



# wwPDB EM Validation Summary Report ⓘ

Jun 19, 2026 – 05:43 am BST

PDB ID : 9QQA / pdb\_00009qqa  
EMDB ID : EMD-53295  
Title : Ternary complex of translating ribosome, NAC and NMT1  
Authors : Echeverria, B.; Jaskolowski, M.; Scaiola, A.; Ban, N.  
Deposited on : 2025-03-31  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

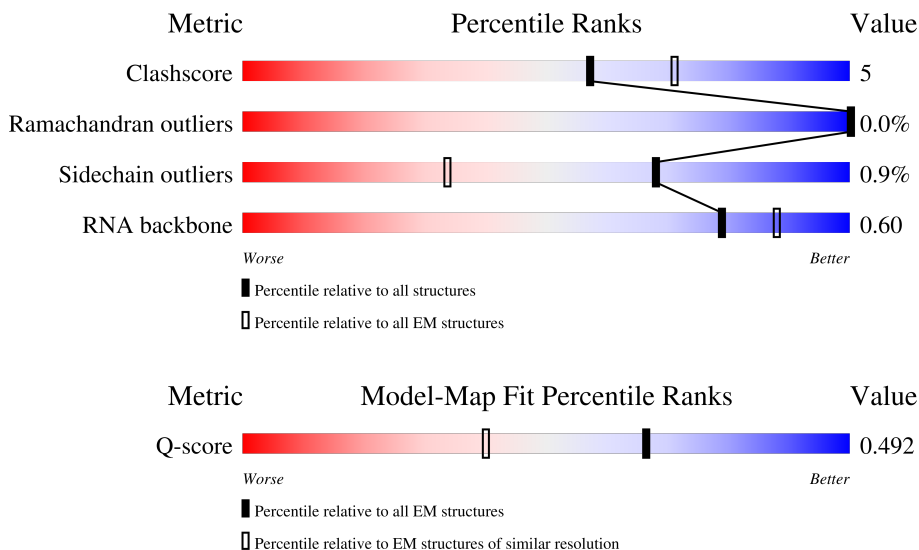
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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	11806 ( 2.30 - 3.30 )

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  $\geq 3$ , 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	A2	1870	
2	AA	84	
3	AB	69	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	AC	156	
5	AD	133	
6	AE	115	
7	AF	317	
8	AG	56	
9	AT	76	
10	AZ	295	
11	Aa	264	
12	Ab	293	
13	Ac	281	
14	Ad	263	
15	Ae	204	
16	Af	249	
17	Ag	432	
18	Ah	208	
19	Ai	194	
20	Aj	165	
21	Ak	158	
22	Al	132	
23	Am	151	
24	An	151	
25	Ao	145	
26	Ap	172	
27	Aq	135	
28	Ar	152	



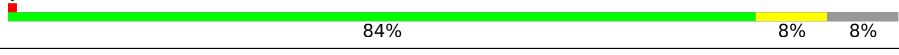
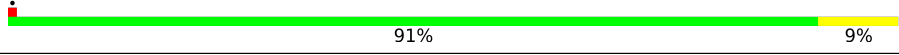


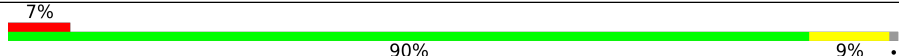
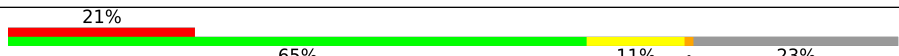
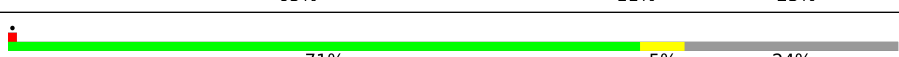

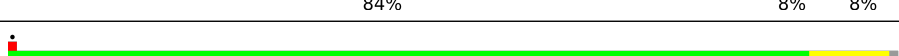
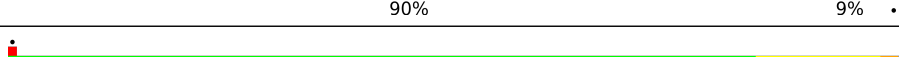
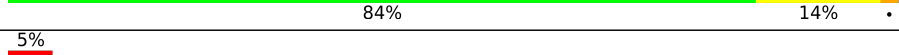



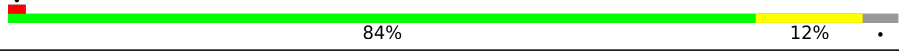
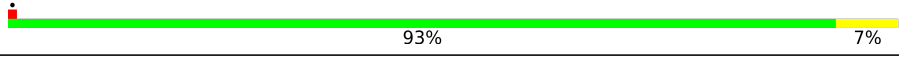
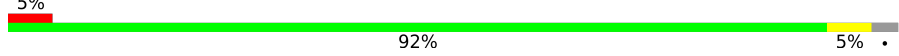

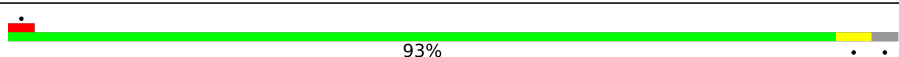

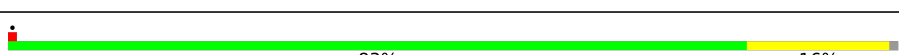
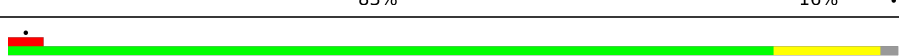

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	As	145	88% 11%
30	At	119	8% 78% 8% 13%
31	Au	84	89% 11%
32	Av	130	96%
33	Aw	143	89% 10%
34	Ax	130	85% 8%
35	Ay	124	12% 58% 10% 31%
36	Az	25	92% 8%
37	B5	4808	55% 18% 23%
38	B7	120	88% 12%
39	B8	158	79% 16%
40	BA	257	86% 12%
41	BB	403	87% 11%
42	BC	413	78% 9% 12%
43	BE	291	8% 73% 9% 16%
44	BF	247	79% 12% 9%
45	BG	266	6% 81% 6% 12%
46	BH	192	90% 9%
47	BI	214	6% 87% 13%
48	BJ	178	80% 15%
49	BK	12	83% 100%
50	BL	211	93% 6%
51	BM	218	57% 6% 37%
52	BN	204	87% 13%
53	BO	203	91% 7%

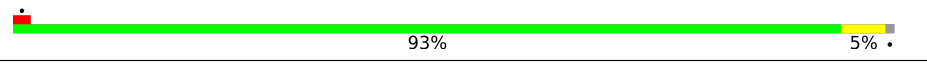


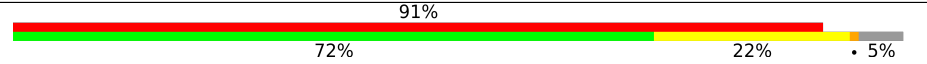
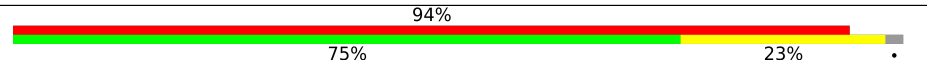
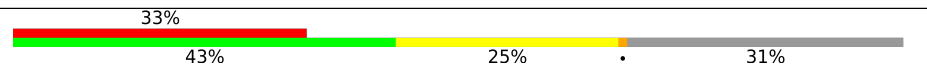

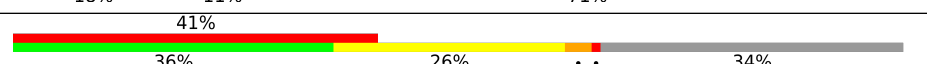
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	BP	184	
55	BQ	188	
56	BR	196	
57	BS	176	
58	BT	160	
59	BU	128	
60	BV	140	
61	BW	157	
62	BX	156	
63	BY	145	
64	BZ	136	
65	Ba	148	
66	Bb	245	
67	Bc	115	
68	Bd	125	
69	Be	135	
70	Bf	110	
71	Bg	117	
72	Bh	123	
73	Bi	105	
74	Bj	97	
75	Bk	70	
76	Bl	51	
77	Bm	128	
78	Bo	106	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
79	Bp	92	
80	Br	137	
81	Bs	318	
82	Bt	165	
83	Bv	217	
84	MA	496	
85	Nt	215	
86	Nu	162	

## 2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 226637 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A2	1770	37833	16911	6781	12371	1770	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 3 is a protein called Small ribosomal subunit protein eS28.

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

- Molecule 4 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

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

- Molecule 5 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

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

- Molecule 6 is a protein called eS26.

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

- Molecule 7 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 9 is a RNA chain called P site Phe tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	AT	76	1621	724	290	531	76	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein uS2.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	2	ACE	-	acetylation	UNP G1TLT8

- Molecule 11 is a protein called 40S ribosomal protein S3a.

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

- Molecule 12 is a protein called 40S ribosomal protein S2.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 13 is a protein called 40S ribosomal protein S3.

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

- Molecule 14 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 16 is a protein called 40S ribosomal protein S6.

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

- Molecule 17 is a protein called 40S ribosomal protein S7.

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

- Molecule 18 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 20 is a protein called S10\_ plectin domain-containing protein.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 22 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 24 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	An	122	899	556	166	171	6	0	0

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Ao	128	1048	665	197	179	7	0	0

- Molecule 26 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 27 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Ar	149	1217	763	245	208	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ar	2	ACE	-	acetylation	UNP G1TPG3

- Molecule 29 is a protein called 40S ribosomal protein S19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
As	119	GLY	TRP	conflict	UNP G1TN62

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
As	142	ASN	LYS	conflict	UNP G1TN62

- Molecule 30 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 31 is a protein called Small ribosomal subunit protein eS21.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 32 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 33 is a protein called 40S ribosomal protein S23.

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

- Molecule 34 is a protein called 40S ribosomal protein S24.

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

- Molecule 35 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Ay	85	683	439	128	115	1	0	0

- Molecule 36 is a protein called Small ribosomal subunit protein eS32.

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

- Molecule 37 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	B5	3706	79525	35447	14532	25840	3706	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 38 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	B7	120	2561	1141	456	844	120	0	0

- Molecule 39 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	B8	156	3319	1481	585	1097	156	0	0

- Molecule 40 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 41 is a protein called Ribosomal protein L3.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL4.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 43 is a protein called 60S ribosomal protein L6.

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

- Molecule 44 is a protein called Ribosomal Protein uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	61	ARG	GLY	conflict	UNP G1TUB1
BF	93	ARG	GLY	conflict	UNP G1TUB1
BF	131	MET	VAL	conflict	UNP G1TUB1
BF	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 45 is a protein called 60S ribosomal protein L7a.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 46 is a protein called 60S ribosomal protein L9.

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

- Molecule 47 is a protein called 60S ribosomal protein L10.

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

- Molecule 48 is a protein called 60S ribosomal protein L11.

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

- Molecule 49 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	BK	12	60	36	12	12	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein eL13.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 51 is a protein called 60S ribosomal protein L14.

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

- Molecule 52 is a protein called Ribosomal protein L15.

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

- Molecule 53 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 54 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	BP	153	1242	777	241	215	9	0	0

- Molecule 55 is a protein called eL18.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 56 is a protein called Ribosomal protein L19.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	38	ARG	CYS	conflict	UNP G1TJR3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
BR	64	ARG	GLN	conflict	UNP G1TJR3
BR	94	THR	LYS	conflict	UNP G1TJR3

- Molecule 57 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 58 is a protein called 60S ribosomal protein L21.

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

- Molecule 59 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	BU	102	831	531	146	152	2	0	0

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 60 is a protein called Ribosomal protein L23.

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

- Molecule 61 is a protein called Ribosomal protein L24.

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

- Molecule 62 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 63 is a protein called Ribosomal protein L26.

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

- Molecule 64 is a protein called 60S ribosomal protein L27.

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

- Molecule 65 is a protein called 60S ribosomal protein L27a.

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

- Molecule 66 is a protein called 60S ribosomal protein L29.

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

- Molecule 67 is a protein called 60S ribosomal protein L30.

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

- Molecule 68 is a protein called 60S ribosomal protein L31.

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

- Molecule 69 is a protein called Ribosomal protein L32.

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

- Molecule 70 is a protein called 60S ribosomal protein L35a.

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

- Molecule 71 is a protein called 60S ribosomal protein L34.

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

- Molecule 72 is a protein called 60S ribosomal protein L35.

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

- Molecule 73 is a protein called 60S ribosomal protein L36.

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

- Molecule 74 is a protein called Ribosomal protein L37.

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

- Molecule 75 is a protein called 60S ribosomal protein L38.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 76 is a protein called 60S ribosomal protein L39-like.

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

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

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

- Molecule 78 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 79 is a protein called 60S ribosomal protein L37a.

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

- Molecule 80 is a protein called [histone H4]-N-methyl-L-lysine20 N-methyltransferase KMT5B.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Br	2	ACE	-	acetylation	UNP A0A8C0DF35

- Molecule 81 is a protein called Large ribosomal subunit protein uL10.

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

- Molecule 82 is a protein called 60S ribosomal protein L12.

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

- Molecule 83 is a protein called Ribosomal protein uL1.

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

- Molecule 84 is a protein called Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	MA	341	2797	1815	475	491	16	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
MA	180	ALA	TYR	engineered mutation	UNP P30419

- Molecule 85 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Nt	63	499	316	91	91	1	0	0

- Molecule 86 is a protein called Isoform 2 of Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	Nu	107	828	518	154	153	3	0	0

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	A2	108	Total 108	Mg 108	0
87	Aw	1	Total 1	Mg 1	0
87	B5	273	Total 273	Mg 273	0
87	B7	9	Total 9	Mg 9	0
87	B8	8	Total 8	Mg 8	0
87	BB	3	Total 3	Mg 3	0
87	BI	1	Total 1	Mg 1	0
87	BP	1	Total 1	Mg 1	0
87	BR	1	Total 1	Mg 1	0
87	BV	1	Total 1	Mg 1	0
87	Bj	1	Total 1	Mg 1	0

- Molecule 88 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

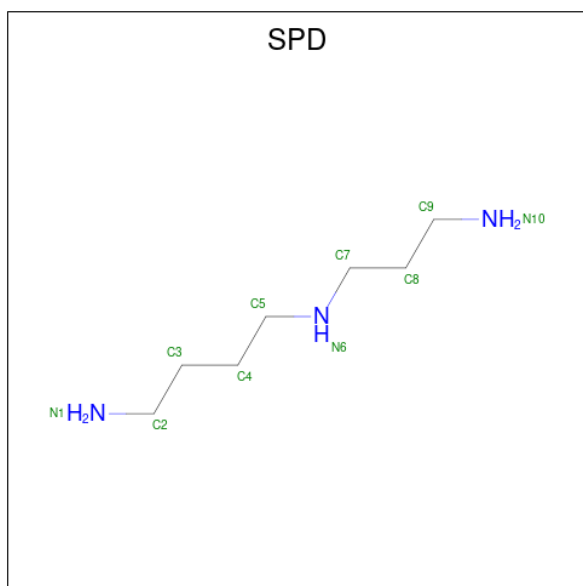
Mol	Chain	Residues	Atoms		AltConf
88	A2	31	Total 31	X 31	0
88	Ad	1	Total 1	X 1	0
88	B5	130	Total 130	X 130	0
88	B7	6	Total 6	X 6	0
88	B8	4	Total 4	X 4	0
88	BA	2	Total 2	X 2	0
88	BH	1	Total 1	X 1	0
88	BI	1	Total 1	X 1	0
88	BL	1	Total 1	X 1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
88	BN	2	Total	X	0
			2	2	
88	BQ	1	Total	X	0
			1	1	
88	BT	1	Total	X	0
			1	1	
88	BY	1	Total	X	0
			1	1	
88	Bb	2	Total	X	0
			2	2	
88	Be	2	Total	X	0
			2	2	
88	Bo	1	Total	X	0
			1	1	

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
89	A2	1	Total	C	N	0
			10	7	3	
89	A2	1	Total	C	N	0
			10	7	3	
89	A2	1	Total	C	N	0
			10	7	3	
89	A2	1	Total	C	N	0
			10	7	3	

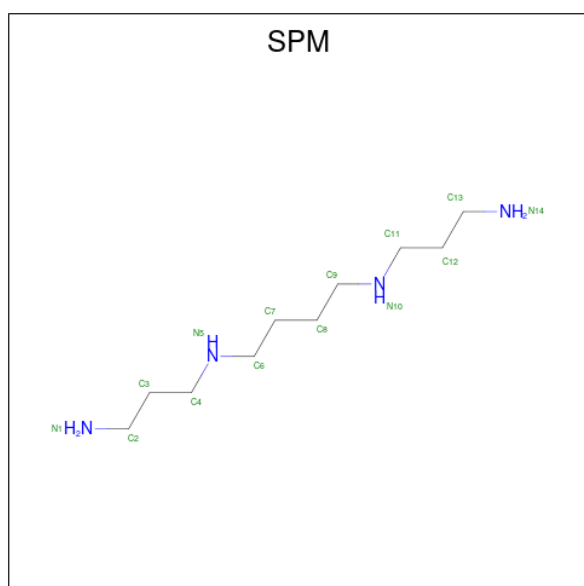
Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
89	B5	1	10	7	3	0
89	B5	1	10	7	3	0
89	B5	1	10	7	3	0
89	B5	1	10	7	3	0
89	B5	1	10	7	3	0

- Molecule 90 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
90	A2	1	14	10	4	0
90	B5	1	14	10	4	0
90	B5	1	14	10	4	0

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
91	AC	1	1	1	0

Continued on next page...

*Continued from previous page...*

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

- Molecule 92 is water.

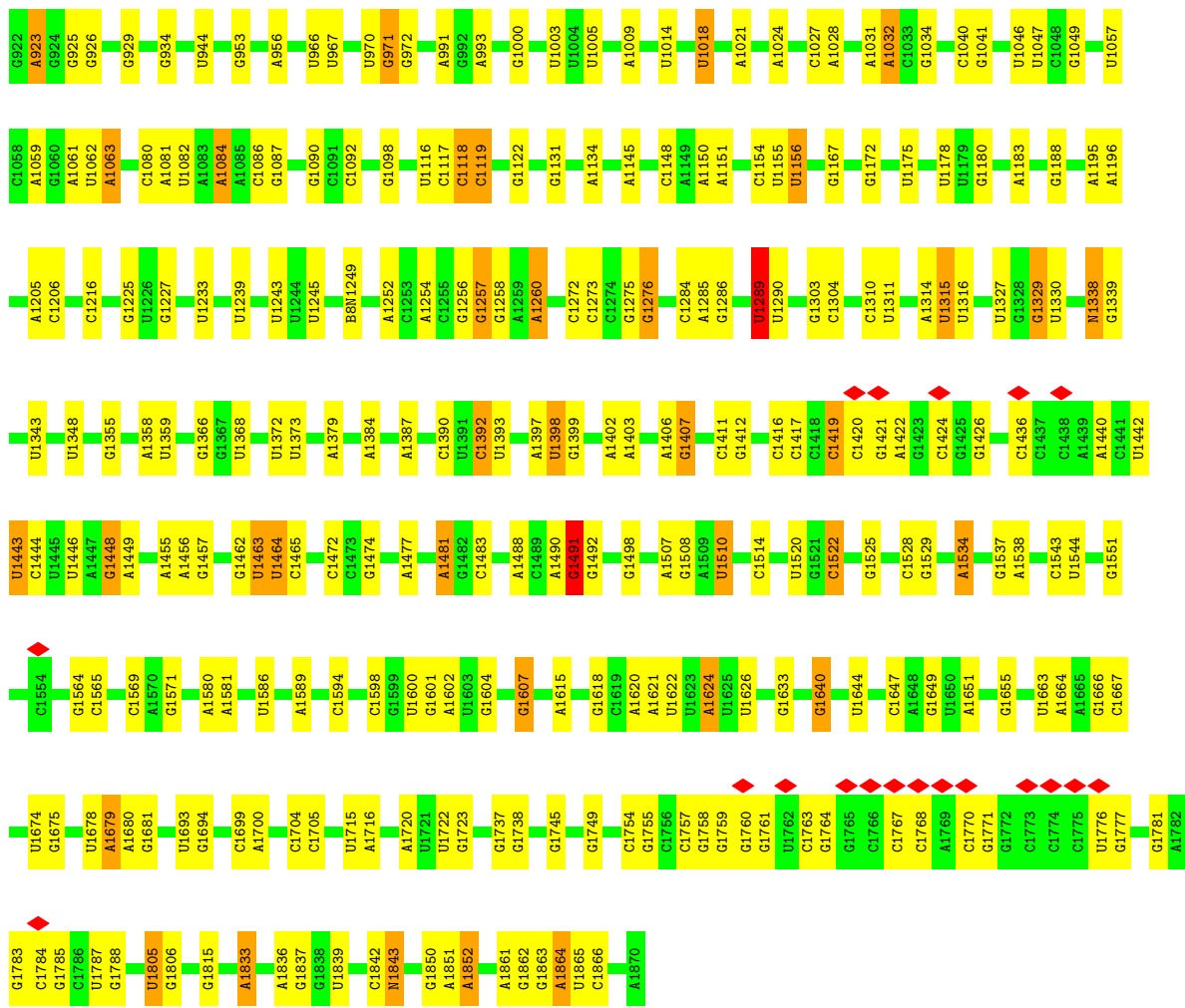
Mol	Chain	Residues	Atoms		AltConf
92	A2	514	Total 514	O 514	0
92	AE	1	Total 1	O 1	0
92	AT	4	Total 4	O 4	0
92	Aa	3	Total 3	O 3	0
92	Af	2	Total 2	O 2	0
92	Ak	2	Total 2	O 2	0
92	An	2	Total 2	O 2	0
92	Ap	1	Total 1	O 1	0
92	Ar	2	Total 2	O 2	0
92	As	2	Total 2	O 2	0
92	At	1	Total 1	O 1	0
92	Aw	4	Total 4	O 4	0

*Continued on next page...*

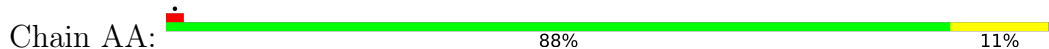
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
92	B5	1359	Total 1359	O 1359	0
92	B7	38	Total 38	O 38	0
92	B8	49	Total 49	O 49	0
92	BA	4	Total 4	O 4	0
92	BC	6	Total 6	O 6	0
92	BH	1	Total 1	O 1	0
92	BI	3	Total 3	O 3	0
92	BL	1	Total 1	O 1	0
92	BN	2	Total 2	O 2	0
92	BP	4	Total 4	O 4	0
92	BR	2	Total 2	O 2	0
92	BV	3	Total 3	O 3	0
92	BX	1	Total 1	O 1	0
92	BY	1	Total 1	O 1	0
92	Ba	4	Total 4	O 4	0
92	Bd	1	Total 1	O 1	0
92	Be	3	Total 3	O 3	0
92	Bg	2	Total 2	O 2	0
92	Bj	5	Total 5	O 5	0
92	Bo	1	Total 1	O 1	0

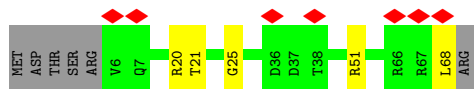
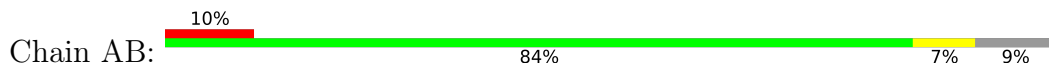




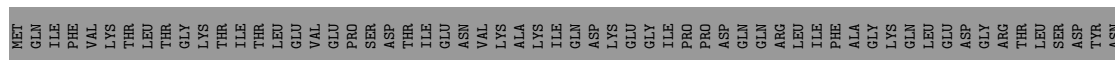
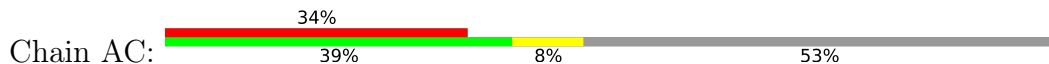
• Molecule 2: Small ribosomal subunit protein eS27

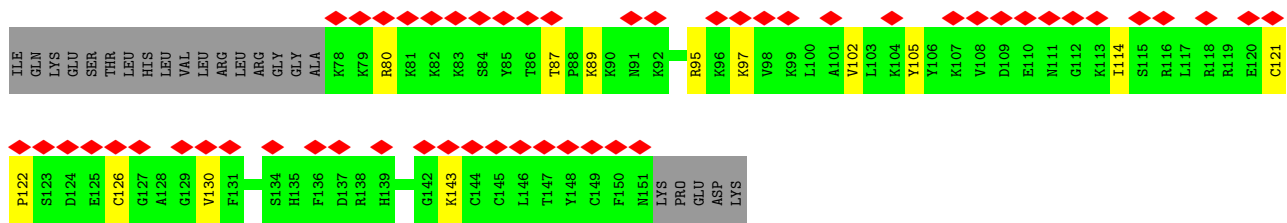


• Molecule 3: Small ribosomal subunit protein eS28

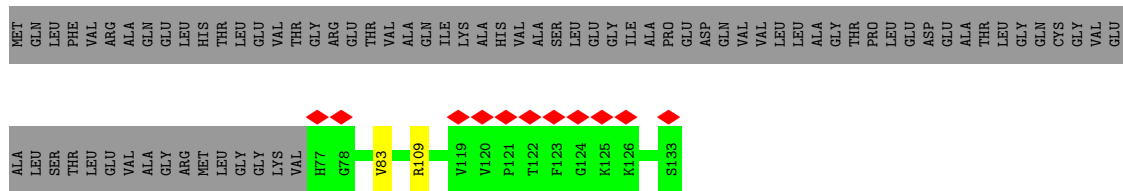


• Molecule 4: Ubiquitin-ribosomal protein eS31 fusion protein

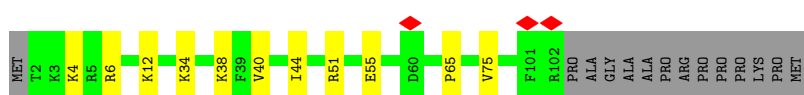
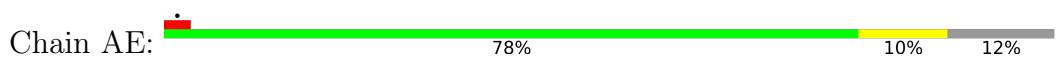




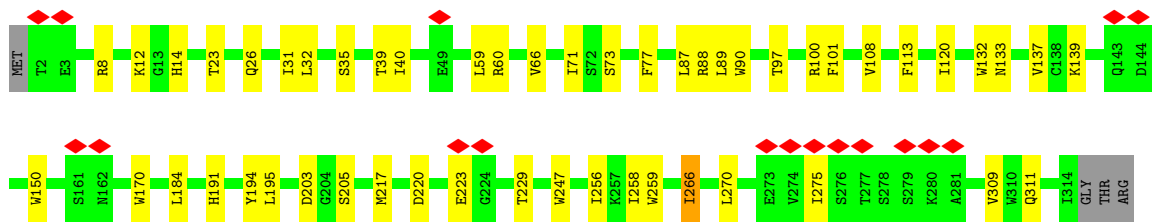
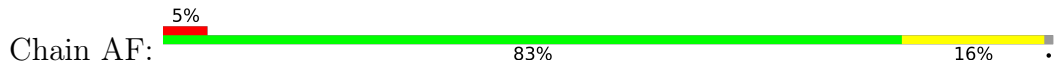
• Molecule 5: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



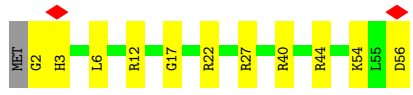
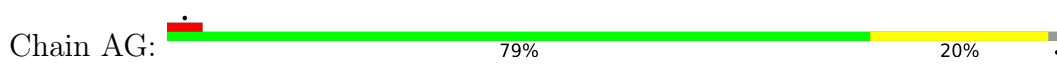
• Molecule 6: eS26



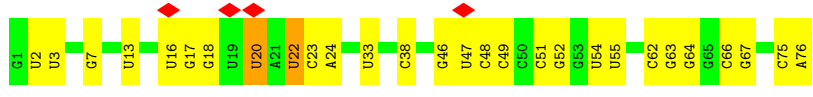
• Molecule 7: Small ribosomal subunit protein RACK1



• Molecule 8: Small ribosomal subunit protein uS14

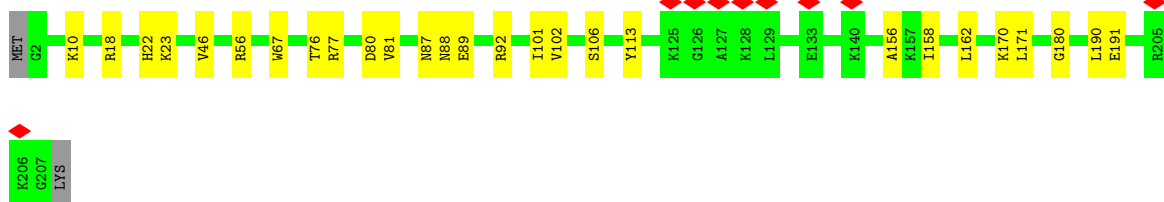
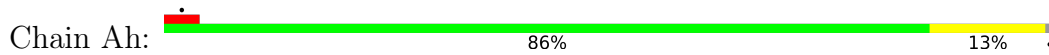


• Molecule 9: P site Phe tRNA

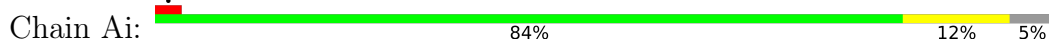




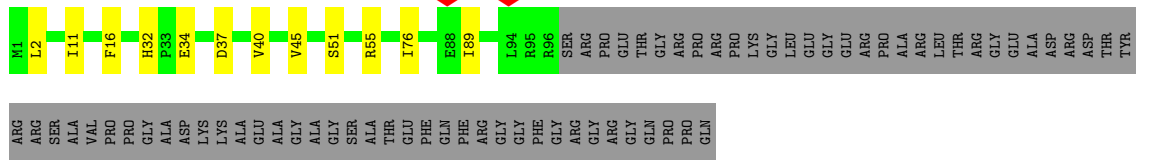




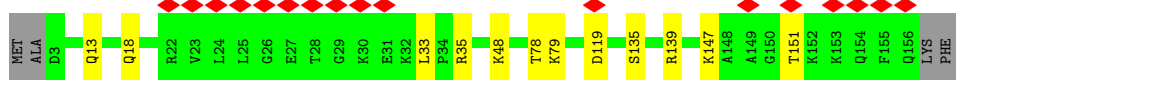
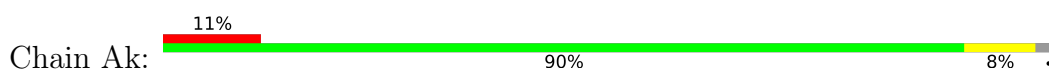
- Molecule 19: Small ribosomal subunit protein uS4



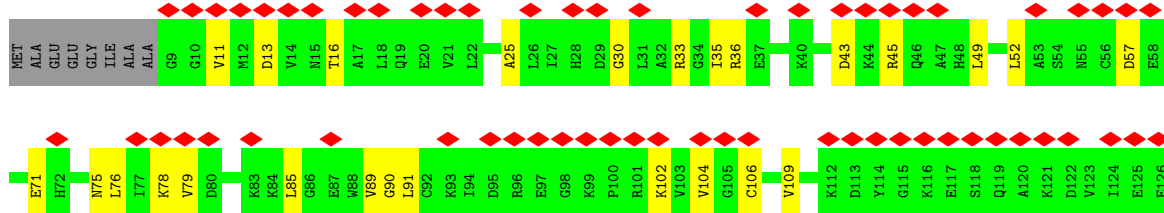
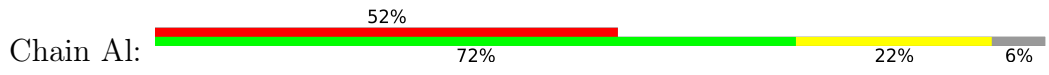
- Molecule 20: S10\_ plectin domain-containing protein



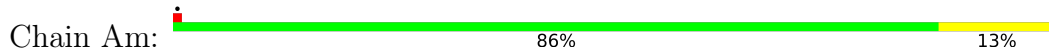
- Molecule 21: Small ribosomal subunit protein uS17

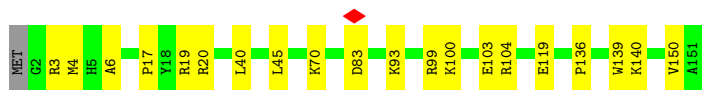


- Molecule 22: Small ribosomal subunit protein eS12

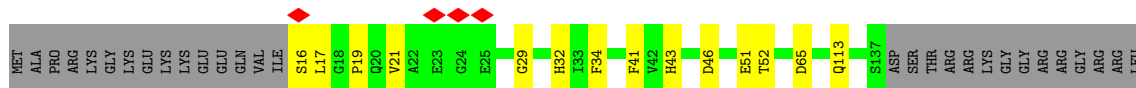
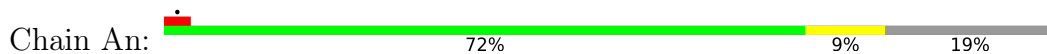


- Molecule 23: Small ribosomal subunit protein uS15

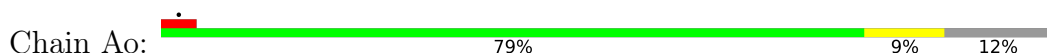




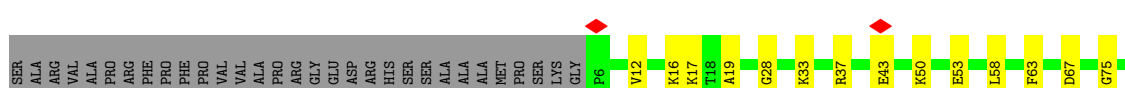
• Molecule 24: Small ribosomal subunit protein uS11



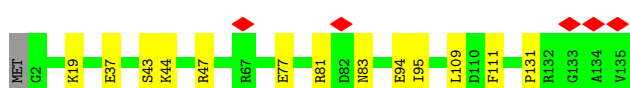
• Molecule 25: Small ribosomal subunit protein uS19



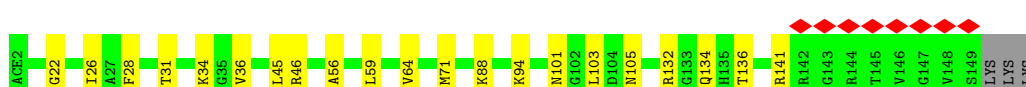
• Molecule 26: Small ribosomal subunit protein uS9



• Molecule 27: Small ribosomal subunit protein eS17



• Molecule 28: Small ribosomal subunit protein uS13

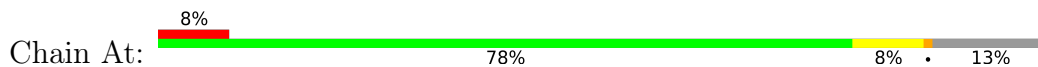


• Molecule 29: 40S ribosomal protein S19





• Molecule 30: Small ribosomal subunit protein uS10



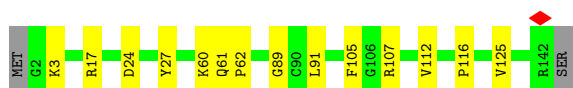
• Molecule 31: Small ribosomal subunit protein eS21



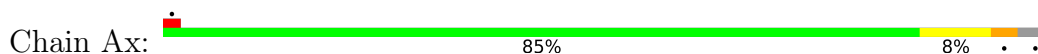
• Molecule 32: Small ribosomal subunit protein uS8



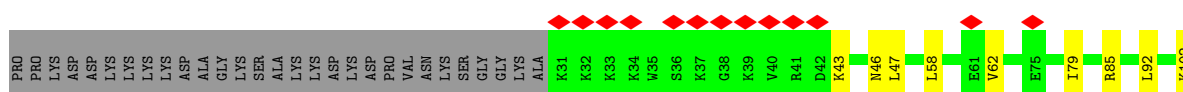
• Molecule 33: 40S ribosomal protein S23

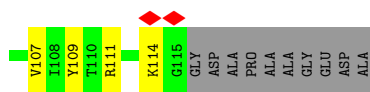


• Molecule 34: 40S ribosomal protein S24

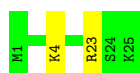


• Molecule 35: Small ribosomal subunit protein eS25

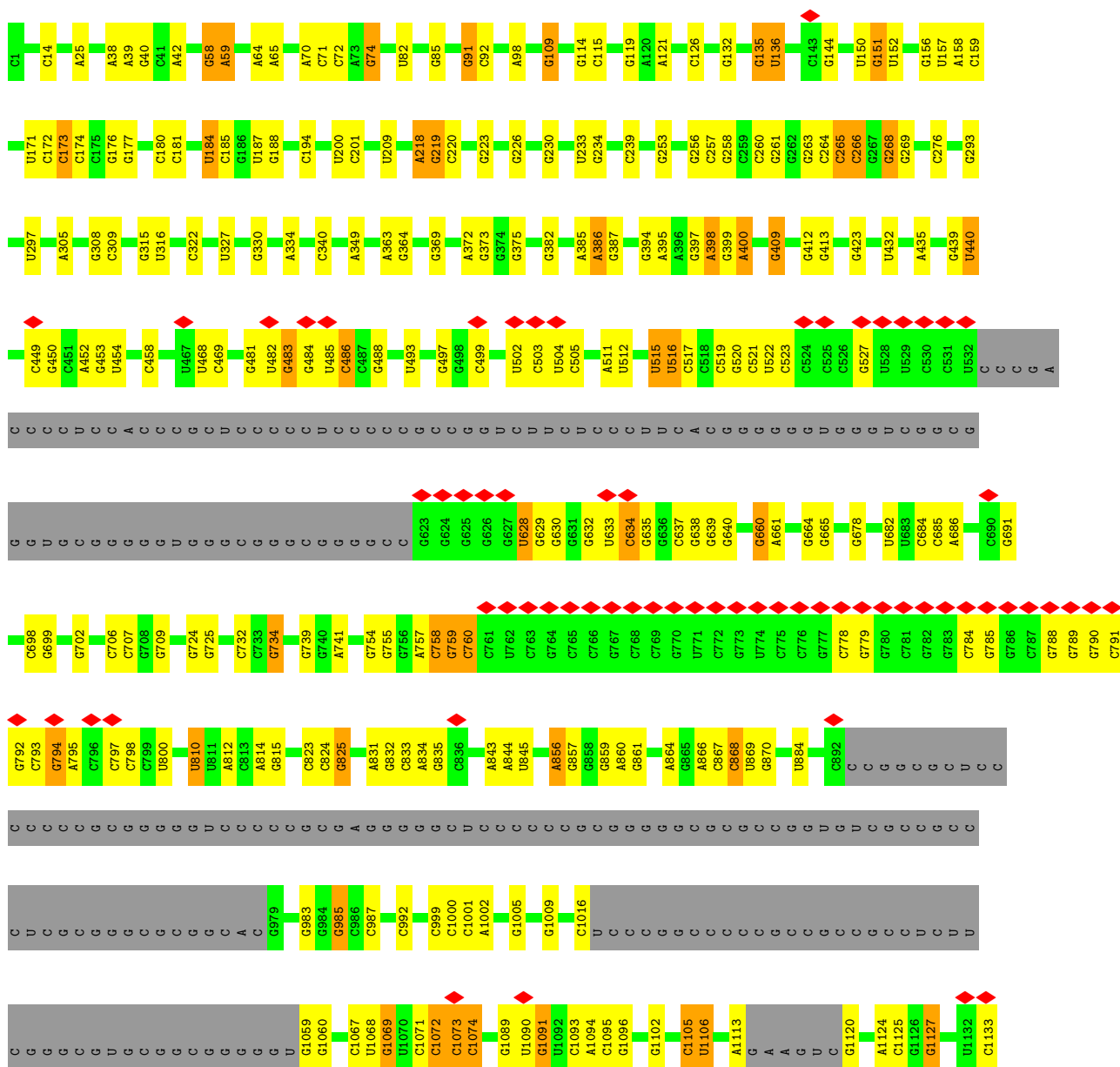


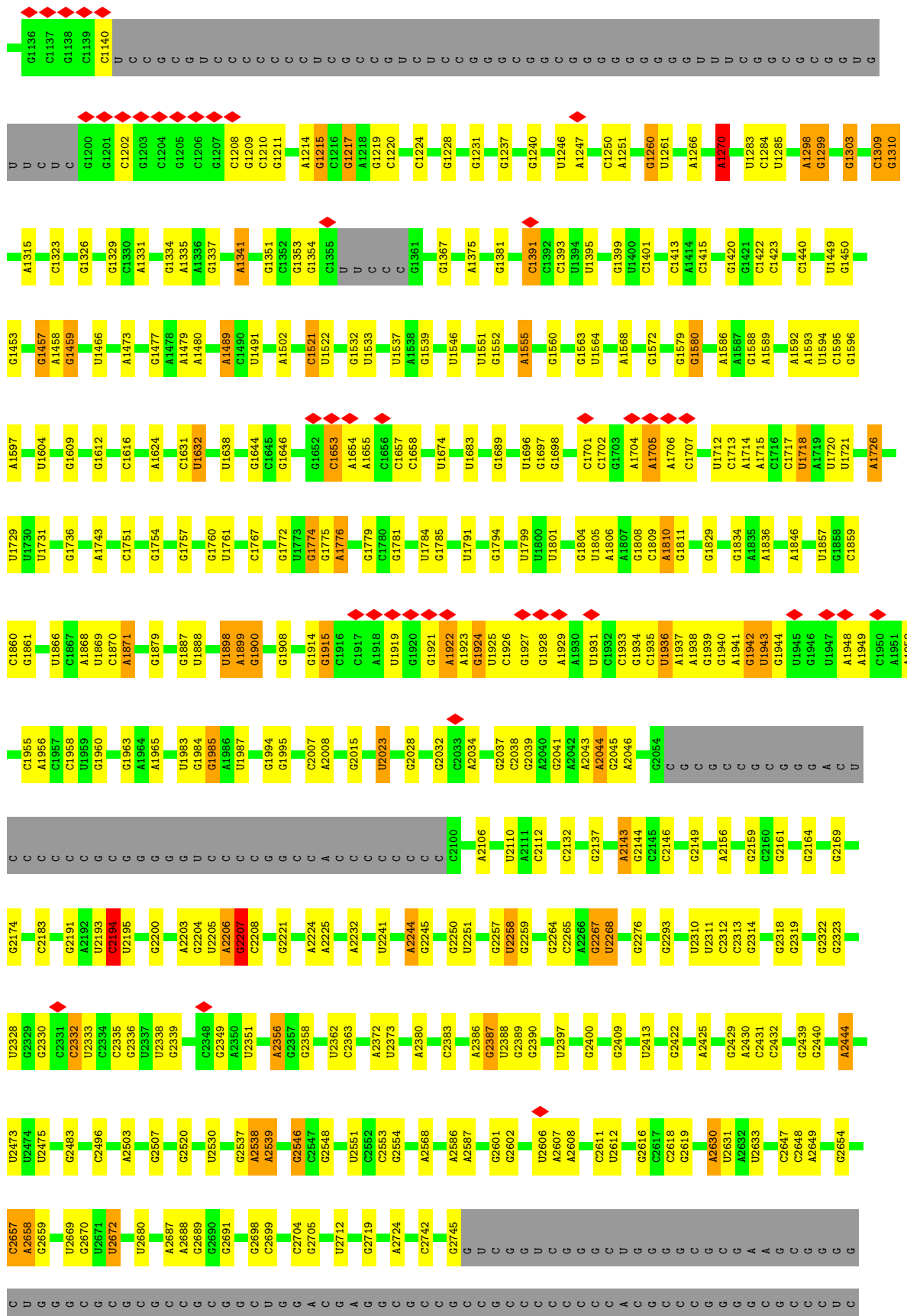


- Molecule 36: Small ribosomal subunit protein eS32

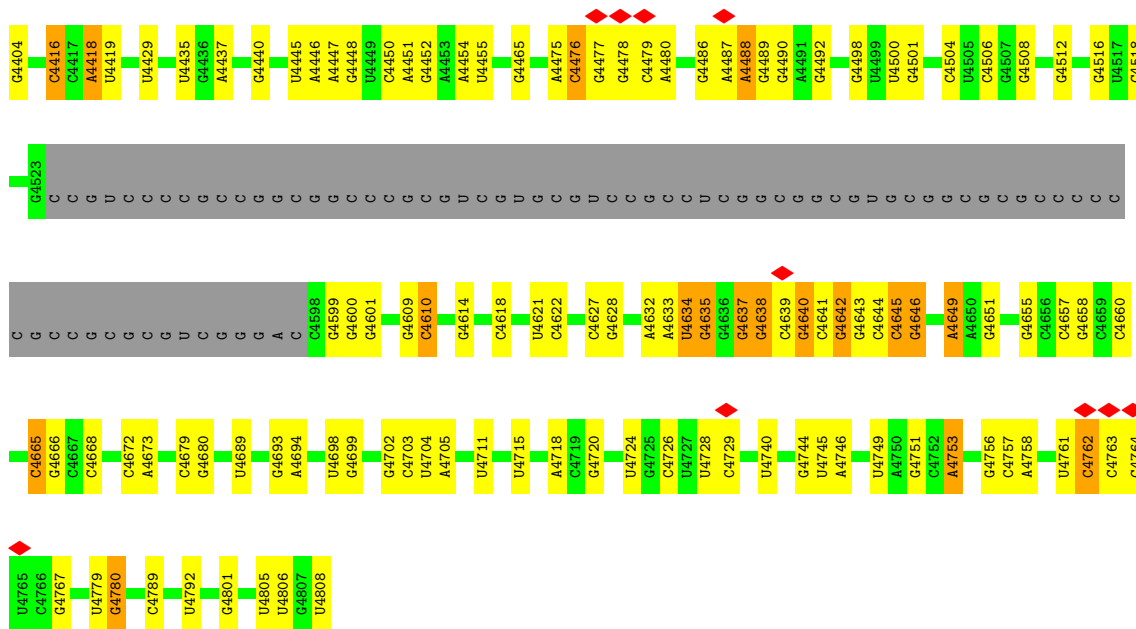


- Molecule 37: 28S rRNA

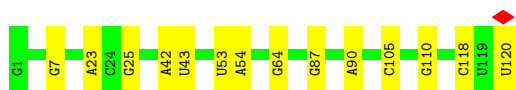




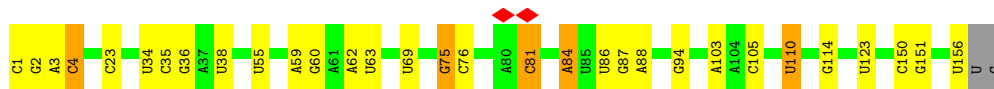
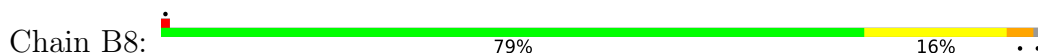




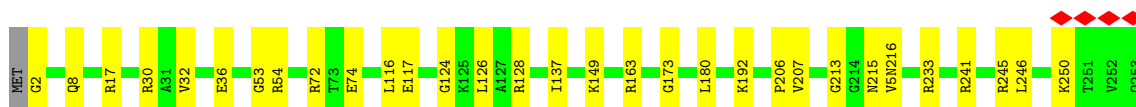
• Molecule 38: 5S rRNA



• Molecule 39: 5.8S rRNA

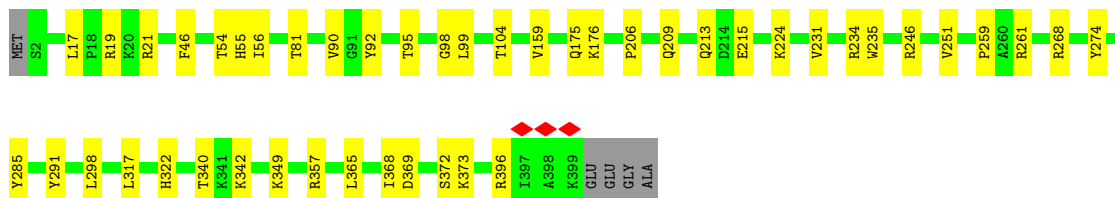


• Molecule 40: Large ribosomal subunit protein uL2

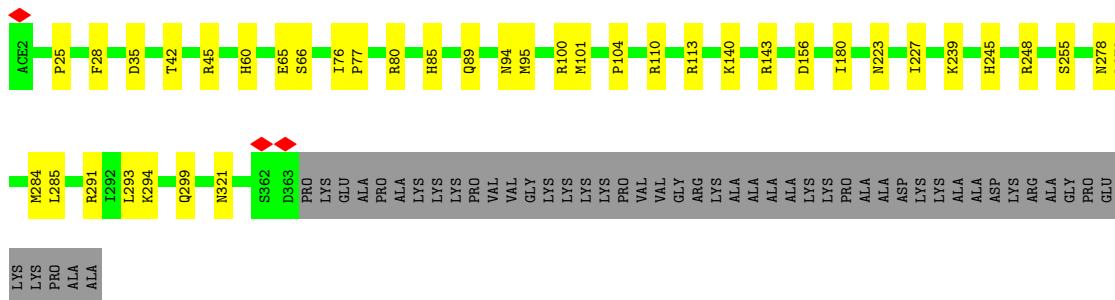
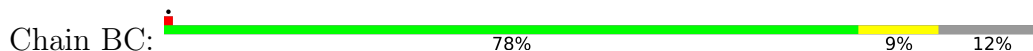


• Molecule 41: Ribosomal protein L3

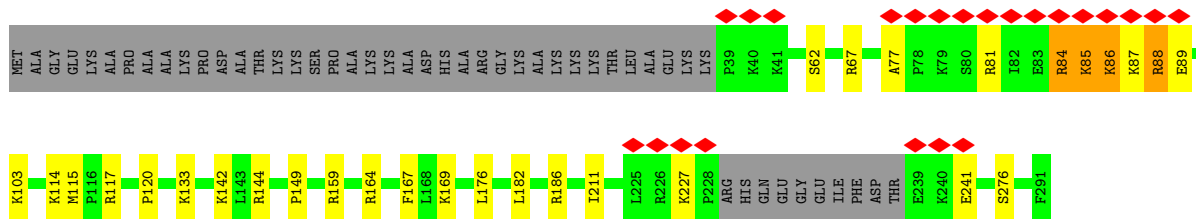
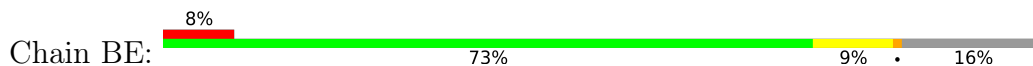




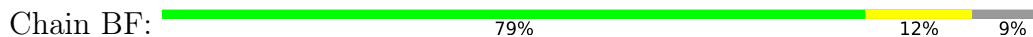
• Molecule 42: Large ribosomal subunit protein uL4



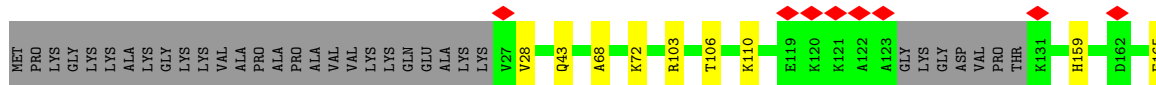
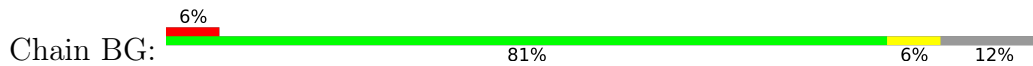
• Molecule 43: 60S ribosomal protein L6

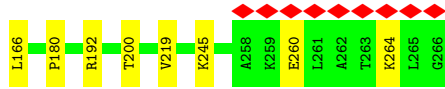


• Molecule 44: Ribosomal Protein uL30

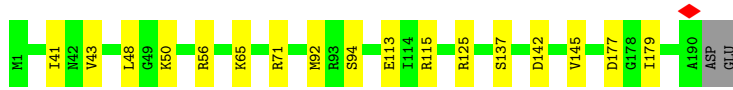
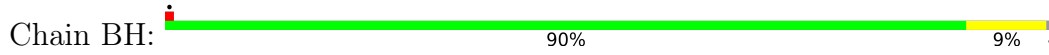


• Molecule 45: 60S ribosomal protein L7a

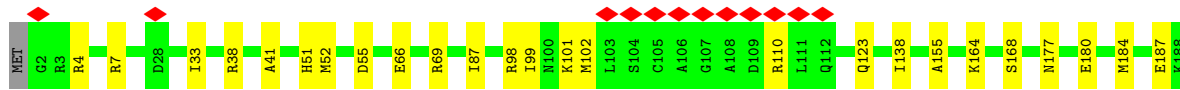
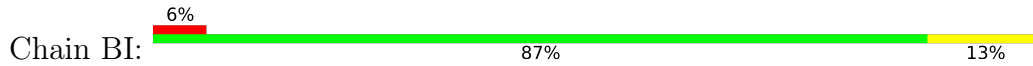




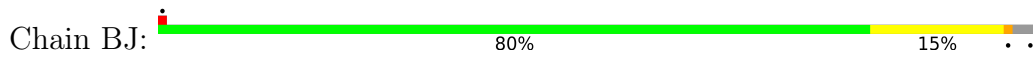
• Molecule 46: 60S ribosomal protein L9



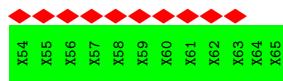
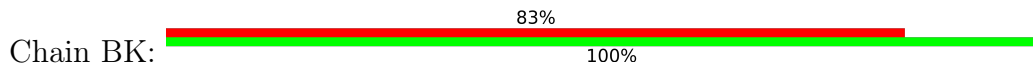
• Molecule 47: 60S ribosomal protein L10



• Molecule 48: 60S ribosomal protein L11



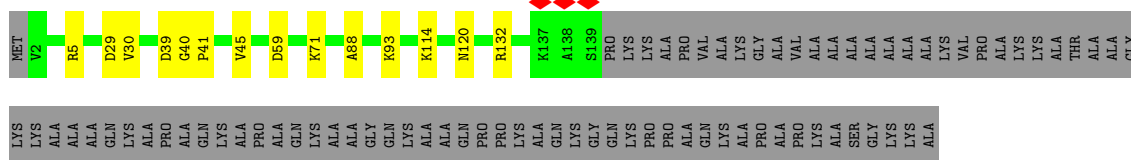
• Molecule 49: Nascent chain



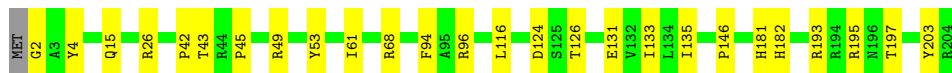
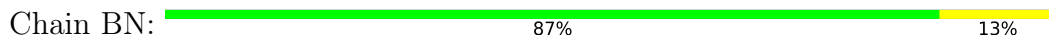
• Molecule 50: Large ribosomal subunit protein eL13



• Molecule 51: 60S ribosomal protein L14



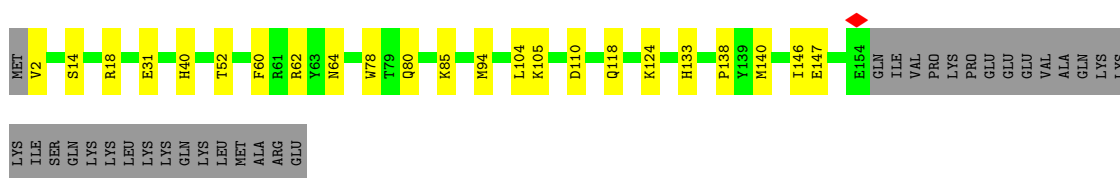
• Molecule 52: Ribosomal protein L15



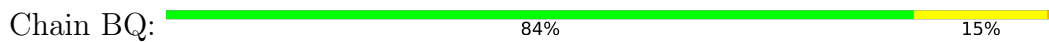
• Molecule 53: Large ribosomal subunit protein uL13



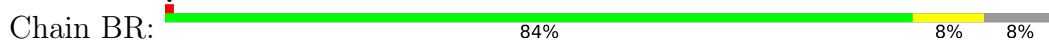
• Molecule 54: Large ribosomal subunit protein uL22



• Molecule 55: eL18



• Molecule 56: Ribosomal protein L19

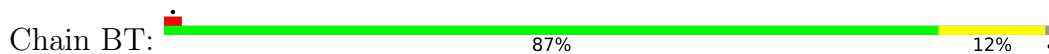


• Molecule 57: Large ribosomal subunit protein eL20

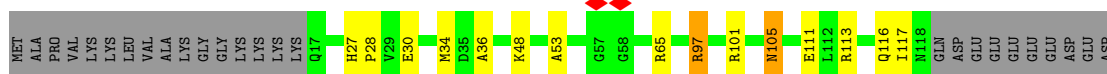




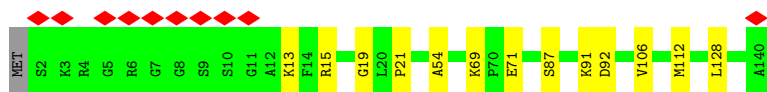
• Molecule 58: 60S ribosomal protein L21



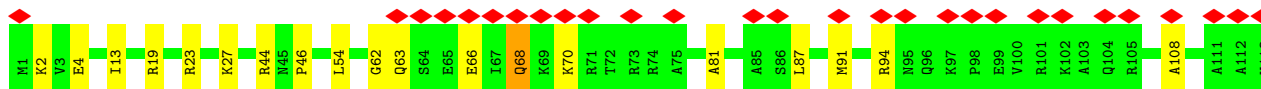
• Molecule 59: 60S ribosomal protein L22



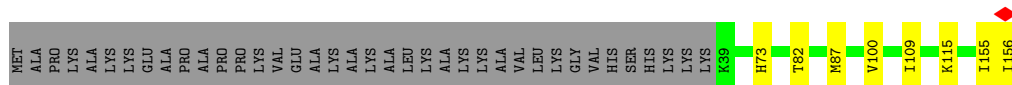
• Molecule 60: Ribosomal protein L23



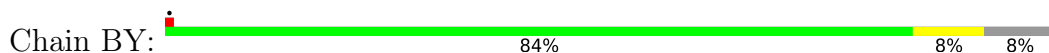
• Molecule 61: Ribosomal protein L24

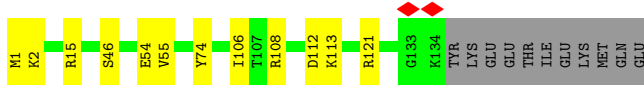


• Molecule 62: Large ribosomal subunit protein uL23

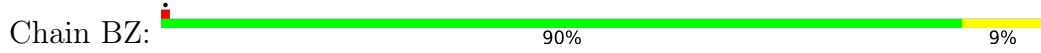


• Molecule 63: Ribosomal protein L26

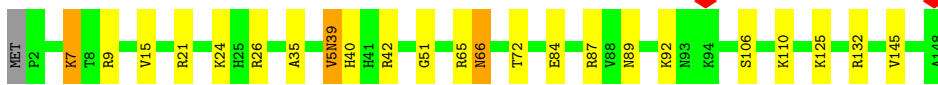
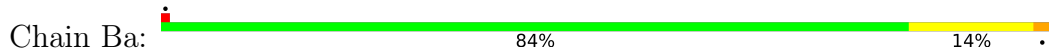




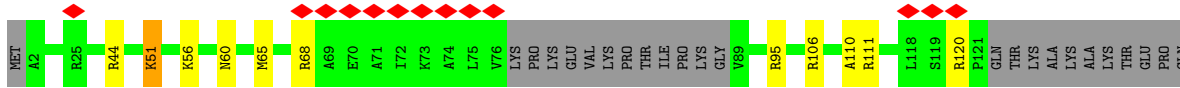
• Molecule 64: 60S ribosomal protein L27



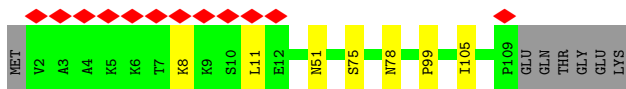
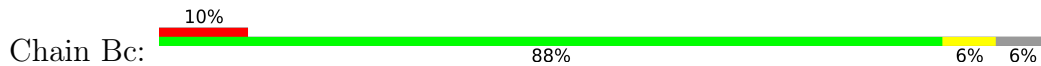
• Molecule 65: 60S ribosomal protein L27a



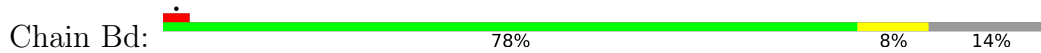
• Molecule 66: 60S ribosomal protein L29



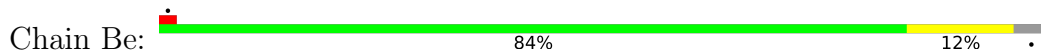
• Molecule 67: 60S ribosomal protein L30



• Molecule 68: 60S ribosomal protein L31



• Molecule 69: Ribosomal protein L32

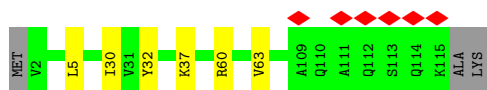




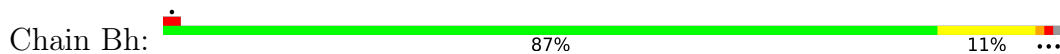
- Molecule 70: 60S ribosomal protein L35a



- Molecule 71: 60S ribosomal protein L34



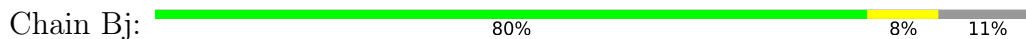
- Molecule 72: 60S ribosomal protein L35



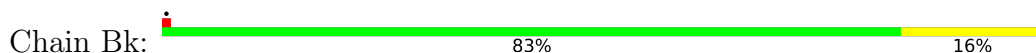
- Molecule 73: 60S ribosomal protein L36



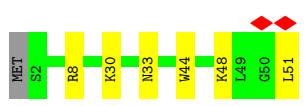
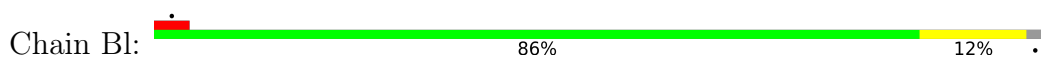
- Molecule 74: Ribosomal protein L37



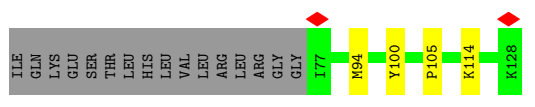
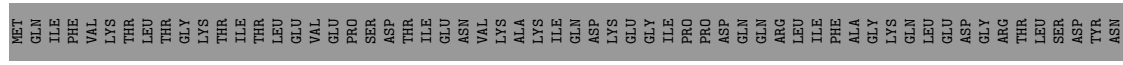
- Molecule 75: 60S ribosomal protein L38



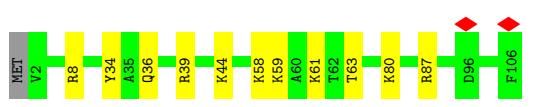
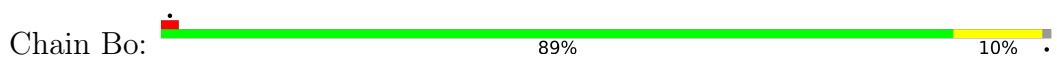
- Molecule 76: 60S ribosomal protein L39-like



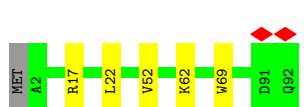
• Molecule 77: Ubiquitin-ribosomal protein eL40 fusion protein



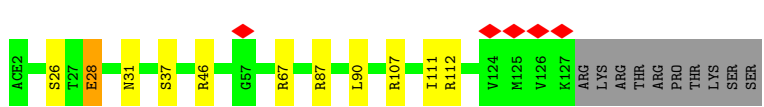
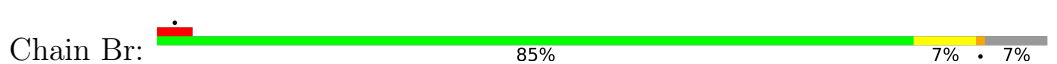
• Molecule 78: Large ribosomal subunit protein eL42



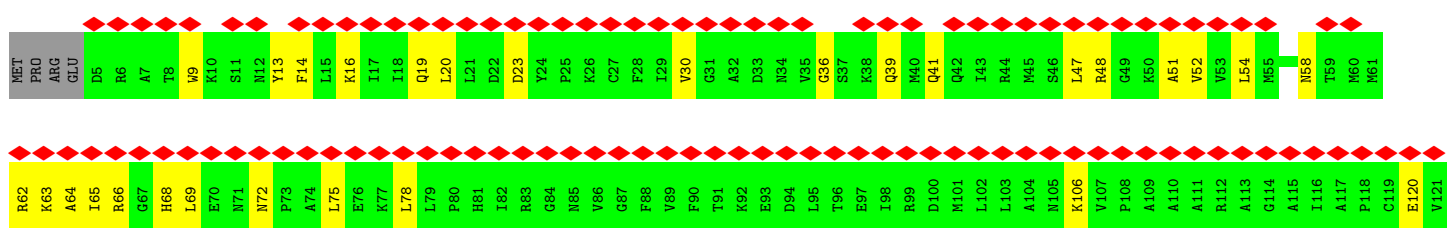
• Molecule 79: 60S ribosomal protein L37a

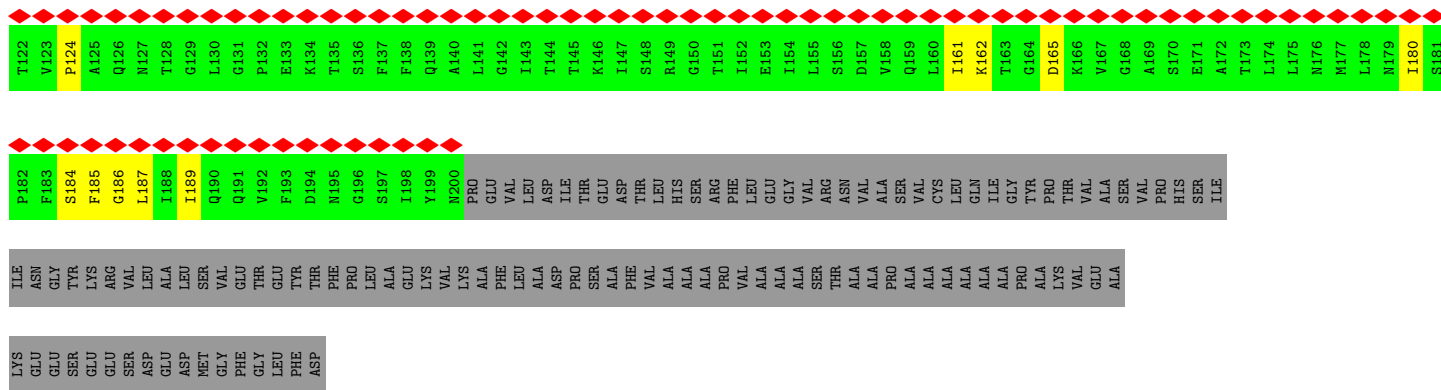


• Molecule 80: [histone H4]-N-methyl-L-lysine20 N-methyltransferase KMT5B

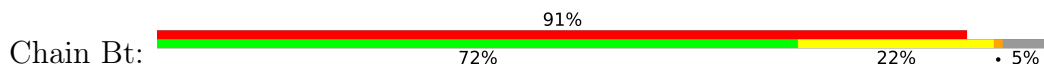


• Molecule 81: Large ribosomal subunit protein uL10

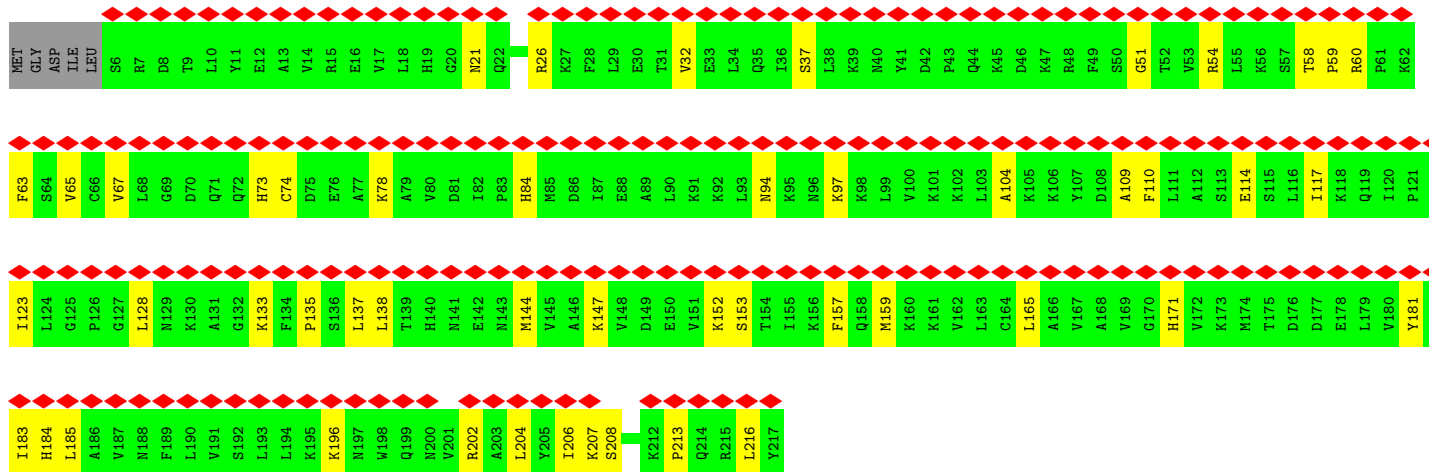
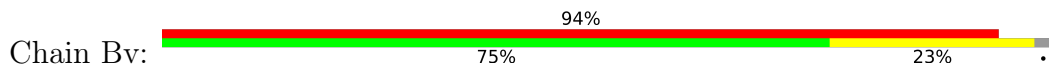




• Molecule 82: 60S ribosomal protein L12

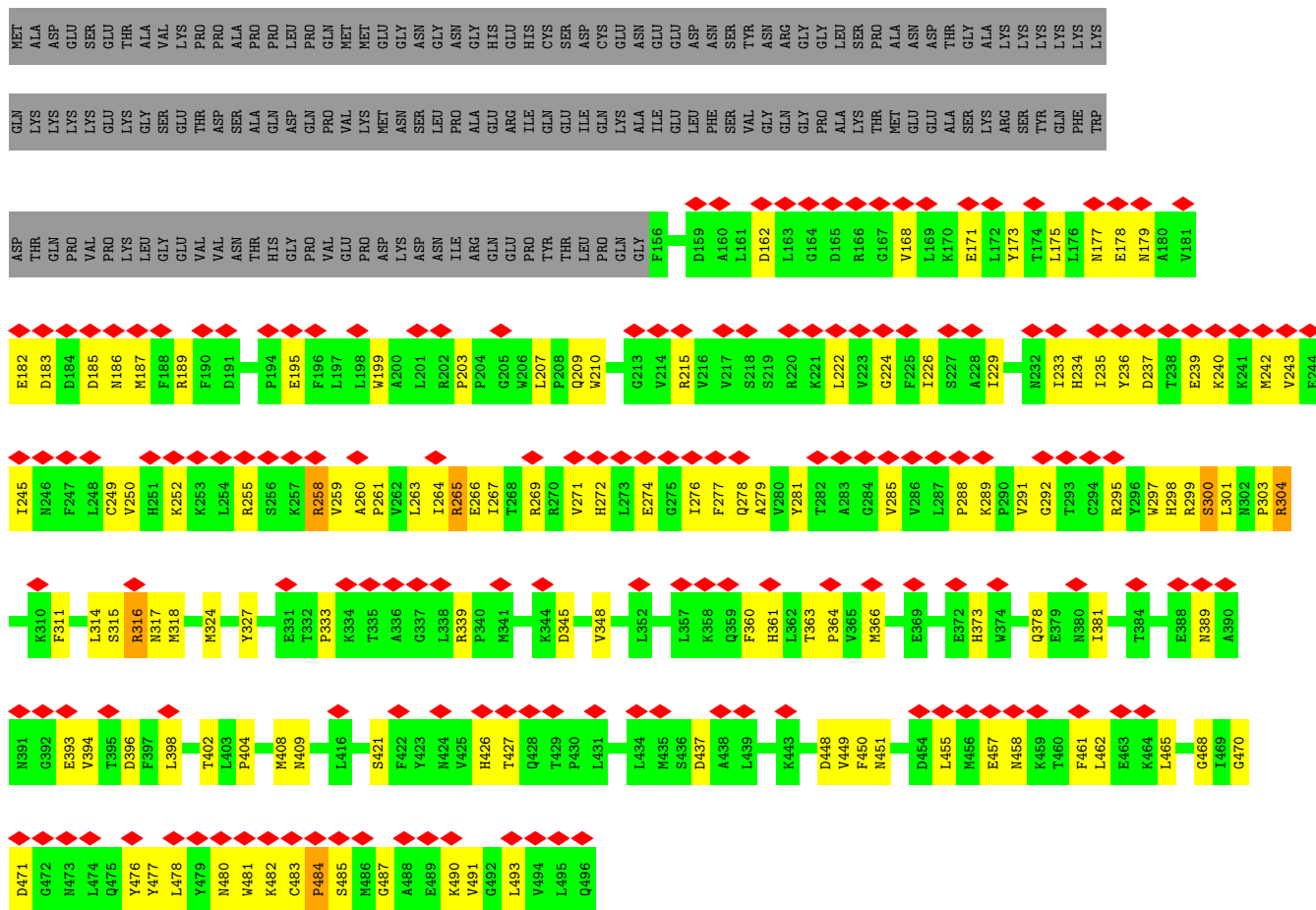


• Molecule 83: Ribosomal protein uL1

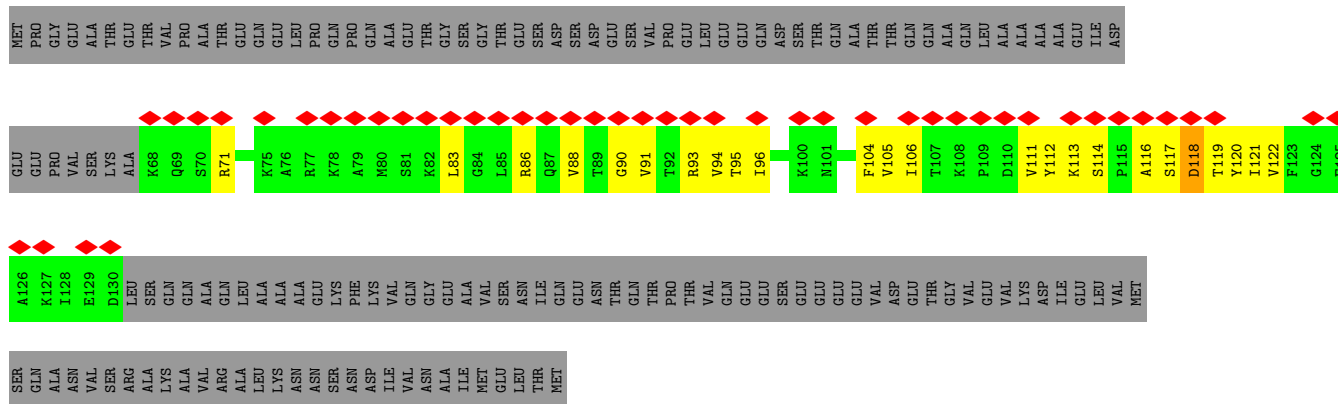


• Molecule 84: Glycylpeptide N-tetradecanoyltransferase 1

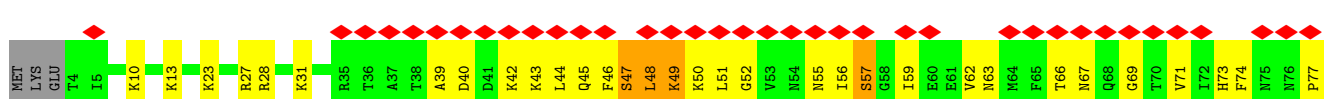
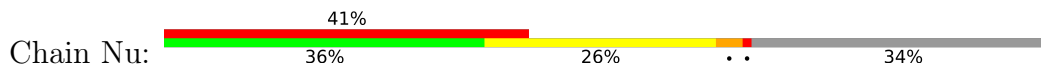




• Molecule 85: Nascent polypeptide-associated complex subunit alpha



• Molecule 86: Isoform 2 of Transcription factor BTF3



K78	V79	Q80	A81	S82	L83	A84	A85	N86	T87	F88	T89	I90	T91	G92	H93	A94	E95	T96	K97	Q98	L99	T100	E101	M102	L103	P104	S105	I106	L107	M108	Q109	L110	GLY	ALA	ASP	SER	LEU	THR	SER	SER	LEU	ARG	ARG	LEU	ALA	GLU	ALA	LEU	PRO	LYS	GLN	SER	VAL	ASP	GLY	LYS	ALA	PRO	LEU	ALA
THR	GLY	GLU	ASP	ASP	ASP	GLU	VAL	PRO	ASP	LEU	VAL	GLU	ASN	PHE	ASP	GLU	ALA	SER	LYS	ASN	GLU	ALA	ASN	THR	GLY	GLU	ASP	SER	LEU	THR	SER	SER	LEU	ARG	ARG	LEU	ALA	GLU	ALA	LEU	PRO	LYS	GLN	SER	VAL	ASP	GLY	LYS	ALA	PRO	LEU	ALA								

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87143	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.108	Depositor
Minimum map value	-0.454	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	A2	0.17	2/40342 (0.0%)	0.19	1/62877 (0.0%)
2	AA	0.08	0/665	0.20	0/891
3	AB	0.07	0/497	0.19	0/666
4	AC	0.07	0/622	0.22	0/822
5	AD	0.09	0/462	0.20	0/607
6	AE	0.09	0/828	0.21	0/1109
7	AF	0.15	0/2493	0.24	0/3394
8	AG	0.08	0/470	0.21	0/623
9	AT	0.17	0/1766	0.22	0/2749
10	AZ	0.13	0/1778	0.26	0/2416
11	Aa	0.09	0/1841	0.21	0/2459
12	Ab	0.08	0/1742	0.21	0/2354
13	Ac	0.22	0/1779	0.37	0/2395
14	Ad	0.15	0/2118	0.30	0/2849
15	Ae	0.09	0/1531	0.26	0/2059
16	Af	0.07	0/1946	0.20	0/2590
17	Ag	0.08	0/1552	0.20	0/2079
18	Ah	0.08	0/1715	0.21	0/2287
19	Ai	0.08	0/1550	0.21	0/2069
20	Aj	0.08	0/834	0.22	0/1125
21	Ak	0.08	0/1284	0.20	0/1717
22	Al	0.07	0/968	0.20	0/1296
23	Am	0.09	0/1232	0.22	0/1656
24	An	0.08	0/912	0.21	0/1230
25	Ao	0.08	0/1069	0.25	0/1429
26	Ap	0.09	0/1142	0.25	0/1528
27	Aq	0.08	0/1094	0.21	0/1469
28	Ar	0.15	0/1233	0.27	0/1653
29	As	0.08	0/1119	0.19	0/1498
30	At	0.08	0/832	0.20	0/1117
31	Au	0.26	0/645	0.34	0/864

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Av	0.09	0/1051	0.20	0/1406
33	Aw	0.09	0/1107	0.21	0/1475
34	Ax	0.35	0/1032	0.50	0/1371
35	Ay	0.07	0/691	0.20	0/922
36	Az	0.07	0/240	0.15	0/305
37	B5	0.17	2/86006 (0.0%)	0.21	0/134179
38	B7	0.27	0/2861	0.37	0/4459
39	B8	0.14	0/3635	0.18	0/5661
40	BA	0.10	0/1965	0.26	0/2633
41	BB	0.09	0/3261	0.23	0/4364
42	BC	0.09	0/2938	0.21	0/3948
43	BE	0.22	0/1998	0.33	0/2673
44	BF	0.24	0/1922	0.37	0/2563
45	BG	0.08	0/1908	0.22	0/2566
46	BH	0.09	0/1535	0.20	0/2063
47	BI	0.08	0/1756	0.21	0/2346
48	BJ	0.30	0/1385	0.42	1/1852 (0.1%)
50	BL	0.26	0/1733	0.42	0/2316
51	BM	0.08	0/1158	0.22	0/1547
52	BN	0.10	0/1746	0.23	0/2338
53	BO	0.09	0/1662	0.20	0/2222
54	BP	0.09	0/1268	0.23	0/1700
55	BQ	0.09	0/1539	0.22	0/2054
56	BR	0.07	0/1524	0.18	0/2013
57	BS	0.10	0/1497	0.23	0/2008
58	BT	0.22	0/1326	0.36	0/1770
59	BU	0.38	0/845	0.54	0/1134
60	BV	0.10	0/1048	0.24	0/1402
61	BW	0.15	0/1006	0.28	0/1334
62	BX	0.09	0/984	0.22	0/1323
63	BY	0.09	0/1132	0.22	0/1504
64	BZ	0.08	0/1130	0.19	0/1507
65	Ba	0.43	0/1179	0.66	3/1572 (0.2%)
66	Bb	0.23	0/884	0.32	0/1169
67	Bc	0.09	0/847	0.20	0/1134
68	Bd	0.09	0/903	0.21	0/1216
69	Be	0.08	0/1088	0.21	0/1451
70	Bf	0.10	0/903	0.22	0/1208
71	Bg	0.08	0/916	0.22	0/1220
72	Bh	0.18	0/1021	0.30	0/1348
73	Bi	0.07	0/841	0.18	0/1112
74	Bj	0.09	0/720	0.24	0/952
75	Bk	0.08	0/575	0.19	0/761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	Bl	0.09	0/459	0.20	0/608
77	Bm	0.09	0/426	0.23	0/564
78	Bo	0.09	0/866	0.21	0/1141
79	Bp	0.09	0/718	0.22	0/953
80	Br	0.11	0/1027	0.23	0/1376
81	Bs	0.08	0/1530	0.21	0/2064
82	Bt	0.07	0/1193	0.23	0/1609
83	Bv	0.09	0/1735	0.28	0/2328
84	MA	0.51	2/2876 (0.1%)	0.70	8/3901 (0.2%)
85	Nt	0.12	0/504	0.22	0/672
86	Nu	0.60	0/836	0.88	5/1122 (0.4%)
All	All	0.17	6/234997 (0.0%)	0.25	18/344316 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	AZ	0	1
13	Ac	0	2
14	Ad	0	1
34	Ax	0	1
43	BE	0	3
44	BF	0	1
48	BJ	0	2
50	BL	0	1
59	BU	0	2
65	Ba	0	4
72	Bh	0	1
84	MA	0	4
86	Nu	0	1
All	All	0	24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	MA	300[A]	SER	C-O	8.21	1.33	1.23
84	MA	300[B]	SER	C-O	8.21	1.33	1.23
37	B5	4052	OMU	O3'-P	5.16	1.61	1.56
1	A2	628	OMU	O3'-P	5.10	1.61	1.56
1	A2	166	A2M	O3'-P	5.08	1.61	1.56

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	MA	484	PRO	N-CA-C	-13.97	88.32	110.95
84	MA	300[A]	SER	CA-C-O	7.38	129.51	121.02
84	MA	300[B]	SER	CA-C-O	7.38	129.51	121.02
65	Ba	15	VAL	N-CA-C	6.49	117.18	110.36
86	Nu	104	PRO	CB-CA-C	6.45	122.20	111.56

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	AZ	53	ARG	Sidechain
13	Ac	40	ARG	Sidechain
13	Ac	45	ARG	Sidechain
14	Ad	68	ARG	Sidechain
34	Ax	20	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	37833	0	19168	237	0
2	AA	651	0	672	5	0
3	AB	495	0	523	3	0
4	AC	610	0	634	14	0
5	AD	457	0	502	4	0
6	AE	814	0	863	7	0
7	AF	2436	0	2393	29	0
8	AG	459	0	448	10	0
9	AT	1621	0	823	13	0
10	AZ	1743	0	1748	22	0
11	Aa	1815	0	1908	19	0
12	Ab	1706	0	1796	16	0
13	Ac	1751	0	1846	29	0
14	Ad	2076	0	2177	26	0
15	Ae	1509	0	1563	14	0
16	Af	1923	0	2089	37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Ag	1529	0	1627	16	0
18	Ah	1686	0	1772	18	0
19	Ai	1525	0	1640	15	0
20	Aj	810	0	836	7	0
21	Ak	1262	0	1335	7	0
22	Al	958	0	993	31	0
23	Am	1208	0	1294	14	0
24	An	899	0	912	9	0
25	Ao	1048	0	1093	8	0
26	Ap	1124	0	1193	21	0
27	Aq	1080	0	1135	11	0
28	Ar	1217	0	1279	13	0
29	As	1113	0	1145	14	0
30	At	822	0	887	10	0
31	Au	640	0	633	5	0
32	Av	1034	0	1080	4	0
33	Aw	1099	0	1162	8	0
34	Ax	1015	0	1086	10	0
35	Ay	683	0	761	9	0
36	Az	239	0	289	2	0
37	B5	79525	0	40261	477	0
38	B7	2561	0	1294	4	0
39	B8	3319	0	1684	13	0
40	BA	1940	0	2029	21	0
41	BB	3206	0	3353	32	0
42	BC	2886	0	3057	34	0
43	BE	1960	0	2153	21	0
44	BF	1886	0	2008	25	0
45	BG	1877	0	2023	11	0
46	BH	1516	0	1597	11	0
47	BI	1717	0	1764	17	0
48	BJ	1362	0	1399	14	0
49	BK	60	0	14	0	0
50	BL	1702	0	1820	12	0
51	BM	1137	0	1211	9	0
52	BN	1701	0	1749	18	0
53	BO	1630	0	1778	14	0
54	BP	1242	0	1274	15	0
55	BQ	1515	0	1634	25	0
56	BR	1508	0	1664	12	0
57	BS	1457	0	1492	11	0
58	BT	1298	0	1366	14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	BU	831	0	852	9	0
60	BV	1034	0	1096	10	0
61	BW	991	0	1048	13	0
62	BX	967	0	1040	8	0
63	BY	1115	0	1205	9	0
64	BZ	1107	0	1182	7	0
65	Ba	1163	0	1202	15	0
66	Bb	881	0	957	10	0
67	Bc	836	0	888	4	0
68	Bd	888	0	930	6	0
69	Be	1070	0	1164	11	0
70	Bf	884	0	924	8	0
71	Bg	906	0	998	3	0
72	Bh	1013	0	1147	15	0
73	Bi	830	0	916	2	0
74	Bj	705	0	737	7	0
75	Bk	569	0	637	7	0
76	Bl	447	0	480	4	0
77	Bm	432	0	470	3	0
78	Bo	863	0	929	8	0
79	Bp	708	0	756	4	0
80	Br	1014	0	1083	8	0
81	Bs	1507	0	1564	29	0
82	Bt	1178	0	1235	27	0
83	Bv	1707	0	1815	38	0
84	MA	2797	0	2818	147	0
85	Nt	499	0	541	22	0
86	Nu	828	0	874	53	0
87	A2	108	0	0	0	0
87	Aw	1	0	0	0	0
87	B5	273	0	0	0	0
87	B7	9	0	0	0	0
87	B8	8	0	0	0	0
87	BB	3	0	0	0	0
87	BI	1	0	0	0	0
87	BP	1	0	0	0	0
87	BR	1	0	0	0	0
87	BV	1	0	0	0	0
87	Bj	1	0	0	0	0
88	A2	31	0	0	0	0
88	Ad	1	0	0	0	0
88	B5	130	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	B7	6	0	0	0	0
88	B8	4	0	0	0	0
88	BA	2	0	0	0	0
88	BH	1	0	0	0	0
88	BI	1	0	0	0	0
88	BL	1	0	0	0	0
88	BN	2	0	0	0	0
88	BQ	1	0	0	0	0
88	BT	1	0	0	0	0
88	BY	1	0	0	0	0
88	Bb	2	0	0	0	0
88	Be	2	0	0	0	0
88	Bo	1	0	0	0	0
89	A2	80	0	151	6	0
89	B5	220	0	418	19	0
90	A2	14	0	26	1	0
90	B5	28	0	52	2	0
91	AC	1	0	0	0	0
91	AE	1	0	0	0	0
91	AG	1	0	0	0	0
91	Bg	1	0	0	0	0
91	Bj	1	0	0	0	0
91	Bm	1	0	0	0	0
91	Bo	1	0	0	0	0
91	Bp	1	0	0	0	0
92	A2	514	0	0	3	0
92	AE	1	0	0	0	0
92	AT	4	0	0	0	0
92	Aa	3	0	0	0	0
92	Af	2	0	0	0	0
92	Ak	2	0	0	0	0
92	An	2	0	0	0	0
92	Ap	1	0	0	0	0
92	Ar	2	0	0	0	0
92	As	2	0	0	0	0
92	At	1	0	0	1	0
92	Aw	4	0	0	0	0
92	B5	1359	0	0	5	0
92	B7	38	0	0	1	0
92	B8	49	0	0	0	0
92	BA	4	0	0	0	0
92	BC	6	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	BH	1	0	0	0	0
92	BI	3	0	0	0	0
92	BL	1	0	0	0	0
92	BN	2	0	0	0	0
92	BP	4	0	0	0	0
92	BR	2	0	0	0	0
92	BV	3	0	0	0	0
92	BX	1	0	0	0	0
92	BY	1	0	0	0	0
92	Ba	4	0	0	0	0
92	Bd	1	0	0	0	0
92	Be	3	0	0	0	0
92	Bg	2	0	0	0	0
92	Bj	5	0	0	0	0
92	Bo	1	0	0	0	0
All	All	226637	0	168064	1661	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 5.

The worst 5 of 1661 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)
84:MA:291:VAL:O	84:MA:485:SER:HB2	1.27	1.29
84:MA:250:VAL:CG1	84:MA:258:ARG:HD3	1.65	1.27
84:MA:250:VAL:HG13	84:MA:258:ARG:CD	1.70	1.19
44:BF:87:LYS:NZ	44:BF:196:VAL:HG23	1.58	1.17
84:MA:291:VAL:HA	84:MA:485:SER:CB	1.72	1.17

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	72/156 (46%)	71 (99%)	1 (1%)	0	100	100
5	AD	55/133 (41%)	55 (100%)	0	0	100	100
6	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
7	AF	311/317 (98%)	305 (98%)	6 (2%)	0	100	100
8	AG	53/56 (95%)	53 (100%)	0	0	100	100
10	AZ	220/295 (75%)	217 (99%)	3 (1%)	0	100	100
11	Aa	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
12	Ab	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
13	Ac	223/281 (79%)	220 (99%)	3 (1%)	0	100	100
14	Ad	260/263 (99%)	258 (99%)	2 (1%)	0	100	100
15	Ae	189/204 (93%)	187 (99%)	2 (1%)	0	100	100
16	Af	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
17	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
18	Ah	204/208 (98%)	198 (97%)	6 (3%)	0	100	100
19	Ai	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
20	Aj	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
21	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
22	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
23	Am	148/151 (98%)	148 (100%)	0	0	100	100
24	An	120/151 (80%)	117 (98%)	3 (2%)	0	100	100
25	Ao	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
26	Ap	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
27	Aq	132/135 (98%)	132 (100%)	0	0	100	100
28	Ar	147/152 (97%)	143 (97%)	4 (3%)	0	100	100
29	As	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
30	At	102/119 (86%)	102 (100%)	0	0	100	100
31	Au	82/84 (98%)	82 (100%)	0	0	100	100
32	Av	127/130 (98%)	127 (100%)	0	0	100	100
33	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
34	Ax	123/130 (95%)	122 (99%)	1 (1%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Ay	83/124 (67%)	82 (99%)	1 (1%)	0	100	100
36	Az	23/25 (92%)	23 (100%)	0	0	100	100
40	BA	250/257 (97%)	245 (98%)	5 (2%)	0	100	100
41	BB	395/403 (98%)	386 (98%)	9 (2%)	0	100	100
42	BC	361/413 (87%)	358 (99%)	3 (1%)	0	100	100
43	BE	239/291 (82%)	236 (99%)	3 (1%)	0	100	100
44	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
45	BG	229/266 (86%)	227 (99%)	2 (1%)	0	100	100
46	BH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
47	BI	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
48	BJ	168/178 (94%)	166 (99%)	2 (1%)	0	100	100
50	BL	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
51	BM	136/218 (62%)	132 (97%)	4 (3%)	0	100	100
52	BN	201/204 (98%)	194 (96%)	7 (4%)	0	100	100
53	BO	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
54	BP	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
55	BQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
56	BR	178/196 (91%)	178 (100%)	0	0	100	100
57	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
58	BT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
59	BU	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
60	BV	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
61	BW	119/157 (76%)	119 (100%)	0	0	100	100
62	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
63	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
64	BZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
65	Ba	144/148 (97%)	138 (96%)	6 (4%)	0	100	100
66	Bb	103/245 (42%)	98 (95%)	5 (5%)	0	100	100
67	Bc	106/115 (92%)	106 (100%)	0	0	100	100
68	Bd	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
69	Be	128/135 (95%)	127 (99%)	1 (1%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	Bf	108/110 (98%)	108 (100%)	0	0	100	100
71	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
72	Bh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
73	Bi	100/105 (95%)	100 (100%)	0	0	100	100
74	Bj	84/97 (87%)	84 (100%)	0	0	100	100
75	Bk	67/70 (96%)	67 (100%)	0	0	100	100
76	Bl	48/51 (94%)	48 (100%)	0	0	100	100
77	Bm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
78	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
79	Bp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
80	Br	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
81	Bs	194/318 (61%)	188 (97%)	6 (3%)	0	100	100
82	Bt	154/165 (93%)	151 (98%)	3 (2%)	0	100	100
83	Bv	210/217 (97%)	200 (95%)	10 (5%)	0	100	100
84	MA	340/496 (68%)	322 (95%)	18 (5%)	0	100	100
85	Nt	61/215 (28%)	59 (97%)	2 (3%)	0	100	100
86	Nu	105/162 (65%)	94 (90%)	9 (9%)	2 (2%)	6	22
All	All	12113/14414 (84%)	11903 (98%)	208 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
86	Nu	104	PRO
86	Nu	98	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	75/76 (99%)	74 (99%)	1 (1%)	61	86

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AB	56/62 (90%)	56 (100%)	0	100	100
4	AC	67/140 (48%)	67 (100%)	0	100	100
5	AD	47/106 (44%)	47 (100%)	0	100	100
6	AE	88/98 (90%)	87 (99%)	1 (1%)	65	87
7	AF	272/275 (99%)	268 (98%)	4 (2%)	57	84
8	AG	48/49 (98%)	48 (100%)	0	100	100
10	AZ	183/243 (75%)	181 (99%)	2 (1%)	65	87
11	Aa	203/231 (88%)	201 (99%)	2 (1%)	68	88
12	Ab	185/223 (83%)	185 (100%)	0	100	100
13	Ac	189/232 (82%)	186 (98%)	3 (2%)	55	83
14	Ad	224/225 (100%)	222 (99%)	2 (1%)	70	89
15	Ae	161/170 (95%)	161 (100%)	0	100	100
16	Af	207/218 (95%)	207 (100%)	0	100	100
17	Ag	170/360 (47%)	170 (100%)	0	100	100
18	Ah	178/180 (99%)	177 (99%)	1 (1%)	78	92
19	Ai	161/168 (96%)	160 (99%)	1 (1%)	78	92
20	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	87
21	Ak	139/142 (98%)	139 (100%)	0	100	100
22	Al	104/108 (96%)	103 (99%)	1 (1%)	68	88
23	Am	130/131 (99%)	130 (100%)	0	100	100
24	An	95/119 (80%)	93 (98%)	2 (2%)	47	79
25	Ao	114/130 (88%)	112 (98%)	2 (2%)	51	82
26	Ap	117/140 (84%)	117 (100%)	0	100	100
27	Aq	120/121 (99%)	120 (100%)	0	100	100
28	Ar	128/131 (98%)	127 (99%)	1 (1%)	73	90
29	As	112/114 (98%)	112 (100%)	0	100	100
30	At	94/107 (88%)	93 (99%)	1 (1%)	65	87
31	Au	68/68 (100%)	66 (97%)	2 (3%)	37	73
32	Av	112/113 (99%)	111 (99%)	1 (1%)	70	89
33	Aw	112/114 (98%)	109 (97%)	3 (3%)	39	74
34	Ax	107/112 (96%)	102 (95%)	5 (5%)	23	57

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	Ay	75/102 (74%)	75 (100%)	0	100	100
36	Az	24/24 (100%)	24 (100%)	0	100	100
40	BA	194/198 (98%)	193 (100%)	1 (0%)	81	93
41	BB	344/347 (99%)	344 (100%)	0	100	100
42	BC	302/336 (90%)	302 (100%)	0	100	100
43	BE	216/251 (86%)	210 (97%)	6 (3%)	38	73
44	BF	197/215 (92%)	196 (100%)	1 (0%)	81	93
45	BG	199/223 (89%)	196 (98%)	3 (2%)	57	84
46	BH	169/171 (99%)	169 (100%)	0	100	100
47	BI	180/181 (99%)	180 (100%)	0	100	100
48	BJ	143/149 (96%)	140 (98%)	3 (2%)	47	79
50	BL	175/176 (99%)	174 (99%)	1 (1%)	78	92
51	BM	117/161 (73%)	117 (100%)	0	100	100
52	BN	171/172 (99%)	171 (100%)	0	100	100
53	BO	171/173 (99%)	170 (99%)	1 (1%)	78	92
54	BP	134/163 (82%)	133 (99%)	1 (1%)	76	91
55	BQ	164/165 (99%)	163 (99%)	1 (1%)	78	92
56	BR	159/175 (91%)	158 (99%)	1 (1%)	78	92
57	BS	154/154 (100%)	154 (100%)	0	100	100
58	BT	139/140 (99%)	137 (99%)	2 (1%)	59	85
59	BU	91/113 (80%)	87 (96%)	4 (4%)	25	59
60	BV	106/107 (99%)	106 (100%)	0	100	100
61	BW	100/126 (79%)	99 (99%)	1 (1%)	68	88
62	BX	106/134 (79%)	106 (100%)	0	100	100
63	BY	124/135 (92%)	123 (99%)	1 (1%)	73	90
64	BZ	117/118 (99%)	117 (100%)	0	100	100
65	Ba	118/119 (99%)	117 (99%)	1 (1%)	73	90
66	Bb	87/183 (48%)	86 (99%)	1 (1%)	65	87
67	Bc	92/98 (94%)	92 (100%)	0	100	100
68	Bd	98/110 (89%)	98 (100%)	0	100	100
69	Be	116/121 (96%)	116 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	Bf	89/89 (100%)	89 (100%)	0	100	100
71	Bg	98/100 (98%)	97 (99%)	1 (1%)	68	88
72	Bh	109/110 (99%)	107 (98%)	2 (2%)	51	82
73	Bi	86/89 (97%)	85 (99%)	1 (1%)	63	87
74	Bj	73/80 (91%)	73 (100%)	0	100	100
75	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	83
76	Bl	47/48 (98%)	47 (100%)	0	100	100
77	Bm	47/115 (41%)	47 (100%)	0	100	100
78	Bo	92/93 (99%)	92 (100%)	0	100	100
79	Bp	74/75 (99%)	73 (99%)	1 (1%)	59	85
80	Br	110/120 (92%)	109 (99%)	1 (1%)	70	89
81	Bs	164/258 (64%)	163 (99%)	1 (1%)	78	92
82	Bt	128/137 (93%)	122 (95%)	6 (5%)	23	57
83	Bv	191/195 (98%)	191 (100%)	0	100	100
84	MA	310/442 (70%)	308 (99%)	2 (1%)	78	92
85	Nt	56/183 (31%)	55 (98%)	1 (2%)	51	82
86	Nu	91/136 (67%)	81 (89%)	10 (11%)	6	20
All	All	10564/12217 (86%)	10472 (99%)	92 (1%)	68	89

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	BU	97	ARG
80	Br	28	GLU
59	BU	116	GLN
71	Bg	32	TYR
82	Bt	35	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
55	BQ	7	HIS
65	Ba	28	HIS
55	BQ	57	ASN
58	BT	131	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
66	Bb	11	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1764/1870 (94%)	231 (13%)	0
37	B5	3694/4808 (76%)	477 (12%)	7 (0%)
38	B7	119/120 (99%)	9 (7%)	0
39	B8	155/158 (98%)	20 (12%)	0
9	AT	75/76 (98%)	12 (16%)	0
All	All	5807/7032 (82%)	749 (12%)	7 (0%)

5 of 749 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	3	C
1	A2	17	C
1	A2	33	G
1	A2	41	G
1	A2	46	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
37	B5	2310	U
37	B5	2313	C
37	B5	4634	U
37	B5	4486	G
37	B5	1588	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	UR3	B5	4276	37	19,22,23	0.98	0	26,32,35	1.42	1 (3%)
37	A2M	B5	2244	87,37	22,25,26	1.46	4 (18%)	31,36,39	2.11	9 (29%)
37	PSU	B5	1721	37	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	36	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
37	PSU	B5	3494	37	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
37	OMU	B5	4052	37	19,22,23	0.21	0	26,31,34	0.50	0
1	PSU	A2	652	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
66	MLZ	Bb	5	66	8,9,10	0.49	0	4,9,11	0.18	0
37	PSU	B5	4749	37	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
77	M3L	Bm	98	77	10,11,12	0.83	0	9,14,16	0.55	0
1	4AC	A2	1843	1	21,24,25	1.11	2 (9%)	29,34,37	1.29	3 (10%)
37	OMC	B5	2667	37	19,22,23	0.82	0	26,31,34	0.79	0
37	PSU	B5	1638	37	18,21,22	0.85	1 (5%)	22,30,33	0.69	0
37	A2M	B5	2630	87,37	22,25,26	1.45	4 (18%)	31,36,39	2.15	9 (29%)
39	PSU	B8	55	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	A2	684	1	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
37	OMC	B5	2647	37	19,22,23	0.82	0	26,31,34	0.80	0
1	PSU	A2	210	1	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
37	PSU	B5	3447	37	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
37	PSU	B5	3616	37	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
37	A2M	B5	3562	37	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
1	MA6	A2	1851	1	23,26,27	2.28	5 (21%)	34,38,41	3.72	13 (38%)
1	A2M	A2	513	1	22,25,26	1.45	4 (18%)	31,36,39	2.13	10 (32%)
1	B8N	A2	1249	1	24,29,30	1.28	3 (12%)	29,42,45	1.28	3 (10%)
1	PSU	A2	1693	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	802	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	6MZ	A2	1833	1,87	22,25,26	1.44	4 (18%)	30,36,39	2.15	9 (30%)
40	V5N	BA	216	40	9,11,12	2.08	2 (22%)	9,14,16	1.70	2 (22%)
1	PSU	A2	816	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
37	OMG	B5	3524	37	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
37	OMG	B5	4245	37	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
37	PSU	B5	4107	37	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
37	A2M	B5	4317	37	22,25,26	1.47	4 (18%)	31,36,39	2.10	10 (32%)
37	PSU	B5	1632	37	18,21,22	1.35	2 (11%)	22,30,33	1.88	4 (18%)
37	PSU	B5	3583	37	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	A2	1289	1	19,22,23	1.21	3 (15%)	26,31,34	1.68	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	A2	1057	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1233	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
37	PSU	B5	4298	37	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
1	OMG	A2	1491	1,87	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
37	A2M	B5	3492	1,37	22,25,26	1.47	4 (18%)	31,36,39	2.18	10 (32%)
37	OMC	B5	3573	37	19,22,23	0.81	0	26,31,34	0.93	1 (3%)
37	PSU	B5	4042	37	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
37	A2M	B5	4336	37	22,25,26	1.45	4 (18%)	31,36,39	2.15	10 (32%)
37	PSU	B5	1720	37	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
37	PSU	B5	4711	37	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	A2	1348	1	18,21,22	0.88	1 (5%)	22,30,33	0.67	0
37	1MA	B5	1266	37	21,25,26	1.38	4 (19%)	31,37,40	1.70	5 (16%)
37	PSU	B5	4382	37	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
37	PSU	B5	3369	37	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	1005	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	A2	1704	1	19,22,23	0.82	0	26,31,34	0.80	0
37	OMC	B5	2265	87,37	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
37	PSU	B5	3466	37	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	OMU	A2	1805	1	19,22,23	1.22	3 (15%)	26,31,34	1.71	5 (19%)
37	A2M	B5	3450	37	22,25,26	1.46	4 (18%)	31,36,39	2.08	9 (29%)
65	V5N	Ba	39	65	9,11,12	2.08	2 (22%)	9,14,16	1.69	2 (22%)
37	PSU	B5	3502	37	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
37	A2M	B5	400	37	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
1	PSU	A2	1644	1,87	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	A2	1679	1	22,25,26	1.46	4 (18%)	31,36,39	2.17	10 (32%)
1	PSU	A2	1626	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
37	A2M	B5	4269	87,37	22,25,26	0.20	0	31,36,39	0.46	0
1	PSU	A2	1047	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	3462	37	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
37	OMU	B5	3657	37	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
1	A2M	A2	99	1,87	22,25,26	1.46	4 (18%)	31,36,39	2.14	9 (29%)
37	PSU	B5	1683	37	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
37	PSU	B5	4267	37	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
1	OMC	A2	463	1	19,22,23	0.83	0	26,31,34	0.84	0
37	OMC	B5	3619	37	19,22,23	0.81	0	26,31,34	0.82	0
29	NMM	As	67	29	9,11,12	0.59	0	6,12,14	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	PSU	B5	4177	37	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	OMU	A2	429	1	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
37	OMG	B5	3974	37	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
37	OMG	B5	4369	37	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
37	PSU	B5	4039	37	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
37	5MC	B5	4193	37	18,22,23	1.00	2 (11%)	26,32,35	1.19	2 (7%)
1	OMU	A2	172	1	19,22,23	1.20	2 (10%)	26,31,34	1.70	4 (15%)
1	OMG	A2	1329	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
37	PSU	B5	4322	37	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	OMU	A2	1443	1,87	19,22,23	1.23	4 (21%)	26,31,34	1.69	5 (19%)
37	PSU	B5	3500	37	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
37	PSU	B5	1491	37	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	A2	602	1	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
37	OMG	B5	2719	37	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
37	OMG	B5	3476	37	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	A2	815	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
9	PSU	AT	55	9	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	A2	1392	1	19,22,23	0.83	0	26,31,34	0.87	1 (3%)
37	OMG	B5	4116	37	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
37	PSU	B5	4325	37	18,21,22	1.35	2 (11%)	22,30,33	1.93	3 (13%)
1	OMU	A2	1327	1,87	19,22,23	1.17	2 (10%)	26,31,34	1.71	5 (19%)
1	OMG	A2	868	1	23,26,27	1.19	3 (13%)	33,38,41	1.91	6 (18%)
1	A2M	A2	591	1	22,25,26	1.47	4 (18%)	31,36,39	2.19	7 (22%)
37	A2M	B5	2206	87,37	22,25,26	1.45	4 (18%)	31,36,39	2.14	10 (32%)
37	PSU	B5	1718	37	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	A2	1032	1	22,25,26	1.46	4 (18%)	31,36,39	2.15	10 (32%)
37	OMC	B5	2208	87,37	19,22,23	0.81	0	26,31,34	0.78	0
37	OMG	B5	4138	37	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
37	PSU	B5	4740	37	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
37	A2M	B5	2658	87,37	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
1	PSU	A2	1239	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	A2	1384	1	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
37	A2M	B5	1489	87,37	22,25,26	1.45	4 (18%)	31,36,39	2.11	9 (29%)
37	PSU	B5	4058	37	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMU	A2	116	1	19,22,23	1.21	2 (10%)	26,31,34	1.67	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	A2	682	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	OMG	B8	75	39	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMC	A2	174	1,87	19,22,23	0.81	0	26,31,34	0.81	0
37	OMC	B5	2704	37	19,22,23	0.81	0	26,31,34	0.81	0
1	PSU	A2	1245	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
37	OMG	B5	4240	37	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
37	A2M	B5	3517	37	22,25,26	1.44	4 (18%)	31,36,39	2.19	11 (35%)
33	HY3	Aw	62	33	6,8,9	6.51	4 (66%)	5,10,12	0.96	0
37	OMC	B5	4202	37	19,22,23	0.82	0	26,31,34	0.83	0
37	PSU	B5	4278	37	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
37	OMG	B5	4383	37	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	A2	93	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	967	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
37	PSU	B5	4166	37	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
37	OMC	B5	2194	87,37	19,22,23	0.82	0	26,31,34	0.91	1 (3%)
37	PSU	B5	4217	37	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
37	PSU	B5	3576	37	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
37	OMC	B5	4282	87,37	19,22,23	0.81	0	26,31,34	0.82	0
37	PSU	B5	4419	37	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	A2	1046	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
37	A2M	B5	3456	37	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
37	OMU	B5	2258	37	19,22,23	1.22	3 (15%)	26,31,34	1.68	4 (15%)
1	PSU	A2	105	1	18,21,22	1.33	2 (11%)	22,30,33	1.90	4 (18%)
37	OMG	B5	1477	37	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
37	PSU	B5	4169	37	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	4045	37	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	A2	166	1	22,25,26	1.46	4 (18%)	31,36,39	2.15	10 (32%)
37	PSU	B5	3496	37	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	650	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	1446	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	3371	37	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B8	69	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
37	PSU	B5	1799	37	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
37	A2M	B5	1479	37	22,25,26	1.45	4 (18%)	31,36,39	2.14	9 (29%)
37	OMG	B5	3631	87,37	23,26,27	1.19	3 (13%)	33,38,41	1.96	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	5MU	AT	54	9	19,22,23	1.40	6 (31%)	28,32,35	2.05	6 (21%)
37	PSU	B5	4203	37	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	A2M	A2	159	1	22,25,26	1.46	4 (18%)	31,36,39	2.15	10 (32%)
37	UY1	B5	3550	37	19,22,23	1.36	3 (15%)	22,31,34	1.90	5 (22%)
1	PSU	A2	573	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
37	OMG	B5	3942	9,37	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	A2	687	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
37	OMU	B5	4244	37	19,22,23	1.20	2 (10%)	26,31,34	1.70	5 (19%)
37	OMG	B5	4364	37	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
37	OMG	B5	1580	37	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
37	PSU	B5	4374	37	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
78	MLZ	Bo	53	78	8,9,10	0.49	0	4,9,11	0.14	0
1	PSU	A2	34	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
37	OMC	B5	3433	37	19,22,23	0.79	0	26,31,34	0.77	0
1	OMU	A2	628	1	19,22,23	0.24	0	26,31,34	0.51	0
1	PSU	A2	864	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
37	OMC	B5	3540	37	19,22,23	0.82	0	26,31,34	0.80	0
37	A2M	B5	1810	87,37	22,25,26	1.46	4 (18%)	31,36,39	2.15	10 (32%)
37	OMG	B5	1260	37	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	A2M	A2	485	1	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
37	PSU	B5	3554	37	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	4188	37	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	109	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1175	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	823	1	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
37	OMC	B5	1820	87,37	19,22,23	0.81	0	26,31,34	0.80	0
37	PSU	B5	3427	37	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
37	OMU	B5	4366	37	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
1	PSU	A2	1178	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
37	PSU	B5	1537	37	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	A2	610	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	MA6	A2	1852	1	23,26,27	2.24	5 (21%)	34,38,41	3.67	13 (38%)
37	OMU	B5	2680	37	19,22,23	1.23	2 (10%)	26,31,34	1.71	4 (15%)
37	PSU	B5	1801	37	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
37	A2M	B5	1270	37	22,25,26	1.45	4 (18%)	31,36,39	2.09	10 (32%)
37	6MZ	B5	3966	37	22,25,26	1.43	4 (18%)	30,36,39	2.19	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	A2M	A2	469	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
1	OMG	A2	1448	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
37	PSU	B5	4149	37	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
37	PSU	B5	3585	87,37	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
37	OMC	B5	1284	37	19,22,23	0.82	0	26,31,34	0.83	0
1	OMU	A2	121	1	19,22,23	1.22	3 (15%)	26,31,34	1.70	4 (15%)
1	PSU	A2	1082	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
37	PSU	B5	1731	37	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	4246	37	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
1	A2M	A2	27	1,87	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
1	OMG	A2	510	1,87	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	A2M	A2	577	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
1	PSU	A2	218	1	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
37	PSU	B5	2475	37	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
37	OMG	B5	3359	37	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	A2	867	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
37	A2M	B5	398	37	22,25,26	1.45	4 (18%)	31,36,39	2.16	10 (32%)
37	PSU	B5	4099	37	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
37	A2M	B5	3557	37	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
1	PSU	A2	1368	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
37	5MC	B5	3514	87,37	18,22,23	0.97	2 (11%)	26,32,35	1.18	3 (11%)
37	OMG	B5	2267	37	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	A2	1338	1	21,24,25	1.09	2 (9%)	29,34,37	1.17	3 (10%)
1	OMG	A2	437	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	A2	119	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
37	OMC	B5	3601	37	19,22,23	0.81	0	26,31,34	0.84	0
1	OMG	A2	645	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
37	PSU	B5	2351	37	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
37	OMG	B5	3676	37	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	OMU	A2	355	1	19,22,23	1.23	2 (10%)	26,31,34	1.72	4 (15%)
37	PSU	B5	4435	37	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	A2	669	1,87	22,25,26	1.44	4 (18%)	31,36,39	2.10	9 (29%)
37	OMU	B5	3973	37	19,22,23	1.23	3 (15%)	26,31,34	1.69	4 (15%)
41	HIC	BB	245	41	10,11,12	0.60	0	8,14,16	0.39	0
1	OMC	A2	518	1	19,22,23	0.82	0	26,31,34	0.85	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	OMG	B5	2207	37	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
37	PSU	B5	3490	37	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
37	A2M	B5	3599	37	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
1	PSU	A2	407	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	G7M	A2	1640	9,1	23,26,27	3.13	9 (39%)	35,39,42	3.31	13 (37%)
37	PSU	B5	3652	87,37	18,21,22	1.35	2 (11%)	22,30,33	1.85	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
37	UR3	B5	4276	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	2244	87,37	-	0/9/27/28	0/3/3/3
37	PSU	B5	1721	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	3494	37	-	0/7/25/26	0/2/2/2
37	OMU	B5	4052	37	-	0/9/27/28	0/2/2/2
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
66	MLZ	Bb	5	66	-	1/7/8/10	-
37	PSU	B5	4749	37	-	0/7/25/26	0/2/2/2
77	M3L	Bm	98	77	-	0/9/10/12	-
1	4AC	A2	1843	1	-	4/11/29/30	0/2/2/2
37	OMC	B5	2667	37	-	3/9/27/28	0/2/2/2
37	PSU	B5	1638	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	2630	87,37	-	2/9/27/28	0/3/3/3
39	PSU	B8	55	39	-	0/7/25/26	0/2/2/2
1	OMG	A2	684	1	-	2/9/27/28	0/3/3/3
37	OMC	B5	2647	37	-	0/9/27/28	0/2/2/2
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	3447	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	3616	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	3562	37	-	0/9/27/28	0/3/3/3
1	MA6	A2	1851	1	-	0/11/29/30	0/3/3/3
1	A2M	A2	513	1	-	2/9/27/28	0/3/3/3
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	802	1	-	0/7/25/26	0/2/2/2
1	6MZ	A2	1833	1,87	-	0/9/27/28	0/3/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	V5N	BA	216	40	-	2/9/10/12	0/1/1/1
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
37	OMG	B5	3524	37	-	0/9/27/28	0/3/3/3
37	OMG	B5	4245	37	-	0/9/27/28	0/3/3/3
37	PSU	B5	4107	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	4317	37	-	0/9/27/28	0/3/3/3
37	PSU	B5	1632	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	3583	37	-	0/7/25/26	0/2/2/2
1	OMU	A2	1289	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	4298	37	-	0/7/25/26	0/2/2/2
1	OMG	A2	1491	1,87	-	0/9/27/28	0/3/3/3
37	A2M	B5	3492	1,37	-	2/9/27/28	0/3/3/3
37	OMC	B5	3573	37	-	1/9/27/28	0/2/2/2
37	PSU	B5	4042	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	4336	37	-	1/9/27/28	0/3/3/3
37	PSU	B5	1720	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4711	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
37	1MA	B5	1266	37	-	0/7/25/26	0/3/3/3
37	PSU	B5	4382	37	-	4/7/25/26	0/2/2/2
37	PSU	B5	3369	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
1	OMC	A2	1704	1	-	2/9/27/28	0/2/2/2
37	OMC	B5	2265	87,37	-	1/9/27/28	0/2/2/2
37	PSU	B5	3466	37	-	0/7/25/26	0/2/2/2
1	OMU	A2	1805	1	-	0/9/27/28	0/2/2/2
37	A2M	B5	3450	37	-	0/9/27/28	0/3/3/3
65	V5N	Ba	39	65	-	0/9/10/12	0/1/1/1
37	PSU	B5	3502	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	400	37	-	0/9/27/28	0/3/3/3
1	PSU	A2	1644	1,87	-	0/7/25/26	0/2/2/2
1	A2M	A2	1679	1	-	0/9/27/28	0/3/3/3
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
37	A2M	B5	4269	87,37	-	1/9/27/28	0/3/3/3
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	3462	37	-	0/7/25/26	0/2/2/2
37	OMU	B5	3657	37	-	0/9/27/28	0/2/2/2
1	A2M	A2	99	1,87	-	1/9/27/28	0/3/3/3
37	PSU	B5	1683	37	-	0/7/25/26	0/2/2/2

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PSU	B5	4267	37	-	0/7/25/26	0/2/2/2
1	OMC	A2	463	1	-	0/9/27/28	0/2/2/2
37	OMC	B5	3619	37	-	2/9/27/28	0/2/2/2
29	NMM	As	67	29	-	0/9/11/13	-
37	PSU	B5	4177	37	-	0/7/25/26	0/2/2/2
1	OMU	A2	429	1	-	4/9/27/28	0/2/2/2
37	OMG	B5	3974	37	-	0/9/27/28	0/3/3/3
37	OMG	B5	4369	37	-	0/9/27/28	0/3/3/3
37	PSU	B5	4039	37	-	0/7/25/26	0/2/2/2
37	5MC	B5	4193	37	-	4/7/25/26	0/2/2/2
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
1	OMG	A2	1329	1	-	0/9/27/28	0/3/3/3
37	PSU	B5	4322	37	-	0/7/25/26	0/2/2/2
1	OMU	A2	1443	1,87	-	0/9/27/28	0/2/2/2
37	PSU	B5	3500	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	1491	37	-	0/7/25/26	0/2/2/2
1	OMG	A2	602	1	-	0/9/27/28	0/3/3/3
37	OMG	B5	2719	37	-	0/9/27/28	0/3/3/3
37	OMG	B5	3476	37	-	1/9/27/28	0/3/3/3
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
9	PSU	AT	55	9	-	0/7/25/26	0/2/2/2
1	OMC	A2	1392	1	-	0/9/27/28	0/2/2/2
37	OMG	B5	4116	37	-	0/9/27/28	0/3/3/3
37	PSU	B5	4325	37	-	0/7/25/26	0/2/2/2
1	OMU	A2	1327	1,87	-	0/9/27/28	0/2/2/2
1	OMG	A2	868	1	-	1/9/27/28	0/3/3/3
1	A2M	A2	591	1	-	4/9/27/28	0/3/3/3
37	A2M	B5	2206	87,37	-	0/9/27/28	0/3/3/3
37	PSU	B5	1718	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	1032	1	-	0/9/27/28	0/3/3/3
37	OMC	B5	2208	87,37	-	0/9/27/28	0/2/2/2
37	OMG	B5	4138	37	-	0/9/27/28	0/3/3/3
37	PSU	B5	4740	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	2658	87,37	-	0/9/27/28	0/3/3/3
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	1384	1	-	0/9/27/28	0/3/3/3
37	A2M	B5	1489	87,37	-	2/9/27/28	0/3/3/3
37	PSU	B5	4058	37	-	0/7/25/26	0/2/2/2
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
39	OMG	B8	75	39	-	2/9/27/28	0/3/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	A2	174	1,87	-	0/9/27/28	0/2/2/2
37	OMC	B5	2704	37	-	0/9/27/28	0/2/2/2
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
37	OMG	B5	4240	37	-	0/9/27/28	0/3/3/3
37	A2M	B5	3517	37	-	2/9/27/28	0/3/3/3
33	HY3	Aw	62	33	-	1/1/12/14	0/1/1/1
37	OMC	B5	4202	37	-	0/9/27/28	0/2/2/2
37	PSU	B5	4278	37	-	0/7/25/26	0/2/2/2
37	OMG	B5	4383	37	-	1/9/27/28	0/3/3/3
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	4166	37	-	0/7/25/26	0/2/2/2
37	OMC	B5	2194	87,37	-	2/9/27/28	0/2/2/2
37	PSU	B5	4217	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	3576	37	-	1/7/25/26	0/2/2/2
37	OMC	B5	4282	87,37	-	1/9/27/28	0/2/2/2
37	PSU	B5	4419	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
37	A2M	B5	3456	37	-	0/9/27/28	0/3/3/3
37	OMU	B5	2258	37	-	0/9/27/28	0/2/2/2
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
37	OMG	B5	1477	37	-	0/9/27/28	0/3/3/3
37	PSU	B5	4169	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4045	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	166	1	-	0/9/27/28	0/3/3/3
37	PSU	B5	3496	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	3371	37	-	0/7/25/26	0/2/2/2
39	PSU	B8	69	39	-	0/7/25/26	0/2/2/2
37	PSU	B5	1799	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	1479	37	-	0/9/27/28	0/3/3/3
37	OMG	B5	3631	87,37	-	1/9/27/28	0/3/3/3
9	5MU	AT	54	9	-	0/7/25/26	0/2/2/2
37	PSU	B5	4203	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	159	1	-	1/9/27/28	0/3/3/3
37	UY1	B5	3550	37	-	1/9/27/28	0/2/2/2
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
37	OMG	B5	3942	9,37	-	0/9/27/28	0/3/3/3
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
37	OMU	B5	4244	37	-	0/9/27/28	0/2/2/2
37	OMG	B5	4364	37	-	0/9/27/28	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OMG	B5	1580	37	-	0/9/27/28	0/3/3/3
37	PSU	B5	4374	37	-	0/7/25/26	0/2/2/2
78	MLZ	B <sub>0</sub>	53	78	-	0/7/8/10	-
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
37	OMC	B5	3433	37	-	4/9/27/28	0/2/2/2
1	OMU	A2	628	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
37	OMC	B5	3540	37	-	0/9/27/28	0/2/2/2
37	A2M	B5	1810	87,37	-	0/9/27/28	0/3/3/3
37	OMG	B5	1260	37	-	0/9/27/28	0/3/3/3
1	A2M	A2	485	1	-	1/9/27/28	0/3/3/3
37	PSU	B5	3554	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4188	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	823	1	-	0/7/25/26	0/2/2/2
37	OMC	B5	1820	87,37	-	1/9/27/28	0/2/2/2
37	PSU	B5	3427	37	-	0/7/25/26	0/2/2/2
37	OMU	B5	4366	37	-	1/9/27/28	0/2/2/2
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	1537	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2
1	MA6	A2	1852	1	-	2/11/29/30	0/3/3/3
37	OMU	B5	2680	37	-	0/9/27/28	0/2/2/2
37	PSU	B5	1801	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	1270	37	-	0/9/27/28	0/3/3/3
37	6MZ	B5	3966	37	-	0/9/27/28	0/3/3/3
1	A2M	A2	469	1	-	1/9/27/28	0/3/3/3
1	OMG	A2	1448	1	-	2/9/27/28	0/3/3/3
37	PSU	B5	4149	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	3585	87,37	-	0/7/25/26	0/2/2/2
37	OMC	B5	1284	37	-	1/9/27/28	0/2/2/2
1	OMU	A2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	A2	1082	1	-	1/7/25/26	0/2/2/2
37	PSU	B5	1731	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4246	37	-	1/7/25/26	0/2/2/2
1	A2M	A2	27	1,87	-	0/9/27/28	0/3/3/3
1	OMG	A2	510	1,87	-	1/9/27/28	0/3/3/3
1	A2M	A2	577	1	-	0/9/27/28	0/3/3/3
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	2475	37	-	0/7/25/26	0/2/2/2
37	OMG	B5	3359	37	-	0/9/27/28	0/3/3/3

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2
37	A2M	B5	398	37	-	2/9/27/28	0/3/3/3
37	PSU	B5	4099	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	3557	37	-	0/9/27/28	0/3/3/3
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
37	5MC	B5	3514	87,37	-	0/7/25/26	0/2/2/2
37	OMG	B5	2267	37	-	0/9/27/28	0/3/3/3
1	4AC	A2	1338	1	-	4/11/29/30	0/2/2/2
1	OMG	A2	437	1	-	1/9/27/28	0/3/3/3
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
37	OMC	B5	3601	37	-	0/9/27/28	0/2/2/2
1	OMG	A2	645	1	-	3/9/27/28	0/3/3/3
37	PSU	B5	2351	37	-	0/7/25/26	0/2/2/2
37	OMG	B5	3676	37	-	1/9/27/28	0/3/3/3
1	OMU	A2	355	1	-	1/9/27/28	0/2/2/2
37	PSU	B5	4435	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	669	1,87	-	2/9/27/28	0/3/3/3
37	OMU	B5	3973	37	-	0/9/27/28	0/2/2/2
41	HIC	BB	245	41	-	2/5/6/8	0/1/1/1
1	OMC	A2	518	1	-	0/9/27/28	0/2/2/2
37	OMG	B5	2207	37	-	2/9/27/28	0/3/3/3
37	PSU	B5	3490	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	3599	37	-	0/9/27/28	0/3/3/3
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
1	G7M	A2	1640	9,1	-	2/7/25/26	0/3/3/3
37	PSU	B5	3652	87,37	-	0/7/25/26	0/2/2/2

The worst 5 of 507 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Aw	62	HY3	C4-C3	-11.35	1.32	1.52
33	Aw	62	HY3	C3-CA	10.43	1.65	1.55
1	A2	1640	G7M	C4-N9	7.83	1.58	1.38
1	A2	1640	G7M	O6-C6	7.68	1.38	1.23
1	A2	1851	MA6	C5-N7	6.83	1.51	1.39

The worst 5 of 938 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1851	MA6	C4-N9-C8	14.75	121.71	105.73

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1852	MA6	C4-N9-C8	14.47	121.42	105.73
1	A2	1640	G7M	C8-N7-C5	11.41	122.04	107.78
1	A2	591	A2M	C5-C4-N3	-6.89	117.76	126.75
1	A2	1852	MA6	N3-C4-N9	6.83	138.34	127.08

There are no chirality outliers.

5 of 103 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	Aw	62	HY3	O-C-CA-C3
37	B5	1489	A2M	O4'-C4'-C5'-O5'
37	B5	2207	OMG	O4'-C4'-C5'-O5'
37	B5	3433	OMC	C2'-C1'-N1-C2
37	B5	3433	OMC	C2'-C1'-N1-C6

There are no ring outliers.

82 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	B5	2244	A2M	1	0
1	A2	1843	4AC	2	0
37	B5	2647	OMC	1	0
37	B5	3562	A2M	2	0
1	A2	513	A2M	1	0
1	A2	1833	6MZ	1	0
37	B5	3524	OMG	1	0
1	A2	1289	OMU	2	0
1	A2	1491	OMG	1	0
37	B5	3573	OMC	1	0
37	B5	4336	A2M	1	0
1	A2	1704	OMC	1	0
1	A2	1805	OMU	1	0
37	B5	3450	A2M	2	0
65	Ba	39	V5N	1	0
37	B5	3502	PSU	1	0
37	B5	400	A2M	1	0
1	A2	1679	A2M	2	0
37	B5	3462	PSU	1	0
1	A2	99	A2M	2	0
1	A2	463	OMC	1	0
37	B5	3619	OMC	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	B5	3974	OMG	1	0
37	B5	4039	PSU	1	0
37	B5	4193	5MC	1	0
1	A2	172	OMU	1	0
1	A2	1329	OMG	1	0
1	A2	1443	OMU	1	0
1	A2	602	OMG	1	0
37	B5	3476	OMG	1	0
1	A2	1392	OMC	1	0
1	A2	868	OMG	1	0
37	B5	2206	A2M	1	0
37	B5	1718	PSU	1	0
1	A2	1032	A2M	1	0
37	B5	2208	OMC	1	0
37	B5	4138	OMG	2	0
37	B5	2658	A2M	1	0
37	B5	4058	PSU	1	0
1	A2	116	OMU	1	0
39	B8	75	OMG	2	0
37	B5	2704	OMC	1	0
37	B5	4202	OMC	1	0
37	B5	4383	OMG	1	0
37	B5	2194	OMC	1	0
37	B5	4282	OMC	1	0
37	B5	3456	A2M	1	0
37	B5	2258	OMU	2	0
1	A2	166	A2M	2	0
37	B5	3631	OMG	1	0
37	B5	4203	PSU	1	0
37	B5	3550	UY1	2	0
37	B5	3942	OMG	3	0
1	A2	628	OMU	1	0
37	B5	3540	OMC	1	0
37	B5	1810	A2M	2	0
37	B5	1260	OMG	2	0
1	A2	823	PSU	1	0
37	B5	4366	OMU	2	0
37	B5	1270	A2M	1	0
1	A2	469	A2M	1	0
1	A2	1448	OMG	2	0
37	B5	4149	PSU	1	0
37	B5	3585	PSU	1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	B5	1284	OMC	2	0
1	A2	121	OMU	2	0
1	A2	27	A2M	1	0
1	A2	510	OMG	1	0
1	A2	577	A2M	2	0
37	B5	398	A2M	1	0
37	B5	3557	A2M	1	0
37	B5	2267	OMG	1	0
1	A2	1338	4AC	4	0
1	A2	437	OMG	2	0
37	B5	3676	OMG	1	0
1	A2	355	OMU	1	0
37	B5	3973	OMU	2	0
1	A2	518	OMC	1	0
37	B5	2207	OMG	1	0
37	B5	3599	A2M	1	0
1	A2	1640	G7M	1	0
37	B5	3652	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 635 ligands modelled in this entry, 415 are monoatomic and 187 are unknown - leaving 33 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	$\# Z  > 2$
89	SPD	B5	5185	-	9,9,9	0.15	0	8,8,8	0.17	0
89	SPD	B5	5189	-	9,9,9	0.16	0	8,8,8	0.18	0
89	SPD	B5	5176	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	B5	5190	-	9,9,9	0.16	0	8,8,8	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
90	SPM	B5	5143	-	13,13,13	0.14	0	12,12,12	0.15	0
89	SPD	B5	5175	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	A2	2038	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	B5	5192	-	9,9,9	0.16	0	8,8,8	0.17	0
89	SPD	B5	5196	-	9,9,9	0.16	0	8,8,8	0.18	0
89	SPD	B5	5179	-	9,9,9	0.15	0	8,8,8	0.16	0
89	SPD	B5	5188	-	9,9,9	0.15	0	8,8,8	0.19	0
90	SPM	B5	5142	-	13,13,13	0.15	0	12,12,12	0.24	0
89	SPD	B5	5187	-	9,9,9	0.15	0	8,8,8	0.17	0
89	SPD	A2	2042	-	9,9,9	0.15	0	8,8,8	0.17	0
89	SPD	B5	5195	-	9,9,9	0.15	0	8,8,8	0.19	0
89	SPD	B5	5194	-	9,9,9	0.15	0	8,8,8	0.20	0
89	SPD	B5	5193	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	B5	5180	-	9,9,9	0.15	0	8,8,8	0.17	0
89	SPD	B5	5181	-	9,9,9	0.15	0	8,8,8	0.19	0
89	SPD	A2	2039	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	B5	5183	-	9,9,9	0.15	0	8,8,8	0.19	0
89	SPD	B5	5186	-	9,9,9	0.15	0	8,8,8	0.21	0
89	SPD	A2	2043	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	A2	2036	-	9,9,9	0.15	0	8,8,8	0.15	0
89	SPD	A2	2041	-	9,9,9	0.16	0	8,8,8	0.18	0
89	SPD	B5	5191	-	9,9,9	0.15	0	8,8,8	0.14	0
89	SPD	B5	5184	-	9,9,9	0.16	0	8,8,8	0.18	0
90	SPM	A2	2044	-	13,13,13	0.15	0	12,12,12	0.14	0
89	SPD	B5	5177	-	9,9,9	0.15	0	8,8,8	0.20	0
89	SPD	A2	2037	-	9,9,9	0.15	0	8,8,8	0.20	0
89	SPD	A2	2040	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	B5	5178	-	9,9,9	0.16	0	8,8,8	0.18	0
89	SPD	B5	5182	-	9,9,9	0.15	0	8,8,8	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	B5	5185	-	-	0/7/7/7	-
89	SPD	B5	5189	-	-	0/7/7/7	-
89	SPD	B5	5176	-	-	0/7/7/7	-
89	SPD	B5	5190	-	-	1/7/7/7	-
90	SPM	B5	5143	-	-	0/11/11/11	-
89	SPD	B5	5175	-	-	0/7/7/7	-
89	SPD	A2	2038	-	-	0/7/7/7	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	B5	5192	-	-	2/7/7/7	-
89	SPD	B5	5196	-	-	1/7/7/7	-
89	SPD	B5	5179	-	-	1/7/7/7	-
89	SPD	B5	5188	-	-	1/7/7/7	-
90	SPM	B5	5142	-	-	1/11/11/11	-
89	SPD	B5	5187	-	-	0/7/7/7	-
89	SPD	A2	2042	-	-	1/7/7/7	-
89	SPD	B5	5195	-	-	1/7/7/7	-
89	SPD	B5	5194	-	-	0/7/7/7	-
89	SPD	B5	5193	-	-	1/7/7/7	-
89	SPD	B5	5180	-	-	0/7/7/7	-
89	SPD	B5	5181	-	-	0/7/7/7	-
89	SPD	A2	2039	-	-	0/7/7/7	-
89	SPD	B5	5183	-	-	0/7/7/7	-
89	SPD	B5	5186	-	-	0/7/7/7	-
89	SPD	A2	2043	-	-	0/7/7/7	-
89	SPD	A2	2036	-	-	0/7/7/7	-
89	SPD	A2	2041	-	-	1/7/7/7	-
89	SPD	B5	5191	-	-	1/7/7/7	-
89	SPD	B5	5184	-	-	0/7/7/7	-
90	SPM	A2	2044	-	-	1/11/11/11	-
89	SPD	B5	5177	-	-	0/7/7/7	-
89	SPD	A2	2037	-	-	0/7/7/7	-
89	SPD	A2	2040	-	-	0/7/7/7	-
89	SPD	B5	5178	-	-	0/7/7/7	-
89	SPD	B5	5182	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	A2	2044	SPM	C8-C9-N10-C11
89	B5	5190	SPD	C2-C3-C4-C5
90	B5	5142	SPM	C8-C9-N10-C11
89	B5	5192	SPD	C2-C3-C4-C5
89	A2	2041	SPD	C2-C3-C4-C5

There are no ring outliers.

20 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	B5	5185	SPD	3	0
89	B5	5176	SPD	1	0
89	B5	5190	SPD	1	0
89	B5	5175	SPD	1	0
89	A2	2038	SPD	2	0
89	B5	5179	SPD	1	0
89	B5	5188	SPD	1	0
90	B5	5142	SPM	2	0
89	A2	2042	SPD	1	0
89	B5	5195	SPD	1	0
89	B5	5193	SPD	1	0
89	A2	2039	SPD	1	0
89	B5	5183	SPD	3	0
89	B5	5186	SPD	1	0
89	A2	2041	SPD	1	0
90	A2	2044	SPM	1	0
89	B5	5177	SPD	1	0
89	A2	2037	SPD	1	0
89	B5	5178	SPD	3	0
89	B5	5182	SPD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

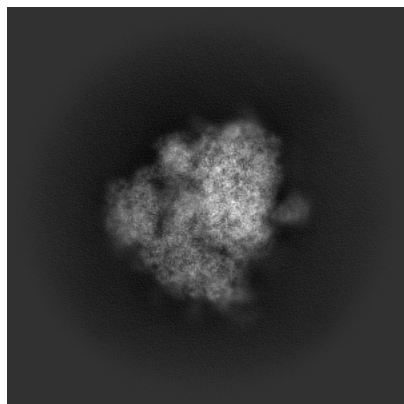
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53295. These allow visual inspection of the internal detail of the map and identification of artifacts.

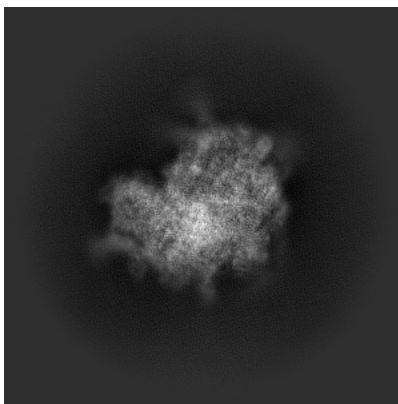
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

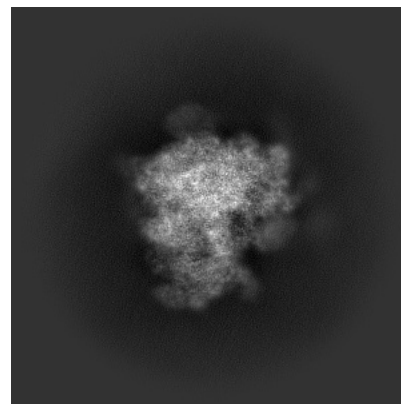
#### 6.1.1 Primary map



X

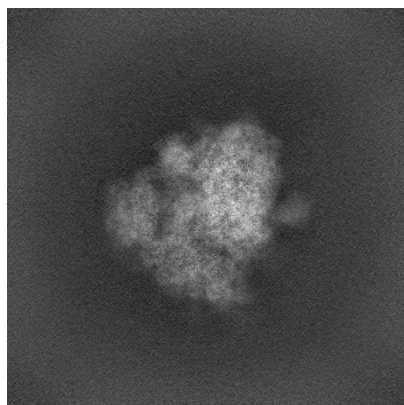


Y

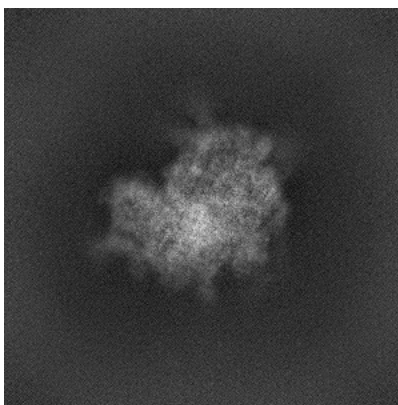


Z

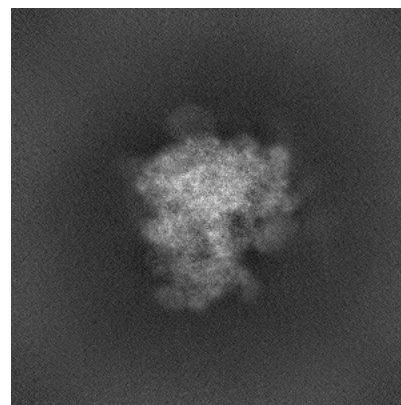
#### 6.1.2 Raw map



X



Y

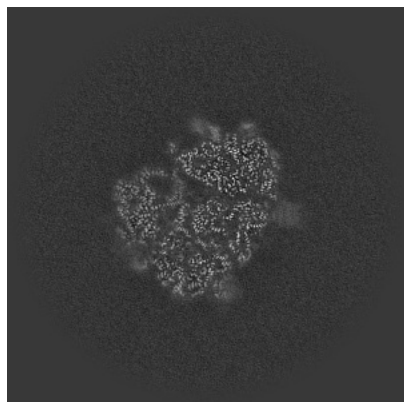


Z

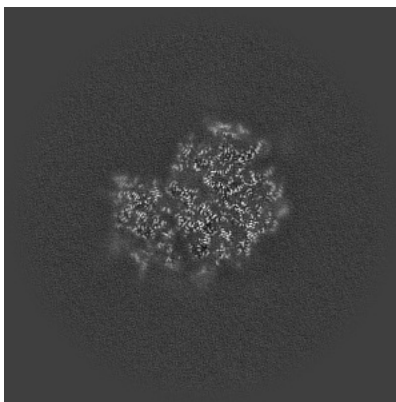
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

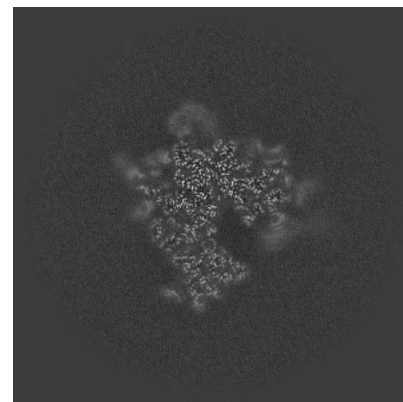
### 6.2.1 Primary map



X Index: 280

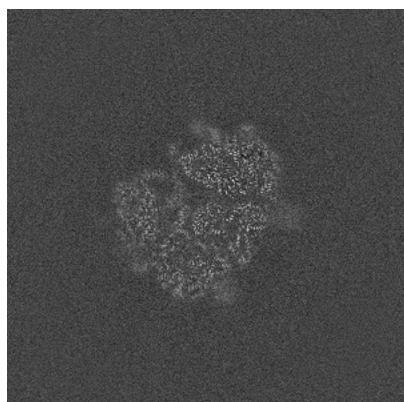


Y Index: 280

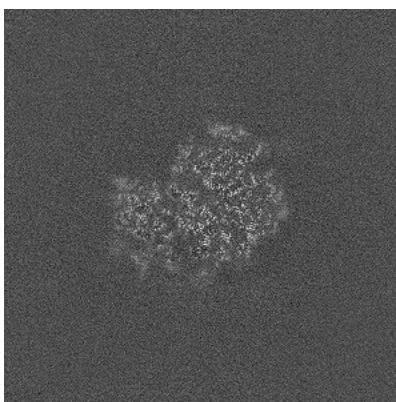


Z Index: 280

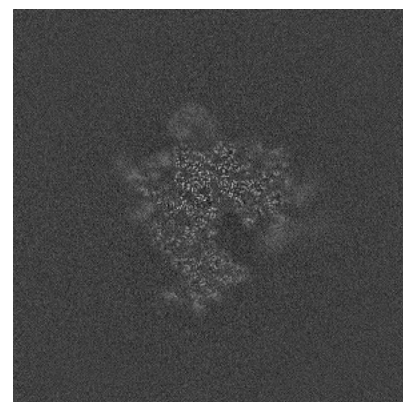
### 6.2.2 Raw map



X Index: 280



Y Index: 280

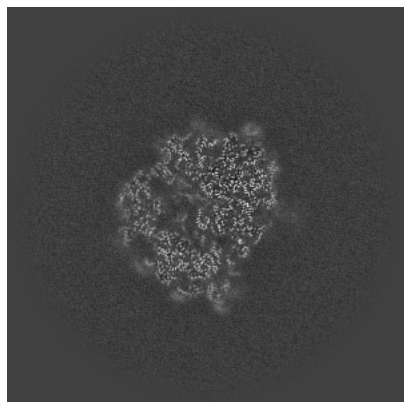


Z Index: 280

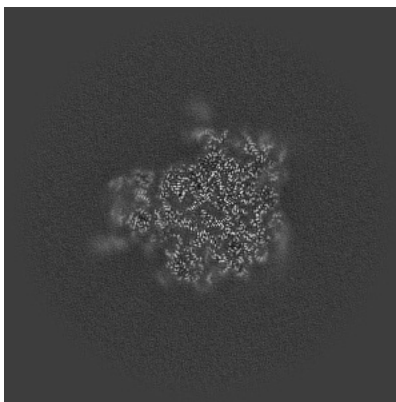
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

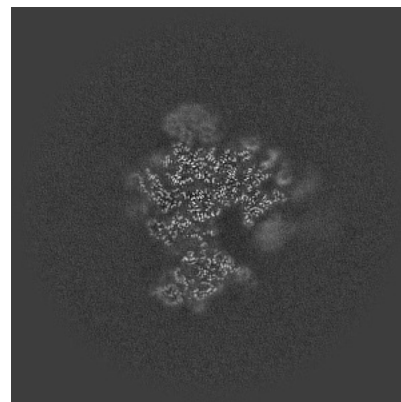
### 6.3.1 Primary map



X Index: 288

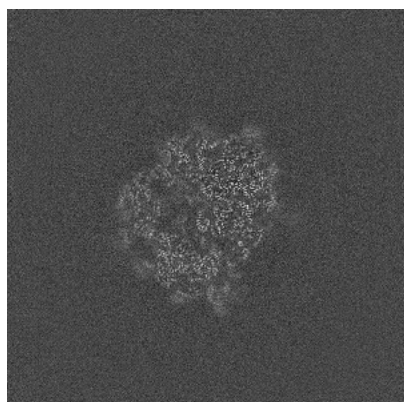


Y Index: 313

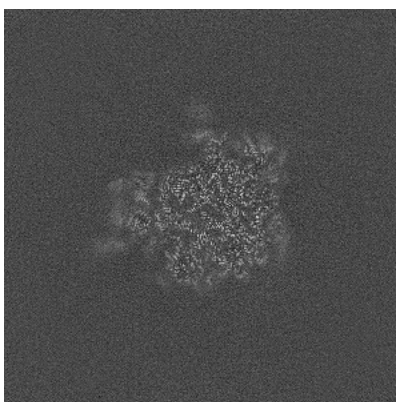


Z Index: 272

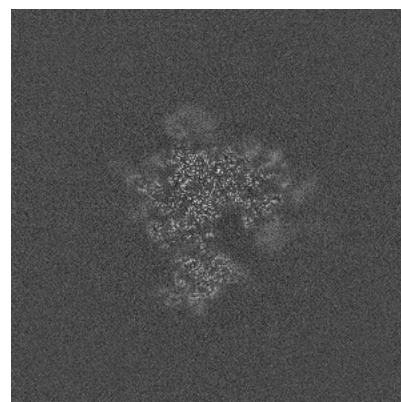
### 6.3.2 Raw map



X Index: 288



Y Index: 313

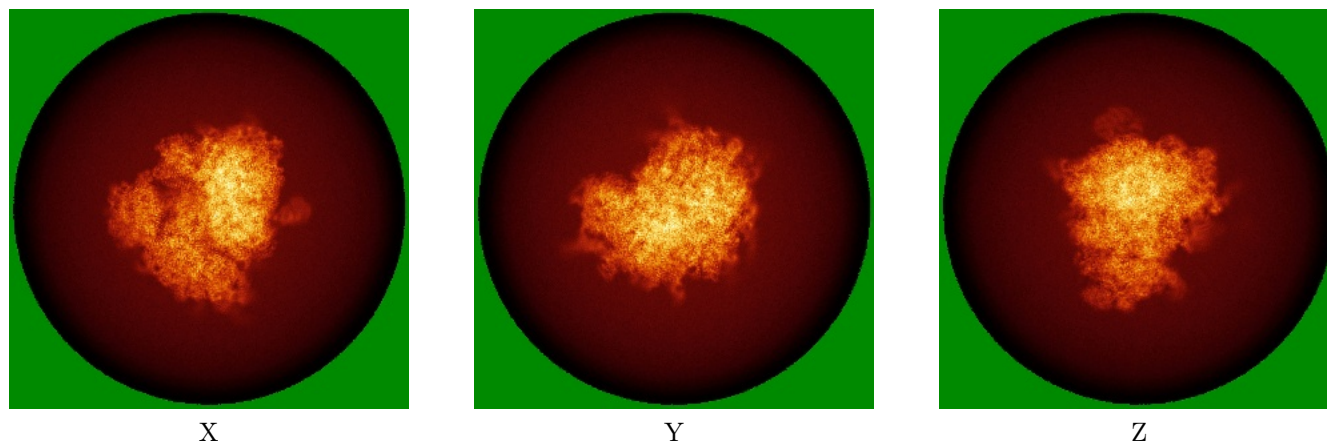


Z Index: 275

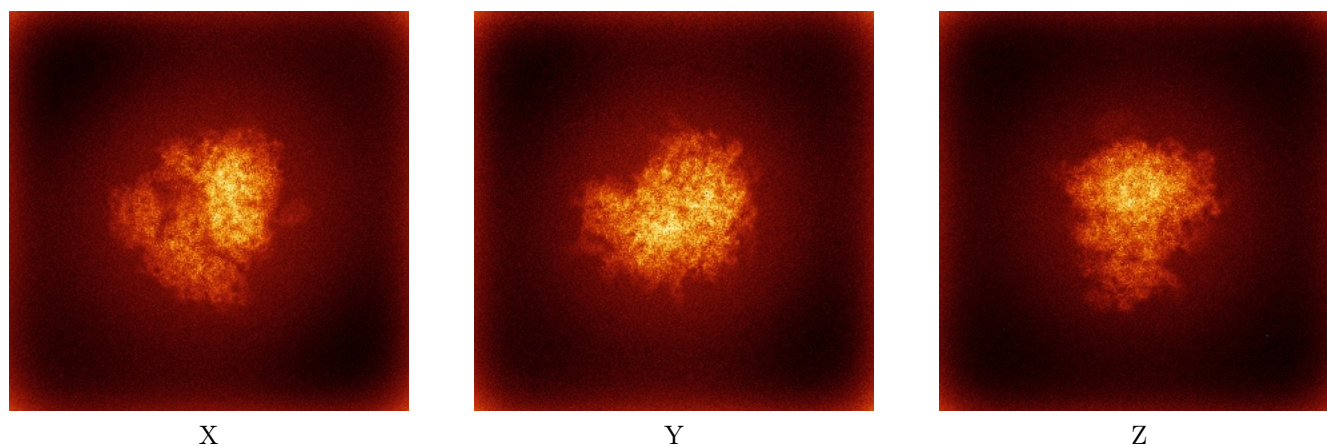
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



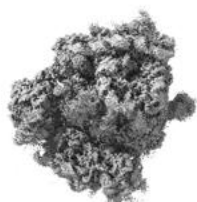
### 6.4.2 Raw map



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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



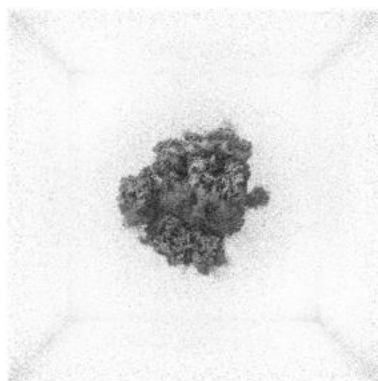
Y



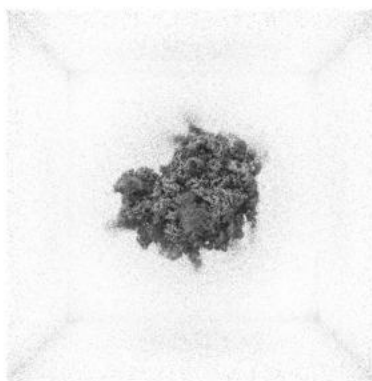
Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

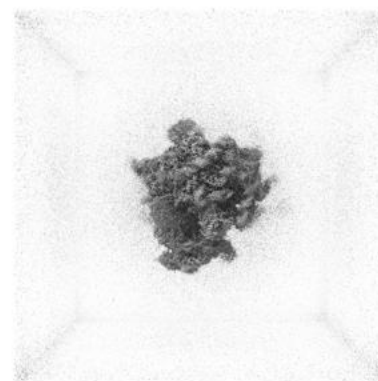
### 6.5.2 Raw map



X



Y



Z

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

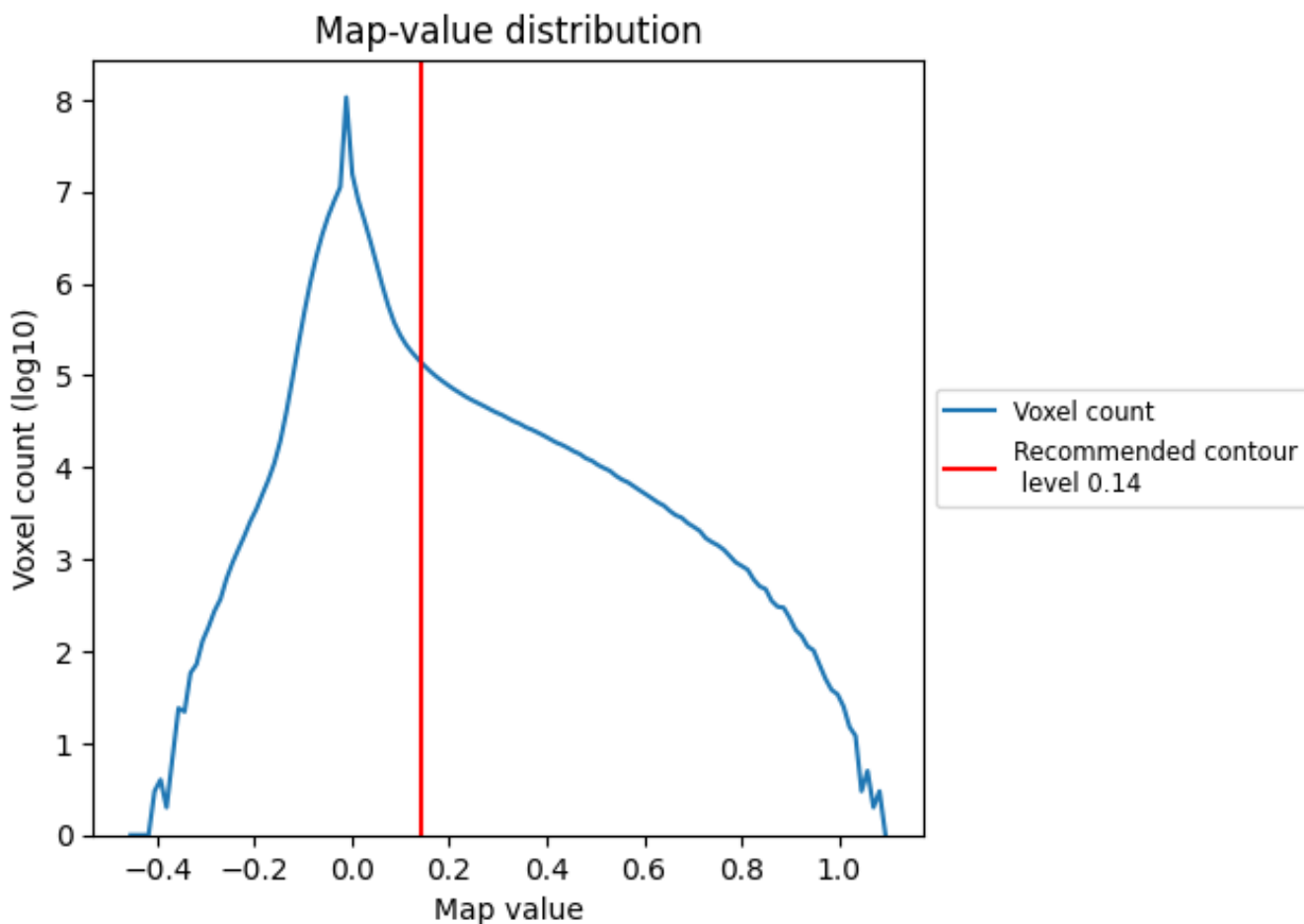
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

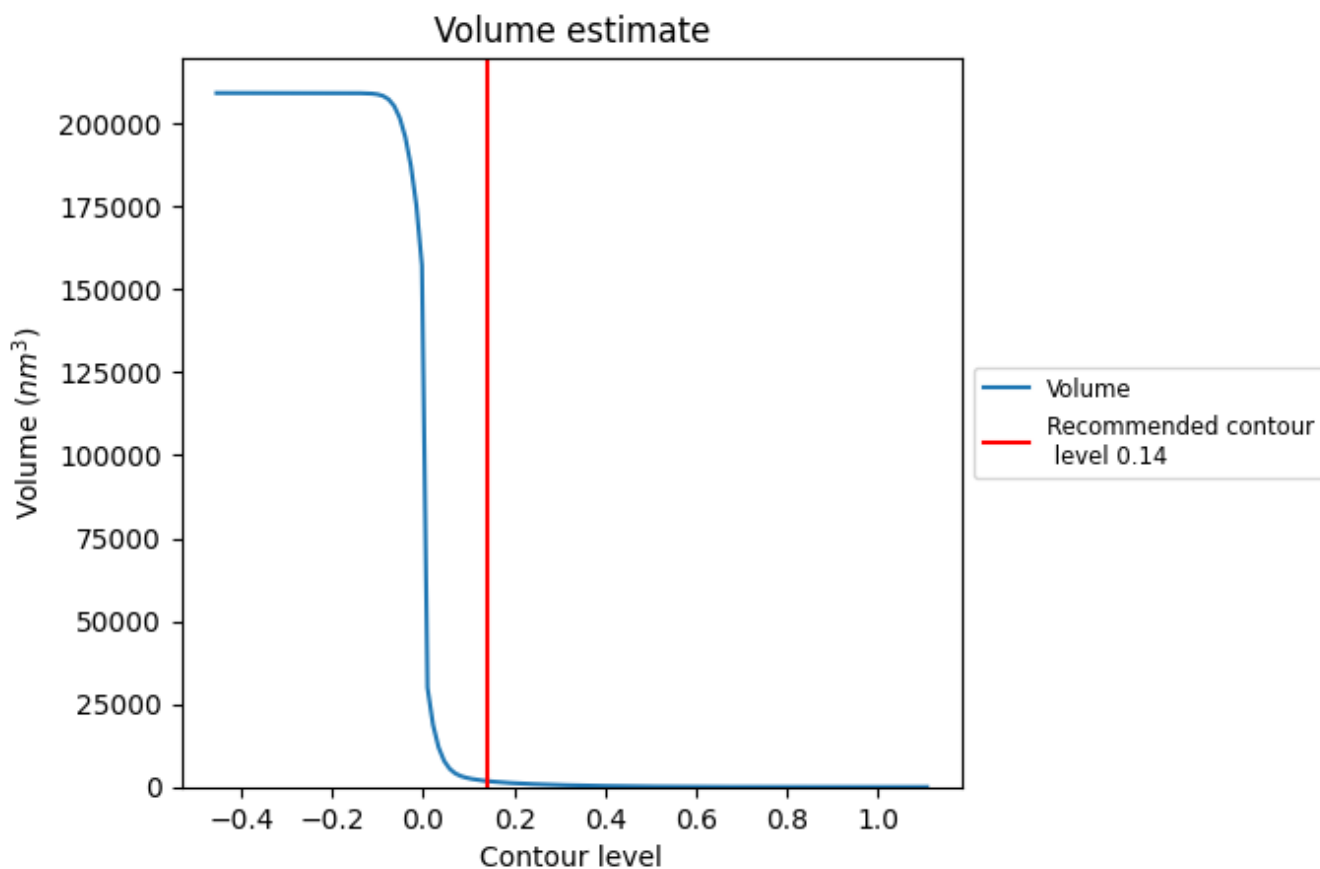
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

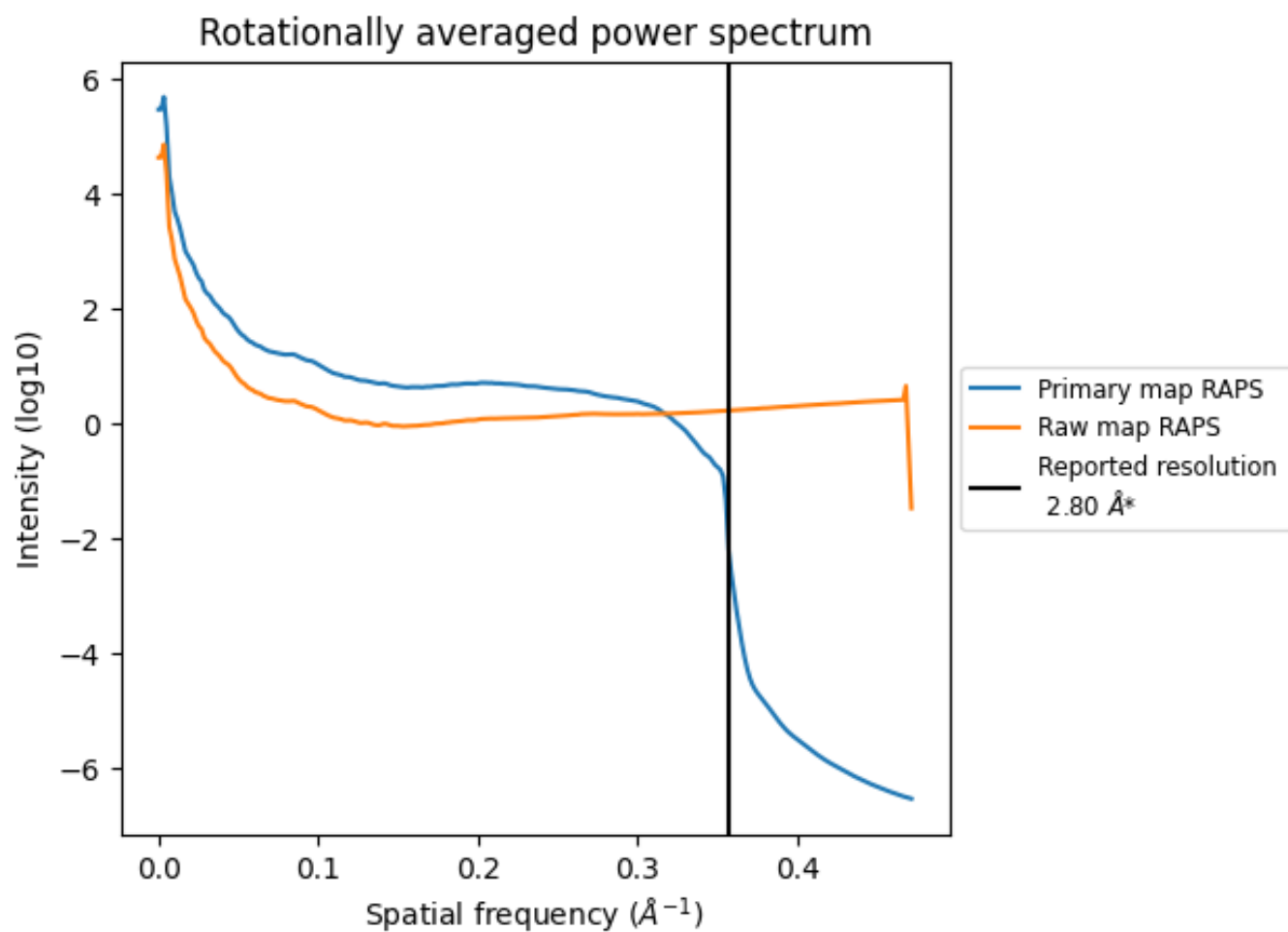
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1787  $\text{nm}^3$ ; this corresponds to an approximate mass of 1614 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 i

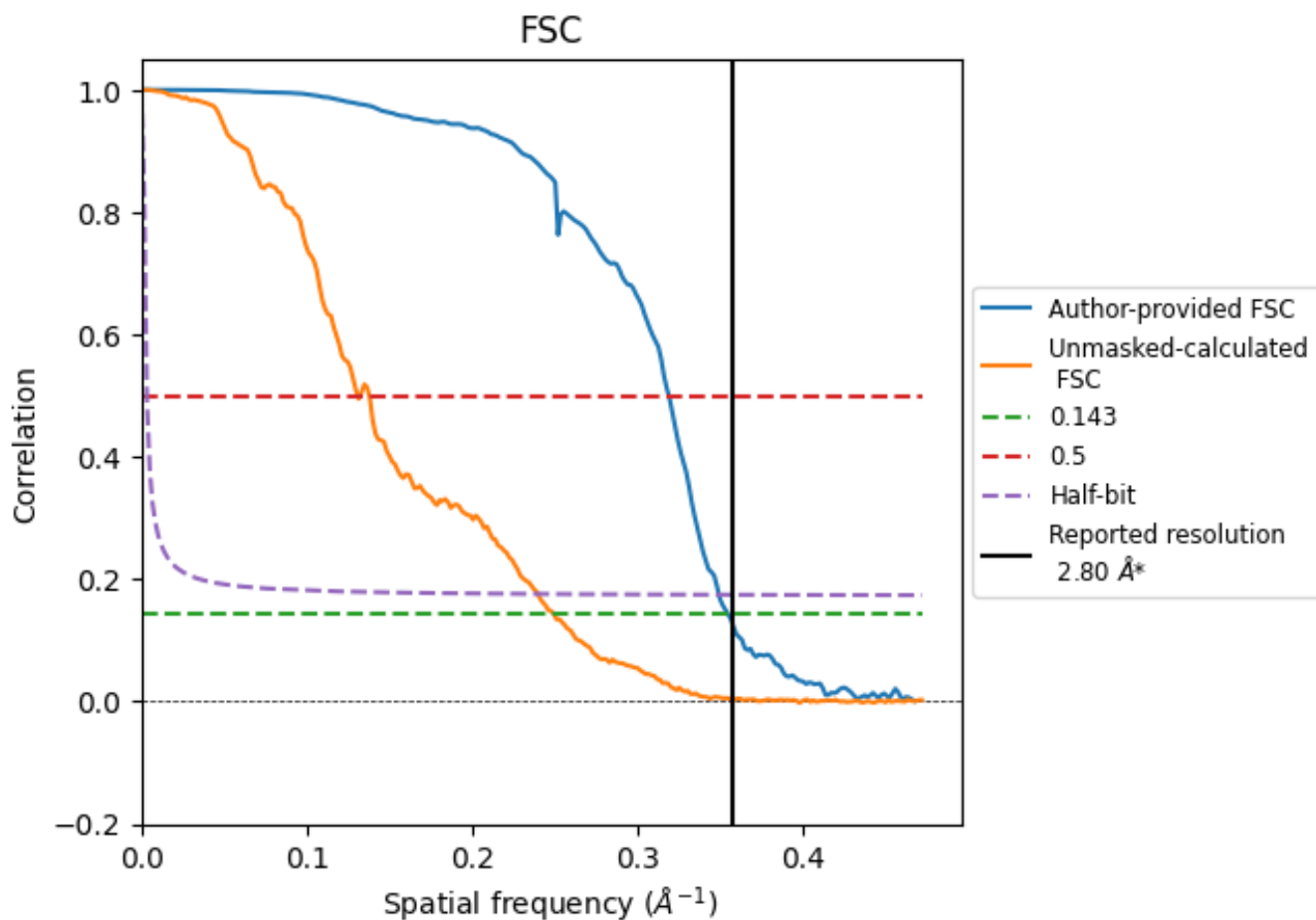


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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  $0.357 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

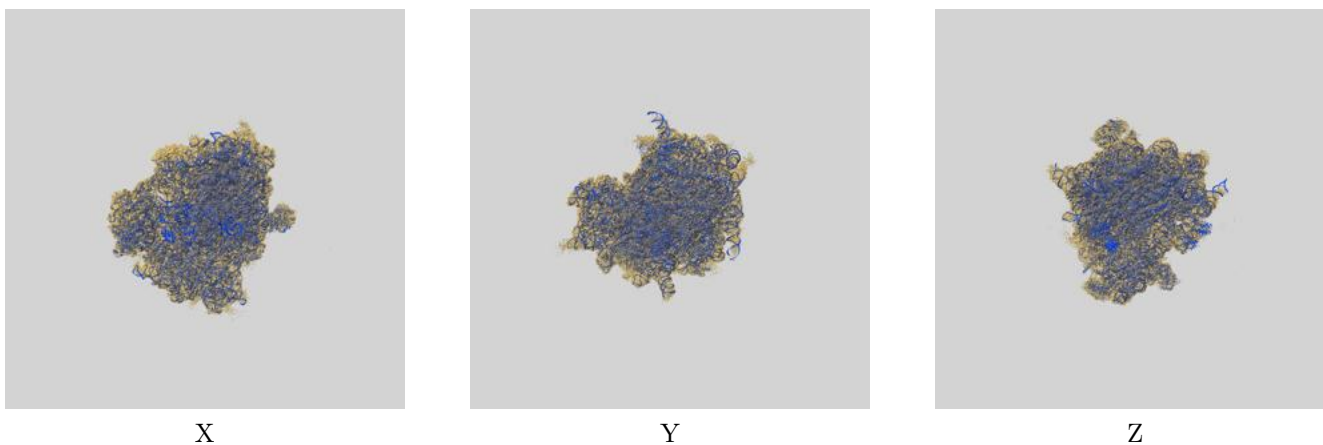
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.14	2.87
Unmasked-calculated*	4.01	7.65	4.17

\*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 4.01 differs from the reported value 2.8 by more than 10 %

## 9 Map-model fit [i](#)

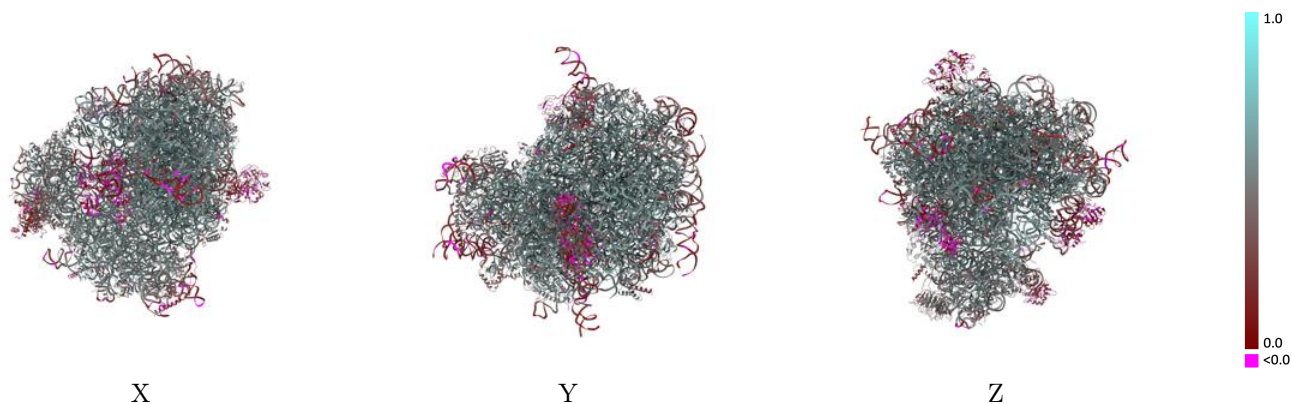
This section contains information regarding the fit between EMDB map EMD-53295 and PDB model 9QQA. Per-residue inclusion information can be found in section [3](#) on page [28](#).

### 9.1 Map-model overlay [i](#)



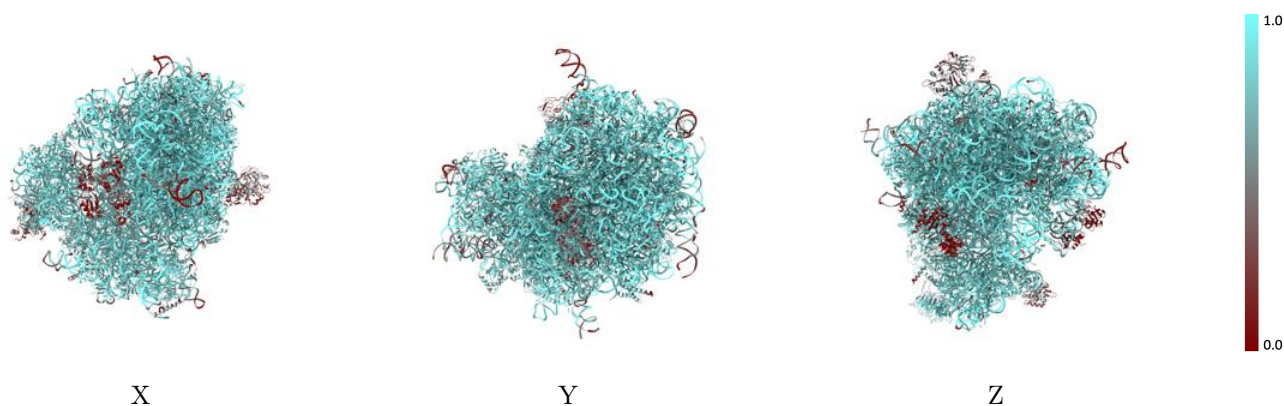
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



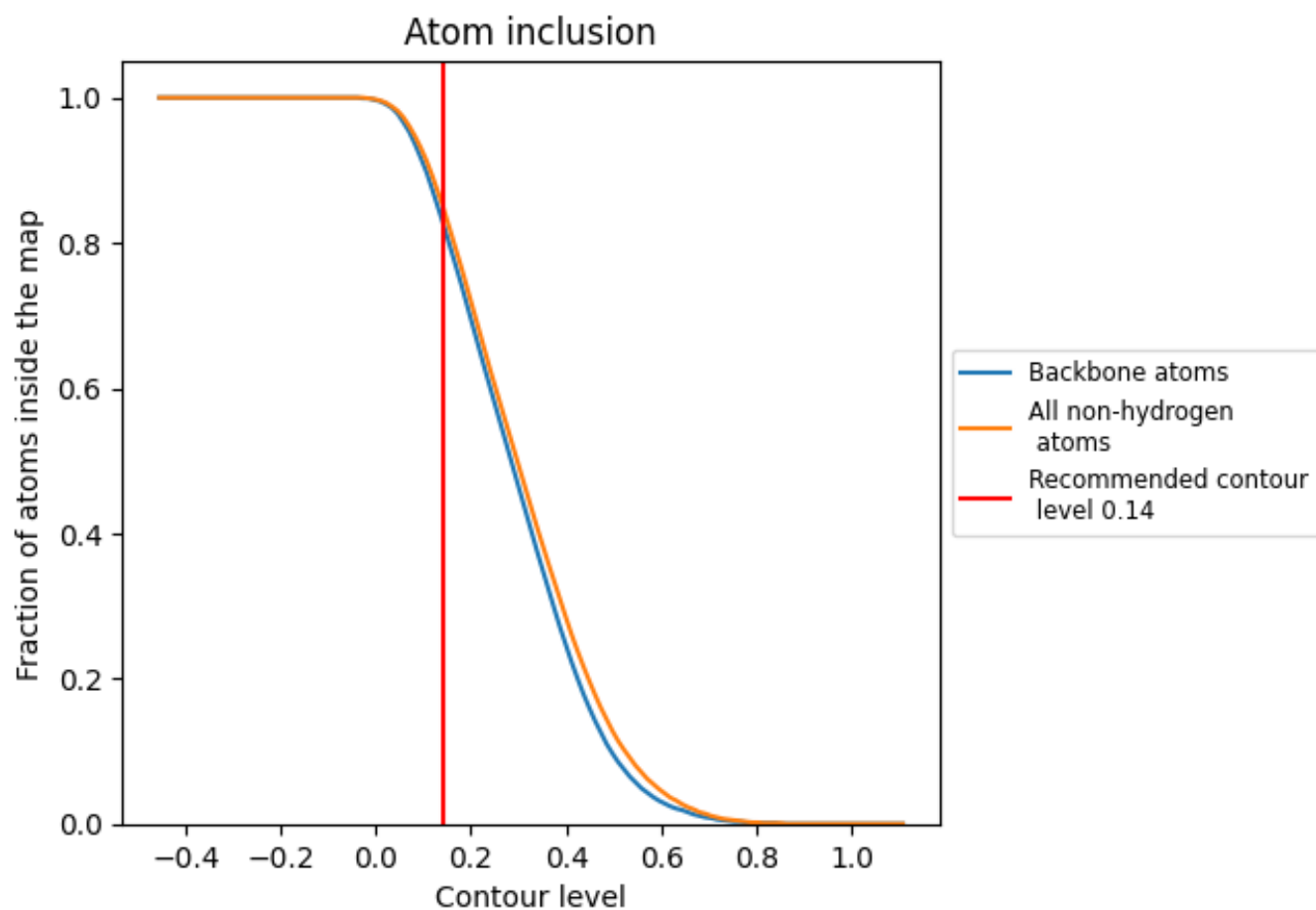
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.4920
A2	 0.9200	 0.4970
AA	 0.7950	 0.4760
AB	 0.7250	 0.4680
AC	 0.2860	 0.1350
AD	 0.6590	 0.4430
AE	 0.8450	 0.5290
AF	 0.7700	 0.3990
AG	 0.8640	 0.5070
AT	 0.7720	 0.4740
AZ	 0.8400	 0.4960
Aa	 0.8070	 0.5000
Ab	 0.8420	 0.5200
Ac	 0.7470	 0.4420
Ad	 0.8450	 0.5090
Ae	 0.7730	 0.4710
Af	 0.7810	 0.4290
Ag	 0.7480	 0.4250
Ah	 0.8320	 0.4910
Ai	 0.8420	 0.4960
Aj	 0.7960	 0.4200
Ak	 0.7860	 0.5040
Al	 0.3630	 0.1640
Am	 0.8400	 0.5270
An	 0.8360	 0.5130
Ao	 0.7730	 0.4340
Ap	 0.8280	 0.4930
Aq	 0.7750	 0.4520
Ar	 0.7920	 0.4690
As	 0.8380	 0.4860
At	 0.7250	 0.4110
Au	 0.8160	 0.5130
Av	 0.8530	 0.5510
Aw	 0.8500	 0.5360
Ax	 0.8160	 0.4780























*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
Ay	0.6840	0.4380
Az	0.8490	0.5460
B5	0.9180	0.5130
B7	0.9870	0.5790
B8	0.9540	0.5440
BA	0.8770	0.5700
BB	0.8850	0.5490
BC	0.8940	0.5540
BE	0.7980	0.4810
BF	0.8790	0.5550
BG	0.8140	0.4850
BH	0.8540	0.5260
BI	0.8400	0.5360
BJ	0.8340	0.4970
BK	0.1670	0.2710
BL	0.8510	0.5220
BM	0.8870	0.5290
BN	0.9290	0.5830
BO	0.9000	0.5570
BP	0.8920	0.5580
BQ	0.8840	0.5580
BR	0.8510	0.5110
BS	0.9080	0.5580
BT	0.8460	0.5360
BU	0.8340	0.4840
BV	0.8250	0.5280
BW	0.6570	0.3630
BX	0.8560	0.5330
BY	0.8810	0.5320
BZ	0.8840	0.5340
Ba	0.9260	0.5760
Bb	0.7410	0.4680
Bc	0.7700	0.4810
Bd	0.8750	0.5420
Be	0.8550	0.5580
Bf	0.9120	0.5720
Bg	0.8580	0.5330
Bh	0.8550	0.5160
Bi	0.8330	0.5090
Bj	0.9240	0.5750
Bk	0.7920	0.4730
Bl	0.8600	0.5490

*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
Bm	 0.8520	 0.5380
Bo	 0.8320	 0.5340
Bp	 0.8260	 0.5380
Br	 0.8950	 0.5600
Bs	 0.0770	 0.0650
Bt	 0.0560	 0.0430
Bv	 0.0600	 0.0550
MA	 0.4200	 0.1470
Nt	 0.2480	 0.1120
Nu	 0.3780	 0.2430