-CZ-NH1	4.25	128.22	120.26
46	A2	647	PSU	O2-C2-N1	-3.64	118.78	122.79

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B5	399	A2M	C1'-C2'-O2'-CM'
1	B5	2536	A2M	C1'-C2'-O2'-CM'
1	B5	3178	OMC	C2'-C1'-N1-C6
1	B5	3192	PSU	C3'-C4'-C5'-O5'
1	B5	3201	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

50 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	2564	A2M	1	0
1	B5	3344	A2M	2	0
46	A2	109	PSU	1	0
1	B5	3172	PSU	3	0
1	B5	399	A2M	2	0
1	B5	3979	OMC	1	0
1	B5	3890	5MC	2	0
1	B5	3295	UY1	1	0
46	A2	1295	4AC	2	0
1	B5	3885	PSU	1	0
1	B5	4066	OMG	1	0
1	B5	2100	OMC	2	0
1	B5	2625	OMG	1	0
1	B5	2173	OMG	1	0
1	B5	1265	OMC	1	0
2	B8	75	OMG	1	0
46	A2	478	OMC	1	0
1	B5	3975	PSU	1	0
1	B5	1457	A2M	1	0
1	B5	1600	PSU	1	0
1	B5	3639	OMG	1	0
46	A2	99	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	4019	PSU	1	0
1	B5	3874	PSU	1	0
46	A2	470	OMG	2	0
1	B5	3900	PSU	1	0
1	B5	4022	PSU	1	0
1	B5	4063	OMU	2	0
1	B5	3195	A2M	3	0
1	B5	4080	OMG	2	0
1	B5	3663	6MZ	1	0
46	A2	27	A2M	1	0
1	B5	3201	A2M	2	0
46	A2	1658	OMC	1	0
1	B5	1251	A2M	1	0
1	B5	4071	PSU	1	0
1	B5	3835	OMG	1	0
1	B5	1780	A2M	1	0
1	B5	3739	PSU	1	0
1	B5	3262	A2M	1	0
1	B5	3749	OMU	1	0
1	B5	2610	OMC	1	0
1	B5	1447	A2M	1	0
1	B5	3671	OMG	1	0
1	B5	3942	OMG	1	0
82	A	715	DDE	2	0
46	A2	116	OMU	1	0
1	B5	3995	PSU	3	0
1	B5	2112	A2M	1	0
46	A2	647	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 501 ligands modelled in this entry, 500 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	GDP	A	901	-	28,30,30	0.41	0	44,47,47	0.66	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	GDP	A	901	-	-	1/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A	901	GDP	PA-O3A-PB	3.35	144.33	132.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	A	901	GDP	C4'-C5'-O5'-PA

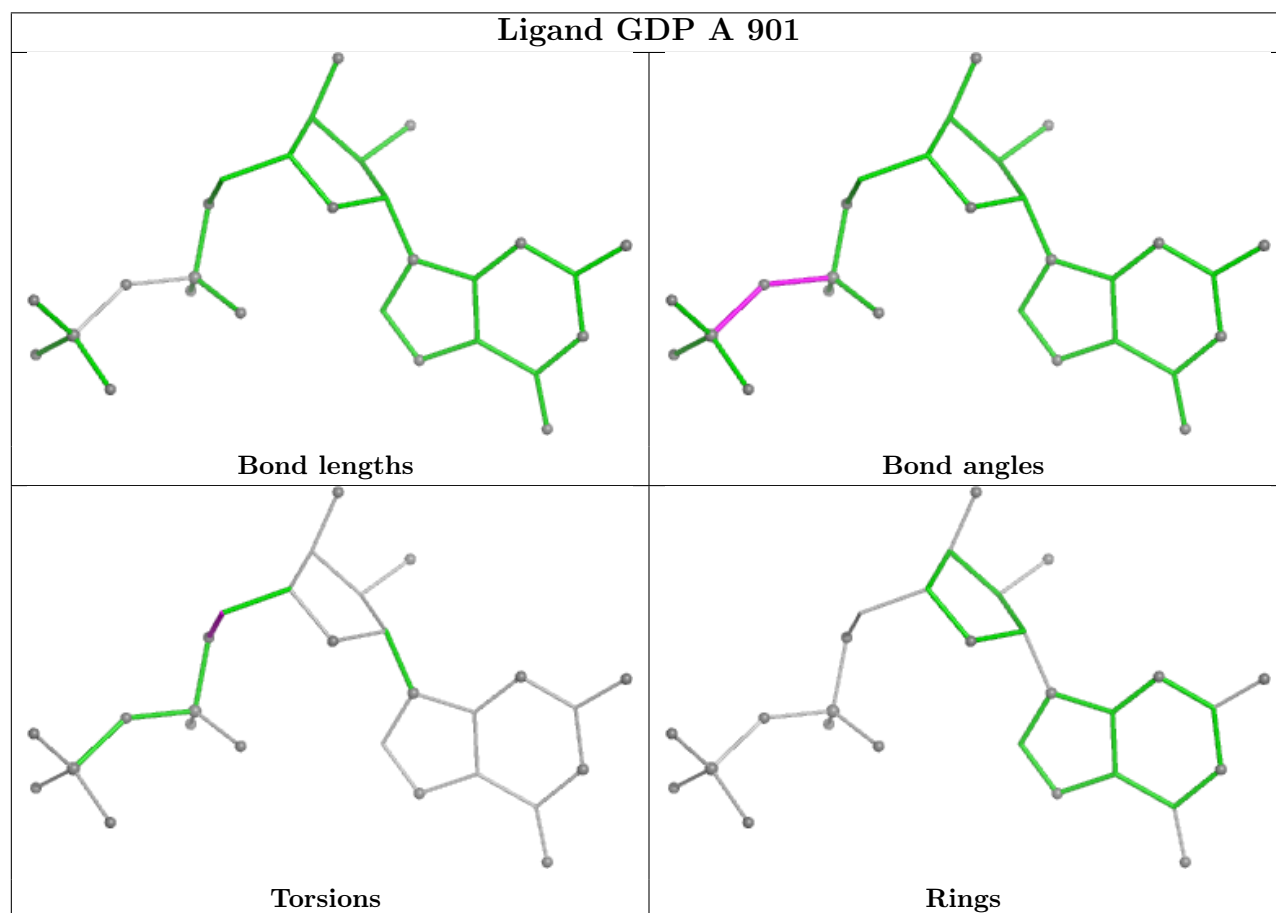
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	A	901	GDP	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](#)

There are no chain breaks in this entry.

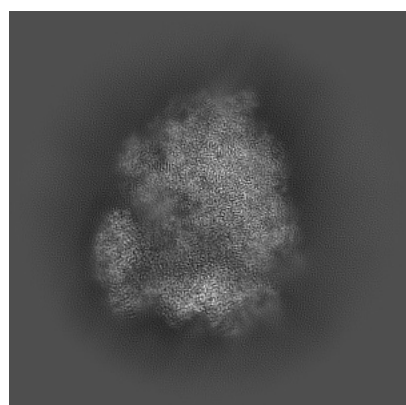
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18169. These allow visual inspection of the internal detail of the map and identification of artifacts.

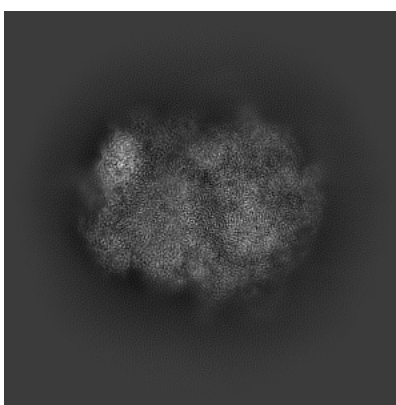
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

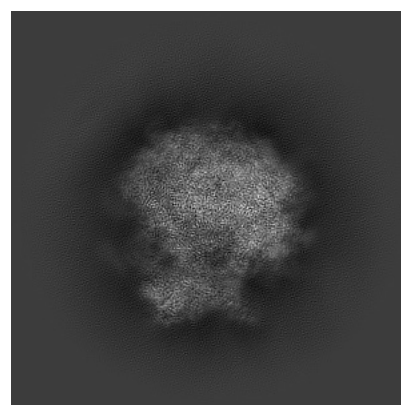
6.1.1 Primary map



X



Y

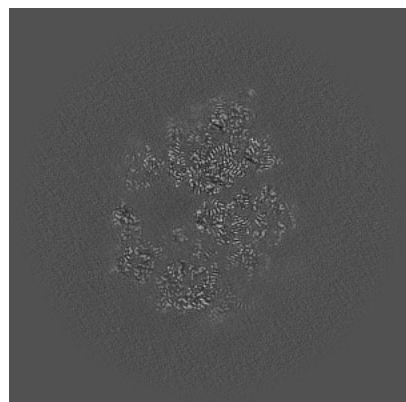


Z

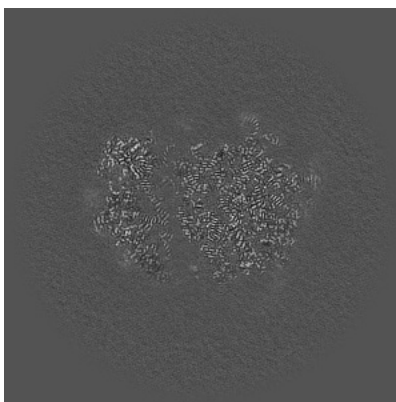
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

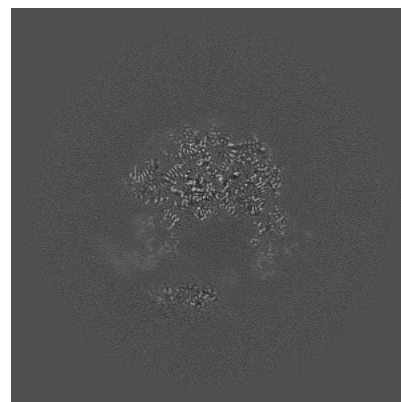
6.2.1 Primary map



X Index: 290



Y Index: 290

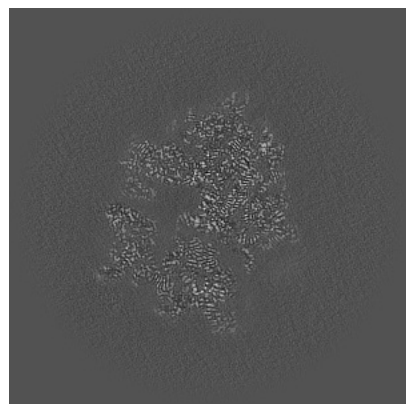


Z Index: 290

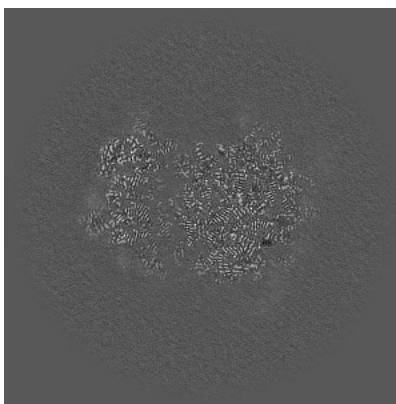
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

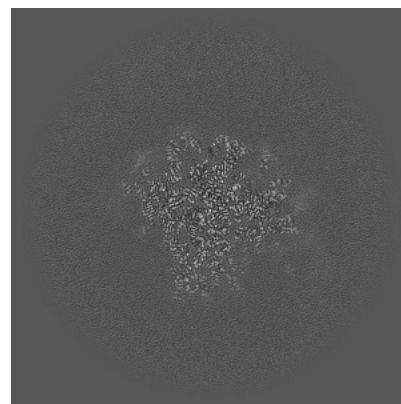
6.3.1 Primary map



X Index: 270



Y Index: 298

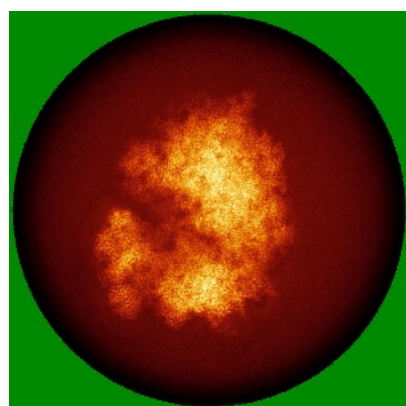


Z Index: 348

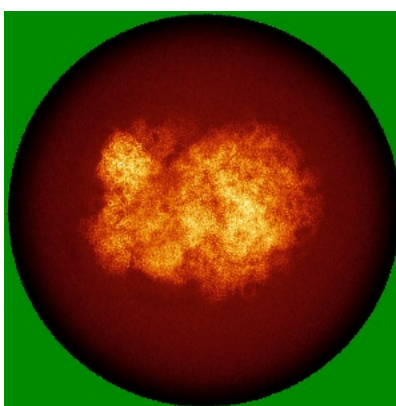
The images above show the largest variance slices of the map in three orthogonal directions.

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

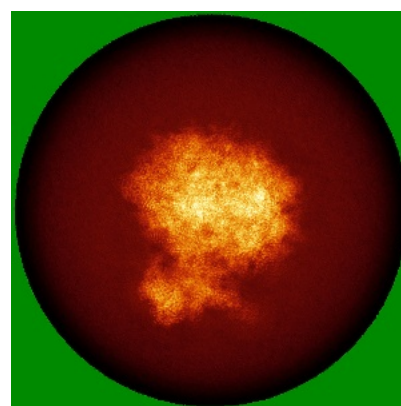
6.4.1 Primary map



X



Y

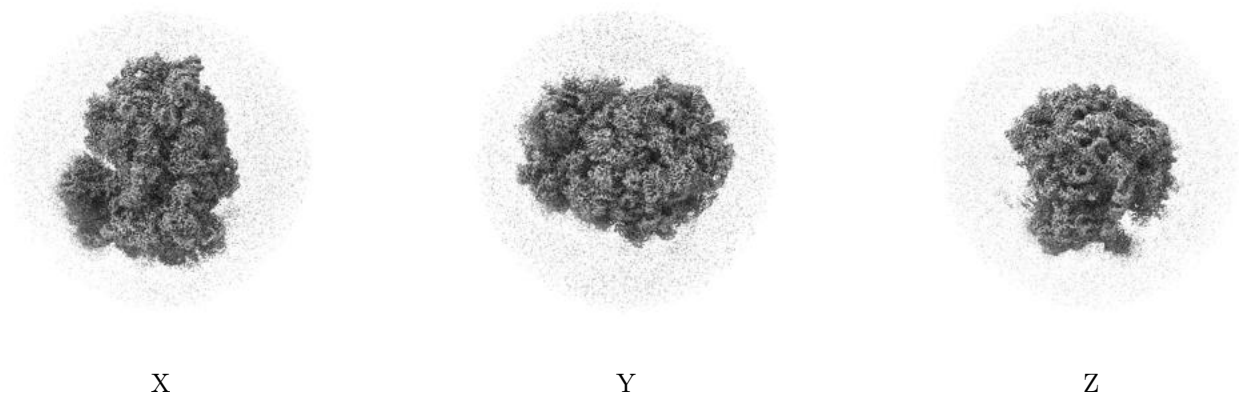


Z

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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

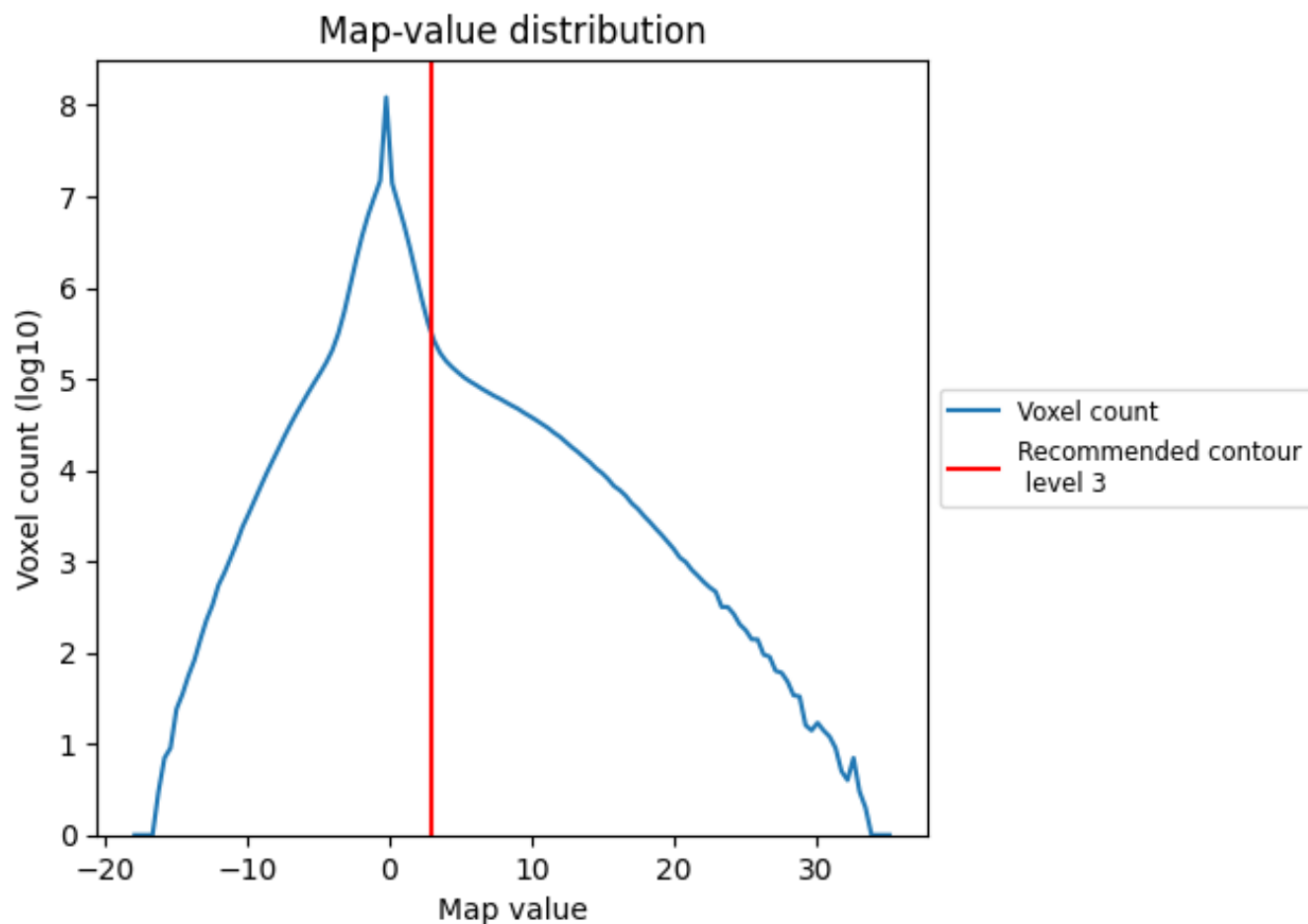
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

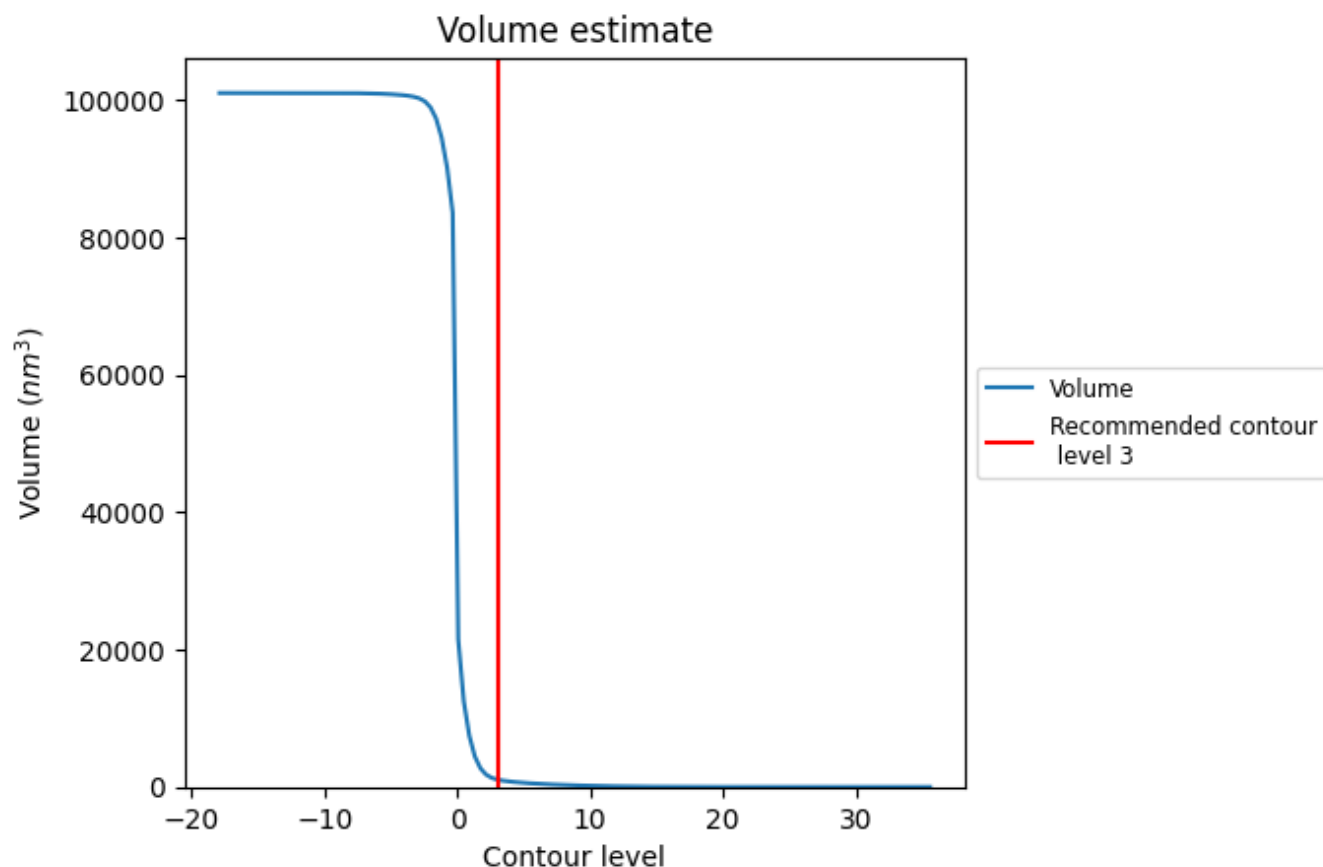
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

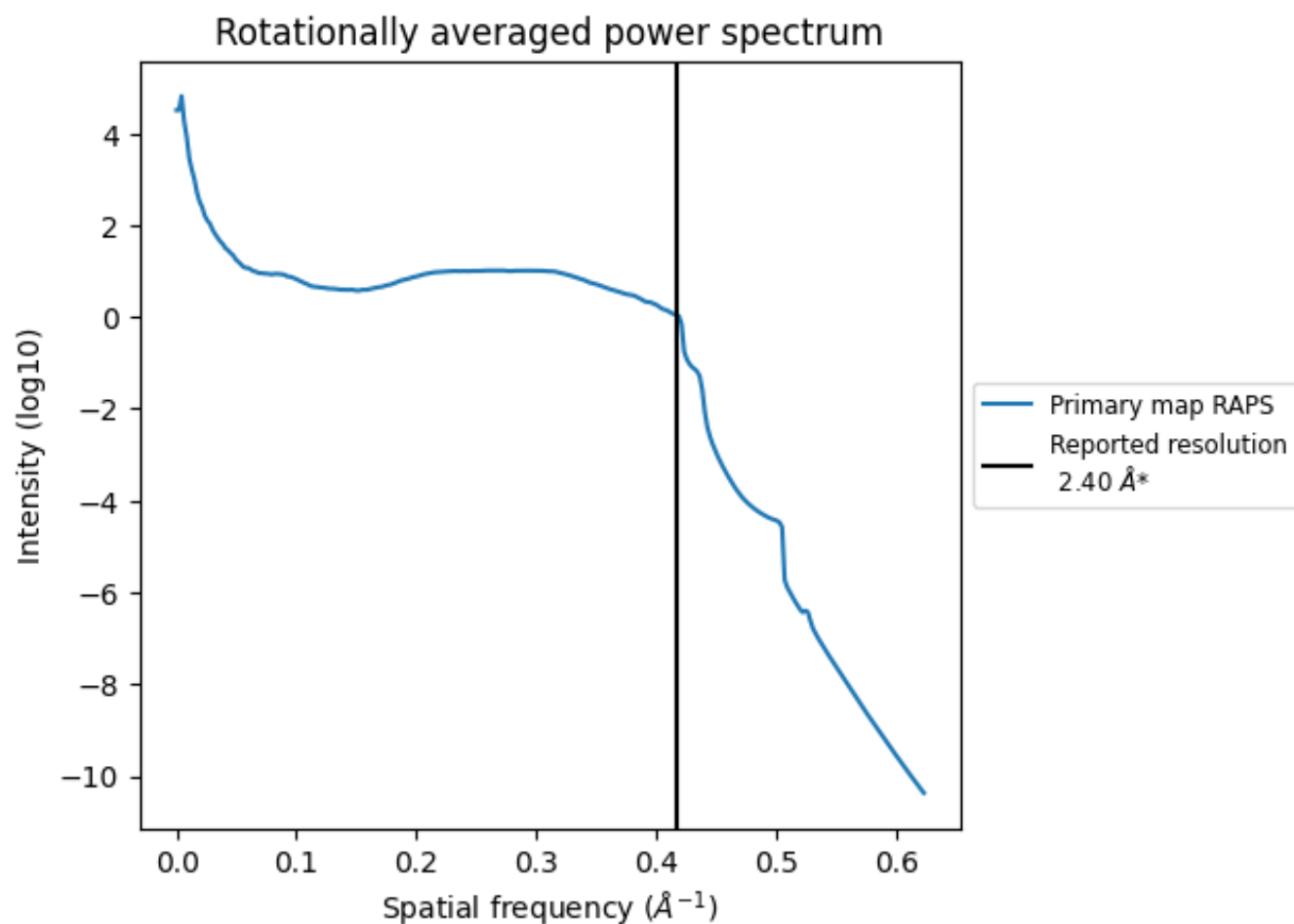
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1075 nm^3 ; this corresponds to an approximate mass of 971 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 0.417 Å⁻¹

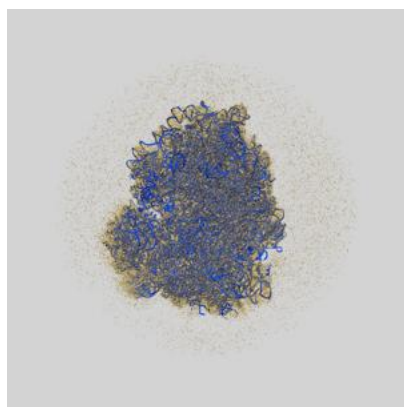
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

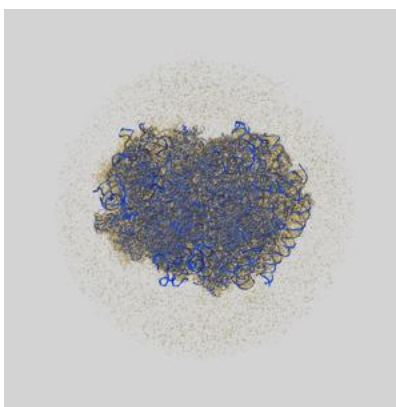
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18169 and PDB model 8Q87. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

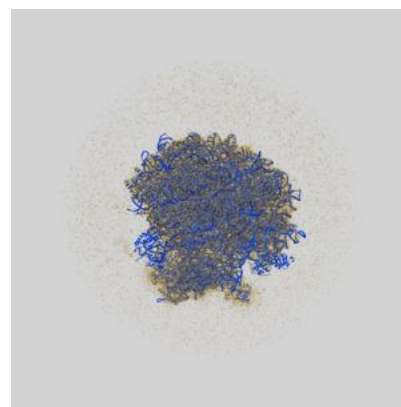
9.1 Map-model overlay [i](#)



X



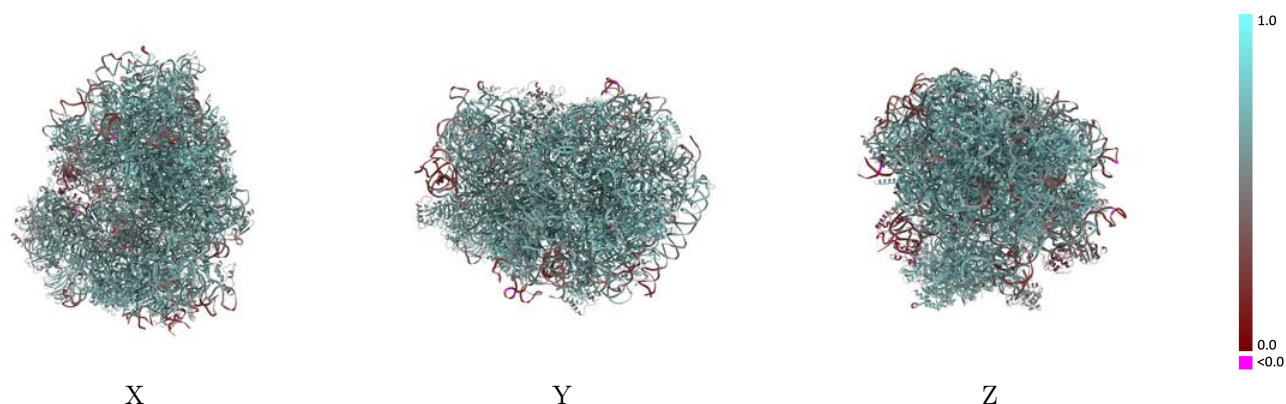
Y



Z

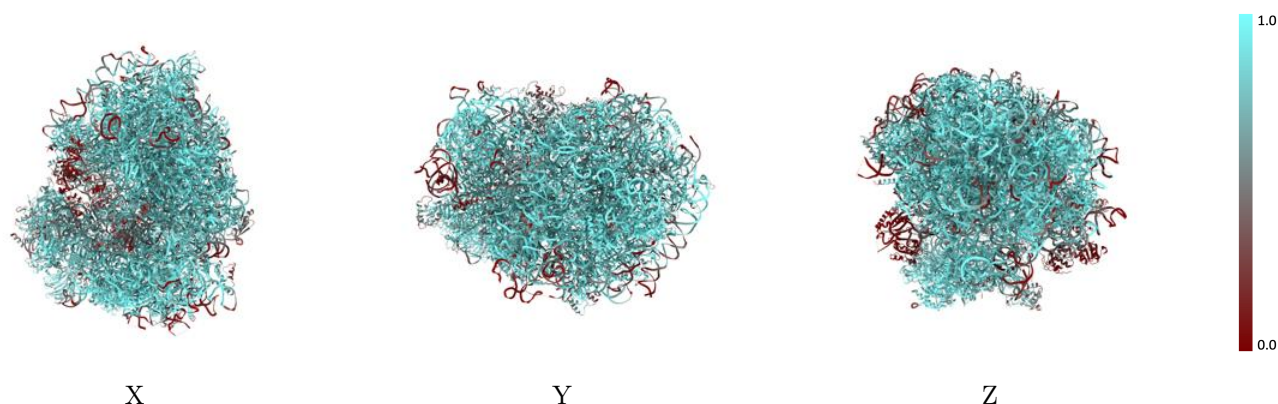
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



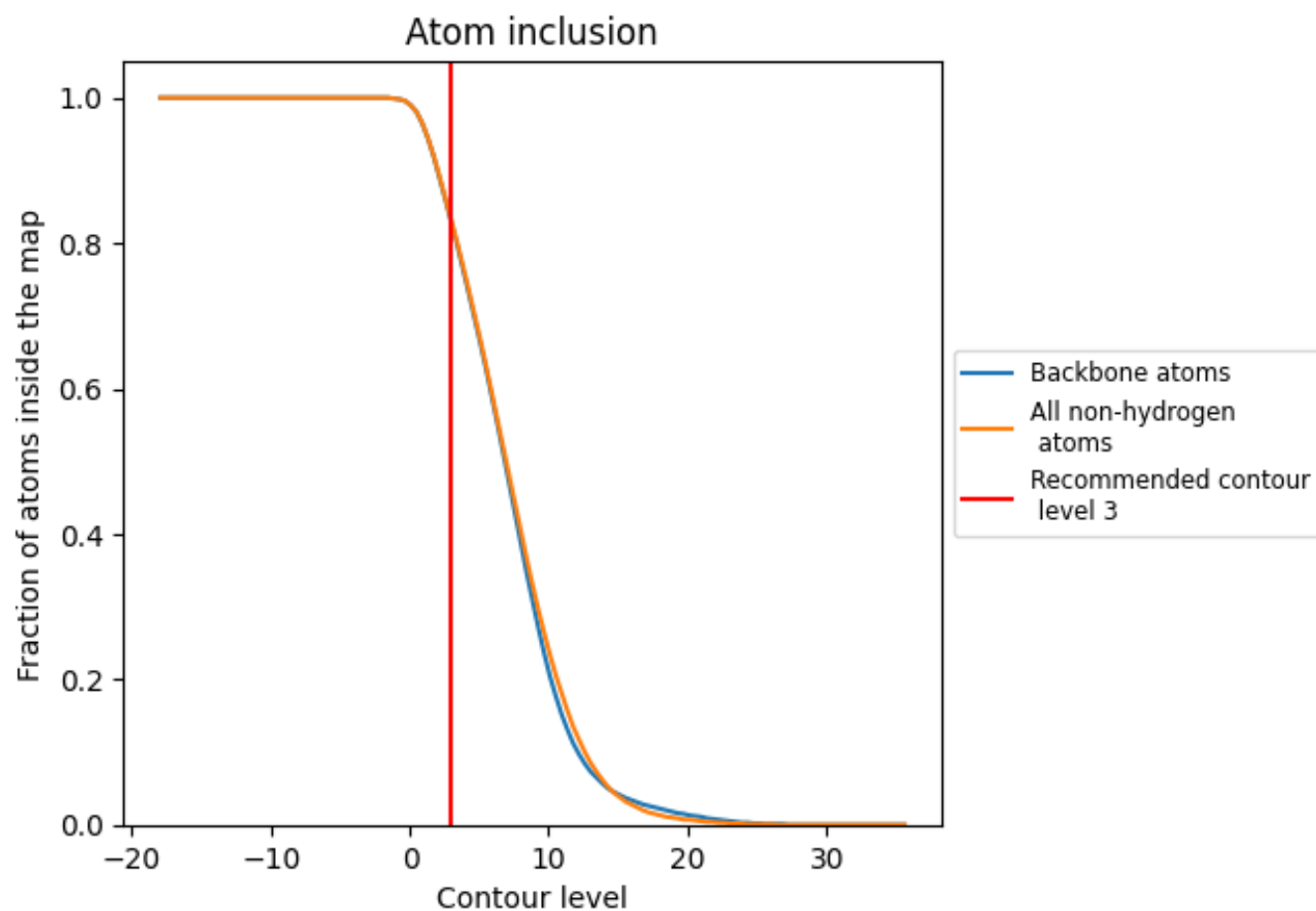
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.6210
A	 0.5550	 0.5490
A2	 0.8430	 0.6100
AA	 0.7770	 0.5950
AB	 0.6130	 0.5490
AC	 0.5290	 0.4900
AD	 0.6680	 0.5920
AE	 0.7950	 0.6360
AF	 0.8910	 0.6120
AG	 0.9460	 0.6720
AZ	 0.9240	 0.6550
Aa	 0.7530	 0.5970
Ab	 0.9070	 0.6600
Ac	 0.8050	 0.6120
Ad	 0.9730	 0.6610
Ae	 0.8900	 0.6330
Af	 0.7970	 0.5950
Ag	 0.6480	 0.5430
Ah	 0.8140	 0.6110
Ai	 0.9560	 0.6540
Aj	 0.9380	 0.6270
Ak	 0.8510	 0.6340
Al	 0.5210	 0.4410
Am	 0.8190	 0.6330
An	 0.7150	 0.6000
Ao	 0.8360	 0.6320
Ap	 0.9520	 0.6600
Aq	 0.7090	 0.5810
Ar	 0.8930	 0.6360
As	 0.9510	 0.6630
At	 0.8530	 0.5940
Au	 0.9390	 0.6510
Av	 0.9770	 0.6730
Aw	 0.8600	 0.6540
Ax	 0.9240	 0.6420



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Chain	Atom inclusion	Q-score
Ay	 0.9150	 0.6300
Az	 0.7250	 0.6440
B5	 0.8480	 0.6160
B7	 0.9710	 0.6670
B8	 0.8960	 0.6430
BA	 0.9500	 0.6980
BB	 0.9380	 0.6910
BC	 0.9400	 0.6880
BD	 0.8500	 0.6400
BE	 0.8610	 0.6510
BF	 0.9430	 0.6940
BG	 0.7900	 0.6220
BH	 0.9170	 0.6810
BI	 0.8870	 0.6640
BJ	 0.6850	 0.5990
BL	 0.8750	 0.6540
BM	 0.9460	 0.6900
BN	 0.9930	 0.7100
BO	 0.9520	 0.6890
BP	 0.9350	 0.6860
BQ	 0.9700	 0.7020
BR	 0.8430	 0.6510
BS	 0.9710	 0.6970
BT	 0.8890	 0.6670
BU	 0.5960	 0.5680
BV	 0.8720	 0.6810
BW	 0.8760	 0.6750
BX	 0.8990	 0.6610
BY	 0.9050	 0.6640
BZ	 0.8600	 0.6500
Ba	 0.9590	 0.7010
Bb	 0.7950	 0.6340
Bc	 0.8290	 0.6570
Bd	 0.8780	 0.6650
Be	 0.9620	 0.6960
Bf	 0.9650	 0.7040
Bg	 0.9220	 0.6730
Bh	 0.8900	 0.6600
Bi	 0.8690	 0.6590
Bj	 0.9780	 0.7000
Bk	 0.6550	 0.5910
Bl	 0.9050	 0.6660

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Chain	Atom inclusion	Q-score
Bm	 0.9380	 0.6810
Bo	 0.8970	 0.6760
Bp	 0.8640	 0.6760
Br	 0.9360	 0.6780
Bs	 0.1530	 0.4360
Bt	 0.0510	 0.2570
Bv	 0.0170	 0.2360
S	 0.6620	 0.6280
V	 0.6090	 0.5160