



wwPDB EM Validation Summary Report ⓘ

Sep 29, 2026 – 05:58 am BST

PDB ID : 30HI / pdb_000030hi
EMDB ID : EMD-57771
Title : Ternary complex of translating ribosome, NAC and NatB
Authors : Knejski, P.; Scaiola, A.; Leibundgut, M.; Ban, N.
Deposited on : 2026-04-25
Resolution : 3.20 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:

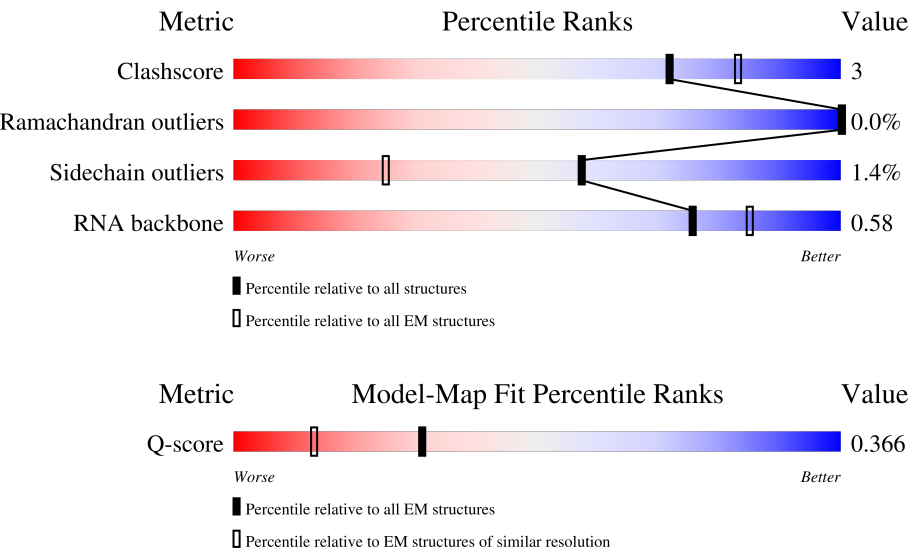
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.51

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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.



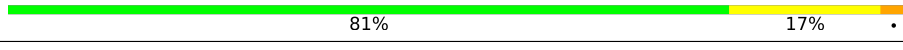
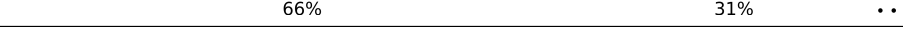
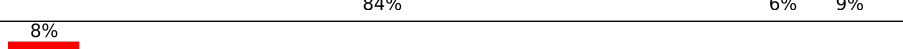
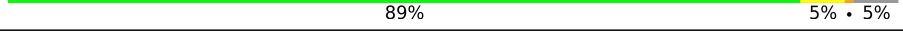
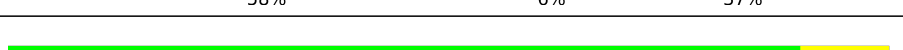
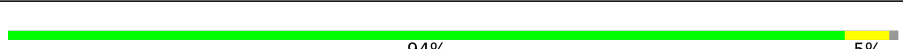
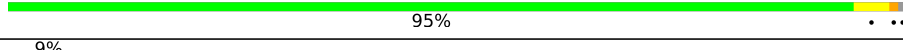
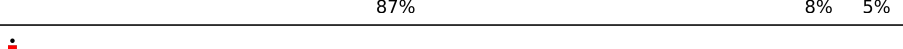
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	B1	60	
2	B2	76	
3	B4	6	

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Mol	Chain	Length	Quality of chain
4	B5	5069	
5	B7	119	
6	B8	157	
7	BA	257	
8	BB	403	
9	BC	427	
10	BD	297	
11	BE	288	
12	BF	248	
13	BG	266	
14	BH	192	
15	BI	214	
16	BJ	178	
17	BL	211	
18	BM	215	
19	BN	204	
20	BO	203	
21	BP	184	
22	BQ	188	
23	BR	196	
24	BS	176	
25	BT	160	
26	BU	128	
27	BV	140	
28	BW	157	

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Mol	Chain	Length	Quality of chain
29	BX	156	
30	BY	145	
31	BZ	136	
32	Ba	148	
33	Bb	159	
34	Bc	115	
35	Bd	125	
36	Be	135	
37	Bf	110	
38	Bg	117	
39	Bh	123	
40	Bi	105	
41	Bj	97	
42	Bk	70	
43	Bl	51	
44	Bm	128	
45	Bo	106	
46	Bp	92	
47	Br	137	
48	Bs	317	
49	Bt	165	
50	Bu	215	
51	Bv	162	
52	Bw	978	
53	By	178	

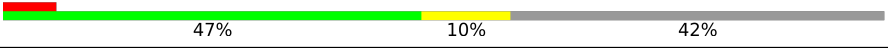
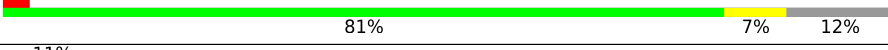
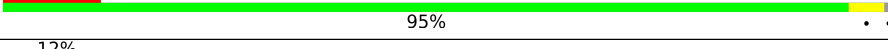
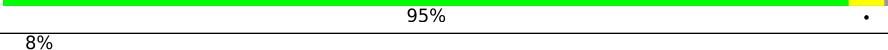
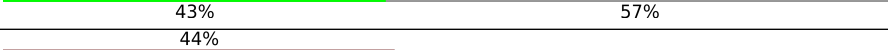
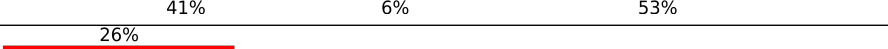
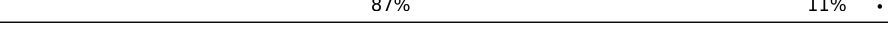
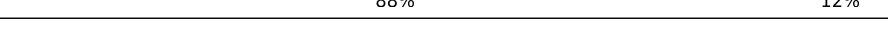
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Mol	Chain	Length	Quality of chain
54	Bz	217	
55	A2	1869	
56	AA	295	
57	AB	264	
58	AC	293	
59	AD	243	
60	AE	263	
61	AF	204	
62	AG	249	
63	AH	194	
64	AI	208	
65	AJ	194	
66	AK	165	
67	AL	158	
68	AM	132	
69	AN	151	
70	AO	151	
71	AP	145	
72	AQ	146	
73	AR	135	
74	AS	152	
75	AT	145	
76	AU	119	
77	AV	84	
78	AW	130	

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Mol	Chain	Length	Quality of chain
79	AX	143	
80	AY	133	
81	AZ	125	
82	Aa	115	
83	Ab	84	
84	Ac	69	
85	Ad	56	
86	Ae	133	
87	Af	156	
88	Ag	317	
89	Ah	25	

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 232781 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Xbp1u stalled ANXA4 nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B1	34	Total	C	N	O	S	0	0
			251	163	45	40	3		

- Molecule 2 is a RNA chain called P-site Met tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B2	76	Total	C	N	O	P	0	0
			1638	736	288	538	76		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B4	6	Total	C	N	O	P	0	0
			127	57	21	43	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B5	3683	Total	C	N	O	P	0	0
			79011	35224	14438	25666	3683		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B7	119	Total	C	N	O	P	0	0
			2538	1131	451	837	119		

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B8	156	Total	C	N	O	P	0	0
			3320	1482	585	1097	156		

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BA	248	Total	C	N	O	S	0	0
			1899	1189	389	315	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 9 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BC	367	Total	C	N	O	S	0	0
			2919	1835	582	488	14		

- Molecule 10 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BD	293	Total	C	N	O	S	0	0
			2386	1510	435	427	14		

- Molecule 11 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BE	223	Total	C	N	O	S	0	0
			1793	1154	341	294	4		

- Molecule 12 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BF	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BG	240	Total	C	N	O	S	0	0
			1927	1229	370	324	4		

- Molecule 14 is a protein called 60S ribosomal protein L9.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BI	205	Total	C	N	O	S	0	0
			1660	1054	319	274	13		

- Molecule 16 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BJ	171	Total	C	N	O	S	0	0
			1371	867	256	242	6		

- Molecule 17 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BL	200	Total	C	N	O	S	0	0
			1621	1016	338	263	4		

- Molecule 18 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 21 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 22 is a protein called 60S ribosomal protein L18.

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

- Molecule 23 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 24 is a protein called 60S ribosomal protein L18a.

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

- Molecule 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BU	104	Total	C	N	O	S	0	0
			851	544	150	155	2		

- Molecule 27 is a protein called 60S ribosomal protein L23.

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

- Molecule 28 is a protein called 60S ribosomal protein L24.

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

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BX	126	Total	C	N	O	S	0	0
			1031	658	196	176	1		

- Molecule 30 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BY	132	Total	C	N	O	S	0	0
			1102	692	223	184	3		

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ba	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 33 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bb	99	Total	C	N	O	S	0	0
			809	503	177	125	4		

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bc	106	Total	C	N	O	S	0	0
			824	523	146	148	7		

- Molecule 35 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bd	107	Total	C	N	O	S	0	0
			886	561	171	152	2		

- Molecule 36 is a protein called 60S ribosomal protein L32.

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

- Molecule 37 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bg	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bi	99	Total	C	N	O	S	0	0
			813	509	173	126	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bk	68	Total	C	N	O	S	0	0
			559	360	101	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bl	50	Total	C	N	O	S	1	0
			451	286	100	64	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bm	51	Total	C	N	O	S	0	0
			419	260	88	65	6		

- Molecule 45 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bo	102	Total	C	N	O	S	0	0
			835	523	171	135	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bp	88	Total	C	N	O	S	0	0
			681	430	131	113	7		

- Molecule 47 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Br	126	Total	C	N	O	S	0	0
			1005	624	207	169	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Br	2	ACE	-	acetylation	UNP P46779

- Molecule 48 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bs	196	Total	C	N	O	S	0	0
			1506	958	263	276	9		

- Molecule 49 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 50 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bu	107	Total	C	N	O	S	0	0
			832	519	151	158	4		

- Molecule 51 is a protein called Isoform 2 of Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bv	109	Total	C	N	O	S	0	0
			846	528	157	157	4		

- Molecule 52 is a protein called N-alpha-acetyltransferase 25, NatB auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bw	949	Total	C	N	O	S	0	0
			7729	4940	1303	1447	39		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bw	-5	MET	-	initiating methionine	UNP Q14CX7
Bw	-4	HIS	-	expression tag	UNP Q14CX7
Bw	-3	HIS	-	expression tag	UNP Q14CX7
Bw	-2	HIS	-	expression tag	UNP Q14CX7
Bw	-1	HIS	-	expression tag	UNP Q14CX7
Bw	0	HIS	-	expression tag	UNP Q14CX7
Bw	1	HIS	-	expression tag	UNP Q14CX7

- Molecule 53 is a protein called N-alpha-acetyltransferase 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	By	178	Total	C	N	O	S	0	0
			1437	923	237	270	7		

- Molecule 54 is a protein called 60S ribosomal protein L10a.

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

- Molecule 55 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	A2	1779	Total	C	N	O	P	0	0
			38027	16999	6818	12431	1779		

- Molecule 56 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AA	217	Total	C	N	O	S	0	0
			1708	1085	299	316	8		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 57 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AB	223	Total	C	N	O	S	0	0
			1806	1146	326	320	14		

- Molecule 58 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AC	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 59 is a protein called 40S ribosomal protein S3.

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

- Molecule 60 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 61 is a protein called 40S ribosomal protein S5.

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

- Molecule 62 is a protein called 40S ribosomal protein S6.

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

- Molecule 63 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AH	188	Total	C	N	O	S	0	0
			1515	966	279	269	1		

- Molecule 64 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AI	203	Total	C	N	O	S	0	0
			1670	1048	329	288	5		

- Molecule 65 is a protein called 40S ribosomal protein S9.

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

- Molecule 66 is a protein called 40S ribosomal protein S10.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 68 is a protein called 40S ribosomal protein S12.

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

- Molecule 69 is a protein called 40S ribosomal protein S13.

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

- Molecule 70 is a protein called 40S ribosomal protein S14.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	138	IAS	ASP	modified residue	UNP P62263

- Molecule 71 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AP	127	Total	C	N	O	S	0	0
			1044	663	197	177	7		

- Molecule 72 is a protein called 40S ribosomal protein S16.

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

- Molecule 73 is a protein called 40S ribosomal protein S17.

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

- Molecule 74 is a protein called Small ribosomal subunit protein uS13.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 75 is a protein called Small ribosomal subunit protein eS19.

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

- Molecule 76 is a protein called 40S ribosomal protein S20.

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

- Molecule 77 is a protein called Small ribosomal subunit protein eS21.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 78 is a protein called 40S ribosomal protein S15a.

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

- Molecule 79 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AX	141	Total	C	N	O	S	1	0
			1105	698	220	184	3		

- Molecule 80 is a protein called 40S ribosomal protein S24.

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

- Molecule 81 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 82 is a protein called 40S ribosomal protein S26.

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

- Molecule 83 is a protein called 40S ribosomal protein S27.

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

- Molecule 84 is a protein called 40S ribosomal protein S28.

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

- Molecule 85 is a protein called 40S ribosomal protein S29.

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

- Molecule 86 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ae	57	Total	C	N	O	S	0	0
			451	279	99	72	1		

- Molecule 87 is a protein called Ubiquitin.

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

- Molecule 88 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 89 is a protein called 60S ribosomal protein L41.

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

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

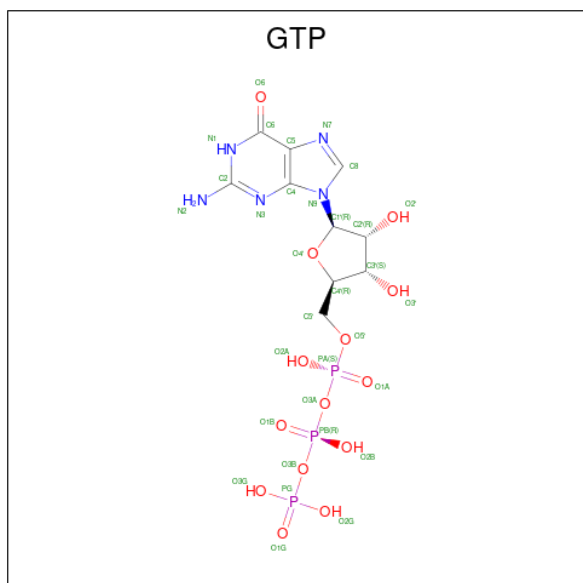
Mol	Chain	Residues	Atoms		AltConf
90	B5	302	Total	Mg	0
			302	302	
90	B7	6	Total	Mg	0
			6	6	
90	B8	9	Total	Mg	0
			9	9	
90	BA	3	Total	Mg	0
			3	3	
90	BN	1	Total	Mg	0
			1	1	
90	BP	1	Total	Mg	0
			1	1	

Continued on next page...

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Mol	Chain	Residues	Atoms		AltConf
90	BV	1	Total	Mg	0
			1	1	
90	Ba	1	Total	Mg	0
			1	1	
90	Bc	1	Total	Mg	0
			1	1	
90	Be	1	Total	Mg	0
			1	1	
90	Bf	1	Total	Mg	0
			1	1	
90	Bg	1	Total	Mg	0
			1	1	
90	A2	122	Total	Mg	0
			122	122	
90	AI	1	Total	Mg	0
			1	1	
90	AQ	1	Total	Mg	0
			1	1	
90	AX	1	Total	Mg	0
			1	1	

- Molecule 91 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

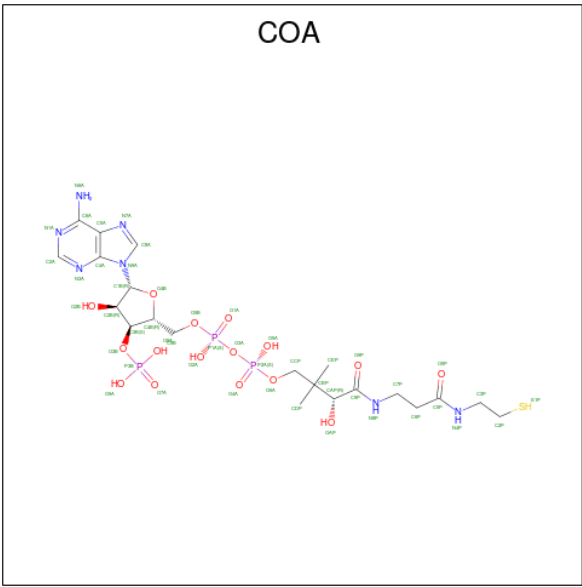


Mol	Chain	Residues	Atoms					AltConf
91	B7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
92	Bg	1	Total	Zn	0
			1	1	
92	Bj	1	Total	Zn	0
			1	1	
92	Bm	1	Total	Zn	0
			1	1	
92	Bo	1	Total	Zn	0
			1	1	
92	Bp	1	Total	Zn	0
			1	1	
92	Aa	1	Total	Zn	0
			1	1	
92	Ad	1	Total	Zn	0
			1	1	
92	Af	1	Total	Zn	0
			1	1	

- Molecule 93 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



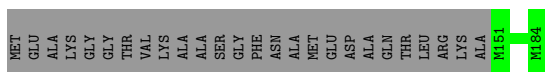
Mol	Chain	Residues	Atoms					AltConf	
93	By	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

3 Residue-property plots [i](#)

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

- Molecule 1: Xbp1u stalled ANXA4 nascent chain

Chain B1: 



- Molecule 2: P-site Met tRNA

Chain B2: 

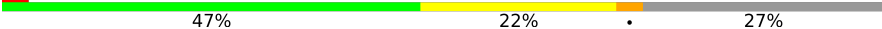


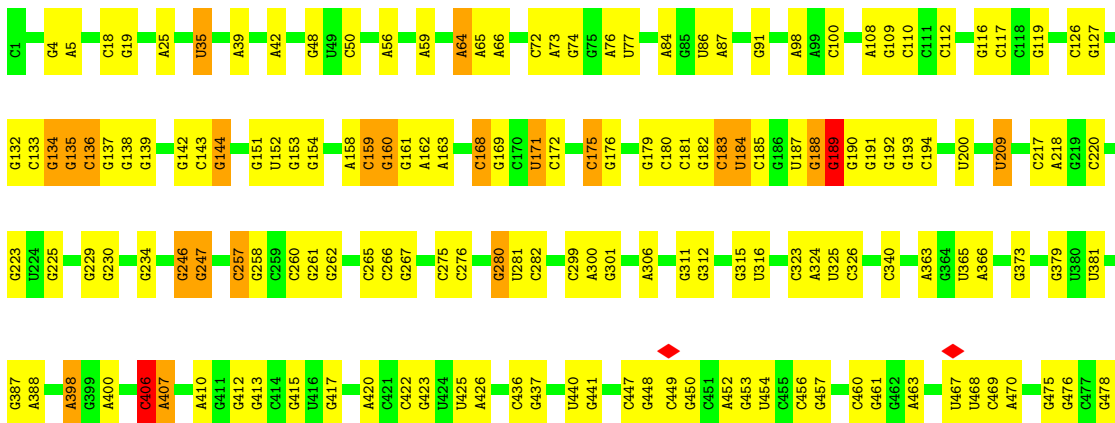
- Molecule 3: mRNA

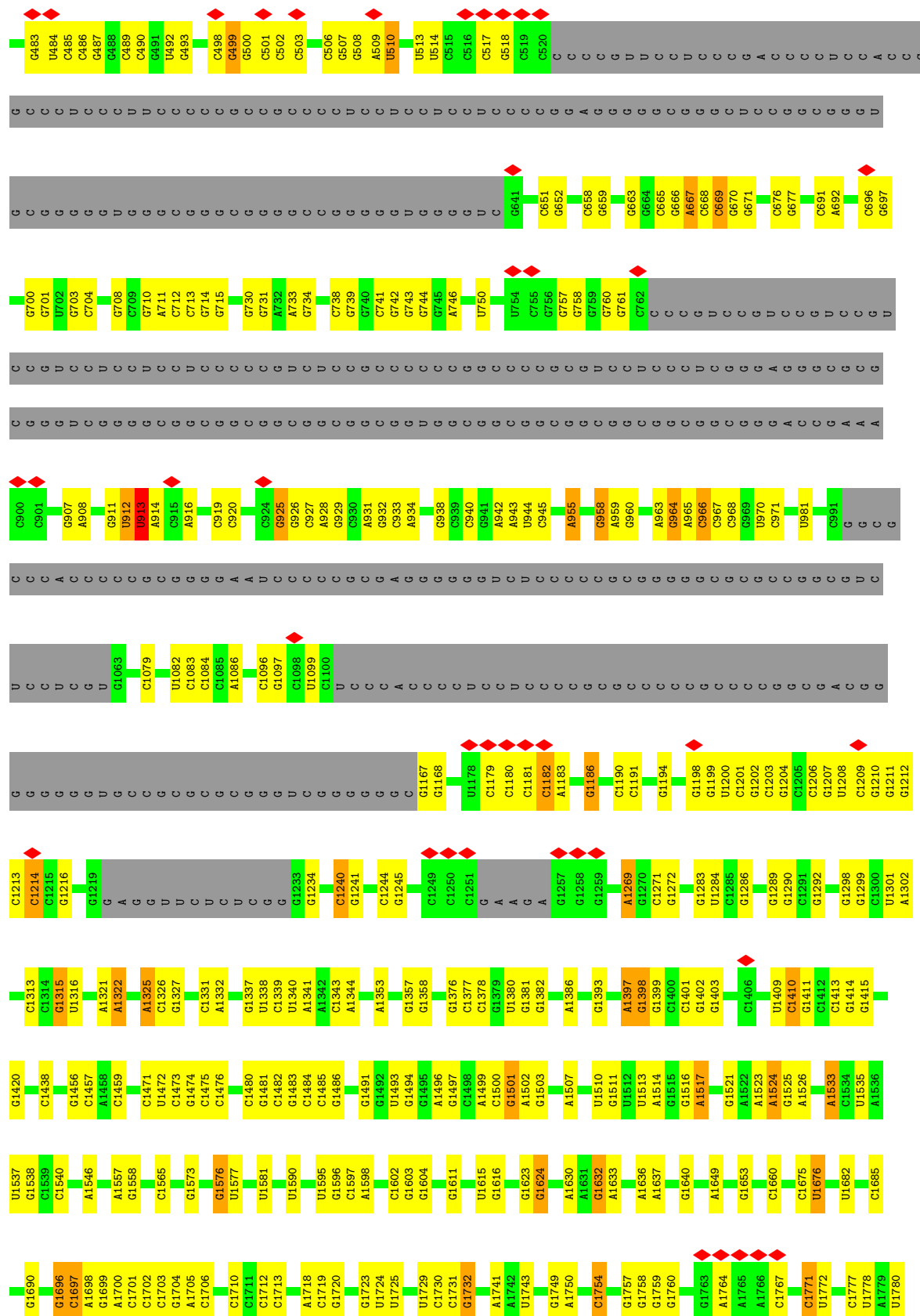
Chain B4: 

There are no outlier residues recorded for this chain.

- Molecule 4: 28S rRNA

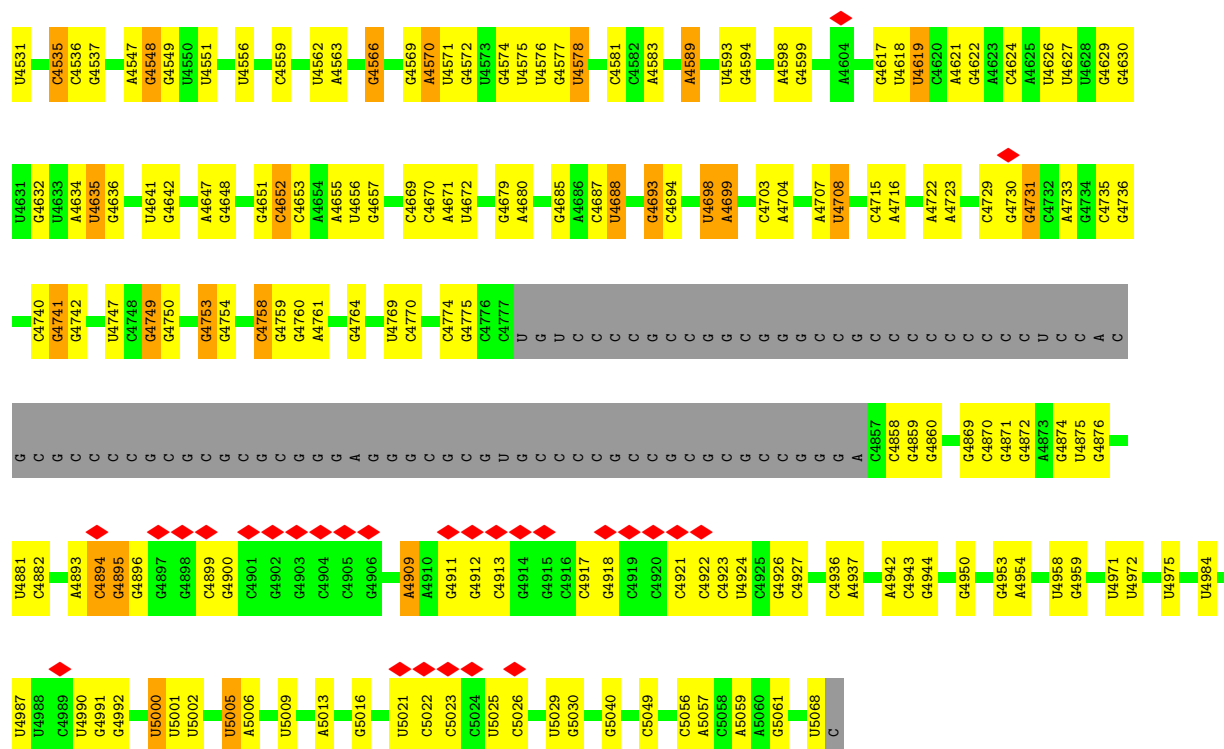
Chain B5: 











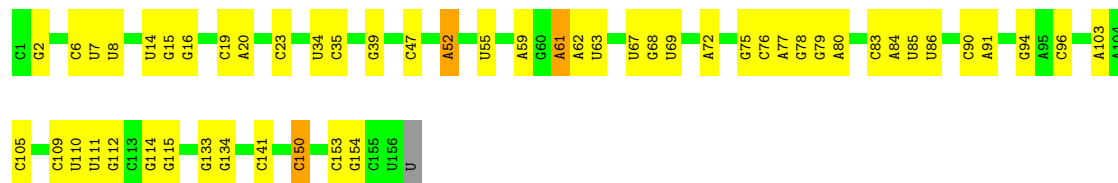
• Molecule 5: 5S rRNA

Chain B7: 81% 17% .



• Molecule 6: 5.8S rRNA

Chain B8: 66% 31% ..



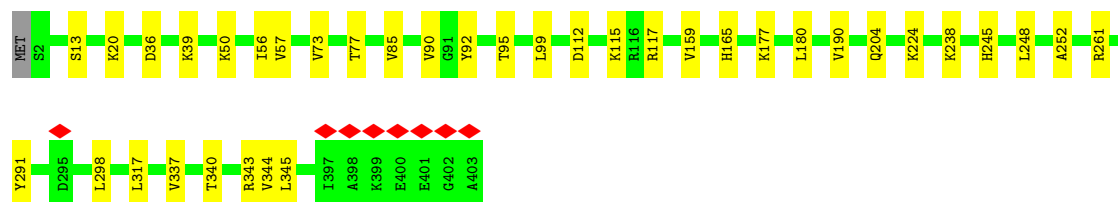
• Molecule 7: Large ribosomal subunit protein uL2

Chain BA: 86% 10% .

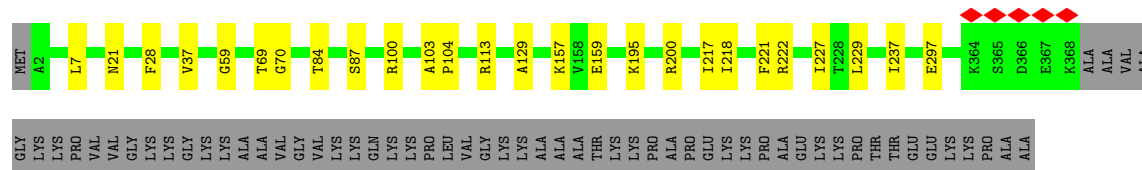
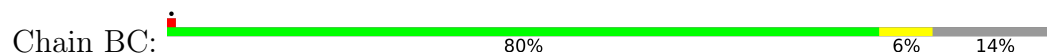


• Molecule 8: Large ribosomal subunit protein uL3

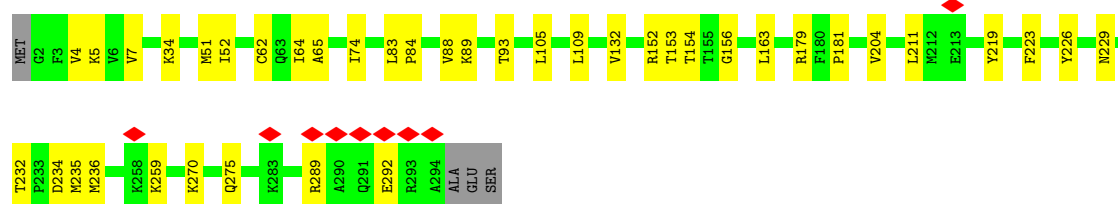
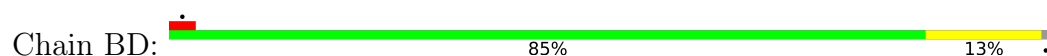
Chain BB: 91% 9%



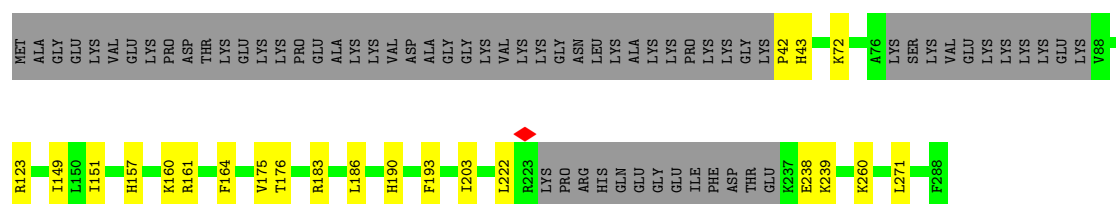
- Molecule 9: 60S ribosomal protein L4



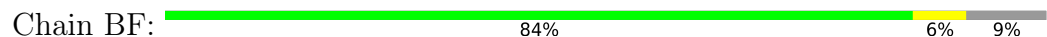
- Molecule 10: 60S ribosomal protein L5



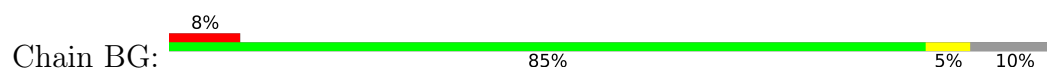
- Molecule 11: Large ribosomal subunit protein eL6



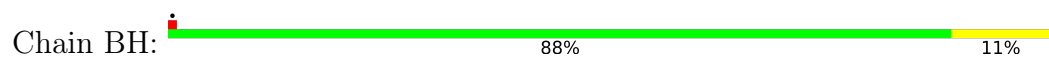
- Molecule 12: Large ribosomal subunit protein uL30



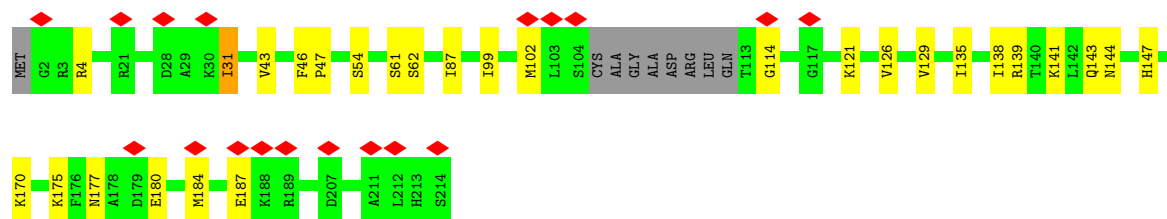
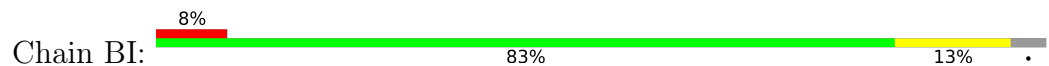
- Molecule 13: 60S ribosomal protein L7a



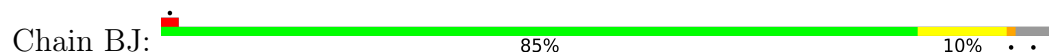
- Molecule 14: 60S ribosomal protein L9



- Molecule 15: 60S ribosomal protein L10



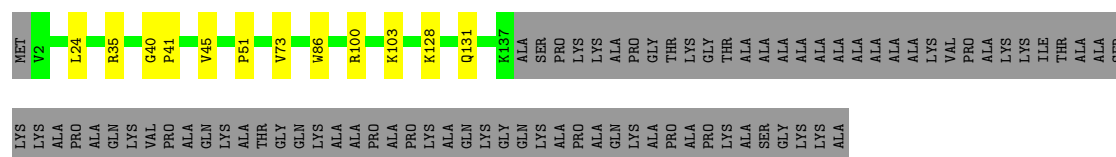
- Molecule 16: 60S ribosomal protein L11



- Molecule 17: 60S ribosomal protein L13



- Molecule 18: 60S ribosomal protein L14

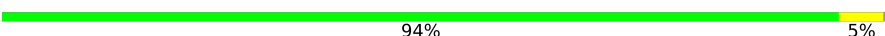


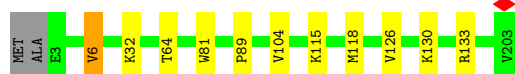
- Molecule 19: 60S ribosomal protein L15

Chain BN:  89% 10%



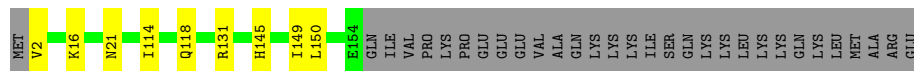
- Molecule 20: 60S ribosomal protein L13a

Chain BO:  94% 5%

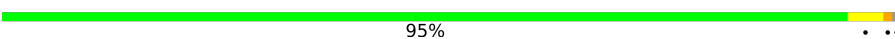


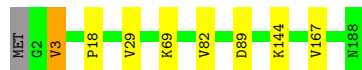
- Molecule 21: 60S ribosomal protein L17

Chain BP:  78% 5% 17%



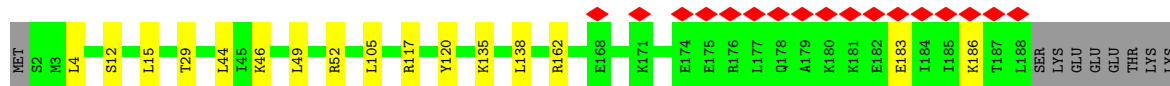
- Molecule 22: 60S ribosomal protein L18

Chain BQ:  95%



- Molecule 23: 60S ribosomal protein L19

Chain BR:  9% 87% 8% 5%

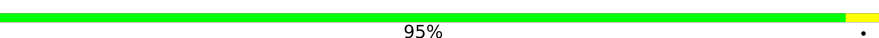


- Molecule 24: 60S ribosomal protein L18a

Chain BS:  93% 7%

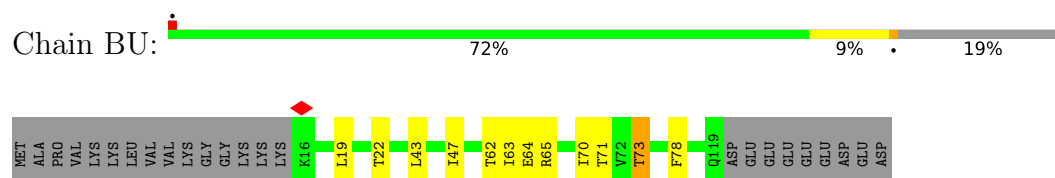


- Molecule 25: 60S ribosomal protein L21

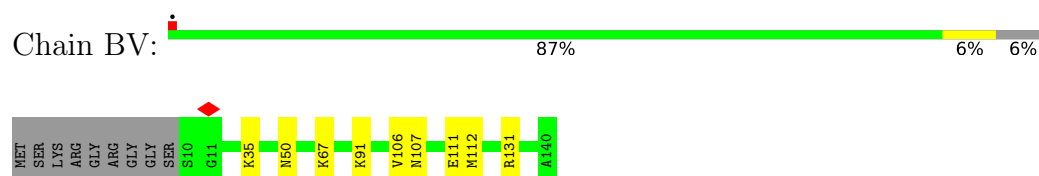
Chain BT:  95%



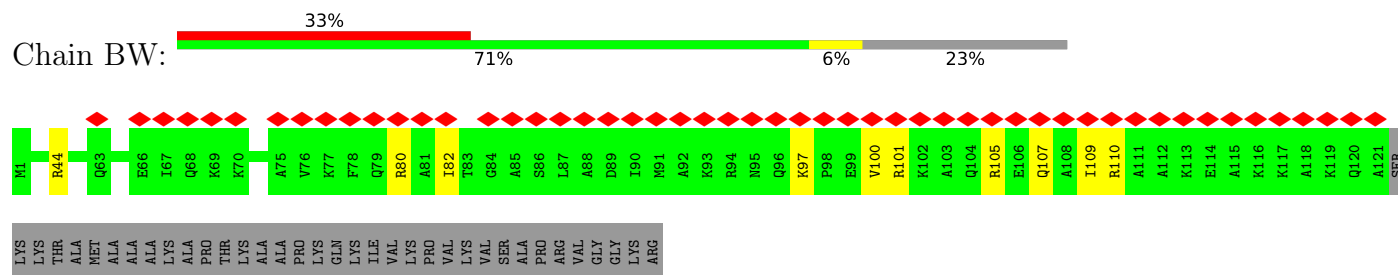
- Molecule 26: 60S ribosomal protein L22



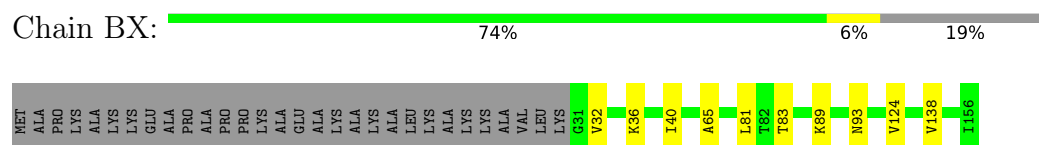
- Molecule 27: 60S ribosomal protein L23



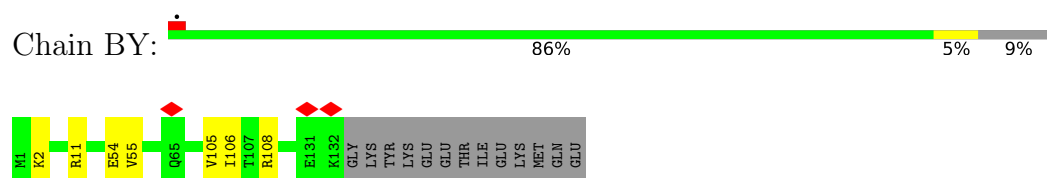
- Molecule 28: 60S ribosomal protein L24



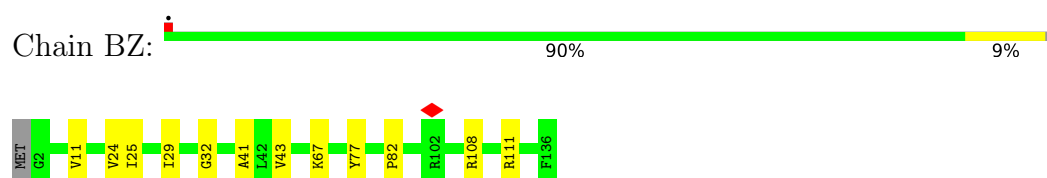
- Molecule 29: 60S ribosomal protein L23a



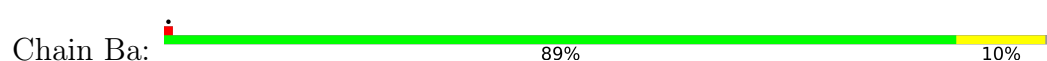
- Molecule 30: 60S ribosomal protein L26

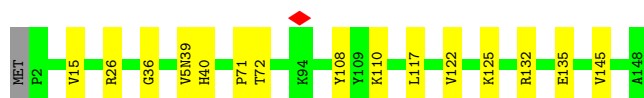


- Molecule 31: 60S ribosomal protein L27

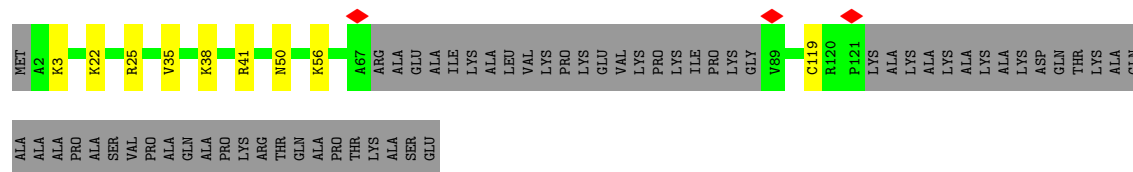


- Molecule 32: Large ribosomal subunit protein uL15

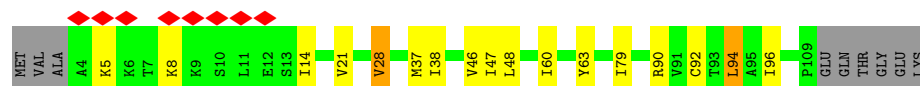
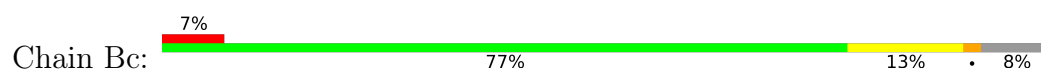




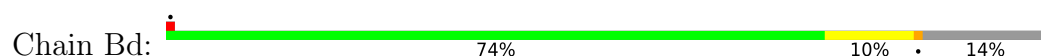
- Molecule 33: Large ribosomal subunit protein eL29



- Molecule 34: 60S ribosomal protein L30



- Molecule 35: 60S ribosomal protein L31



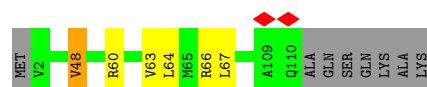
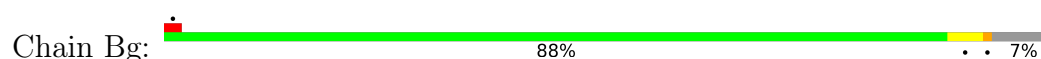
- Molecule 36: 60S ribosomal protein L32



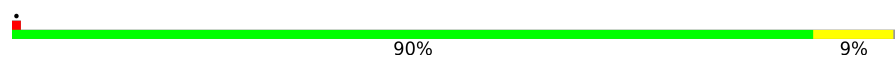
- Molecule 37: Large ribosomal subunit protein eL33



- Molecule 38: 60S ribosomal protein L34

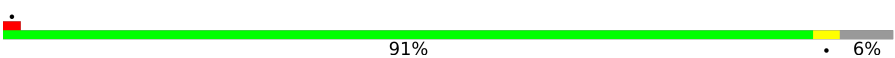


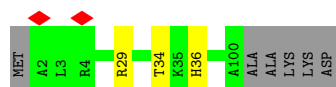
- Molecule 39: 60S ribosomal protein L35

Chain Bh: 



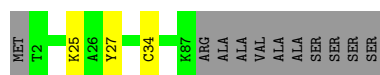
- Molecule 40: 60S ribosomal protein L36

Chain Bi: 



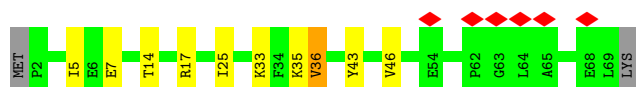
- Molecule 41: Large ribosomal subunit protein eL37

Chain Bj: 



- Molecule 42: 60S ribosomal protein L38

Chain Bk: 



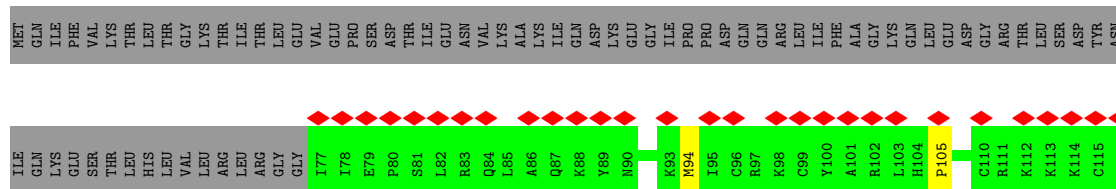
- Molecule 43: 60S ribosomal protein L39

Chain Bl: 



- Molecule 44: Ubiquitin-60S ribosomal protein L40

Chain Bm: 



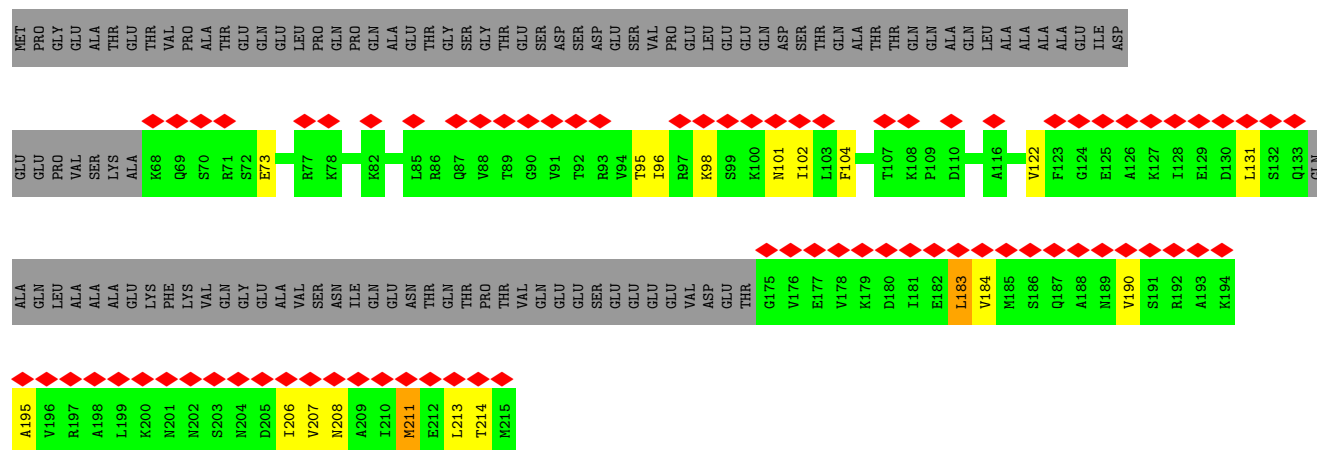
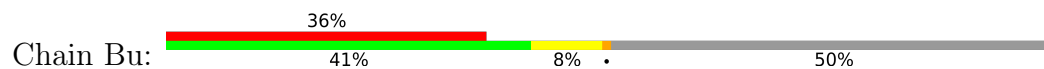
- Molecule 45: Large ribosomal subunit protein eL42

Chain Bo: 

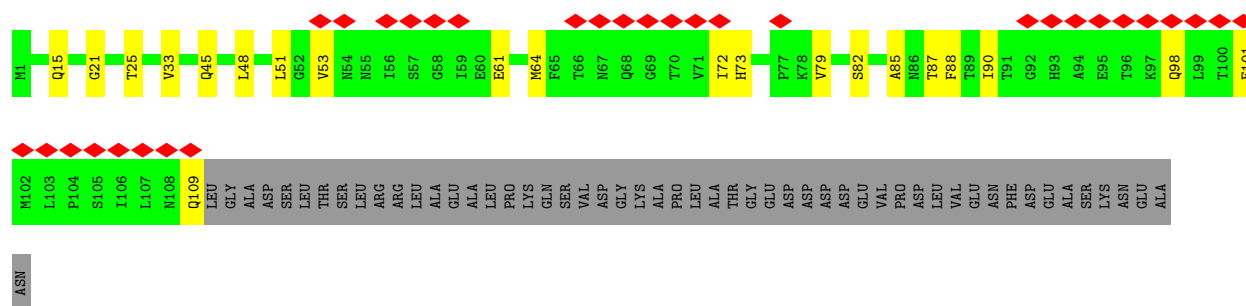




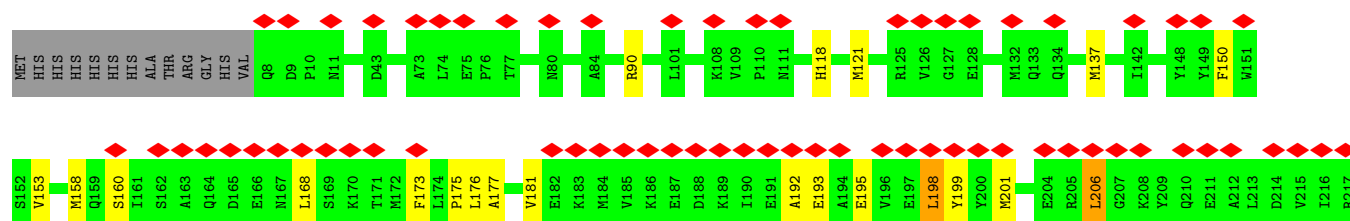
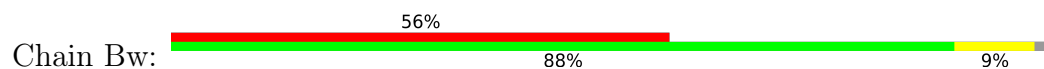
• Molecule 50: Nascent polypeptide-associated complex subunit alpha

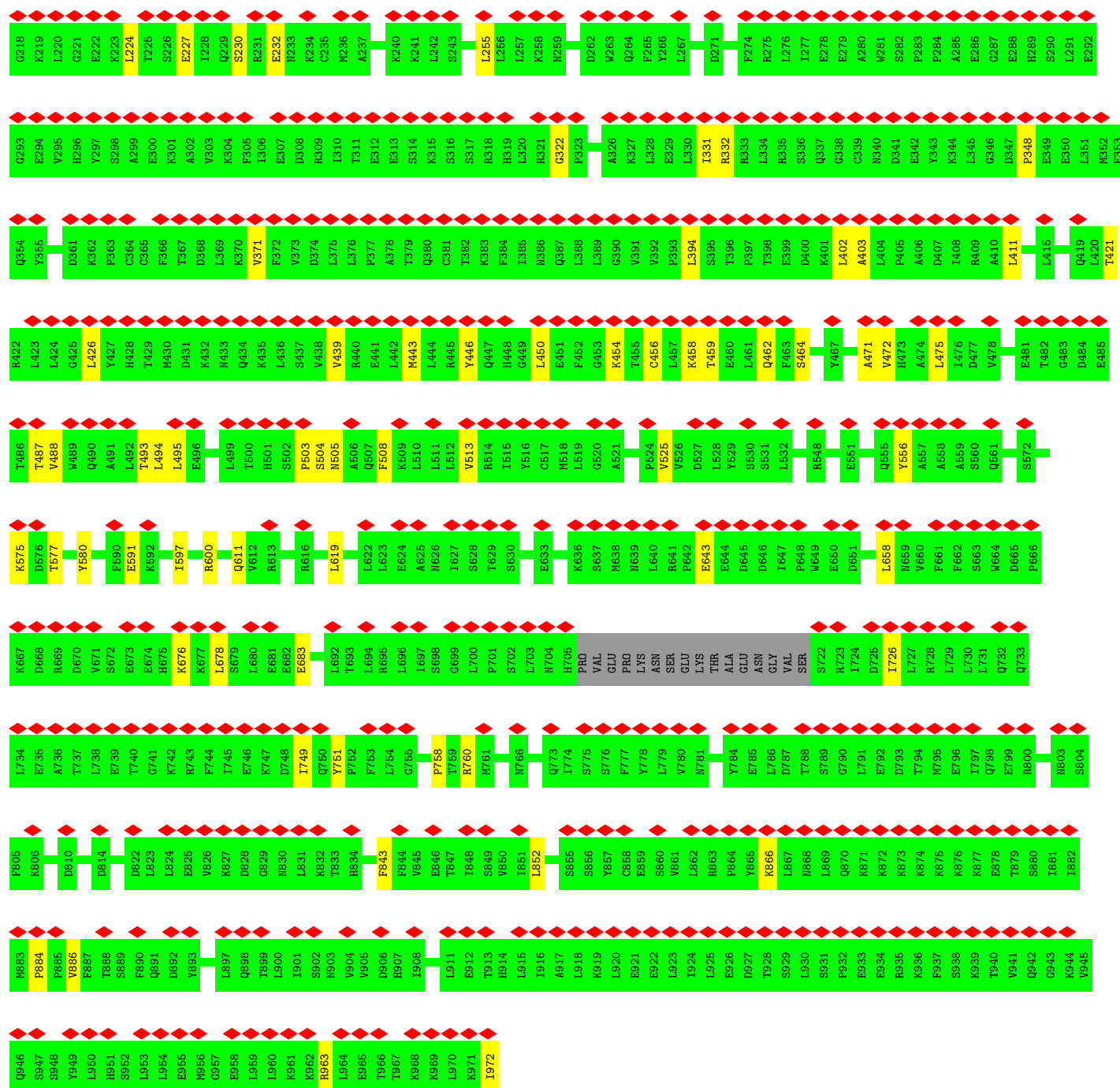


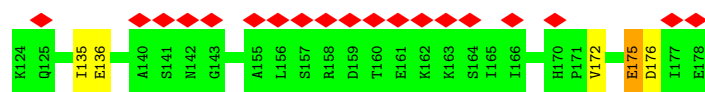
• Molecule 51: Isoform 2 of Transcription factor BTF3



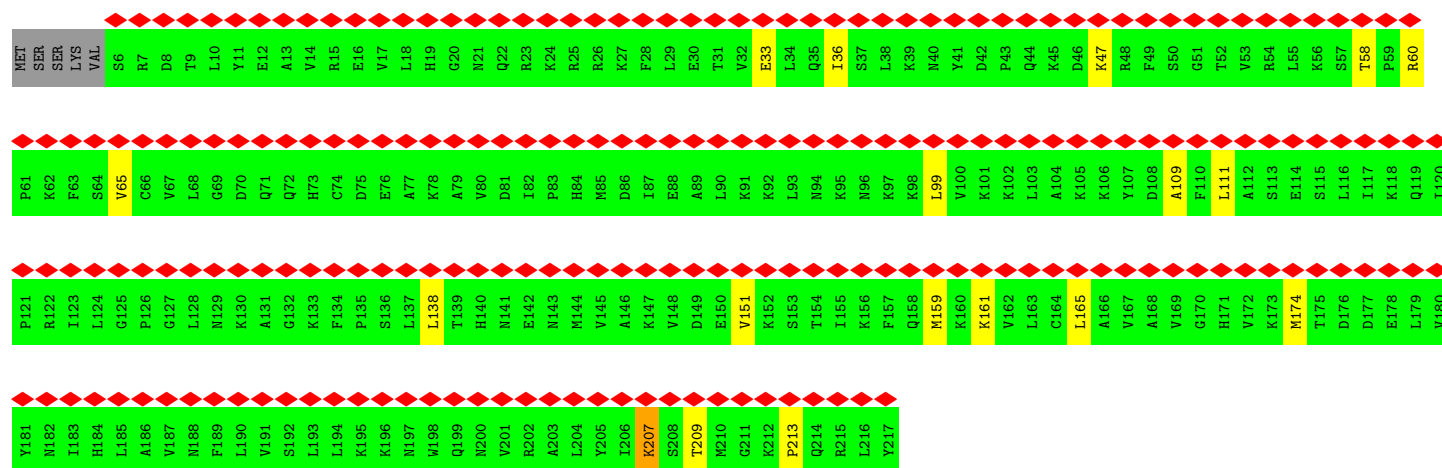
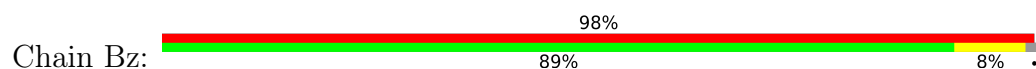
• Molecule 52: N-alpha-acetyltransferase 25, NatB auxiliary subunit



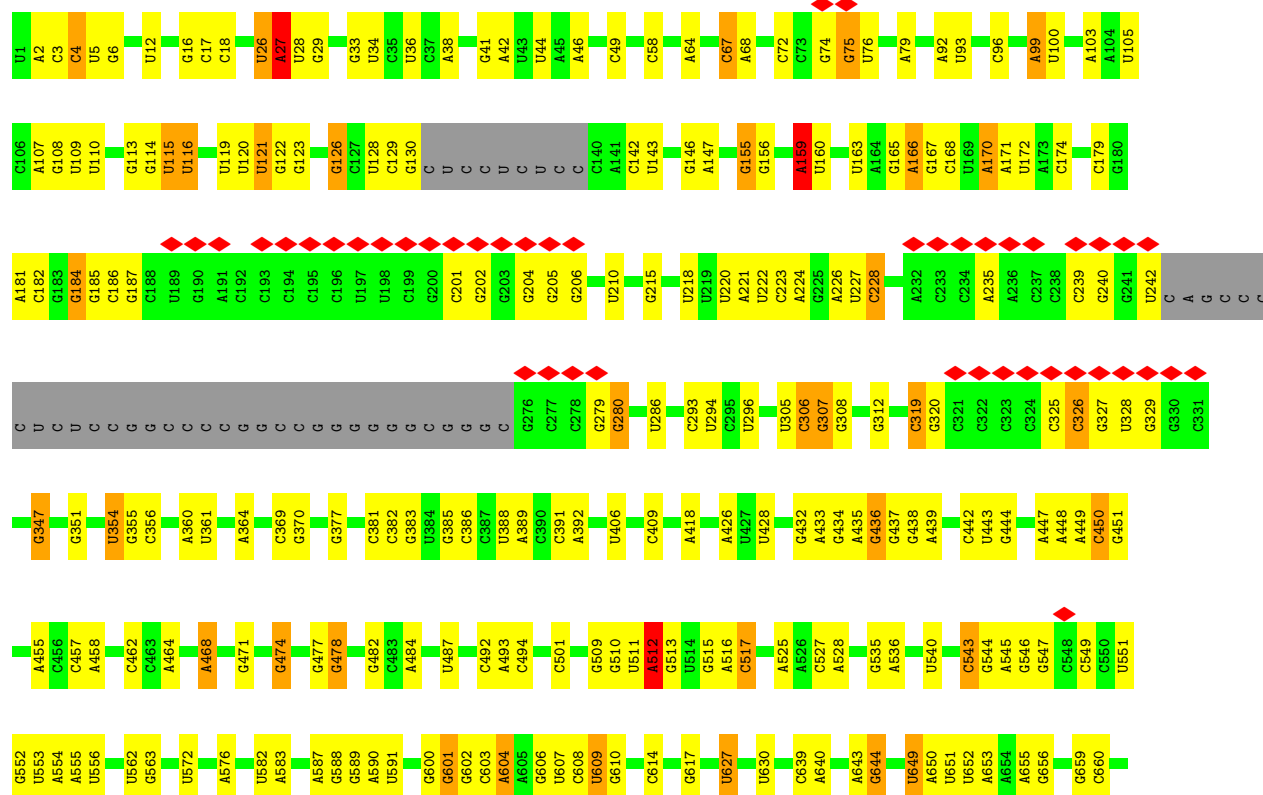


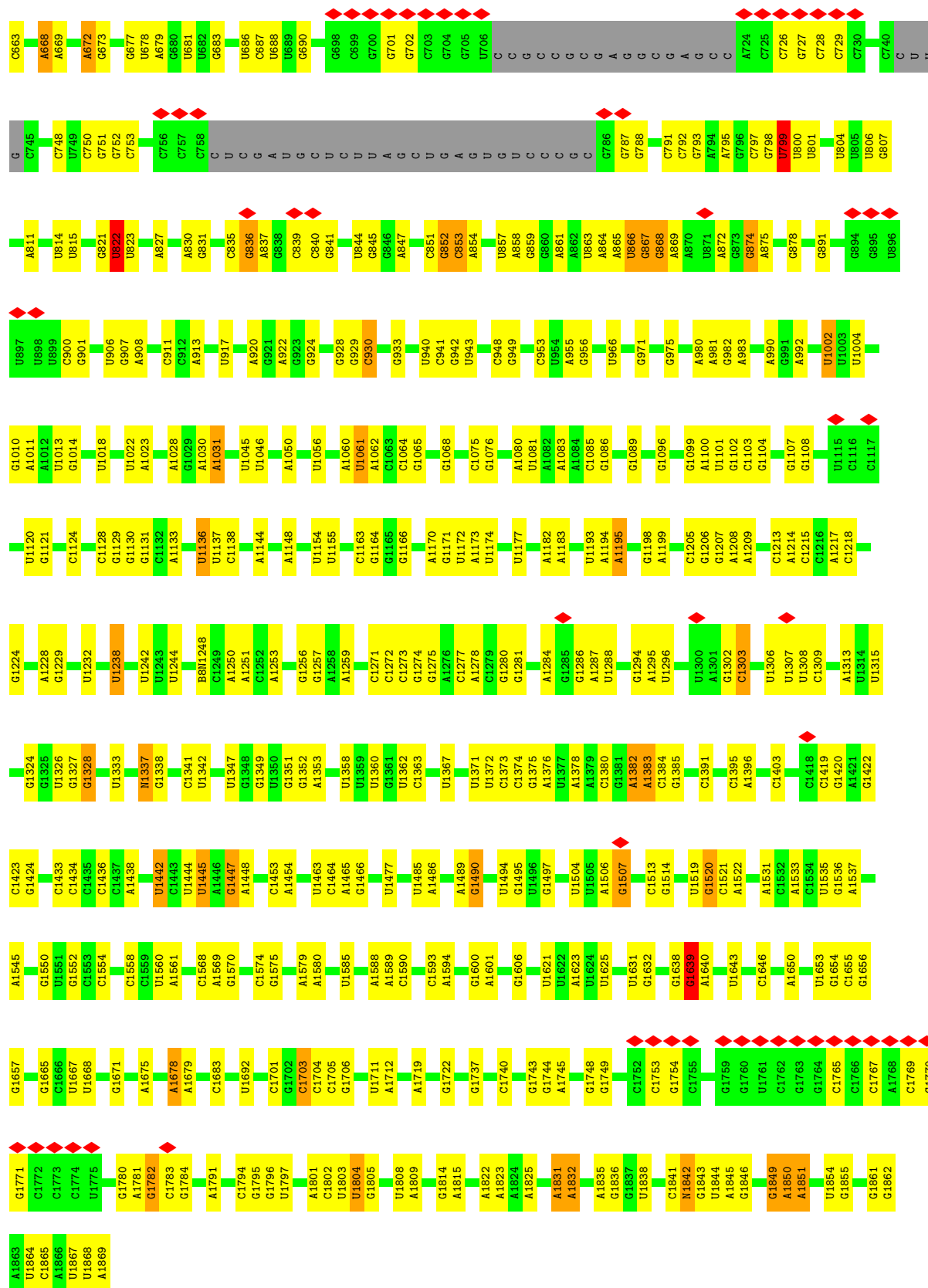


• Molecule 54: 60S ribosomal protein L10a

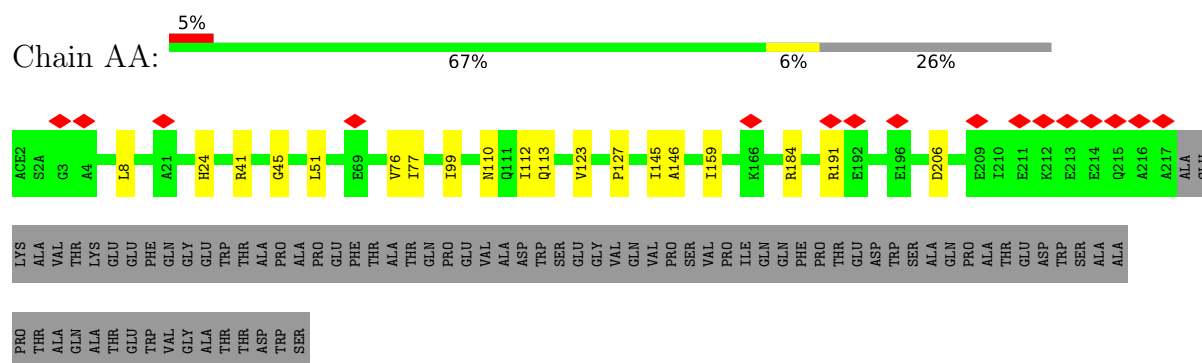


• Molecule 55: 18S rRNA

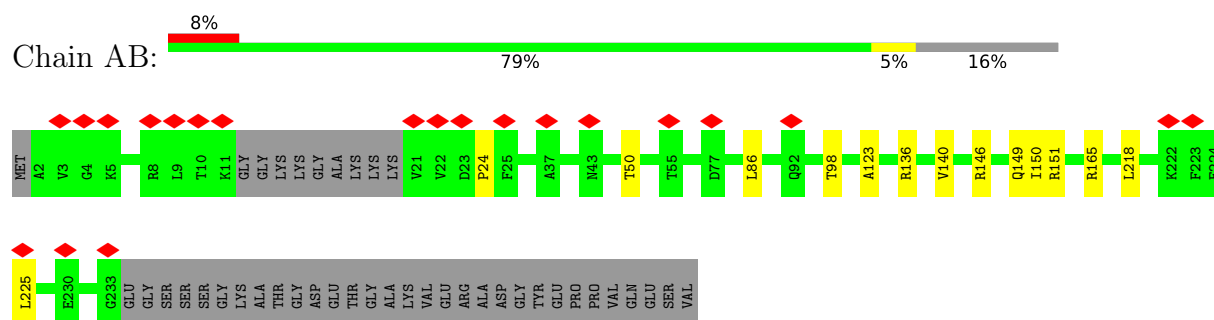




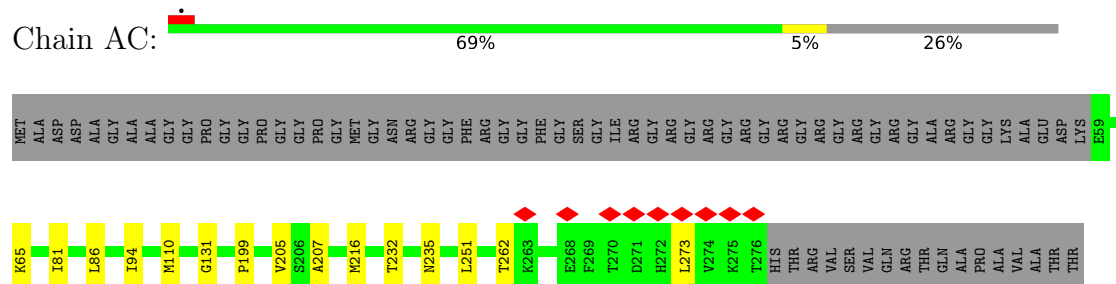
• Molecule 56: Small ribosomal subunit protein uS2



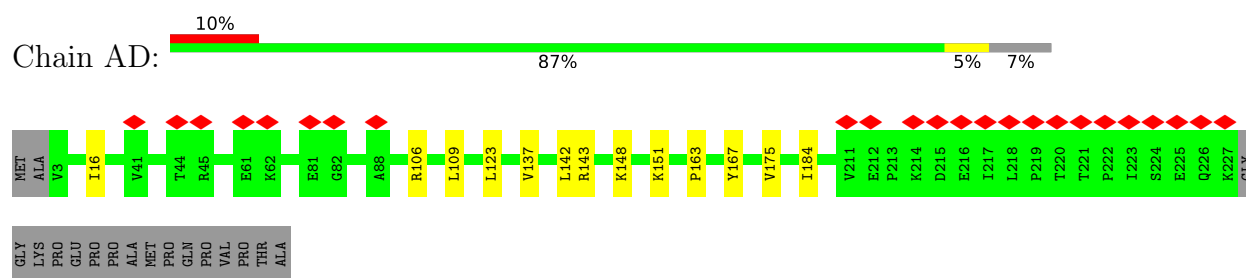
- Molecule 57: 40S ribosomal protein S3a



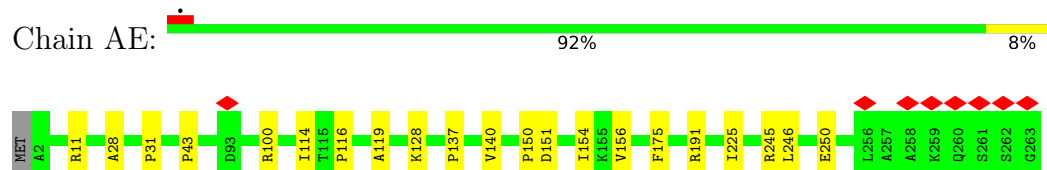
- Molecule 58: 40S ribosomal protein S2



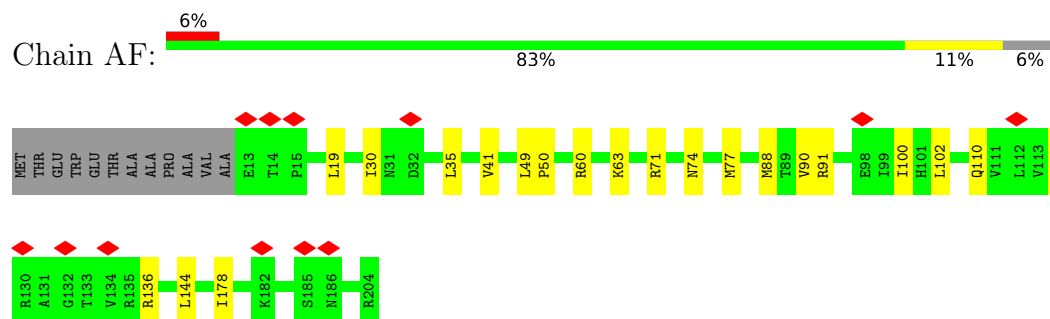
- Molecule 59: 40S ribosomal protein S3



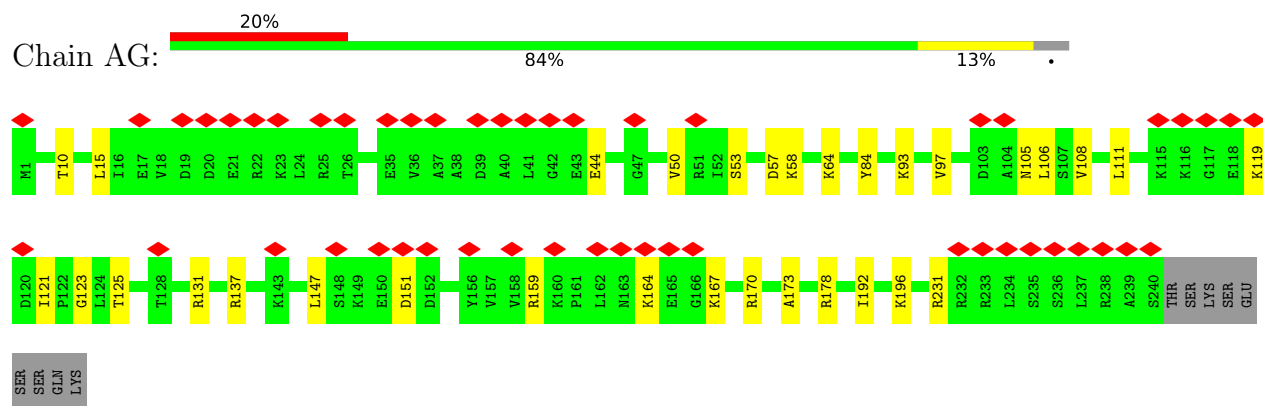
- Molecule 60: Small ribosomal subunit protein eS4, X isoform



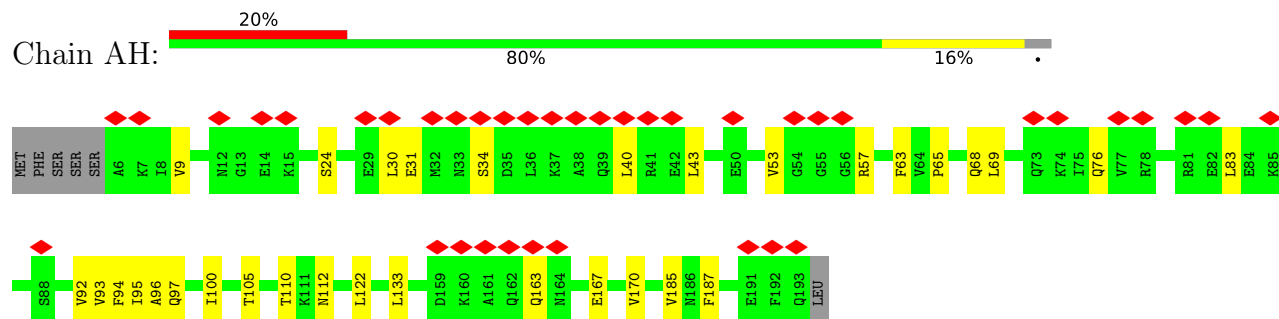
- Molecule 61: 40S ribosomal protein S5



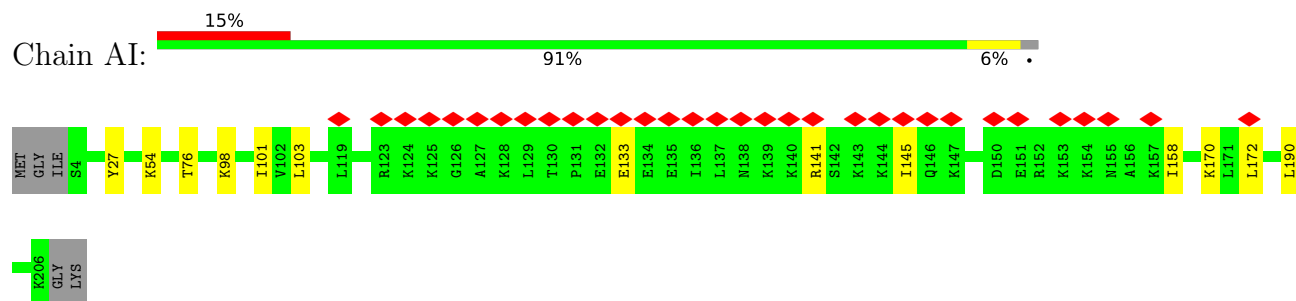
- Molecule 62: 40S ribosomal protein S6



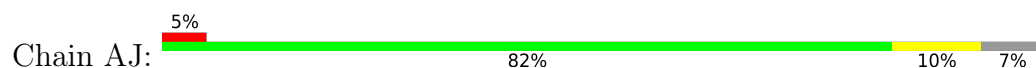
- Molecule 63: 40S ribosomal protein S7



- Molecule 64: 40S ribosomal protein S8



- Molecule 65: 40S ribosomal protein S9





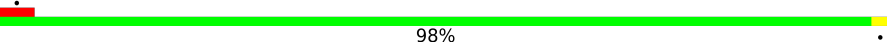
- | |
|-----|
| ARG | GLY | ALA | ASP | ARG | ASP | THR | TYR | ARG | ARG | SER | ALA | VAL | PRO | PRO | GLY | ALA | ASP | LYS | ALA | GLU | ALA | GLY | GLY | SER | ALA | THR | GLU | PHE | GLN | PHE | ARG | GLY | GLY | ARG | GLY | GLN | PRO | GLN | | | | | | | |
| M1 | L2 | K6 | L15 | E18 | M21 | P33 | E34 | L36 | A36 | D37 | K38 | N39 | K47 | K53 | M69 | M73 | D81 | P87 | E98 | I99 | V90 | T93 | L94 | R95 | R96 | S97 | ARG | PRO | GLU | THR | GLY | ARG | PRO | ARG | PRO | LYS | GLY | LEU | GLU | GLY | ARG | PRO | ALA | ARG | LEU |

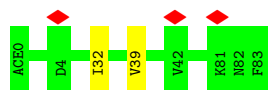
- [illegible]

- | | | | | | |
|------|------|------|------|------|------|
| F128 | K129 | C130 | K131 | K132 | | |
| L64 | V65 | E66 | A67 | L68 | G69 | A70 | E71 | H72 | Q73 | T74 | N75 | L76 | I77 | K78 | V79 | D80 | D81 | N82 | K83 | X84 | L85 | G86 | E87 | W88 | V89 | G90 | L91 | C92 | K93 | I94 | D95 | R96 | E97 | G98 | K99 | P100 | R101 | K102 | V103 | V109 | V110 | K112 | D113 | V114 | G115 | K116 | E117 | S118 | Q119 | A120 | K121 | D122 | V123 | I124 | E125 | E126 | V127 |
| MET | ALA | GLU | GLY | ILE | ALA | ALA | GLY | G10 | V11 | M12 | D13 | V14 | N15 | T16 | A17 | L18 | Q19 | E20 | V21 | L22 | K23 | T24 | A25 | L26 | I27 | H28 | D29 | G30 | L31 | A32 | R33 | A38 | A39 | K40 | A41 | L42 | D43 | K44 | R45 | Q46 | A47 | H48 | L49 | C50 | V51 | L52 | A53 | S54 | N55 | C56 | D57 | E58 | P59 | M60 | V61 | V62 | K63 |

-

- Chain AO: 

Chain AV:  98%



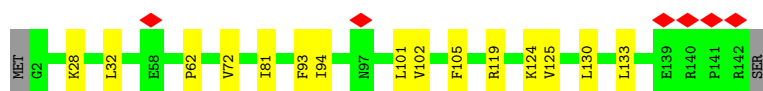
- Molecule 78: 40S ribosomal protein S15a

Chain AW:  88% 11%



- Molecule 79: Small ribosomal subunit protein uS12

Chain AX:  88% 10%

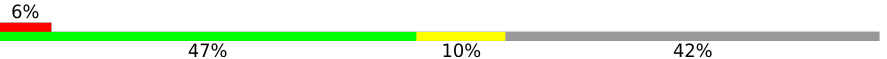


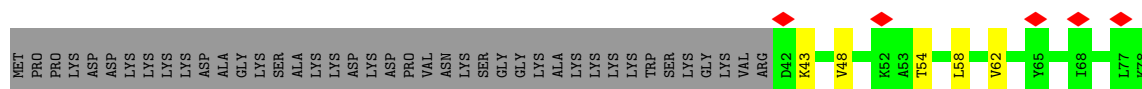
- Molecule 80: 40S ribosomal protein S24

Chain AY:  9% 86% 7% 7%



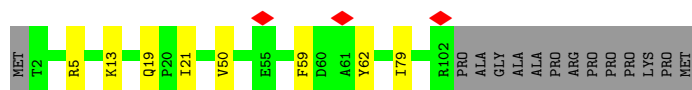
- Molecule 81: Small ribosomal subunit protein eS25

Chain AZ:  6% 47% 10% 42%

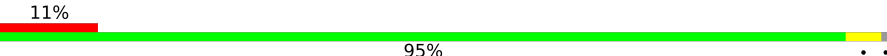


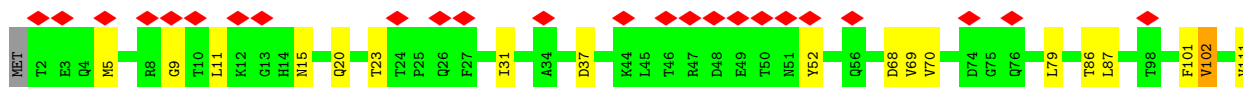
- Molecule 82: 40S ribosomal protein S26

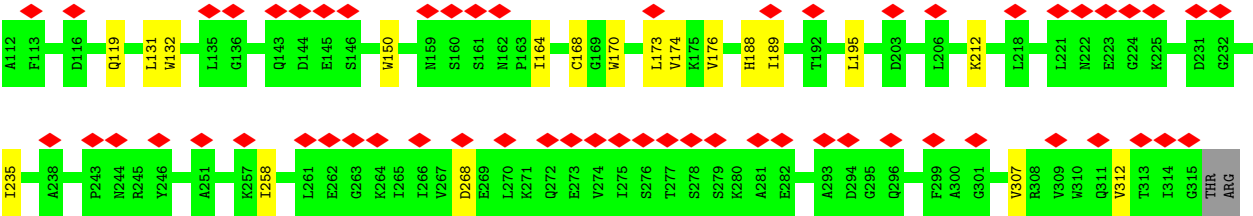
Chain Aa:  81% 7% 12%



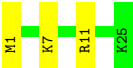
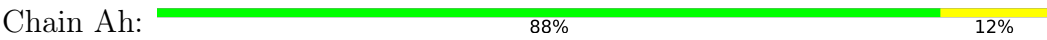
- Molecule 83: 40S ribosomal protein S27

Chain Ab:  11% 95%





• Molecule 89: 60S ribosomal protein L41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63788	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.030	Depositor
Minimum map value	-0.205	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.18	Depositor
Map size ($\text{\AA}$)	587.44, 587.44, 587.44	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.049, 1.049, 1.049	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UY1, OMC, G7M, A2M, GTP, HIC, OMU, V5N, OMG, M2G, IAS, ZN, 2MG, 5MC, MG, B8N, MA6, T6A, ACE, MLZ, COA, NMM, 1MA, UR3, HY3, 6MZ, 4AC, H2U, PSU, 5MU

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	B1	0.18	0/262	0.40	0/360
2	B2	0.29	0/1434	0.85	0/2232
3	B4	0.18	0/141	0.66	0/217
4	B5	0.27	2/85431 (0.0%)	0.81	88/133277 (0.1%)
5	B7	0.23	0/2835	0.76	2/4418 (0.0%)
6	B8	0.27	0/3613	0.80	2/5627 (0.0%)
7	BA	0.11	0/1924	0.30	0/2578
8	BB	0.11	0/3294	0.27	0/4406
9	BC	0.11	0/2973	0.28	0/3992
10	BD	0.11	0/2432	0.26	0/3256
11	BE	0.10	0/1827	0.27	0/2450
12	BF	0.13	0/1916	0.31	0/2553
13	BG	0.13	0/1960	0.32	0/2639
14	BH	0.12	0/1537	0.28	0/2066
15	BI	0.10	0/1698	0.28	0/2266
16	BJ	0.09	0/1394	0.28	0/1863
17	BL	0.12	0/1652	0.31	0/2211
18	BM	0.12	0/1142	0.28	0/1527
19	BN	0.12	0/1746	0.29	0/2338
20	BO	0.13	0/1682	0.30	0/2250
21	BP	0.11	0/1268	0.29	0/1701
22	BQ	0.12	0/1537	0.29	0/2052
23	BR	0.12	0/1582	0.26	0/2091
24	BS	0.10	0/1501	0.25	0/2013
25	BT	0.09	0/1326	0.24	0/1770
26	BU	0.13	0/865	0.31	0/1160
27	BV	0.10	0/993	0.27	0/1332
28	BW	0.11	0/1006	0.26	0/1334
29	BX	0.10	0/1050	0.26	0/1409
30	BY	0.11	0/1119	0.28	0/1488
31	BZ	0.10	0/1130	0.24	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ba	0.12	0/1179	0.31	0/1573
33	Bb	0.23	0/811	0.34	0/1070
34	Bc	0.13	0/835	0.29	0/1118
35	Bd	0.12	0/901	0.31	0/1214
36	Be	0.11	0/1071	0.28	0/1429
37	Bf	0.11	0/895	0.26	0/1198
38	Bg	0.11	0/878	0.29	0/1170
39	Bh	0.13	0/1023	0.30	0/1351
40	Bi	0.11	0/824	0.29	0/1090
41	Bj	0.11	0/720	0.30	0/952
42	Bk	0.08	0/565	0.22	0/750
43	Bl	0.12	0/465	0.25	0/614
44	Bm	0.11	0/425	0.28	0/564
45	Bo	0.08	0/837	0.23	0/1102
46	Bp	0.11	0/691	0.27	0/919
47	Br	0.13	0/1018	0.33	0/1366
48	Bs	0.12	0/1529	0.29	0/2063
49	Bt	0.14	0/1193	0.34	0/1609
50	Bu	0.13	0/836	0.35	0/1116
51	Bv	0.11	0/854	0.31	0/1144
52	Bw	0.16	0/7881	0.31	0/10630
53	By	0.14	0/1474	0.32	0/1997
54	Bz	0.14	0/1735	0.34	0/2328
55	A2	0.26	1/40445 (0.0%)	0.78	40/63039 (0.1%)
56	AA	0.11	0/1743	0.26	0/2369
57	AB	0.11	0/1832	0.28	0/2448
58	AC	0.11	0/1726	0.29	0/2332
59	AD	0.10	0/1780	0.25	0/2397
60	AE	0.10	0/2118	0.29	0/2849
61	AF	0.12	0/1539	0.32	0/2071
62	AG	0.11	0/1968	0.25	0/2619
63	AH	0.12	0/1538	0.27	0/2060
64	AI	0.11	0/1699	0.27	0/2266
65	AJ	0.10	0/1524	0.25	0/2035
66	AK	0.12	0/840	0.29	0/1133
67	AL	0.08	0/1250	0.24	0/1673
68	AM	0.13	0/963	0.35	0/1291
69	AN	0.11	0/1226	0.26	0/1649
70	AO	0.10	0/1014	0.26	0/1358
71	AP	0.09	0/1065	0.23	0/1424
72	AQ	0.13	0/1146	0.31	0/1534
73	AR	0.11	0/1097	0.29	0/1474
74	AS	0.13	0/1216	0.32	0/1630

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	AT	0.10	0/1130	0.24	0/1513
76	AU	0.10	0/813	0.25	0/1092
77	AV	0.10	0/644	0.25	0/862
78	AW	0.11	0/1051	0.26	0/1406
79	AX	0.10	0/1116	0.29	0/1486
80	AY	0.10	0/1031	0.25	0/1370
81	AZ	0.24	0/580	0.37	0/780
82	Aa	0.10	0/828	0.30	0/1109
83	Ab	0.09	0/664	0.25	0/891
84	Ac	0.07	0/514	0.21	0/688
85	Ad	0.10	0/469	0.27	0/623
86	Ae	0.08	0/457	0.26	0/602
87	Af	0.09	0/622	0.28	0/822
88	Ag	0.10	0/2497	0.31	0/3399
89	Ah	0.12	0/240	0.24	0/305
All	All	0.21	3/243295 (0.0%)	0.64	132/355349 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B5	4522	A2M	O3'-P	5.14	1.61	1.56
4	B5	2814	A2M	O3'-P	5.11	1.61	1.56
55	A2	668	A2M	O3'-P	5.04	1.61	1.56

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A2	1453	C	C2-N1-C1'	9.43	129.18	118.80
55	A2	1453	C	N1-C2-O2	9.38	124.53	118.90
4	B5	1214	C	N1-C2-O2	9.30	124.48	118.90
4	B5	2408	U	C2-N1-C1'	9.15	128.68	117.70
4	B5	1214	C	C2-N1-C1'	8.91	128.60	118.80

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	B1	251	0	216	0	0
2	B2	1638	0	850	21	0
3	B4	127	0	64	0	0
4	B5	79011	0	40013	522	0
5	B7	2538	0	1284	8	0
6	B8	3320	0	1686	20	0
7	BA	1899	0	1986	17	0
8	BB	3239	0	3377	22	0
9	BC	2919	0	3092	17	0
10	BD	2386	0	2421	21	0
11	BE	1793	0	1954	12	0
12	BF	1878	0	2009	10	0
13	BG	1927	0	2080	7	0
14	BH	1518	0	1601	11	0
15	BI	1660	0	1710	14	0
16	BJ	1371	0	1412	12	0
17	BL	1621	0	1736	6	0
18	BM	1120	0	1187	6	0
19	BN	1701	0	1749	13	0
20	BO	1650	0	1794	6	0
21	BP	1242	0	1267	4	0
22	BQ	1513	0	1628	5	0
23	BR	1566	0	1729	11	0
24	BS	1461	0	1502	10	0
25	BT	1298	0	1366	4	0
26	BU	851	0	877	5	0
27	BV	979	0	1039	5	0
28	BW	991	0	1048	7	0
29	BX	1031	0	1110	4	0
30	BY	1102	0	1189	4	0
31	BZ	1107	0	1182	6	0
32	Ba	1163	0	1206	7	0
33	Bb	809	0	876	6	0
34	Bc	824	0	874	10	0
35	Bd	886	0	932	9	0
36	Be	1053	0	1147	3	0
37	Bf	876	0	912	4	0
38	Bg	868	0	959	4	0
39	Bh	1015	0	1148	7	0
40	Bi	813	0	894	1	0
41	Bj	705	0	737	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	Bk	559	0	624	5	0
43	Bl	451	0	490	4	0
44	Bm	419	0	452	1	0
45	Bo	835	0	901	5	0
46	Bp	681	0	731	6	0
47	Br	1005	0	1072	7	0
48	Bs	1506	0	1562	10	0
49	Bt	1178	0	1235	10	0
50	Bu	832	0	890	14	0
51	Bv	846	0	894	10	0
52	Bw	7729	0	7808	47	0
53	By	1437	0	1398	10	0
54	Bz	1707	0	1815	8	0
55	A2	38027	0	19275	279	0
56	AA	1708	0	1710	10	0
57	AB	1806	0	1895	8	0
58	AC	1690	0	1777	9	0
59	AD	1752	0	1848	6	0
60	AE	2076	0	2177	10	0
61	AF	1517	0	1569	14	0
62	AG	1945	0	2112	20	0
63	AH	1515	0	1611	16	0
64	AI	1670	0	1755	7	0
65	AJ	1499	0	1618	11	0
66	AK	816	0	841	1	0
67	AL	1229	0	1302	7	0
68	AM	953	0	990	10	0
69	AN	1202	0	1289	4	0
70	AO	1010	0	1033	5	0
71	AP	1044	0	1089	4	0
72	AQ	1128	0	1195	9	0
73	AR	1082	0	1137	3	0
74	AS	1200	0	1262	5	0
75	AT	1123	0	1152	7	0
76	AU	803	0	873	6	0
77	AV	639	0	638	1	0
78	AW	1034	0	1080	8	0
79	AX	1105	0	1175	5	0
80	AY	1014	0	1082	5	0
81	AZ	574	0	627	8	0
82	Aa	814	0	863	4	0
83	Ab	650	0	672	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	Ac	512	0	541	5	0
85	Ad	458	0	448	2	0
86	Ae	451	0	494	0	0
87	Af	610	0	634	5	0
88	Ag	2440	0	2396	18	0
89	Ah	239	0	289	2	0
90	A2	122	0	0	0	0
90	AI	1	0	0	0	0
90	AQ	1	0	0	0	0
90	AX	1	0	0	0	0
90	B5	302	0	0	0	0
90	B7	6	0	0	0	0
90	B8	9	0	0	0	0
90	BA	3	0	0	0	0
90	BN	1	0	0	0	0
90	BP	1	0	0	0	0
90	BV	1	0	0	0	0
90	Ba	1	0	0	0	0
90	Bc	1	0	0	0	0
90	Be	1	0	0	0	0
90	Bf	1	0	0	0	0
90	Bg	1	0	0	0	0
91	B7	32	0	11	0	0
92	Aa	1	0	0	0	0
92	Ad	1	0	0	0	0
92	Af	1	0	0	0	0
92	Bg	1	0	0	0	0
92	Bj	1	0	0	0	0
92	Bm	1	0	0	0	0
92	Bo	1	0	0	0	0
92	Bp	1	0	0	0	0
93	By	48	0	32	3	0
All	All	232781	0	176207	1375	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 1375 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)
4:B5:2646:A:H62	4:B5:2685:G:N2	1.56	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:A2:536:A:H61	55:A2:547:G:H1	1.10	0.97
55:A2:1743:G:N2	55:A2:1791:A:H62	1.61	0.97
4:B5:2646:A:N6	4:B5:2685:G:H21	1.65	0.95
55:A2:442:C:H42	55:A2:449:A:H62	1.01	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B1	32/60 (53%)	32 (100%)	0	0	100	100
7	BA	245/257 (95%)	237 (97%)	8 (3%)	0	100	100
8	BB	399/403 (99%)	396 (99%)	3 (1%)	0	100	100
9	BC	365/427 (86%)	362 (99%)	3 (1%)	0	100	100
10	BD	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
11	BE	217/288 (75%)	210 (97%)	7 (3%)	0	100	100
12	BF	224/248 (90%)	219 (98%)	4 (2%)	1 (0%)	30	62
13	BG	238/266 (90%)	235 (99%)	3 (1%)	0	100	100
14	BH	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
15	BI	201/214 (94%)	199 (99%)	2 (1%)	0	100	100
16	BJ	169/178 (95%)	168 (99%)	1 (1%)	0	100	100
17	BL	198/211 (94%)	194 (98%)	4 (2%)	0	100	100
18	BM	134/215 (62%)	133 (99%)	1 (1%)	0	100	100
19	BN	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
20	BO	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
21	BP	151/184 (82%)	149 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	BQ	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
23	BR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
24	BS	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
25	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
26	BU	102/128 (80%)	99 (97%)	3 (3%)	0	100	100
27	BV	129/140 (92%)	127 (98%)	2 (2%)	0	100	100
28	BW	119/157 (76%)	117 (98%)	2 (2%)	0	100	100
29	BX	124/156 (80%)	122 (98%)	2 (2%)	0	100	100
30	BY	130/145 (90%)	128 (98%)	2 (2%)	0	100	100
31	BZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
32	Ba	144/148 (97%)	136 (94%)	7 (5%)	1 (1%)	18	52
33	Bb	94/159 (59%)	89 (95%)	5 (5%)	0	100	100
34	Bc	104/115 (90%)	104 (100%)	0	0	100	100
35	Bd	105/125 (84%)	102 (97%)	3 (3%)	0	100	100
36	Be	126/135 (93%)	126 (100%)	0	0	100	100
37	Bf	107/110 (97%)	107 (100%)	0	0	100	100
38	Bg	107/117 (92%)	106 (99%)	1 (1%)	0	100	100
39	Bh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
40	Bi	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
41	Bj	84/97 (87%)	81 (96%)	3 (4%)	0	100	100
42	Bk	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
43	Bl	49/51 (96%)	49 (100%)	0	0	100	100
44	Bm	49/128 (38%)	49 (100%)	0	0	100	100
45	Bo	99/106 (93%)	97 (98%)	2 (2%)	0	100	100
46	Bp	86/92 (94%)	85 (99%)	1 (1%)	0	100	100
47	Br	124/137 (90%)	122 (98%)	2 (2%)	0	100	100
48	Bs	194/317 (61%)	189 (97%)	5 (3%)	0	100	100
49	Bt	154/165 (93%)	152 (99%)	2 (1%)	0	100	100
50	Bu	103/215 (48%)	96 (93%)	7 (7%)	0	100	100
51	Bv	107/162 (66%)	104 (97%)	3 (3%)	0	100	100
52	Bw	945/978 (97%)	938 (99%)	7 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	By	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
54	Bz	210/217 (97%)	201 (96%)	9 (4%)	0	100	100
56	AA	215/295 (73%)	215 (100%)	0	0	100	100
57	AB	219/264 (83%)	219 (100%)	0	0	100	100
58	AC	216/293 (74%)	214 (99%)	2 (1%)	0	100	100
59	AD	223/243 (92%)	222 (100%)	1 (0%)	0	100	100
60	AE	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
61	AF	190/204 (93%)	183 (96%)	7 (4%)	0	100	100
62	AG	238/249 (96%)	236 (99%)	2 (1%)	0	100	100
63	AH	186/194 (96%)	182 (98%)	4 (2%)	0	100	100
64	AI	201/208 (97%)	197 (98%)	4 (2%)	0	100	100
65	AJ	178/194 (92%)	176 (99%)	2 (1%)	0	100	100
66	AK	95/165 (58%)	95 (100%)	0	0	100	100
67	AL	149/158 (94%)	147 (99%)	2 (1%)	0	100	100
68	AM	121/132 (92%)	119 (98%)	2 (2%)	0	100	100
69	AN	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
70	AO	131/151 (87%)	129 (98%)	2 (2%)	0	100	100
71	AP	125/145 (86%)	125 (100%)	0	0	100	100
72	AQ	140/146 (96%)	136 (97%)	4 (3%)	0	100	100
73	AR	132/135 (98%)	132 (100%)	0	0	100	100
74	AS	144/152 (95%)	138 (96%)	6 (4%)	0	100	100
75	AT	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
76	AU	99/119 (83%)	98 (99%)	1 (1%)	0	100	100
77	AV	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
78	AW	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
79	AX	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
80	AY	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
81	AZ	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
82	Aa	99/115 (86%)	99 (100%)	0	0	100	100
83	Ab	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
84	Ac	63/69 (91%)	63 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
85	Ad	53/56 (95%)	53 (100%)	0	0	100	100
86	Ae	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
87	Af	72/156 (46%)	68 (94%)	4 (6%)	0	100	100
88	Ag	312/317 (98%)	297 (95%)	15 (5%)	0	100	100
89	Ah	23/25 (92%)	23 (100%)	0	0	100	100
All	All	13188/15055 (88%)	12957 (98%)	229 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	Ba	15	VAL
12	BF	197	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B1	22/46 (48%)	22 (100%)	0	100	100
7	BA	189/198 (96%)	187 (99%)	2 (1%)	65	79
8	BB	347/348 (100%)	341 (98%)	6 (2%)	53	75
9	BC	305/348 (88%)	304 (100%)	1 (0%)	86	88
10	BD	247/250 (99%)	241 (98%)	6 (2%)	43	70
11	BE	197/252 (78%)	196 (100%)	1 (0%)	81	85
12	BF	195/215 (91%)	195 (100%)	0	100	100
13	BG	205/223 (92%)	203 (99%)	2 (1%)	68	80
14	BH	169/171 (99%)	166 (98%)	3 (2%)	51	74
15	BI	175/181 (97%)	171 (98%)	4 (2%)	44	70
16	BJ	144/149 (97%)	142 (99%)	2 (1%)	59	77
17	BL	168/177 (95%)	163 (97%)	5 (3%)	36	66
18	BM	116/161 (72%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	BN	171/172 (99%)	171 (100%)	0	100	100
20	BO	173/174 (99%)	170 (98%)	3 (2%)	53	75
21	BP	134/163 (82%)	132 (98%)	2 (2%)	57	76
22	BQ	164/165 (99%)	161 (98%)	3 (2%)	51	74
23	BR	166/175 (95%)	164 (99%)	2 (1%)	63	79
24	BS	157/157 (100%)	156 (99%)	1 (1%)	78	84
25	BT	139/140 (99%)	137 (99%)	2 (1%)	59	77
26	BU	94/115 (82%)	91 (97%)	3 (3%)	34	65
27	BV	101/107 (94%)	100 (99%)	1 (1%)	68	80
28	BW	100/126 (79%)	99 (99%)	1 (1%)	68	80
29	BX	113/133 (85%)	110 (97%)	3 (3%)	39	68
30	BY	123/135 (91%)	122 (99%)	1 (1%)	73	82
31	BZ	117/118 (99%)	116 (99%)	1 (1%)	70	81
32	Ba	119/120 (99%)	117 (98%)	2 (2%)	53	75
33	Bb	82/125 (66%)	80 (98%)	2 (2%)	43	70
34	Bc	90/97 (93%)	87 (97%)	3 (3%)	33	65
35	Bd	97/110 (88%)	96 (99%)	1 (1%)	68	80
36	Be	114/121 (94%)	114 (100%)	0	100	100
37	Bf	88/89 (99%)	88 (100%)	0	100	100
38	Bg	94/100 (94%)	93 (99%)	1 (1%)	65	79
39	Bh	109/110 (99%)	109 (100%)	0	100	100
40	Bi	85/89 (96%)	83 (98%)	2 (2%)	43	70
41	Bj	73/80 (91%)	73 (100%)	0	100	100
42	Bk	63/65 (97%)	61 (97%)	2 (3%)	34	65
43	Bl	48/48 (100%)	47 (98%)	1 (2%)	47	71
44	Bm	47/116 (40%)	47 (100%)	0	100	100
45	Bo	89/93 (96%)	87 (98%)	2 (2%)	45	71
46	Bp	71/75 (95%)	69 (97%)	2 (3%)	38	68
47	Br	109/120 (91%)	108 (99%)	1 (1%)	70	81
48	Bs	164/258 (64%)	156 (95%)	8 (5%)	22	55
49	Bt	128/137 (93%)	122 (95%)	6 (5%)	23	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	Bu	94/183 (51%)	92 (98%)	2 (2%)	47	71
51	Bv	93/136 (68%)	89 (96%)	4 (4%)	26	59
52	Bw	862/887 (97%)	856 (99%)	6 (1%)	76	83
53	By	152/152 (100%)	148 (97%)	4 (3%)	40	69
54	Bz	191/196 (97%)	185 (97%)	6 (3%)	35	66
56	AA	180/242 (74%)	178 (99%)	2 (1%)	65	79
57	AB	202/231 (87%)	200 (99%)	2 (1%)	68	80
58	AC	184/225 (82%)	182 (99%)	2 (1%)	65	79
59	AD	189/202 (94%)	187 (99%)	2 (1%)	65	79
60	AE	224/225 (100%)	223 (100%)	1 (0%)	84	86
61	AF	162/170 (95%)	161 (99%)	1 (1%)	78	84
62	AG	209/218 (96%)	208 (100%)	1 (0%)	81	85
63	AH	168/174 (97%)	166 (99%)	2 (1%)	63	79
64	AI	177/180 (98%)	174 (98%)	3 (2%)	53	75
65	AJ	160/168 (95%)	158 (99%)	2 (1%)	61	78
66	AK	88/136 (65%)	85 (97%)	3 (3%)	32	64
67	AL	135/142 (95%)	134 (99%)	1 (1%)	76	83
68	AM	104/108 (96%)	103 (99%)	1 (1%)	68	80
69	AN	130/131 (99%)	128 (98%)	2 (2%)	57	76
70	AO	104/118 (88%)	103 (99%)	1 (1%)	68	80
71	AP	113/130 (87%)	113 (100%)	0	100	100
72	AQ	117/121 (97%)	115 (98%)	2 (2%)	53	75
73	AR	121/122 (99%)	121 (100%)	0	100	100
74	AS	126/131 (96%)	122 (97%)	4 (3%)	34	65
75	AT	113/114 (99%)	113 (100%)	0	100	100
76	AU	93/107 (87%)	90 (97%)	3 (3%)	34	65
77	AV	67/67 (100%)	66 (98%)	1 (2%)	57	76
78	AW	112/113 (99%)	110 (98%)	2 (2%)	51	74
79	AX	113/114 (99%)	109 (96%)	4 (4%)	32	64
80	AY	108/115 (94%)	108 (100%)	0	100	100
81	AZ	64/103 (62%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	Aa	88/98 (90%)	85 (97%)	3 (3%)	32	64
83	Ab	75/76 (99%)	75 (100%)	0	100	100
84	Ac	58/62 (94%)	58 (100%)	0	100	100
85	Ad	48/49 (98%)	48 (100%)	0	100	100
86	Ae	46/104 (44%)	46 (100%)	0	100	100
87	Af	67/140 (48%)	66 (98%)	1 (2%)	57	76
88	Ag	272/275 (99%)	270 (99%)	2 (1%)	76	83
89	Ah	24/24 (100%)	24 (100%)	0	100	100
All	All	11534/12841 (90%)	11376 (99%)	158 (1%)	57	77

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
58	AC	262	THR
76	AU	68	THR
61	AF	41	VAL
66	AK	93	THR
79	AX	119	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
74	AS	42	HIS
78	AW	70	ASN
88	Ag	26	GLN
41	Bj	76	HIS
39	Bh	65	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B2	75/76 (98%)	13 (17%)	0
3	B4	5/6 (83%)	0	0
4	B5	3672/5069 (72%)	568 (15%)	17 (0%)
5	B7	118/119 (99%)	10 (8%)	1 (0%)
55	A2	1773/1869 (94%)	249 (14%)	3 (0%)
6	B8	155/157 (98%)	21 (13%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	5798/7296 (79%)	861 (14%)	21 (0%)

5 of 861 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B2	16	H2U
2	B2	17	A
2	B2	18	G
2	B2	19	G
2	B2	20	H2U

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	B5	4652	C
5	B7	11	A
55	A2	1814	G
55	A2	836	G
4	B5	4895	G

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

239 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
55	PSU	A2	822	55	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
4	PSU	B5	4551	4	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
2	H2U	B2	20	2	18,21,22	0.90	2 (11%)	21,30,33	1.50	1 (4%)
4	PSU	B5	4688	4	18,21,22	1.35	2 (11%)	22,30,33	1.76	3 (13%)
4	A2M	B5	1325	4	22,25,26	1.47	4 (18%)	31,36,39	2.09	8 (25%)
2	PSU	B2	39	2	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
4	A2M	B5	3717	4	22,25,26	1.48	4 (18%)	31,36,39	2.03	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	B5	4589	4	22,25,26	1.47	4 (18%)	31,36,39	2.07	8 (25%)
4	PSU	B5	1676	4	18,21,22	1.38	2 (11%)	22,30,33	1.85	4 (18%)
55	PSU	A2	218	55	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
55	OMU	A2	1804	55	19,22,23	1.27	4 (21%)	26,31,34	1.68	6 (23%)
2	H2U	B2	47	2	18,21,22	0.64	0	21,30,33	1.57	1 (4%)
4	OMC	B5	4535	4	19,22,23	0.85	0	26,31,34	0.95	1 (3%)
4	PSU	B5	1780	4	18,21,22	1.39	2 (11%)	22,30,33	1.82	3 (13%)
4	A2M	B5	1523	4	22,25,26	1.45	4 (18%)	31,36,39	2.15	10 (32%)
4	OMU	B5	2836	4	19,22,23	1.23	3 (15%)	26,31,34	1.69	4 (15%)
4	OMG	B5	1624	4	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
55	OMU	A2	172	55	19,22,23	1.19	3 (15%)	26,31,34	1.69	5 (19%)
6	OMU	B8	14	4,6	19,22,23	1.28	4 (21%)	26,31,34	1.78	6 (23%)
2	T6A	B2	37	2	31,34,35	0.52	0	44,49,52	0.65	1 (2%)
55	PSU	A2	1177	55	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
4	PSU	B5	2842	4	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
55	PSU	A2	681	55	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
55	6MZ	A2	1832	55,90	22,25,26	1.47	4 (18%)	30,36,39	2.24	9 (30%)
55	PSU	A2	34	55	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
55	PSU	A2	1367	55	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
4	6MZ	B5	4219	4	22,25,26	1.43	4 (18%)	30,36,39	2.29	10 (33%)
55	A2M	A2	159	55	22,25,26	1.48	4 (18%)	31,36,39	2.15	9 (29%)
55	PSU	A2	1232	55	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
55	PSU	A2	1004	55	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
55	A2M	A2	468	55	22,25,26	1.47	4 (18%)	31,36,39	2.07	8 (25%)
4	A2M	B5	2362	4,90	22,25,26	1.48	4 (18%)	31,36,39	2.13	9 (29%)
4	PSU	B5	1682	4	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
4	OMU	B5	3924	4	19,22,23	1.20	3 (15%)	26,31,34	1.66	4 (15%)
55	PSU	A2	863	55	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
55	A2M	A2	1678	55	22,25,26	1.47	4 (18%)	31,36,39	2.14	9 (29%)
4	PSU	B5	3636	4	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
4	OMC	B5	3700	4,90	19,22,23	0.78	0	26,31,34	0.75	0
4	PSU	B5	4295	4	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
4	OMU	B5	4305	4	19,22,23	1.26	4 (21%)	26,31,34	1.64	5 (19%)
55	PSU	A2	1046	55	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
55	PSU	A2	1174	55	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	A2	814	55	18,21,22	1.37	2 (11%)	22,30,33	1.79	4 (18%)
4	OMG	B5	3743	4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
2	5MC	B2	48	2	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
55	A2M	A2	1383	55	22,25,26	1.48	4 (18%)	31,36,39	2.07	8 (25%)
4	OMG	B5	4622	4	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
4	A2M	B5	1870	4,90	22,25,26	1.46	4 (18%)	31,36,39	2.06	9 (29%)
55	4AC	A2	1337	55	21,24,25	1.10	2 (9%)	29,34,37	1.15	3 (10%)
4	OMC	B5	3807	4	19,22,23	0.84	0	26,31,34	1.03	2 (7%)
55	PSU	A2	686	55	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	4578	4	18,21,22	1.32	2 (11%)	22,30,33	1.93	3 (13%)
79	HY3	AX	62	79	6,8,9	2.61	3 (50%)	5,10,12	1.22	0
55	PSU	A2	801	55	18,21,22	1.36	2 (11%)	22,30,33	1.82	4 (18%)
55	OMU	A2	1442	55,90	19,22,23	1.28	3 (15%)	26,31,34	1.75	6 (23%)
55	PSU	A2	296	55	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
4	PSU	B5	3638	4	18,21,22	1.37	2 (11%)	22,30,33	1.83	3 (13%)
4	PSU	B5	3852	4,90	18,21,22	1.37	2 (11%)	22,30,33	1.90	4 (18%)
6	PSU	B8	69	6	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
2	H2U	B2	16	2	18,21,22	1.07	2 (11%)	21,30,33	1.73	2 (9%)
4	PSU	B5	4499	4	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
55	PSU	A2	1445	55	18,21,22	1.33	2 (11%)	22,30,33	1.93	4 (18%)
55	PSU	A2	966	55	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
55	OMG	A2	601	55	23,26,27	1.23	3 (13%)	33,38,41	2.06	6 (18%)
55	A2M	A2	27	55	22,25,26	1.49	4 (18%)	31,36,39	2.08	9 (29%)
55	OMC	A2	174	55	19,22,23	0.82	0	26,31,34	0.83	1 (3%)
55	A2M	A2	99	55,90	22,25,26	1.45	4 (18%)	31,36,39	2.16	8 (25%)
55	PSU	A2	1238	55	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
2	2MG	B2	10	2	23,26,27	1.25	4 (17%)	32,38,41	2.25	6 (18%)
4	5MC	B5	3781	4,90	18,22,23	0.95	2 (11%)	26,32,35	1.18	3 (11%)
55	PSU	A2	1625	55	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
4	1MA	B5	1321	4,90	21,25,26	1.38	4 (19%)	31,37,40	1.74	6 (19%)
2	PSU	B2	31	2	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	4470	4	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
4	OMC	B5	1339	4	19,22,23	0.83	0	26,31,34	0.84	0
55	PSU	A2	406	55	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
4	A2M	B5	3829	4	22,25,26	1.46	4 (18%)	31,36,39	2.07	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	B5	3866	4	22,25,26	1.48	4 (18%)	31,36,39	2.08	8 (25%)
4	PSU	B5	3919	4,90	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
55	PSU	A2	119	55	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
55	PSU	A2	109	55	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
4	PSU	B5	4627	4	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
4	PSU	B5	1581	4	18,21,22	1.39	2 (11%)	22,30,33	1.81	4 (18%)
55	A2M	A2	484	55	22,25,26	1.48	4 (18%)	31,36,39	2.08	8 (25%)
55	OMG	A2	1447	55	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
4	PSU	B5	3714	4	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
4	PSU	B5	4672	4	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
4	A2M	B5	3784	4	22,25,26	1.44	4 (18%)	31,36,39	2.26	11 (35%)
4	PSU	B5	4456	4	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
6	PSU	B8	55	6	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
4	A2M	B5	2786	4,90	22,25,26	1.45	4 (18%)	31,36,39	2.17	9 (29%)
4	OMC	B5	3840	4	19,22,23	0.79	0	26,31,34	0.78	0
55	PSU	A2	1643	55,90	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
4	OMG	B5	3898	4,90	23,26,27	1.20	3 (13%)	33,38,41	1.90	6 (18%)
4	PSU	B5	4441	4	18,21,22	1.37	2 (11%)	22,30,33	1.90	4 (18%)
55	OMC	A2	517	55	19,22,23	0.83	0	26,31,34	0.90	1 (3%)
4	PSU	B5	1781	4	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
55	PSU	A2	815	55	18,21,22	1.29	2 (11%)	22,30,33	1.79	4 (18%)
4	PSU	B5	1791	4	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
55	OMU	A2	116	55	19,22,23	1.20	4 (21%)	26,31,34	1.67	5 (19%)
4	PSU	B5	4430	4	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
4	A2M	B5	3824	4	22,25,26	1.49	4 (18%)	31,36,39	2.04	8 (25%)
4	PSU	B5	4492	4,90	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
55	PSU	A2	1244	55	18,21,22	1.38	2 (11%)	22,30,33	1.84	3 (13%)
55	OMU	A2	121	55	19,22,23	1.21	3 (15%)	26,31,34	1.71	5 (19%)
55	PSU	A2	649	55	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
55	OMG	A2	1328	55	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
55	MA6	A2	1850	55	23,26,27	0.26	0	34,38,41	0.68	1 (2%)
4	PSU	B5	3769	4	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
4	OMU	B5	4619	4	19,22,23	1.25	4 (21%)	26,31,34	1.66	5 (19%)
4	PSU	B5	4311	4	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
55	OMU	A2	1326	55,90	19,22,23	1.17	2 (10%)	26,31,34	1.69	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OMG	B8	75	6	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
55	4AC	A2	1842	55	21,24,25	1.07	2 (9%)	29,34,37	1.23	3 (10%)
2	1MA	B2	58	2	21,25,26	1.41	4 (19%)	31,37,40	1.73	4 (12%)
4	PSU	B5	4575	4	18,21,22	1.35	2 (11%)	22,30,33	1.85	4 (18%)
4	OMG	B5	4636	4	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
4	OMC	B5	1880	4	19,22,23	0.80	0	26,31,34	0.79	0
4	OMG	B5	2423	4	23,26,27	1.20	3 (13%)	33,38,41	1.91	6 (18%)
55	OMC	A2	462	55	19,22,23	0.84	0	26,31,34	0.94	2 (7%)
4	A2M	B5	398	4	22,25,26	1.47	4 (18%)	31,36,39	2.20	10 (32%)
4	A2M	B5	1322	4	22,25,26	1.47	4 (18%)	31,36,39	2.05	8 (25%)
4	A2M	B5	400	4	22,25,26	1.47	4 (18%)	31,36,39	2.06	8 (25%)
4	OMU	B5	4226	4	19,22,23	1.24	3 (15%)	26,31,34	1.66	4 (15%)
4	A2M	B5	2400	4	22,25,26	1.46	4 (18%)	31,36,39	2.09	10 (32%)
2	5MU	B2	54	2	19,22,23	1.45	6 (31%)	28,32,35	1.92	7 (25%)
4	OMG	B5	4369	4	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
4	PSU	B5	4360	4	18,21,22	1.38	2 (11%)	22,30,33	1.83	3 (13%)
4	OMG	B5	3943	4	23,26,27	1.19	3 (13%)	33,38,41	1.96	6 (18%)
4	A2M	B5	4570	4	22,25,26	1.48	4 (18%)	31,36,39	2.09	8 (25%)
4	UR3	B5	4529	4	19,22,23	1.01	1 (5%)	26,32,35	1.43	2 (7%)
55	OMU	A2	1288	55	19,22,23	1.25	3 (15%)	26,31,34	1.67	5 (19%)
4	A2M	B5	4522	4,90	22,25,26	1.45	4 (18%)	31,36,39	2.12	10 (32%)
4	PSU	B5	3850	4	18,21,22	1.38	2 (11%)	22,30,33	1.83	3 (13%)
4	PSU	B5	1859	4	18,21,22	1.38	2 (11%)	22,30,33	1.81	3 (13%)
4	OMG	B5	4617	4	23,26,27	1.17	3 (13%)	33,38,41	1.98	6 (18%)
4	5MC	B5	4446	4,90	18,22,23	0.97	2 (11%)	26,32,35	1.17	2 (7%)
55	PSU	A2	651	55	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	3729	4	18,21,22	1.39	2 (11%)	22,30,33	1.86	3 (13%)
4	PSU	B5	4520	4,90	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
55	PSU	A2	105	55	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
55	OMG	A2	867	55	23,26,27	1.21	3 (13%)	33,38,41	1.96	6 (18%)
55	OMC	A2	1391	55	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
55	PSU	A2	572	55	18,21,22	1.36	2 (11%)	22,30,33	1.83	4 (18%)
2	M2G	B2	26	2	24,27,28	1.32	4 (16%)	35,40,43	1.84	6 (17%)
55	PSU	A2	210	55	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
4	OMG	B5	1315	4	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMU	B5	2414	4	19,22,23	1.24	4 (21%)	26,31,34	1.72	5 (19%)
4	OMC	B5	3868	4	19,22,23	0.81	0	26,31,34	0.78	0
4	OMG	B5	3791	4	23,26,27	1.20	3 (13%)	33,38,41	2.01	6 (18%)
55	PSU	A2	36	55	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
55	A2M	A2	668	55,90	22,25,26	1.45	4 (18%)	31,36,39	2.14	9 (29%)
4	PSU	B5	2838	4	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
4	PSU	B5	3883	4	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
4	A2M	B5	2814	4,90	22,25,26	1.47	4 (18%)	31,36,39	2.14	7 (22%)
4	OMG	B5	2363	4	23,26,27	1.19	3 (13%)	33,38,41	1.97	6 (18%)
4	PSU	B5	2631	4	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
2	G7M	B2	46	2	23,26,27	0.71	1 (4%)	35,39,42	0.57	0
55	OMU	A2	428	55	19,22,23	1.23	3 (15%)	26,31,34	1.74	5 (19%)
55	A2M	A2	576	55	22,25,26	1.47	4 (18%)	31,36,39	2.14	8 (25%)
55	OMU	A2	799	55	19,22,23	1.24	3 (15%)	26,31,34	1.66	5 (19%)
55	OMG	A2	644	55	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
4	OMG	B5	2875	4	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
32	V5N	Ba	39	32	9,11,12	2.05	2 (22%)	9,14,16	1.91	3 (33%)
4	OMG	B5	4391	4	23,26,27	1.21	3 (13%)	33,38,41	1.92	5 (15%)
4	OMC	B5	2803	4	19,22,23	0.85	0	26,31,34	1.15	2 (7%)
2	PSU	B2	55	2	18,21,22	1.38	2 (11%)	22,30,33	1.81	3 (13%)
2	PSU	B2	27	2	18,21,22	1.33	2 (11%)	22,30,33	1.84	3 (13%)
55	PSU	A2	1081	55	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	4298	4	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
55	G7M	A2	1639	55,2	23,26,27	0.71	1 (4%)	35,39,42	0.54	0
55	PSU	A2	93	55	18,21,22	1.38	2 (11%)	22,30,33	1.81	3 (13%)
4	PSU	B5	1861	4	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
55	OMG	A2	509	55,90	23,26,27	1.22	3 (13%)	33,38,41	1.89	6 (18%)
4	PSU	B5	4402	4	18,21,22	1.37	2 (11%)	22,30,33	1.90	4 (18%)
55	MA6	A2	1851	55	23,26,27	0.25	0	34,38,41	0.64	1 (2%)
4	OMG	B5	1521	4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
2	OMC	B2	34	2,3	19,22,23	0.87	0	26,31,34	1.35	4 (15%)
4	OMG	B5	4493	4	23,26,27	1.18	3 (13%)	33,38,41	1.91	7 (21%)
70	IAS	AO	138	70	6,7,8	0.97	0	6,8,10	1.27	1 (16%)
55	OMG	A2	1490	55,90	23,26,27	1.18	3 (13%)	33,38,41	1.95	6 (18%)
4	PSU	B5	4422	4	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMC	B5	2860	4	19,22,23	0.85	0	26,31,34	1.13	2 (7%)
4	PSU	B5	3761	4	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
4	PSU	B5	3694	4	18,21,22	1.31	2 (11%)	22,30,33	1.88	3 (13%)
4	PSU	B5	4972	4	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
55	B8N	A2	1248	55	24,29,30	1.26	3 (12%)	29,42,45	1.34	3 (10%)
55	PSU	A2	1136	55	18,21,22	1.31	2 (11%)	22,30,33	1.87	3 (13%)
55	OMC	A2	797	55	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
55	PSU	A2	866	55	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
55	PSU	A2	609	55	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
4	PSU	B5	4531	4	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
4	OMG	B5	3626	4	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
4	PSU	B5	5009	4	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
4	OMG	B5	4498	4	23,26,27	1.18	3 (13%)	33,38,41	1.91	6 (18%)
4	OMC	B5	4455	4	19,22,23	0.86	0	26,31,34	1.14	2 (7%)
4	PSU	B5	4971	4	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
4	PSU	B5	3843	4	18,21,22	1.39	2 (11%)	22,30,33	1.83	3 (13%)
2	2MG	B2	6	2	23,26,27	1.26	4 (17%)	32,38,41	2.17	6 (18%)
4	PSU	B5	1778	4	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
55	PSU	A2	1692	55	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
4	OMG	B5	4227	4	23,26,27	1.18	3 (13%)	33,38,41	1.93	6 (18%)
4	PSU	B5	4292	4	18,21,22	1.33	2 (11%)	22,30,33	1.88	4 (18%)
55	OMU	A2	627	55	19,22,23	1.18	2 (10%)	26,31,34	1.67	4 (15%)
4	PSU	B5	1743	4	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
55	A2M	A2	512	55	22,25,26	1.47	4 (18%)	31,36,39	2.16	8 (25%)
75	NMM	AT	67	75	9,11,12	0.59	0	6,12,14	0.45	0
55	PSU	A2	1056	55	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
45	MLZ	Bo	53	45	8,9,10	0.49	0	4,9,11	0.12	0
4	PSU	B5	4635	4	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
7	V5N	BA	216	7	9,11,12	2.08	2 (22%)	9,14,16	1.70	2 (22%)
4	A2M	B5	3723	4	22,25,26	1.46	4 (18%)	31,36,39	2.09	7 (22%)
4	PSU	B5	5000	4	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
4	OMC	B5	2823	4	19,22,23	0.83	0	26,31,34	0.99	2 (7%)
55	OMG	A2	436	55	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
55	PSU	A2	1347	55	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
55	A2M	A2	166	55	22,25,26	1.48	4 (18%)	31,36,39	2.14	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	B5	1533	4,90	22,25,26	1.47	4 (18%)	31,36,39	2.10	8 (25%)
55	OMU	A2	354	55	19,22,23	1.22	4 (21%)	26,31,34	1.65	4 (15%)
4	PSU	B5	3767	4	18,21,22	1.33	2 (11%)	22,30,33	1.82	3 (13%)
4	OMC	B5	2364	4	19,22,23	0.81	0	26,31,34	0.79	0
33	MLZ	Bb	5	33	8,9,10	0.47	0	4,9,11	0.15	0
4	OMU	B5	4497	4,90	19,22,23	1.20	2 (10%)	26,31,34	1.68	4 (15%)
4	OMC	B5	3886	4	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
4	PSU	B5	3821	4	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
55	A2M	A2	1031	55	22,25,26	1.46	4 (18%)	31,36,39	2.08	7 (22%)
55	OMC	A2	1703	55	19,22,23	0.83	0	26,31,34	0.95	2 (7%)
4	UY1	B5	3817	4	19,22,23	1.37	3 (15%)	22,31,34	1.72	3 (13%)
4	PSU	B5	2507	4	18,21,22	1.35	2 (11%)	22,30,33	1.88	4 (18%)
55	PSU	A2	1045	55	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
55	OMC	A2	1272	55	19,22,23	0.81	0	26,31,34	0.86	1 (3%)
55	A2M	A2	590	55	22,25,26	1.48	4 (18%)	31,36,39	2.27	6 (19%)
55	OMG	A2	683	55	23,26,27	1.18	3 (13%)	33,38,41	1.96	6 (18%)
4	OMC	B5	2421	4,90	19,22,23	0.81	0	26,31,34	0.79	0
4	PSU	B5	1535	4	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
4	OMG	B5	4195	4,90,2	23,26,27	1.21	3 (13%)	33,38,41	1.97	6 (18%)
8	HIC	BB	245	8	10,11,12	0.61	0	8,14,16	0.39	0
4	OMC	B5	2350	4,90	19,22,23	0.81	0	26,31,34	0.83	0
4	PSU	B5	4352	4	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)

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
55	PSU	A2	822	55	-	1/7/25/26	0/2/2/2
4	PSU	B5	4551	4	-	0/7/25/26	0/2/2/2
2	H2U	B2	20	2	-	5/7/38/39	0/2/2/2
4	PSU	B5	4688	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	1325	4	-	3/9/27/28	0/3/3/3
2	PSU	B2	39	2	-	0/7/25/26	0/2/2/2
4	A2M	B5	3717	4	-	0/9/27/28	0/3/3/3
4	A2M	B5	4589	4	-	3/9/27/28	0/3/3/3
4	PSU	B5	1676	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	A2	218	55	-	0/7/25/26	0/2/2/2
55	OMU	A2	1804	55	-	0/9/27/28	0/2/2/2
2	H2U	B2	47	2	-	6/7/38/39	0/2/2/2
4	OMC	B5	4535	4	-	1/9/27/28	0/2/2/2
4	PSU	B5	1780	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	1523	4	-	1/9/27/28	0/3/3/3
4	OMU	B5	2836	4	-	1/9/27/28	0/2/2/2
4	OMG	B5	1624	4	-	1/9/27/28	0/3/3/3
55	OMU	A2	172	55	-	0/9/27/28	0/2/2/2
6	OMU	B8	14	4,6	-	0/9/27/28	0/2/2/2
2	T6A	B2	37	2	-	1/23/41/42	0/3/3/3
55	PSU	A2	1177	55	-	0/7/25/26	0/2/2/2
4	PSU	B5	2842	4	-	0/7/25/26	0/2/2/2
55	PSU	A2	681	55	-	0/7/25/26	0/2/2/2
55	6MZ	A2	1832	55,90	-	0/9/27/28	0/3/3/3
55	PSU	A2	34	55	-	0/7/25/26	0/2/2/2
55	PSU	A2	1367	55	-	0/7/25/26	0/2/2/2
4	6MZ	B5	4219	4	-	2/9/27/28	0/3/3/3
55	A2M	A2	159	55	-	2/9/27/28	0/3/3/3
55	PSU	A2	1232	55	-	0/7/25/26	0/2/2/2
55	PSU	A2	1004	55	-	0/7/25/26	0/2/2/2
55	A2M	A2	468	55	-	1/9/27/28	0/3/3/3
4	A2M	B5	2362	4,90	-	0/9/27/28	0/3/3/3
4	PSU	B5	1682	4	-	0/7/25/26	0/2/2/2
4	OMU	B5	3924	4	-	0/9/27/28	0/2/2/2
55	PSU	A2	863	55	-	0/7/25/26	0/2/2/2
55	A2M	A2	1678	55	-	1/9/27/28	0/3/3/3
4	PSU	B5	3636	4	-	0/7/25/26	0/2/2/2
4	OMC	B5	3700	4,90	-	4/9/27/28	0/2/2/2
4	PSU	B5	4295	4	-	0/7/25/26	0/2/2/2
4	OMU	B5	4305	4	-	0/9/27/28	0/2/2/2
55	PSU	A2	1046	55	-	0/7/25/26	0/2/2/2
55	PSU	A2	1174	55	-	0/7/25/26	0/2/2/2
55	PSU	A2	814	55	-	0/7/25/26	0/2/2/2
4	OMG	B5	3743	4	-	0/9/27/28	0/3/3/3
2	5MC	B2	48	2	-	3/7/25/26	0/2/2/2
55	A2M	A2	1383	55	-	0/9/27/28	0/3/3/3
4	OMG	B5	4622	4	-	0/9/27/28	0/3/3/3
4	A2M	B5	1870	4,90	-	0/9/27/28	0/3/3/3
55	4AC	A2	1337	55	-	4/11/29/30	0/2/2/2
4	OMC	B5	3807	4	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	A2	686	55	-	0/7/25/26	0/2/2/2
4	PSU	B5	4578	4	-	0/7/25/26	0/2/2/2
79	HY3	AX	62	79	-	1/1/12/14	0/1/1/1
55	PSU	A2	801	55	-	0/7/25/26	0/2/2/2
55	OMU	A2	1442	55,90	-	1/9/27/28	0/2/2/2
55	PSU	A2	296	55	-	0/7/25/26	0/2/2/2
4	PSU	B5	3638	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3852	4,90	-	0/7/25/26	0/2/2/2
6	PSU	B8	69	6	-	0/7/25/26	0/2/2/2
2	H2U	B2	16	2	-	7/7/38/39	0/2/2/2
4	PSU	B5	4499	4	-	5/7/25/26	0/2/2/2
55	PSU	A2	1445	55	-	0/7/25/26	0/2/2/2
55	PSU	A2	966	55	-	0/7/25/26	0/2/2/2
55	OMG	A2	601	55	-	2/9/27/28	0/3/3/3
55	A2M	A2	27	55	-	2/9/27/28	0/3/3/3
55	OMC	A2	174	55	-	0/9/27/28	0/2/2/2
55	A2M	A2	99	55,90	-	2/9/27/28	0/3/3/3
55	PSU	A2	1238	55	-	0/7/25/26	0/2/2/2
2	2MG	B2	10	2	-	0/9/27/28	0/3/3/3
4	5MC	B5	3781	4,90	-	0/7/25/26	0/2/2/2
55	PSU	A2	1625	55	-	0/7/25/26	0/2/2/2
4	1MA	B5	1321	4,90	-	0/7/25/26	0/3/3/3
2	PSU	B2	31	2	-	0/7/25/26	0/2/2/2
4	PSU	B5	4470	4	-	0/7/25/26	0/2/2/2
4	OMC	B5	1339	4	-	0/9/27/28	0/2/2/2
55	PSU	A2	406	55	-	0/7/25/26	0/2/2/2
4	A2M	B5	3829	4	-	0/9/27/28	0/3/3/3
4	A2M	B5	3866	4	-	1/9/27/28	0/3/3/3
4	PSU	B5	3919	4,90	-	0/7/25/26	0/2/2/2
55	PSU	A2	119	55	-	0/7/25/26	0/2/2/2
55	PSU	A2	109	55	-	0/7/25/26	0/2/2/2
4	PSU	B5	4627	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	1581	4	-	2/7/25/26	0/2/2/2
55	A2M	A2	484	55	-	0/9/27/28	0/3/3/3
55	OMG	A2	1447	55	-	2/9/27/28	0/3/3/3
4	PSU	B5	3714	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4672	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	3784	4	-	2/9/27/28	0/3/3/3
4	PSU	B5	4456	4	-	0/7/25/26	0/2/2/2
6	PSU	B8	55	6	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A2M	B5	2786	4,90	-	3/9/27/28	0/3/3/3
4	OMC	B5	3840	4	-	1/9/27/28	0/2/2/2
55	PSU	A2	1643	55,90	-	0/7/25/26	0/2/2/2
4	OMG	B5	3898	4,90	-	0/9/27/28	0/3/3/3
4	PSU	B5	4441	4	-	0/7/25/26	0/2/2/2
55	OMC	A2	517	55	-	2/9/27/28	0/2/2/2
4	PSU	B5	1781	4	-	0/7/25/26	0/2/2/2
55	PSU	A2	815	55	-	0/7/25/26	0/2/2/2
4	PSU	B5	1791	4	-	1/7/25/26	0/2/2/2
55	OMU	A2	116	55	-	0/9/27/28	0/2/2/2
4	PSU	B5	4430	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	3824	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	4492	4,90	-	0/7/25/26	0/2/2/2
55	PSU	A2	1244	55	-	0/7/25/26	0/2/2/2
55	OMU	A2	121	55	-	0/9/27/28	0/2/2/2
55	PSU	A2	649	55	-	0/7/25/26	0/2/2/2
55	OMG	A2	1328	55	-	0/9/27/28	0/3/3/3
55	MA6	A2	1850	55	-	3/11/29/30	0/3/3/3
4	PSU	B5	3769	4	-	0/7/25/26	0/2/2/2
4	OMU	B5	4619	4	-	0/9/27/28	0/2/2/2
4	PSU	B5	4311	4	-	0/7/25/26	0/2/2/2
55	OMU	A2	1326	55,90	-	0/9/27/28	0/2/2/2
6	OMG	B8	75	6	-	0/9/27/28	0/3/3/3
55	4AC	A2	1842	55	-	4/11/29/30	0/2/2/2
2	1MA	B2	58	2	-	2/7/25/26	0/3/3/3
4	PSU	B5	4575	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	4636	4	-	0/9/27/28	0/3/3/3
4	OMC	B5	1880	4	-	0/9/27/28	0/2/2/2
4	OMG	B5	2423	4	-	0/9/27/28	0/3/3/3
55	OMC	A2	462	55	-	0/9/27/28	0/2/2/2
4	A2M	B5	398	4	-	2/9/27/28	0/3/3/3
4	A2M	B5	1322	4	-	2/9/27/28	0/3/3/3
4	A2M	B5	400	4	-	0/9/27/28	0/3/3/3
4	OMU	B5	4226	4	-	0/9/27/28	0/2/2/2
4	A2M	B5	2400	4	-	0/9/27/28	0/3/3/3
2	5MU	B2	54	2	-	0/7/25/26	0/2/2/2
4	OMG	B5	4369	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	4360	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	3943	4	-	0/9/27/28	0/3/3/3
4	A2M	B5	4570	4	-	1/9/27/28	0/3/3/3
4	UR3	B5	4529	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	OMU	A2	1288	55	-	1/9/27/28	0/2/2/2
4	A2M	B5	4522	4,90	-	1/9/27/28	0/3/3/3
4	PSU	B5	3850	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	1859	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	4617	4	-	0/9/27/28	0/3/3/3
4	5MC	B5	4446	4,90	-	4/7/25/26	0/2/2/2
55	PSU	A2	651	55	-	0/7/25/26	0/2/2/2
4	PSU	B5	3729	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4520	4,90	-	0/7/25/26	0/2/2/2
55	PSU	A2	105	55	-	0/7/25/26	0/2/2/2
55	OMG	A2	867	55	-	0/9/27/28	0/3/3/3
55	OMC	A2	1391	55	-	0/9/27/28	0/2/2/2
55	PSU	A2	572	55	-	0/7/25/26	0/2/2/2
2	M2G	B2	26	2	-	0/11/29/30	0/3/3/3
55	PSU	A2	210	55	-	0/7/25/26	0/2/2/2
4	OMG	B5	1315	4	-	0/9/27/28	0/3/3/3
4	OMU	B5	2414	4	-	0/9/27/28	0/2/2/2
4	OMC	B5	3868	4	-	1/9/27/28	0/2/2/2
4	OMG	B5	3791	4	-	0/9/27/28	0/3/3/3
55	PSU	A2	36	55	-	0/7/25/26	0/2/2/2
55	A2M	A2	668	55,90	-	4/9/27/28	0/3/3/3
4	PSU	B5	2838	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3883	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	2814	4,90	-	1/9/27/28	0/3/3/3
4	OMG	B5	2363	4	-	3/9/27/28	0/3/3/3
4	PSU	B5	2631	4	-	0/7/25/26	0/2/2/2
2	G7M	B2	46	2	-	3/7/25/26	0/3/3/3
55	OMU	A2	428	55	-	2/9/27/28	0/2/2/2
55	A2M	A2	576	55	-	4/9/27/28	0/3/3/3
55	OMU	A2	799	55	-	2/9/27/28	0/2/2/2
55	OMG	A2	644	55	-	3/9/27/28	0/3/3/3
4	OMG	B5	2875	4	-	0/9/27/28	0/3/3/3
32	V5N	Ba	39	32	-	0/9/10/12	0/1/1/1
4	OMG	B5	4391	4	-	1/9/27/28	0/3/3/3
4	OMC	B5	2803	4	-	1/9/27/28	0/2/2/2
2	PSU	B2	55	2	-	0/7/25/26	0/2/2/2
2	PSU	B2	27	2	-	0/7/25/26	0/2/2/2
55	PSU	A2	1081	55	-	0/7/25/26	0/2/2/2
4	PSU	B5	4298	4	-	0/7/25/26	0/2/2/2
55	G7M	A2	1639	55,2	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	A2	93	55	-	0/7/25/26	0/2/2/2
4	PSU	B5	1861	4	-	0/7/25/26	0/2/2/2
55	OMG	A2	509	55,90	-	0/9/27/28	0/3/3/3
4	PSU	B5	4402	4	-	1/7/25/26	0/2/2/2
55	MA6	A2	1851	55	-	4/11/29/30	0/3/3/3
4	OMG	B5	1521	4	-	0/9/27/28	0/3/3/3
2	OMC	B2	34	2,3	-	2/9/27/28	0/2/2/2
4	OMG	B5	4493	4	-	0/9/27/28	0/3/3/3
70	IAS	AO	138	70	-	1/7/7/8	-
55	OMG	A2	1490	55,90	-	1/9/27/28	0/3/3/3
4	PSU	B5	4422	4	-	0/7/25/26	0/2/2/2
4	OMC	B5	2860	4	-	0/9/27/28	0/2/2/2
4	PSU	B5	3761	4	-	2/7/25/26	0/2/2/2
4	PSU	B5	3694	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4972	4	-	0/7/25/26	0/2/2/2
55	B8N	A2	1248	55	-	4/16/34/35	0/2/2/2
55	PSU	A2	1136	55	-	0/7/25/26	0/2/2/2
55	OMC	A2	797	55	-	0/9/27/28	0/2/2/2
55	PSU	A2	866	55	-	0/7/25/26	0/2/2/2
55	PSU	A2	609	55	-	0/7/25/26	0/2/2/2
4	PSU	B5	4531	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	3626	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	5009	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	4498	4	-	0/9/27/28	0/3/3/3
4	OMC	B5	4455	4	-	1/9/27/28	0/2/2/2
4	PSU	B5	4971	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3843	4	-	1/7/25/26	0/2/2/2
2	2MG	B2	6	2	-	0/9/27/28	0/3/3/3
4	PSU	B5	1778	4	-	0/7/25/26	0/2/2/2
55	PSU	A2	1692	55	-	0/7/25/26	0/2/2/2
4	OMG	B5	4227	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	4292	4	-	0/7/25/26	0/2/2/2
55	OMU	A2	627	55	-	1/9/27/28	0/2/2/2
4	PSU	B5	1743	4	-	0/7/25/26	0/2/2/2
55	A2M	A2	512	55	-	2/9/27/28	0/3/3/3
75	NMM	AT	67	75	-	0/9/11/13	-
55	PSU	A2	1056	55	-	0/7/25/26	0/2/2/2
45	MLZ	Bo	53	45	-	0/7/8/10	-
4	PSU	B5	4635	4	-	3/7/25/26	0/2/2/2
7	V5N	BA	216	7	-	3/9/10/12	0/1/1/1
4	A2M	B5	3723	4	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	B5	5000	4	-	0/7/25/26	0/2/2/2
4	OMC	B5	2823	4	-	0/9/27/28	0/2/2/2
55	OMG	A2	436	55	-	1/9/27/28	0/3/3/3
55	PSU	A2	1347	55	-	0/7/25/26	0/2/2/2
55	A2M	A2	166	55	-	0/9/27/28	0/3/3/3
4	A2M	B5	1533	4,90	-	2/9/27/28	0/3/3/3
55	OMU	A2	354	55	-	1/9/27/28	0/2/2/2
4	PSU	B5	3767	4	-	0/7/25/26	0/2/2/2
4	OMC	B5	2364	4	-	0/9/27/28	0/2/2/2
33	MLZ	Bb	5	33	-	0/7/8/10	-
4	OMU	B5	4497	4,90	-	0/9/27/28	0/2/2/2
4	OMC	B5	3886	4	-	1/9/27/28	0/2/2/2
4	PSU	B5	3821	4	-	0/7/25/26	0/2/2/2
55	A2M	A2	1031	55	-	0/9/27/28	0/3/3/3
55	OMC	A2	1703	55	-	3/9/27/28	0/2/2/2
4	UY1	B5	3817	4	-	1/9/27/28	0/2/2/2
4	PSU	B5	2507	4	-	0/7/25/26	0/2/2/2
55	PSU	A2	1045	55	-	2/7/25/26	0/2/2/2
55	OMC	A2	1272	55	-	0/9/27/28	0/2/2/2
55	A2M	A2	590	55	-	3/9/27/28	0/3/3/3
55	OMG	A2	683	55	-	2/9/27/28	0/3/3/3
4	OMC	B5	2421	4,90	-	1/9/27/28	0/2/2/2
4	PSU	B5	1535	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	4195	4,90,2	-	0/9/27/28	0/3/3/3
8	HIC	BB	245	8	-	2/5/6/8	0/1/1/1
4	OMC	B5	2350	4,90	-	1/9/27/28	0/2/2/2
4	PSU	B5	4352	4	-	0/7/25/26	0/2/2/2

The worst 5 of 551 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	BA	216	V5N	CG-ND1	-4.86	1.33	1.37
32	Ba	39	V5N	CG-ND1	-4.85	1.33	1.37
55	A2	590	A2M	C5-C4	4.71	1.47	1.39
55	A2	576	A2M	C5-C4	4.61	1.47	1.39
55	A2	27	A2M	C5-C4	4.61	1.47	1.39

The worst 5 of 983 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B2	10	2MG	C2-N3-C4	7.55	121.39	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A2	590	A2M	C5-C4-N3	-7.24	117.30	126.75
2	B2	6	2MG	C2-N3-C4	7.17	120.93	112.04
2	B2	16	H2U	C4-N3-C2	-6.88	120.09	125.79
55	A2	601	OMG	C5-C4-N3	-6.84	117.36	128.46

There are no chirality outliers.

5 of 167 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	BA	216	V5N	O-C-CA-CB
2	B2	16	H2U	O4'-C1'-N1-C6
2	B2	20	H2U	O4'-C4'-C5'-O5'
2	B2	20	H2U	C3'-C4'-C5'-O5'
2	B2	47	H2U	O4'-C4'-C5'-O5'

There are no ring outliers.

75 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	A2	822	PSU	1	0
2	B2	20	H2U	1	0
4	B5	4688	PSU	1	0
4	B5	3717	A2M	2	0
55	A2	1804	OMU	2	0
4	B5	4535	OMC	1	0
55	A2	1832	6MZ	1	0
4	B5	4219	6MZ	2	0
55	A2	159	A2M	1	0
55	A2	468	A2M	1	0
4	B5	2362	A2M	1	0
55	A2	1678	A2M	1	0
55	A2	1383	A2M	1	0
4	B5	1870	A2M	1	0
55	A2	1337	4AC	2	0
4	B5	3807	OMC	1	0
4	B5	4578	PSU	2	0
4	B5	3638	PSU	1	0
2	B2	16	H2U	1	0
55	A2	1445	PSU	1	0
55	A2	601	OMG	1	0
55	A2	27	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	A2	99	A2M	1	0
55	A2	1238	PSU	1	0
4	B5	4470	PSU	1	0
4	B5	1339	OMC	1	0
4	B5	3829	A2M	1	0
4	B5	3866	A2M	1	0
55	A2	1447	OMG	1	0
4	B5	3784	A2M	1	0
4	B5	4456	PSU	1	0
4	B5	2786	A2M	1	0
55	A2	116	OMU	2	0
4	B5	4492	PSU	1	0
55	A2	121	OMU	2	0
55	A2	649	PSU	2	0
55	A2	1328	OMG	2	0
55	A2	1850	MA6	1	0
4	B5	4619	OMU	1	0
55	A2	1842	4AC	2	0
4	B5	4226	OMU	1	0
2	B2	54	5MU	1	0
4	B5	3943	OMG	2	0
4	B5	4570	A2M	2	0
4	B5	4522	A2M	1	0
55	A2	867	OMG	1	0
2	B2	26	M2G	1	0
4	B5	1315	OMG	1	0
4	B5	2414	OMU	1	0
4	B5	3791	OMG	1	0
2	B2	46	G7M	1	0
55	A2	799	OMU	1	0
4	B5	2875	OMG	1	0
4	B5	4391	OMG	1	0
4	B5	2803	OMC	1	0
55	A2	1639	G7M	2	0
4	B5	4493	OMG	1	0
4	B5	2860	OMC	1	0
4	B5	3694	PSU	1	0
55	A2	1136	PSU	1	0
55	A2	866	PSU	1	0
55	A2	609	PSU	1	0
4	B5	4455	OMC	1	0
55	A2	512	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B5	3723	A2M	2	0
4	B5	5000	PSU	1	0
55	A2	436	OMG	1	0
55	A2	166	A2M	2	0
55	A2	354	OMU	1	0
55	A2	1031	A2M	1	0
55	A2	1703	OMC	1	0
4	B5	4195	OMG	1	0
8	BB	245	HIC	1	0
4	B5	2350	OMC	1	0
4	B5	4352	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 463 ligands modelled in this entry, 461 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
91	GTP	B7	201	5	30,34,34	0.50	0	46,54,54	0.52	0
93	COA	By	201	-	44,50,50	0.51	0	65,75,75	0.68	1 (1%)

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
91	GTP	B7	201	5	-	2/22/38/38	0/3/3/3
93	COA	By	201	-	-	11/48/64/64	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($^{\circ}$)	Ideal($^{\circ}$)
93	By	201	COA	C7P-N8P-C9P	2.00	126.16	122.59

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

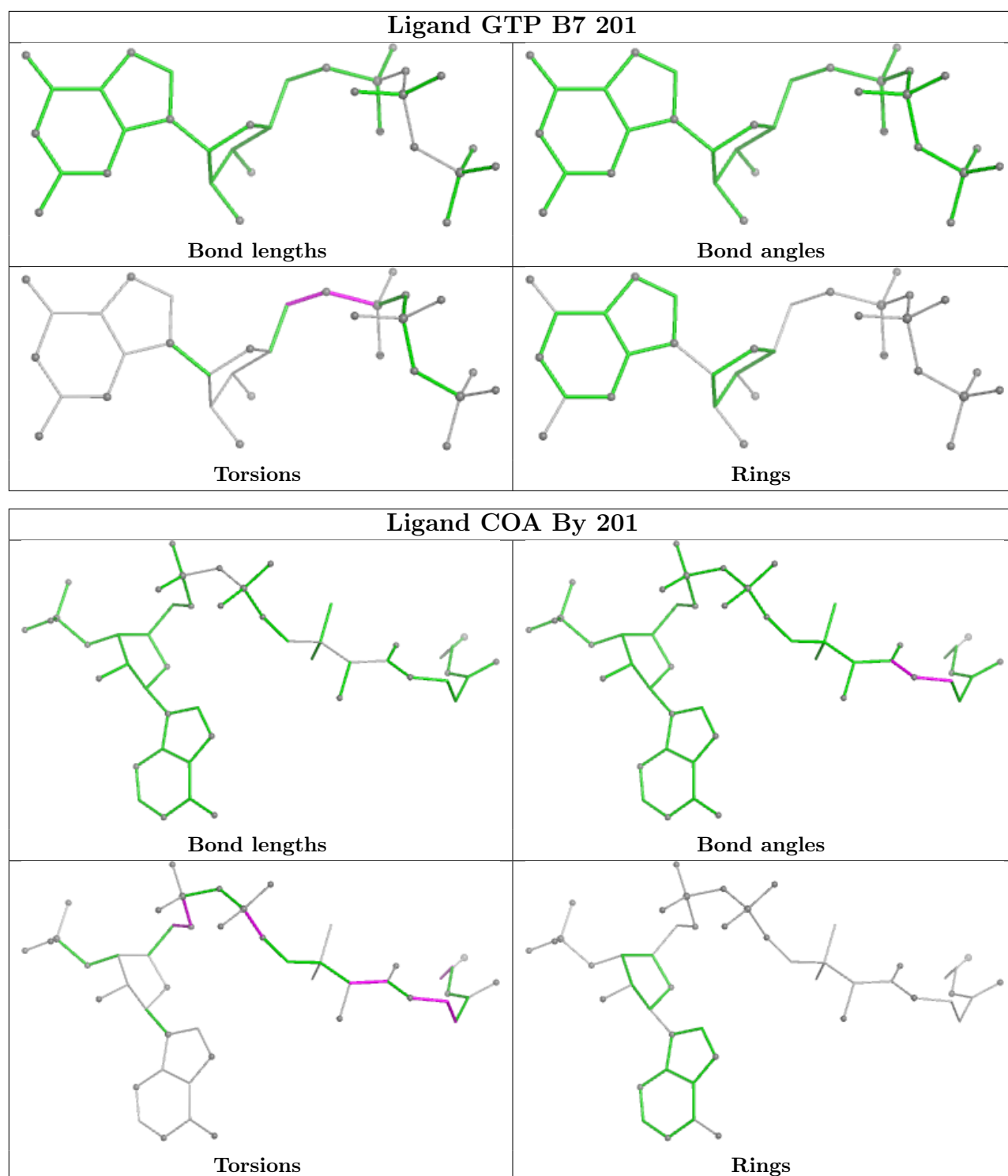
Mol	Chain	Res	Type	Atoms
91	B7	201	GTP	C5'-O5'-PA-O1A
93	By	201	COA	C5B-O5B-P1A-O2A
93	By	201	COA	C5B-O5B-P1A-O3A
93	By	201	COA	O9P-C9P-CAP-CBP
93	By	201	COA	N8P-C9P-CAP-CBP

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
93	By	201	COA	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

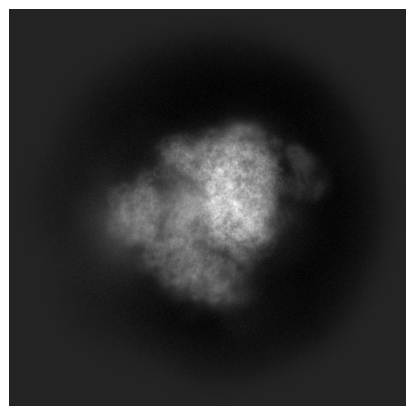
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57771. These allow visual inspection of the internal detail of the map and identification of artifacts.

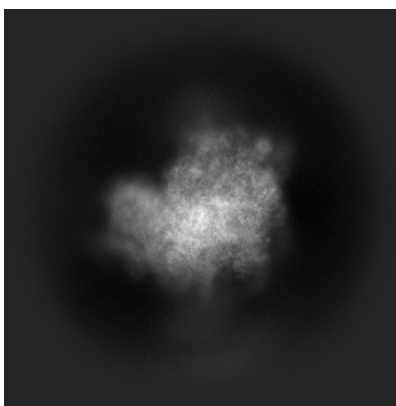
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

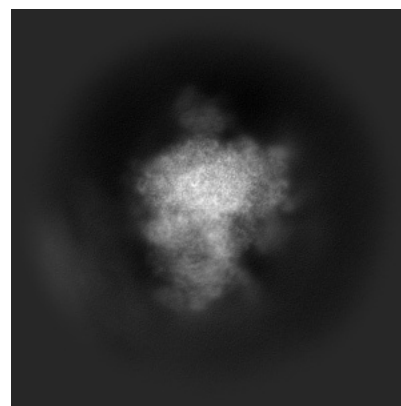
6.1.1 Primary map



X

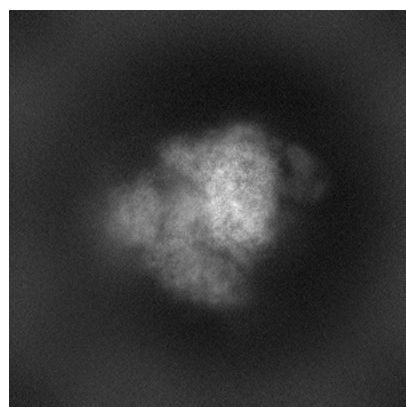


Y

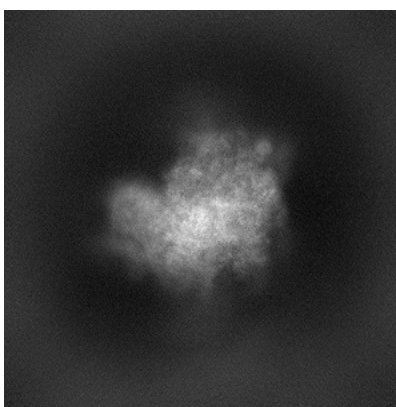


Z

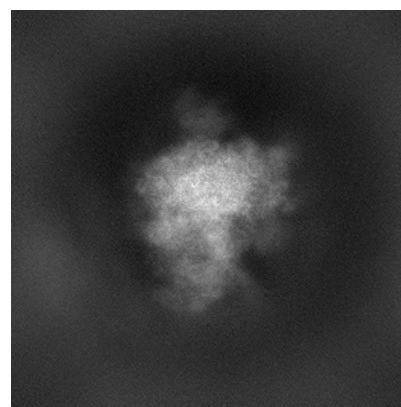
6.1.2 Raw map



X



Y

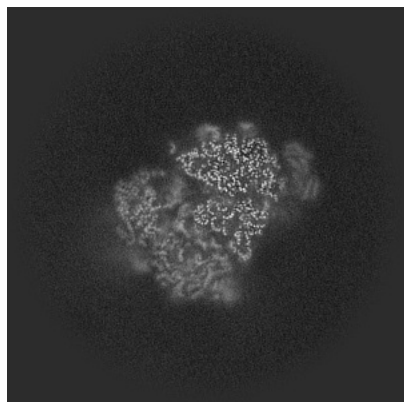


Z

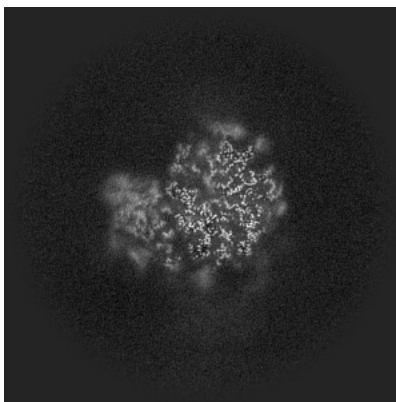
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

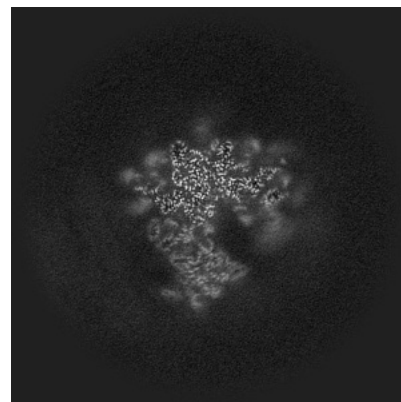
6.2.1 Primary map



X Index: 280

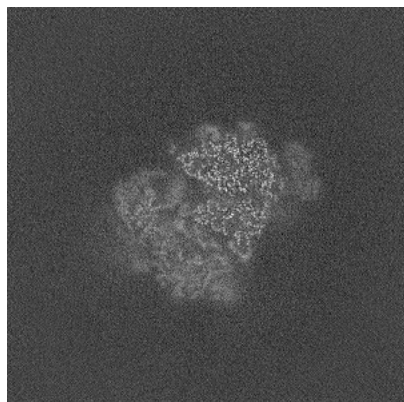


Y Index: 280

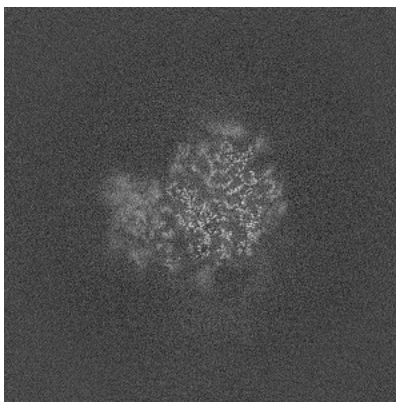


Z Index: 280

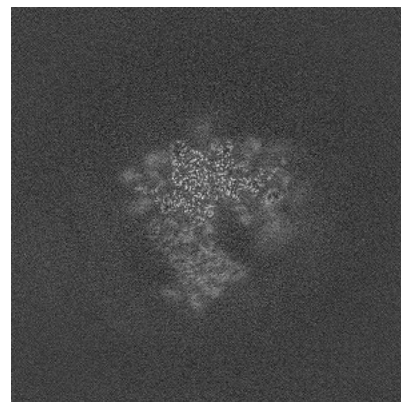
6.2.2 Raw map



X Index: 280



Y Index: 280

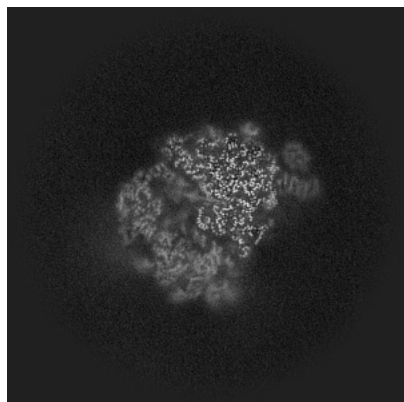


Z Index: 280

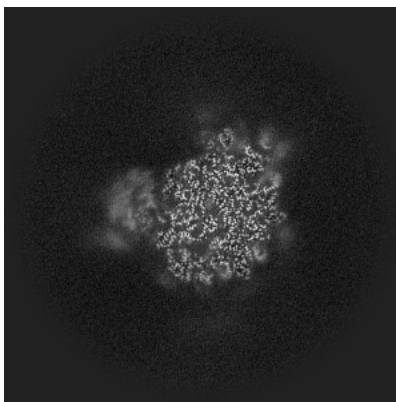
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

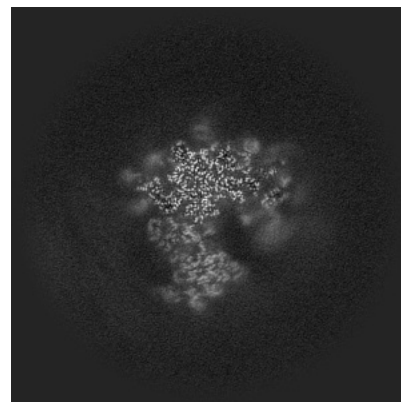
6.3.1 Primary map



X Index: 287

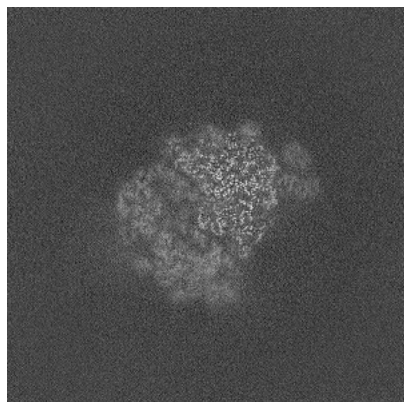


Y Index: 307

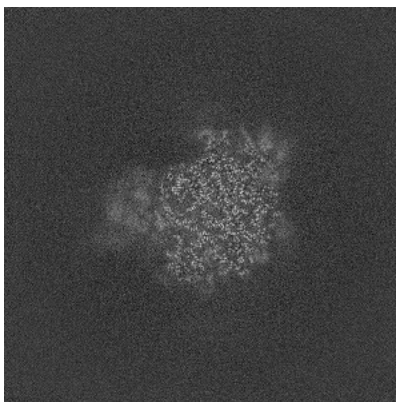


Z Index: 277

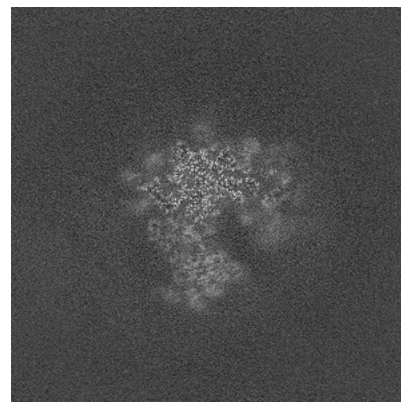
6.3.2 Raw map



X Index: 286



Y Index: 313

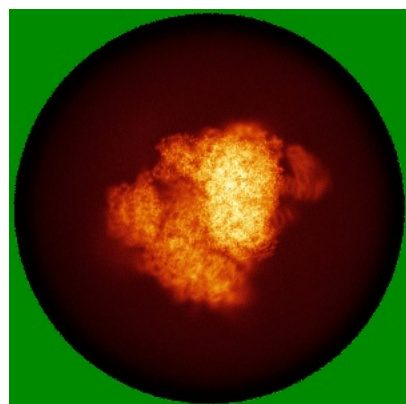


Z Index: 277

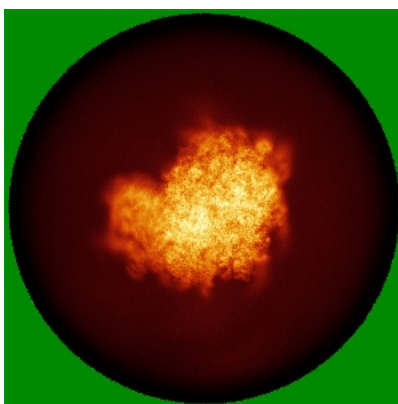
The images above show the largest variance slices of the map in three orthogonal directions.

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

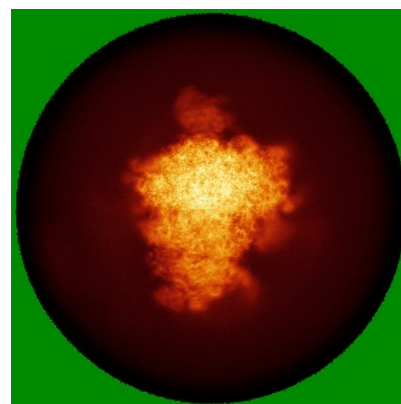
6.4.1 Primary map



X

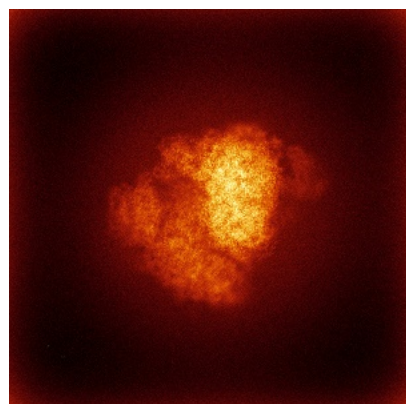


Y

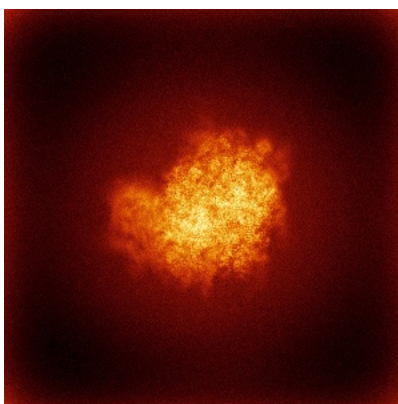


Z

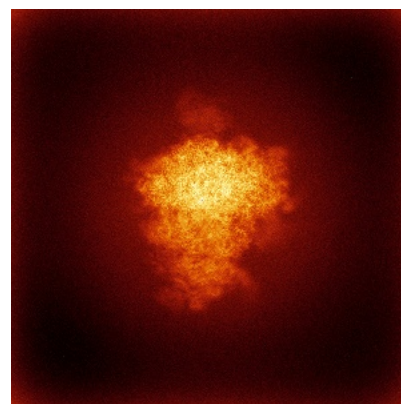
6.4.2 Raw map



X



Y

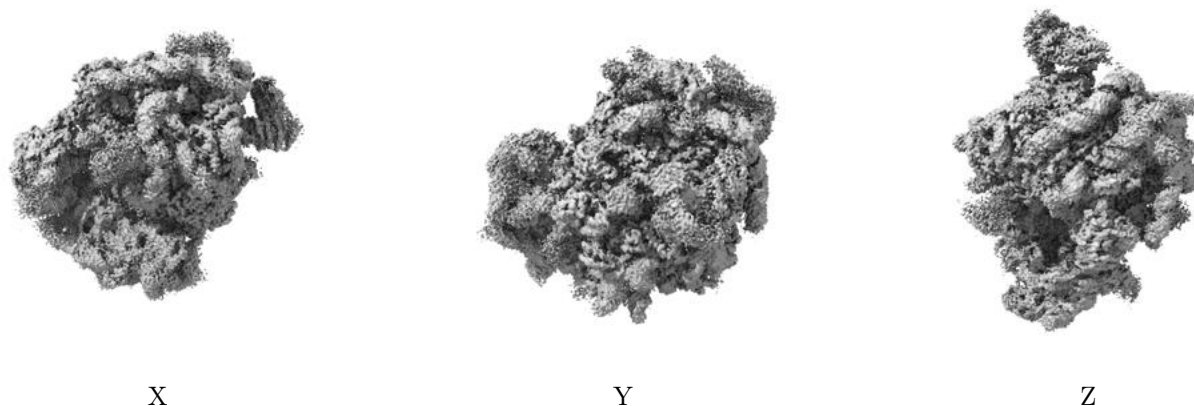


Z

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

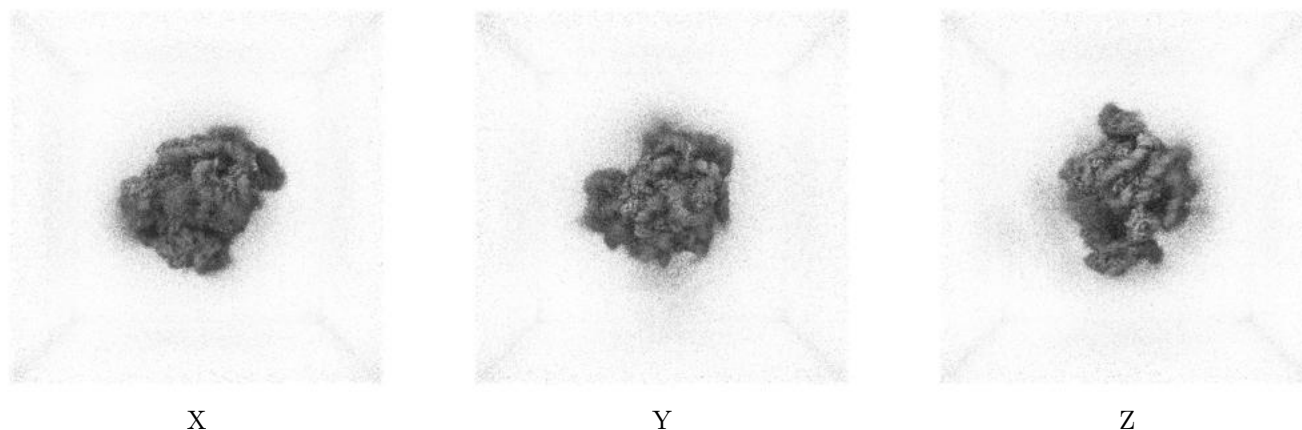
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

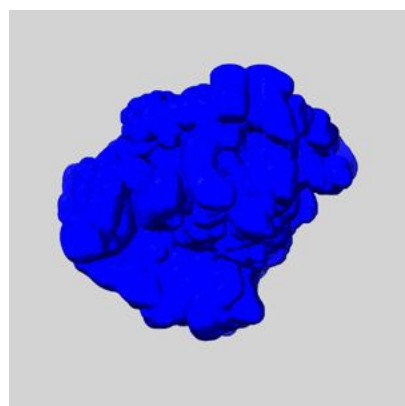
6.6 Mask visualisation [i](#)

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

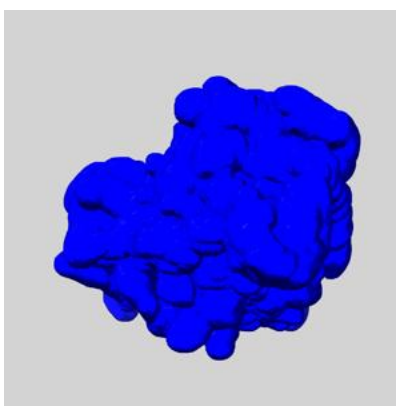
A mask typically either:

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

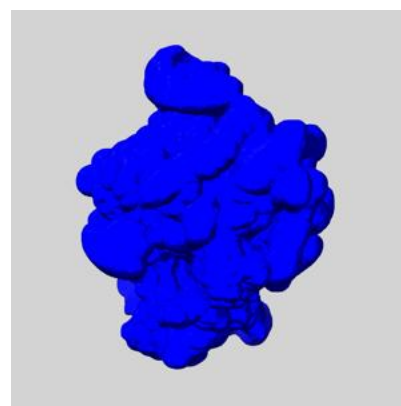
6.6.1 emd_57771_msk_1.map [i](#)



X



Y

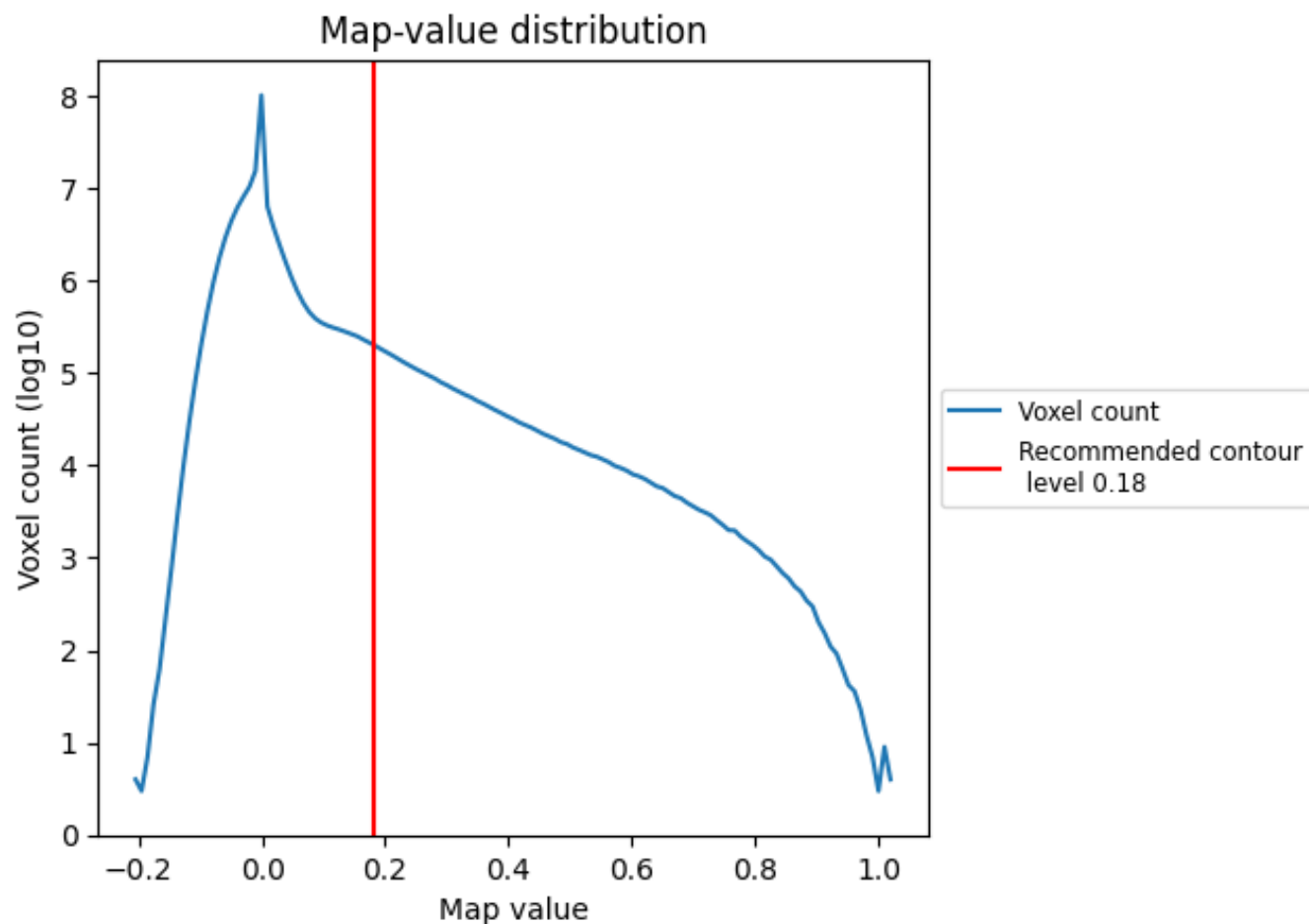


Z

7 Map analysis [i](#)

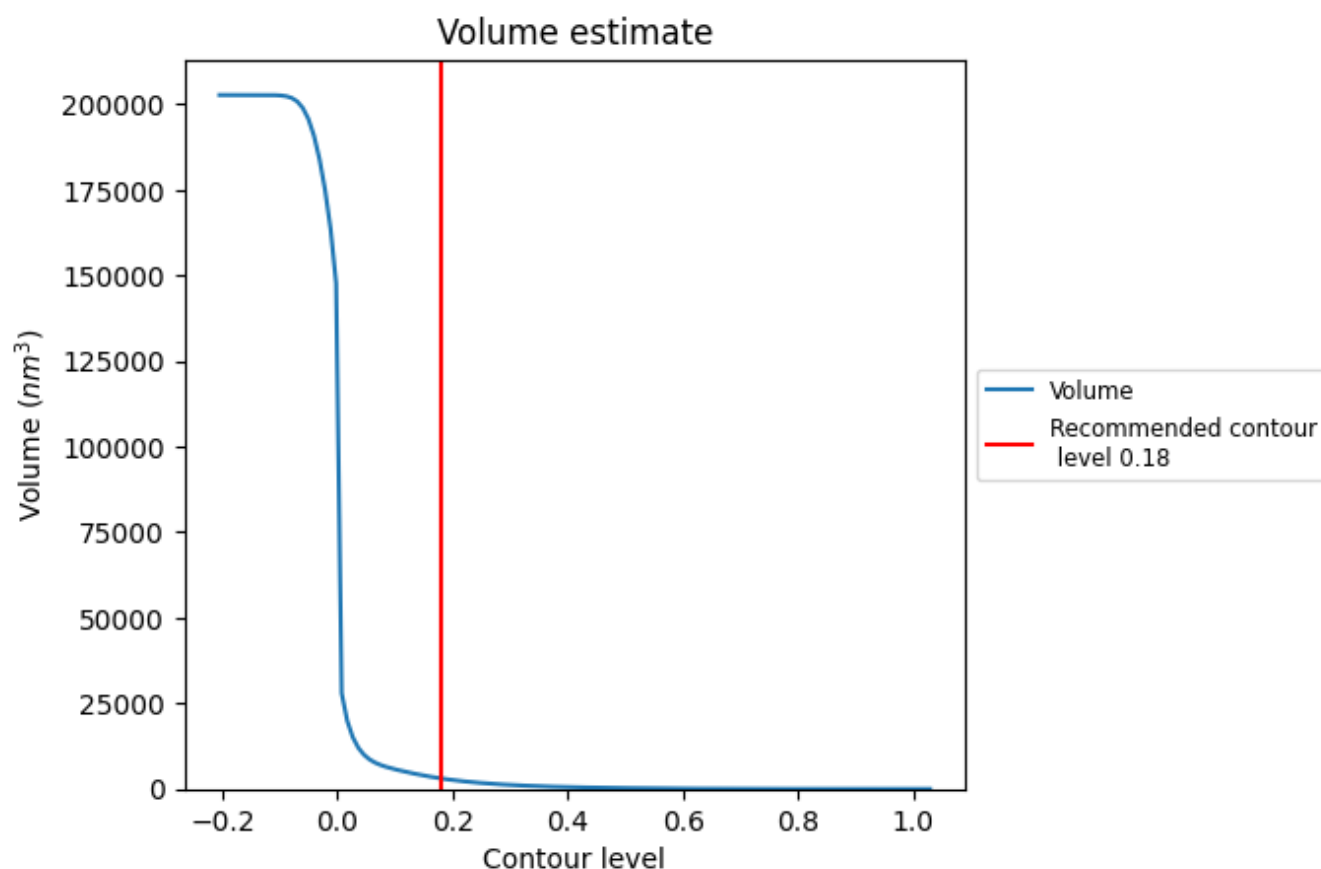
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

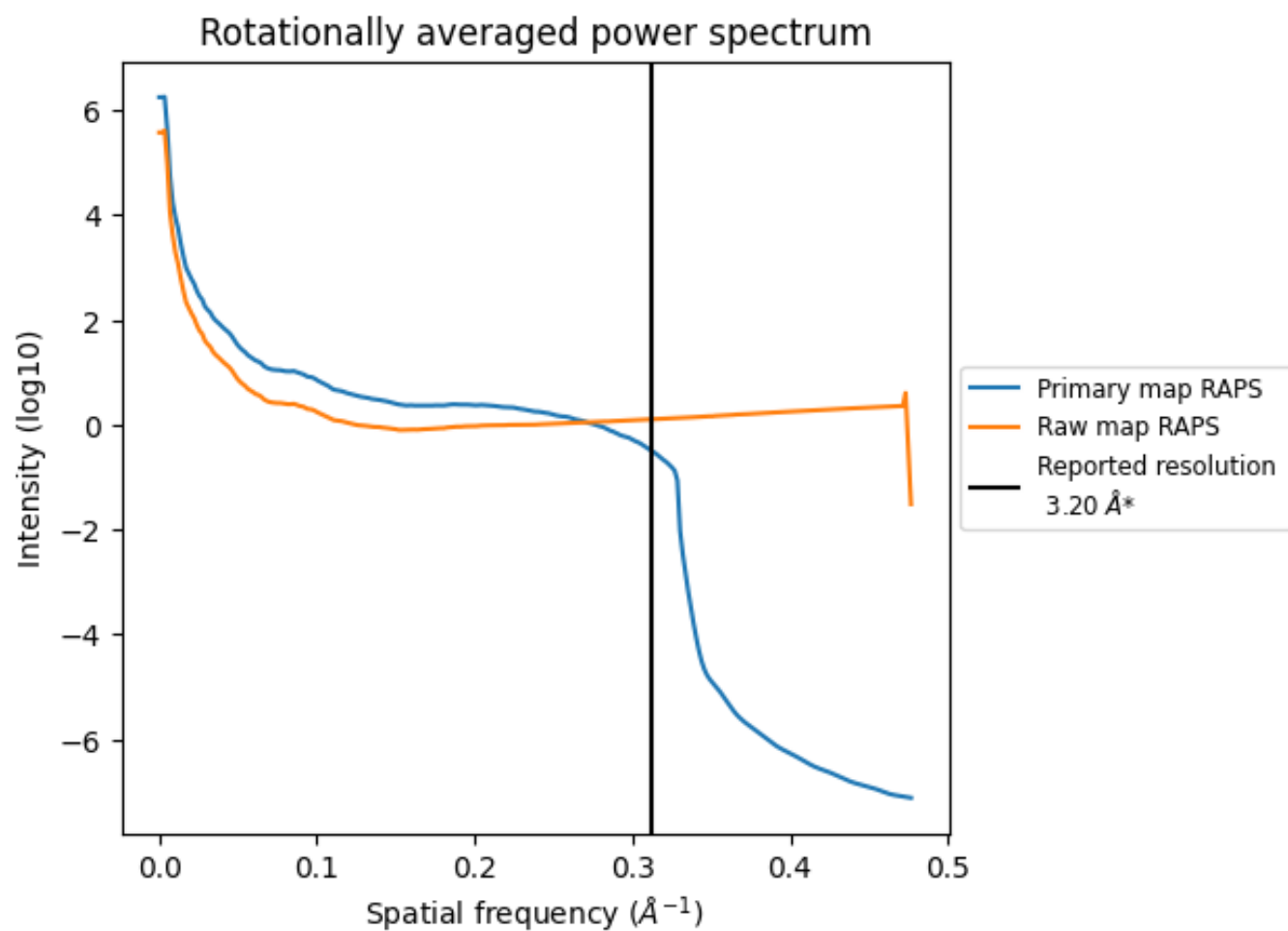
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3069 nm^3 ; this corresponds to an approximate mass of 2772 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 ⓘ

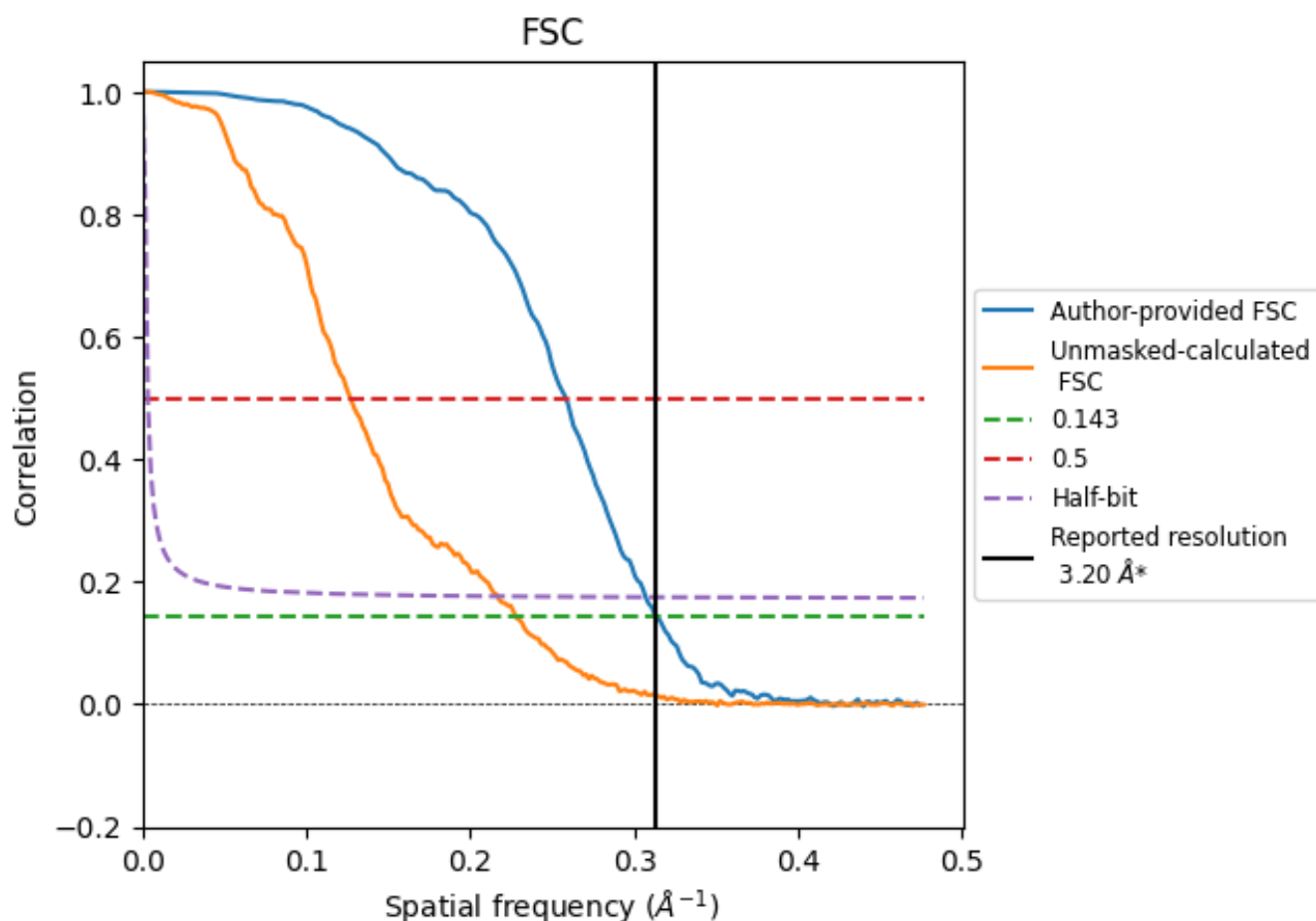


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

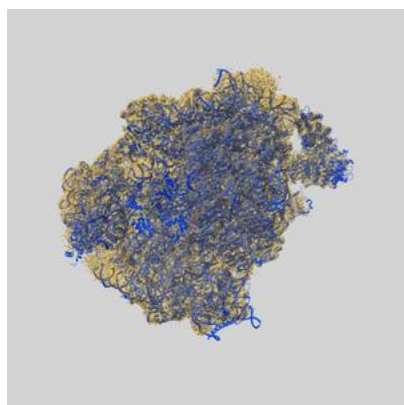
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.87	3.26
Unmasked-calculated*	4.39	7.88	4.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.2 by more than 10 %

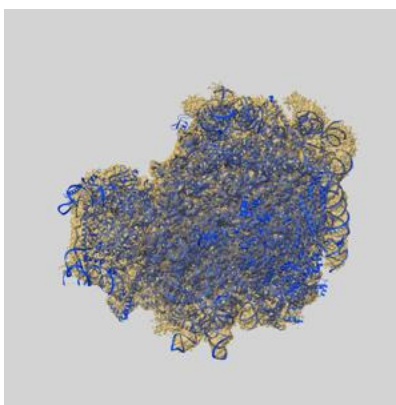
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57771 and PDB model 30HI. Per-residue inclusion information can be found in section 3 on page 23.

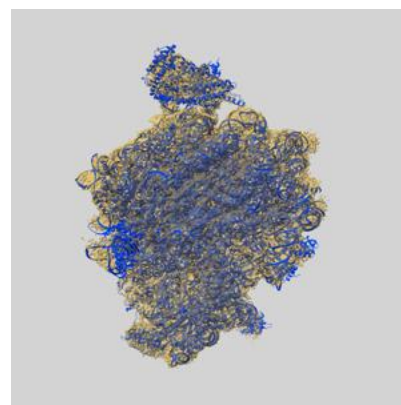
9.1 Map-model overlay [i](#)



X



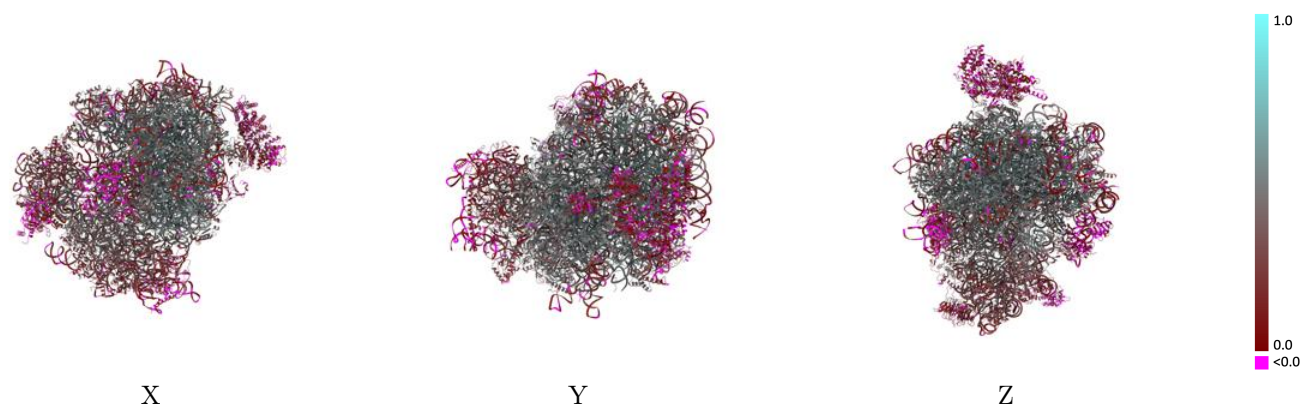
Y



Z

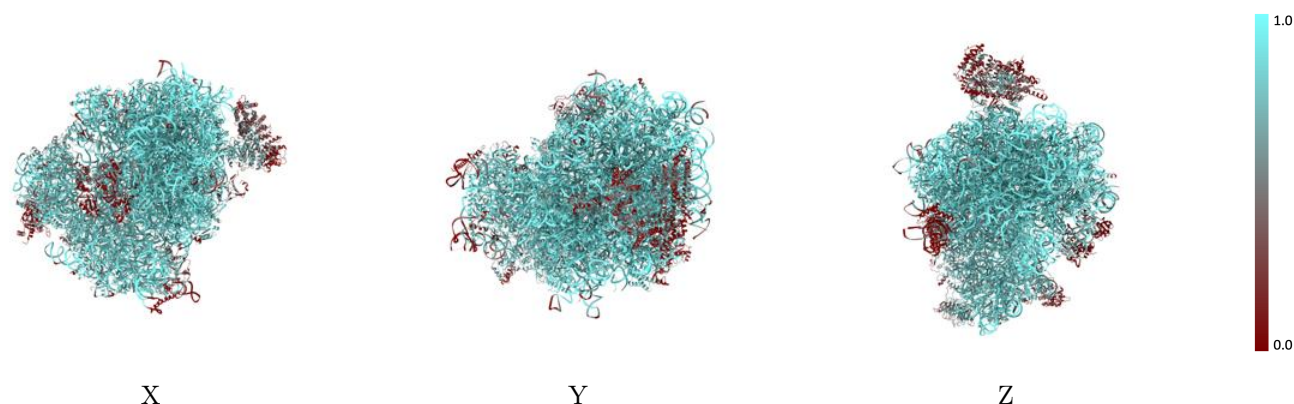
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



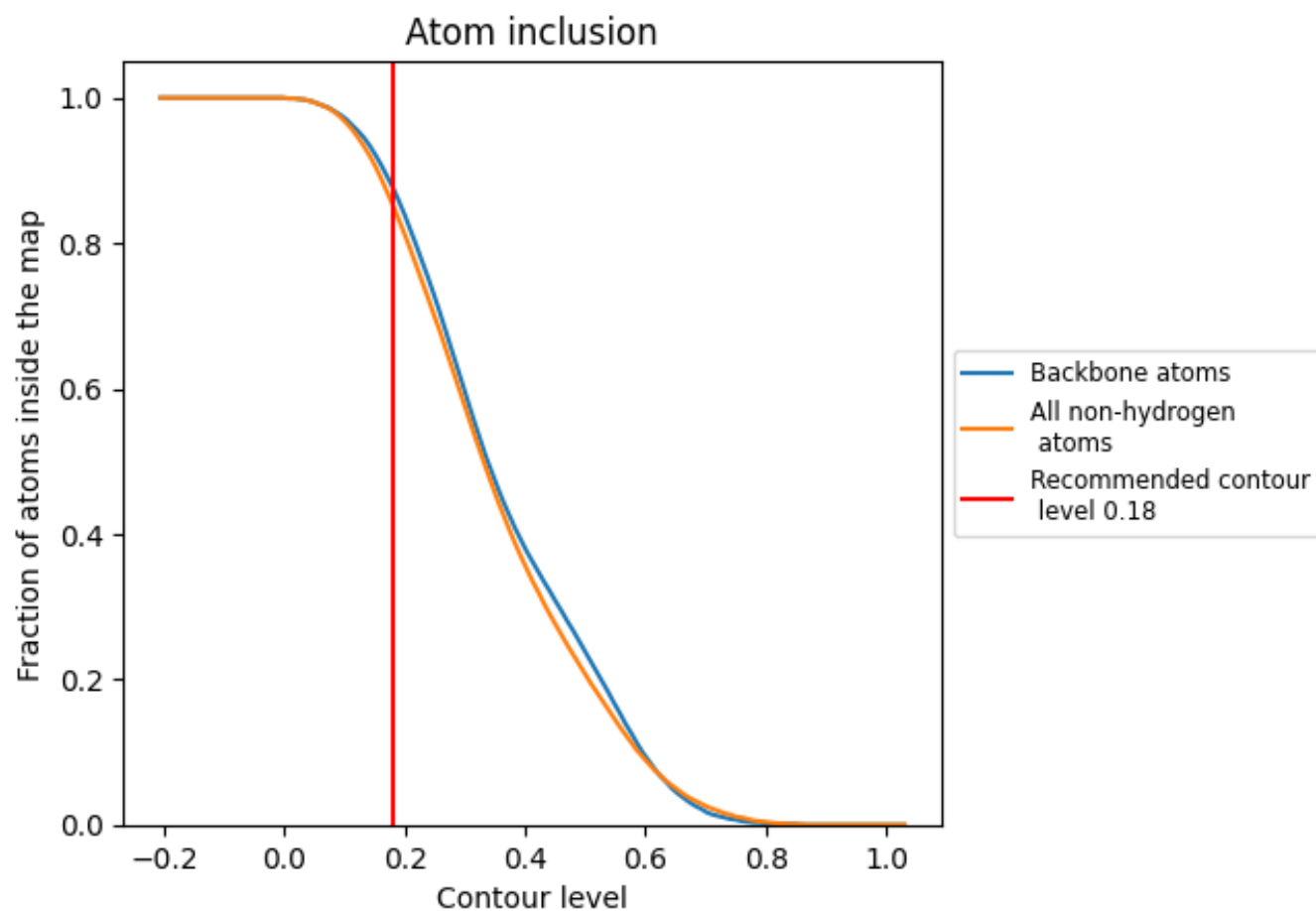
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.3660
A2	 0.9160	 0.3090
AA	 0.7710	 0.3490
AB	 0.7410	 0.3560
AC	 0.8250	 0.3730
AD	 0.7480	 0.2970
AE	 0.8870	 0.2790
AF	 0.7770	 0.2770
AG	 0.6640	 0.1480
AH	 0.6450	 0.2510
AI	 0.7490	 0.2840
AJ	 0.8080	 0.2680
AK	 0.6560	 0.1890
AL	 0.8190	 0.3590
AM	 0.1500	 0.0410
AN	 0.8720	 0.4180
AO	 0.8260	 0.3770
AP	 0.6810	 0.2060
AQ	 0.8390	 0.2710
AR	 0.6020	 0.2410
AS	 0.7730	 0.2370
AT	 0.8180	 0.2540
AU	 0.8160	 0.3180
AV	 0.7790	 0.3720
AW	 0.9290	 0.4080
AX	 0.8590	 0.3650
AY	 0.7720	 0.1820
AZ	 0.7060	 0.2190
Aa	 0.9000	 0.3790
Ab	 0.7880	 0.3520
Ac	 0.7110	 0.2930
Ad	 0.7940	 0.2620
Ae	 0.7230	 0.2670
Af	 0.0980	 0.0390
Ag	 0.6050	 0.1620



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Chain	Atom inclusion	Q-score
Ah	 0.9040	 0.4270
B1	 0.9680	 0.4090
B2	 0.9390	 0.2370
B4	 1.0000	 0.4210
B5	 0.9360	 0.4110
B7	 0.9900	 0.4460
B8	 0.9910	 0.4780
BA	 0.9780	 0.5430
BB	 0.9280	 0.5070
BC	 0.9560	 0.5220
BD	 0.8700	 0.4230
BE	 0.9170	 0.4480
BF	 0.9700	 0.5050
BG	 0.8430	 0.4400
BH	 0.8490	 0.3970
BI	 0.8110	 0.3620
BJ	 0.8270	 0.3630
BL	 0.9230	 0.4940
BM	 0.9230	 0.4520
BN	 0.9900	 0.5470
BO	 0.9560	 0.5010
BP	 0.9600	 0.5250
BQ	 0.9740	 0.5390
BR	 0.8470	 0.4280
BS	 0.9530	 0.4940
BT	 0.9350	 0.4970
BU	 0.8840	 0.4410
BV	 0.9380	 0.5250
BW	 0.5480	 0.2740
BX	 0.9450	 0.4870
BY	 0.9210	 0.5040
BZ	 0.9240	 0.4720
Ba	 0.9650	 0.5280
Bb	 0.9010	 0.4040
Bc	 0.8430	 0.4280
Bd	 0.9370	 0.4870
Be	 0.9690	 0.5370
Bf	 0.9750	 0.5410
Bg	 0.9560	 0.5080
Bh	 0.9260	 0.4870
Bi	 0.8770	 0.4430
Bj	 0.9870	 0.5370

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Chain	Atom inclusion	Q-score
Bk	 0.7480	 0.3920
Bl	 0.9860	 0.5200
Bm	 0.3080	 0.1430
Bo	 0.8580	 0.4430
Bp	 0.9620	 0.5030
Br	 0.9590	 0.5150
Bs	 0.0930	 0.0140
Bt	 0.0360	 0.0380
Bu	 0.2440	 0.0760
Bv	 0.5640	 0.2330
Bw	 0.3530	 0.1180
By	 0.5500	 0.1780
Bz	 0.0100	 0.0430