



## wwPDB EM Validation Summary Report ⓘ

Jul 10, 2025 – 02:51 pm BST

PDB ID : 9QQB / pdb\_00009qqb  
EMDB ID : EMD-53296  
Title : Quaternary complex of a translating ribosome, NAC, NMT1, and NatA  
Authors : Echeverria, B.; Jaskolowski, M.; Scaiola, A.; Ban, N.  
Deposited on : 2025-03-31  
Resolution : 3.43 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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

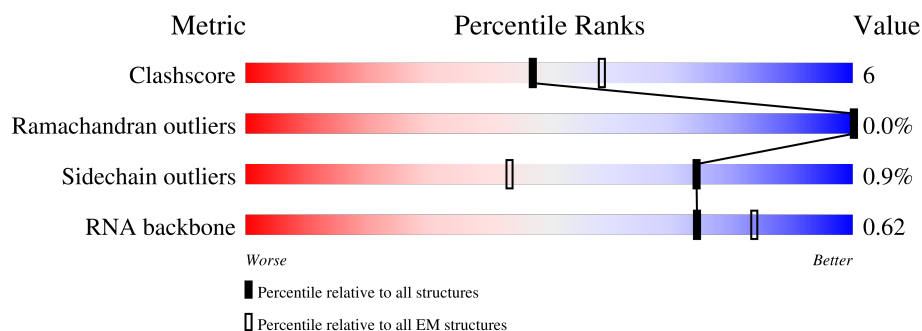
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.43 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	B5	4808	
2	B7	120	
3	B8	158	
4	BA	257	
5	BB	403	
6	BC	413	
7	BD	297	

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Mol	Chain	Length	Quality of chain
8	BE	291	
9	BF	247	
10	BG	266	
11	BH	192	
12	BI	214	
13	BJ	178	
14	BK	12	
15	BL	211	
16	BM	218	
17	BN	204	
18	BO	203	
19	BP	184	
20	BQ	188	
21	BR	196	
22	BS	176	
23	BT	160	
24	BU	128	
25	BV	140	
26	BW	157	
27	BX	156	
28	BY	145	
29	BZ	136	
30	Ba	148	
31	Bb	245	
32	Bc	115	

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Mol	Chain	Length	Quality of chain
33	Bd	125	
34	Be	135	
35	Bf	110	
36	Bg	117	
37	Bh	123	
38	Bi	105	
39	Bj	97	
40	Bk	70	
41	Bl	51	
42	Bm	128	
43	Bo	106	
44	Bp	92	
45	Br	137	
46	Bs	318	
47	Bt	165	
48	Bv	217	
49	Nt	215	
50	Nu	162	
51	XA	866	
52	XB	235	
53	MA	496	
54	A2	1870	
55	AA	84	
56	AB	69	
57	AC	156	


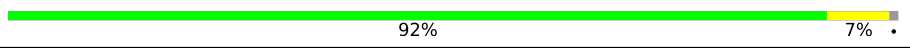



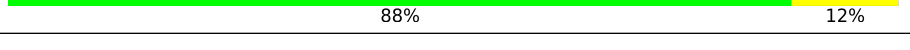
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Mol	Chain	Length	Quality of chain
58	AD	133	
59	AE	115	
60	AF	317	
61	AG	56	
62	AT	76	
63	AZ	295	
64	Aa	264	
65	Ab	293	
66	Ac	281	
67	Ad	263	
68	Ae	204	
69	Af	249	
70	Ag	432	
71	Ah	208	
72	Ai	194	
73	Aj	165	
74	Ak	158	
75	Al	132	
76	Am	151	
77	An	151	
78	Ao	145	
79	Ap	172	
80	Aq	135	
81	Ar	152	
82	As	145	

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Mol	Chain	Length	Quality of chain
83	At	119	
84	Au	84	
85	Av	130	
86	Aw	143	
87	Ax	130	
88	Ay	124	
89	Az	25	

## 2 Entry composition [i](#)

There are 96 unique types of molecules in this entry. The entry contains 239026 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B5	3764	Total	C	N	O	P	0	0
			80772	36003	14762	26243	3764		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a RNA chain called 5.8S rRNA.

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

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 5 is a protein called Ribosomal protein L3.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 8 is a protein called 60S ribosomal protein L6.

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

- Molecule 9 is a protein called Ribosomal Protein uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 10 is a protein called 60S ribosomal protein L7a.

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

There is a discrepancy between the modelled and reference sequences:



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

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called 60S ribosomal protein L10.

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

- Molecule 13 is a protein called 60S ribosomal protein L11.

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

- Molecule 14 is a protein called Nascent chain.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 17 is a protein called Ribosomal protein L15.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL13.

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

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

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

- Molecule 20 is a protein called eL18.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 21 is a protein called Ribosomal protein L19.

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

- Molecule 22 is a protein called Large ribosomal subunit protein eL20.

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

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

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

- Molecule 24 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BU	99	Total	C	N	O	S	0	0
			806	516	141	147	2		

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 25 is a protein called Ribosomal protein L23.

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 28 is a protein called Ribosomal protein L26.

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

- Molecule 29 is a protein called 60S ribosomal protein L27.

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

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

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

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

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

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

- Molecule 34 is a protein called Ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

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

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

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

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

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

- Molecule 39 is a protein called Ribosomal protein L37.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 41 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 42 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

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

- Molecule 43 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called [histone H4]-N-methyl-L-lysine20 N-methyltransferase KMT5B.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL10.

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

- Molecule 47 is a protein called 60S ribosomal protein L12.

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

- Molecule 48 is a protein called Ribosomal protein uL1.

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

- Molecule 49 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Nt	113	Total	C	N	O	S	0	0
			879	550	160	165	4		

- Molecule 50 is a protein called Isoform 2 of Transcription factor BTF3.

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

- Molecule 51 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	XA	837	Total	C	N	O	S	0	0
			6900	4391	1192	1276	41		

- Molecule 52 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	XB	168	Total	C	N	O	S	0	0
			1375	862	247	255	11		

- Molecule 53 is a protein called Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	MA	341	Total	C	N	O	S	1	0
			2804	1821	475	492	16		

- Molecule 54 is a RNA chain called 18S rRNA.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 55 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS28.

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

- Molecule 57 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

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

- Molecule 58 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

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

- Molecule 59 is a protein called eS26.



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

- Molecule 60 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 61 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 62 is a RNA chain called P site Phe tRNA.

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

- Molecule 63 is a protein called Small ribosomal subunit protein uS2.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 64 is a protein called 40S ribosomal protein S3a.

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

- Molecule 65 is a protein called 40S ribosomal protein S2.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 66 is a protein called 40S ribosomal protein S3.

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

- Molecule 67 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 69 is a protein called 40S ribosomal protein S6.

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

- Molecule 70 is a protein called 40S ribosomal protein S7.

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

- Molecule 71 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 73 is a protein called S10\_pectin domain-containing protein.

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

- Molecule 74 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 75 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 76 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 77 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 78 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 79 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 80 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 81 is a protein called Small ribosomal subunit protein uS13.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 82 is a protein called 40S ribosomal protein S19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
As	119	GLY	TRP	variant	UNP G1TN62
As	142	ASN	LYS	variant	UNP G1TN62

- Molecule 83 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	At	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 84 is a protein called Small ribosomal subunit protein eS21.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 85 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 86 is a protein called 40S ribosomal protein S23.

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

- Molecule 87 is a protein called 40S ribosomal protein S24.

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

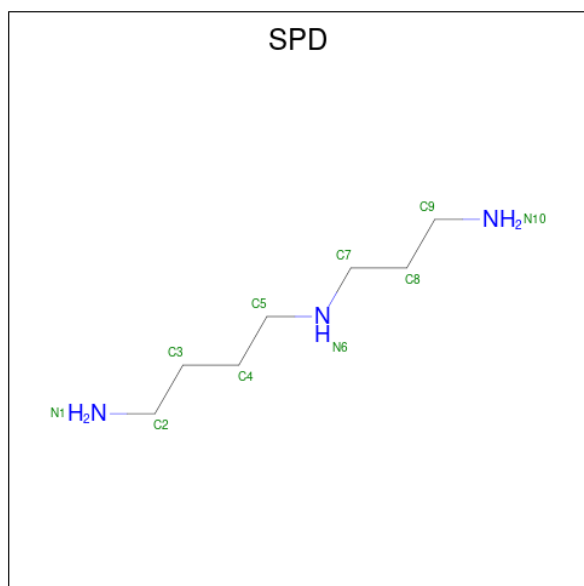
- Molecule 88 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 89 is a protein called Small ribosomal subunit protein eS32.

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

- Molecule 90 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ).



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

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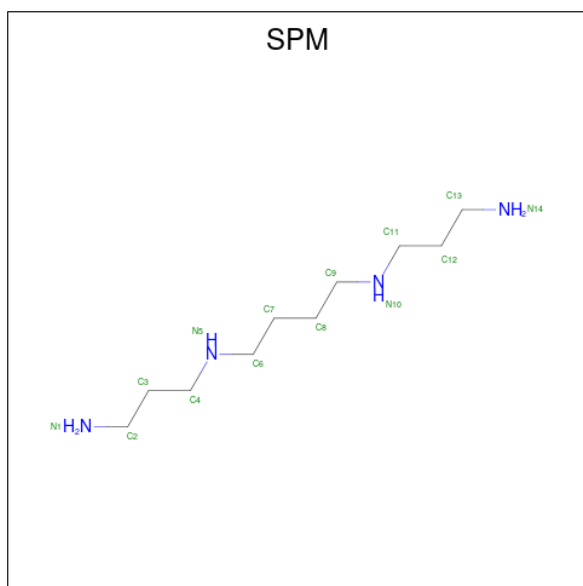
Mol	Chain	Residues	Atoms			AltConf
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	B5	1	Total 10	C 7	N 3	0
90	BS	1	Total 10	C 7	N 3	0
90	A2	1	Total 10	C 7	N 3	0
90	A2	1	Total 10	C 7	N 3	0
90	A2	1	Total 10	C 7	N 3	0



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

- Molecule 91 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



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

- Molecule 92 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
92	B5	278	Total	Mg	0
			278	278	

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Mol	Chain	Residues	Atoms		AltConf
92	B7	9	Total 9	Mg 9	0
92	B8	9	Total 9	Mg 9	0
92	BB	2	Total 2	Mg 2	0
92	BP	1	Total 1	Mg 1	0
92	BR	1	Total 1	Mg 1	0
92	BV	1	Total 1	Mg 1	0
92	Ba	1	Total 1	Mg 1	0
92	Bj	1	Total 1	Mg 1	0
92	A2	108	Total 108	Mg 108	0
92	Aw	1	Total 1	Mg 1	0

- Molecule 93 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
93	B5	117	Total 117	X 117	0
93	B7	3	Total 3	X 3	0
93	B8	5	Total 5	X 5	0
93	BA	1	Total 1	X 1	0
93	BI	1	Total 1	X 1	0
93	BN	1	Total 1	X 1	0
93	BQ	2	Total 2	X 2	0
93	BT	1	Total 1	X 1	0
93	BY	1	Total 1	X 1	0

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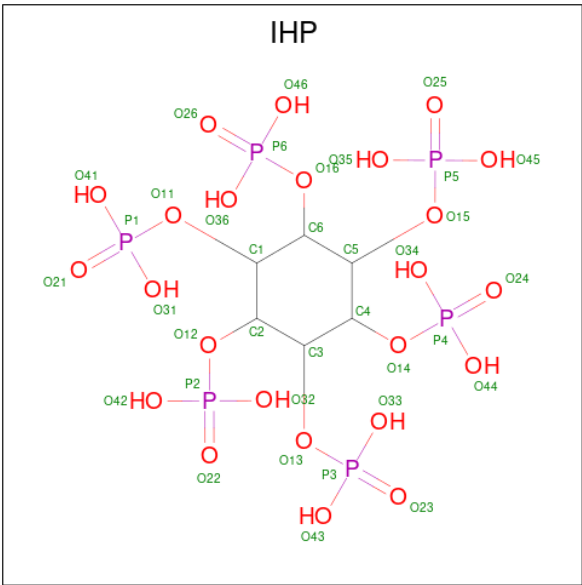
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Mol	Chain	Residues	Atoms		AltConf
93	Bb	2	Total 2	X 2	0
93	Be	1	Total 1	X 1	0
93	Bj	1	Total 1	X 1	0
93	Bo	1	Total 1	X 1	0
93	A2	29	Total 29	X 29	0
93	Ad	1	Total 1	X 1	0
93	Ar	1	Total 1	X 1	0

- Molecule 94 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 95 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
95	XA	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 96 is water.

Mol	Chain	Residues	Atoms		AltConf
96	B5	1379	Total	O	0
			1379	1379	
96	B7	45	Total	O	0
			45	45	
96	B8	50	Total	O	0
			50	50	
96	BA	7	Total	O	0
			7	7	
96	BB	6	Total	O	0
			6	6	
96	BC	2	Total	O	0
			2	2	
96	BF	1	Total	O	0
			1	1	
96	BI	2	Total	O	0
			2	2	
96	BL	2	Total	O	0
			2	2	
96	BN	4	Total	O	0
			4	4	
96	BO	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
96	BP	3	Total 3	O 3	0
96	BR	4	Total 4	O 4	0
96	BT	1	Total 1	O 1	0
96	BV	3	Total 3	O 3	0
96	BX	1	Total 1	O 1	0
96	Ba	5	Total 5	O 5	0
96	Bd	1	Total 1	O 1	0
96	Be	3	Total 3	O 3	0
96	Bg	2	Total 2	O 2	0
96	Bj	3	Total 3	O 3	0
96	Bl	1	Total 1	O 1	0
96	A2	529	Total 529	O 529	0
96	AE	1	Total 1	O 1	0
96	AT	1	Total 1	O 1	0
96	Aa	3	Total 3	O 3	0
96	Ad	1	Total 1	O 1	0
96	Af	2	Total 2	O 2	0
96	Ak	1	Total 1	O 1	0
96	Am	1	Total 1	O 1	0
96	Ap	2	Total 2	O 2	0
96	As	1	Total 1	O 1	0

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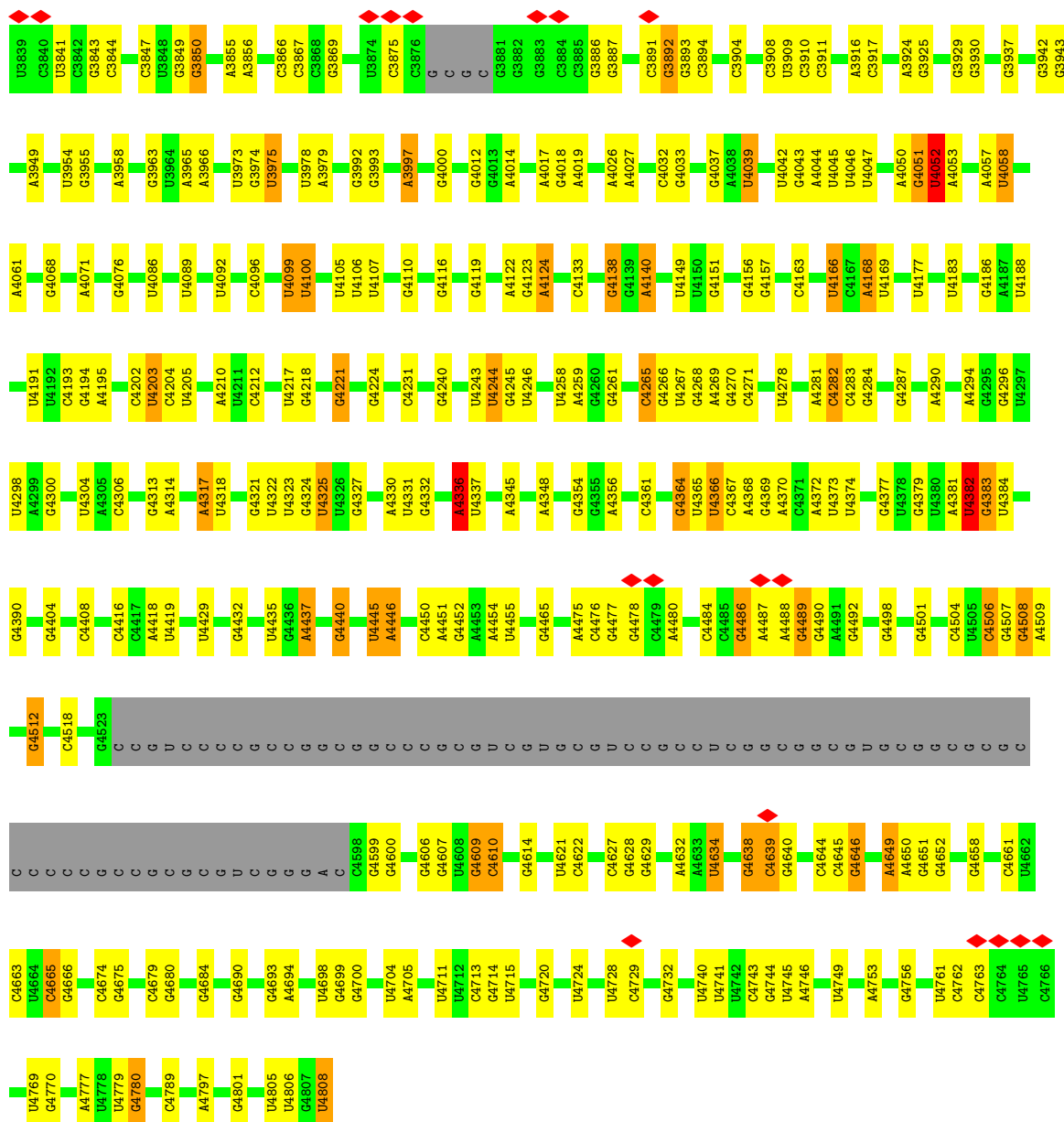
Mol	Chain	Residues	Atoms		AltConf
96	At	1	Total	O	0
			1	1	
96	Aw	5	Total	O	0
			5	5	





WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

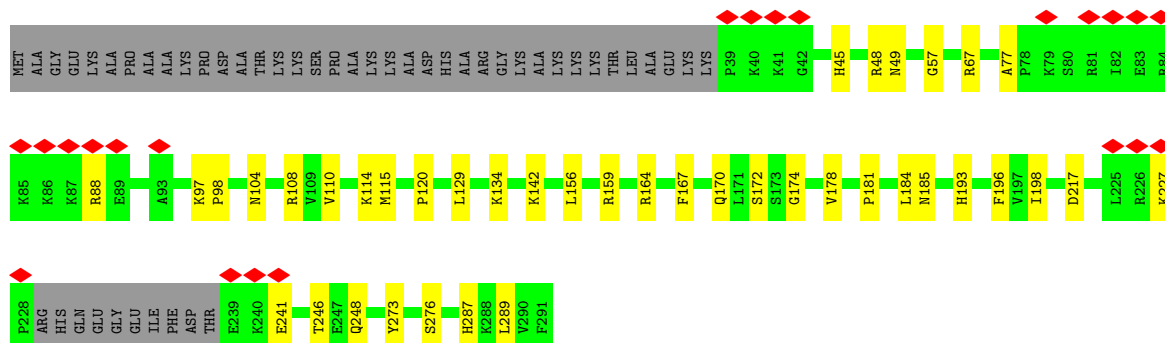
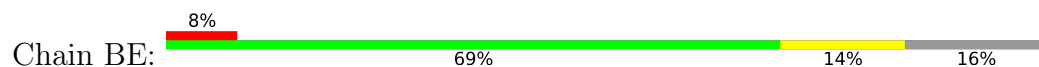




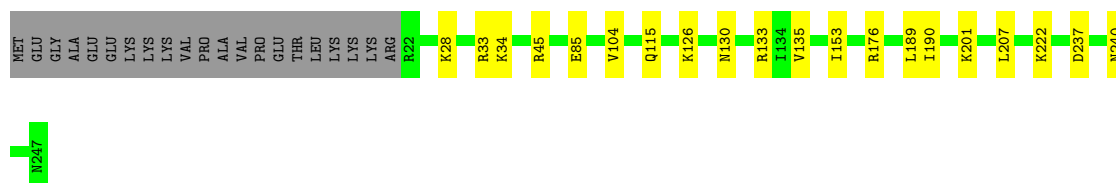
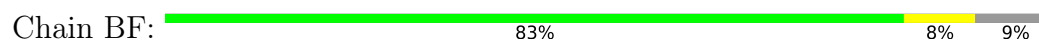




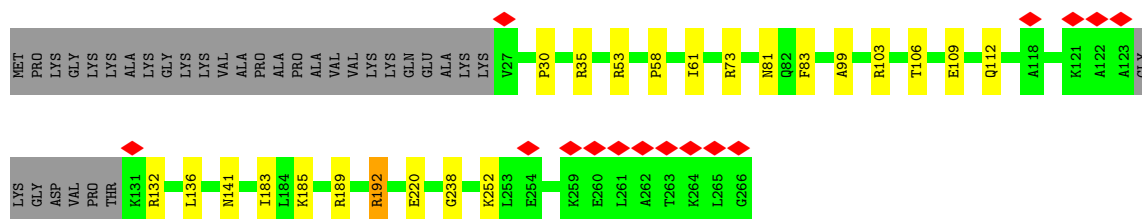
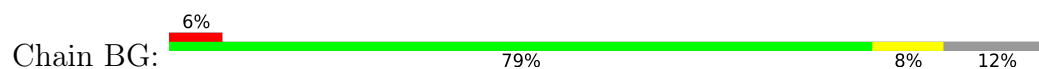
- Molecule 8: 60S ribosomal protein L6



- Molecule 9: Ribosomal Protein uL30



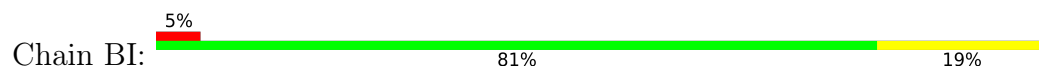
- Molecule 10: 60S ribosomal protein L7a



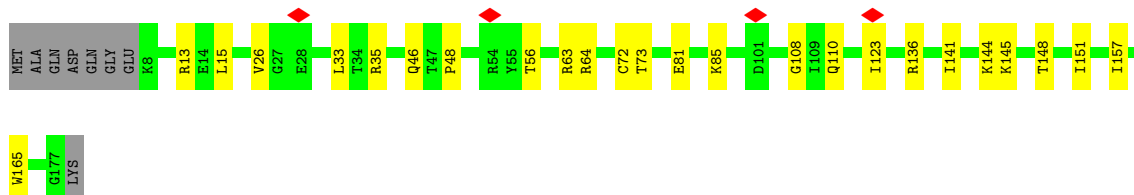
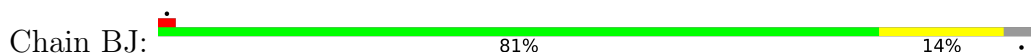
- Molecule 11: 60S ribosomal protein L9



- Molecule 12: 60S ribosomal protein L10



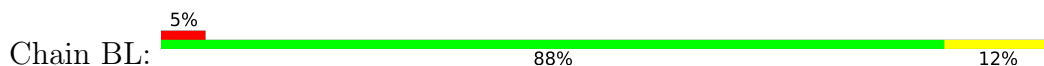
- Molecule 13: 60S ribosomal protein L11



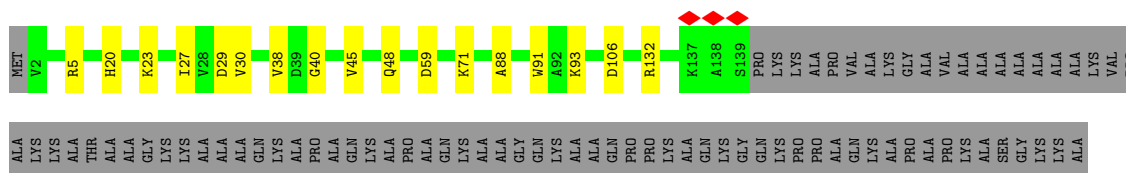
- Molecule 14: Nascent chain



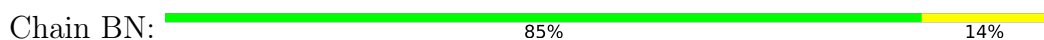
- Molecule 15: Large ribosomal subunit protein eL13




- Molecule 16: 60S ribosomal protein L14



- Molecule 17: Ribosomal protein L15




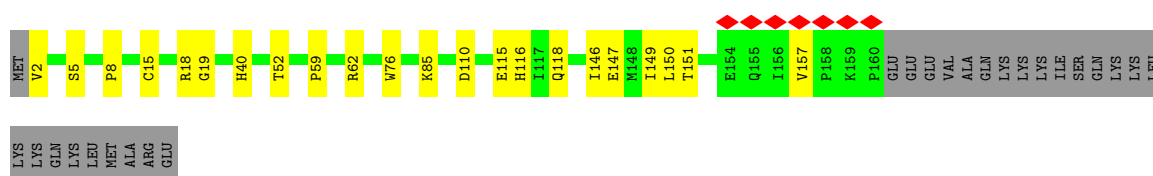
- Molecule 18: Large ribosomal subunit protein uL13

Chain BO:  87% 11%




- Molecule 19: Large ribosomal subunit protein uL22

Chain BP:  74% 12% 14%




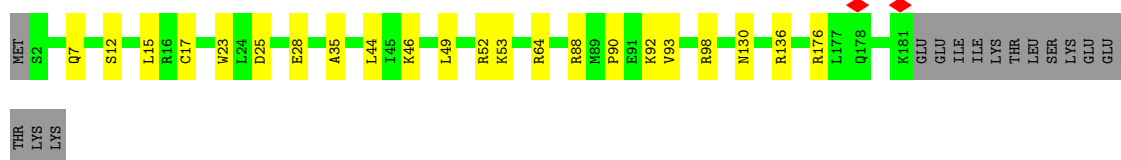
- Molecule 20: eL18

Chain BQ:  83% 16%




- Molecule 21: Ribosomal protein L19

Chain BR:  81% 11% 8%




- Molecule 22: Large ribosomal subunit protein eL20

Chain BS:  89% 11%

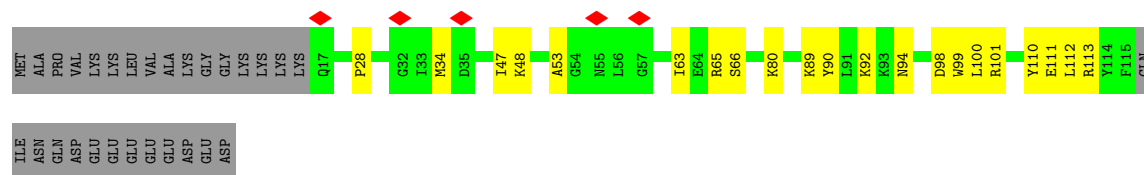


- Molecule 23: 60S ribosomal protein L21

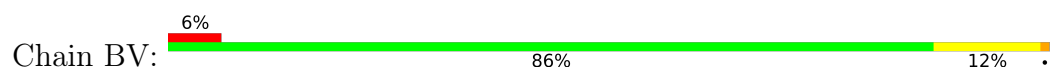
Chain BT:  85% 14%



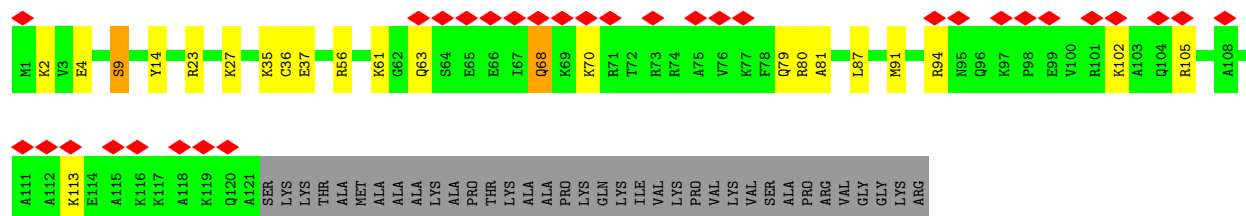
- Molecule 24: 60S ribosomal protein L22



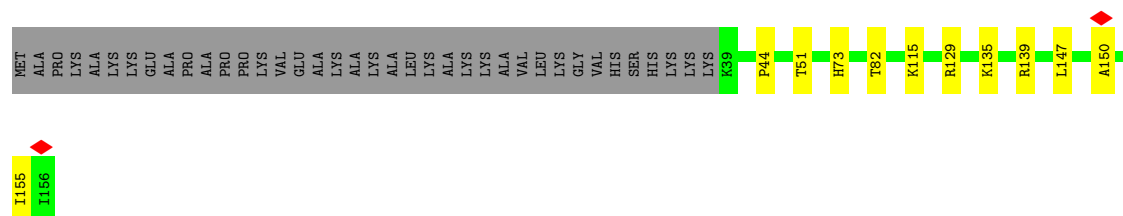
- Molecule 25: Ribosomal protein L23



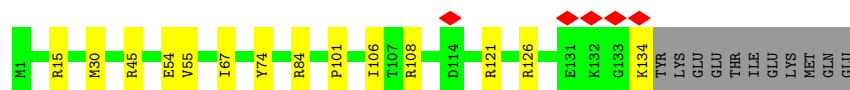
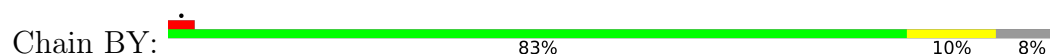
- Molecule 26: Ribosomal protein L24



- Molecule 27: Large ribosomal subunit protein uL23

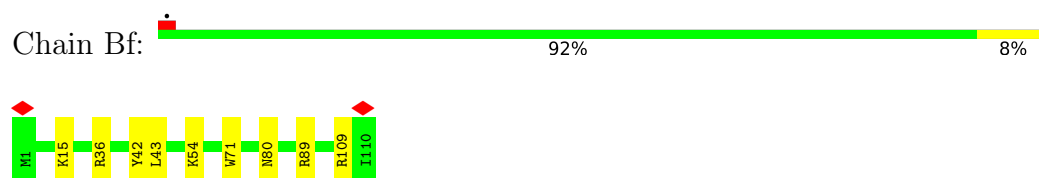


- Molecule 28: Ribosomal protein L26

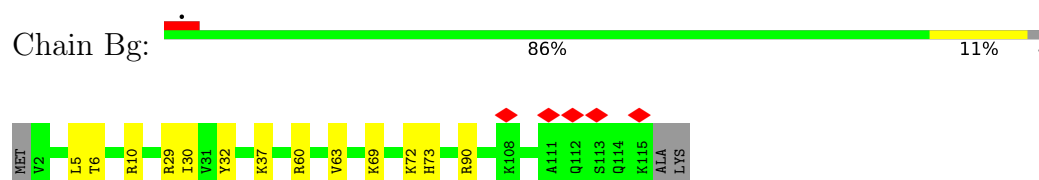


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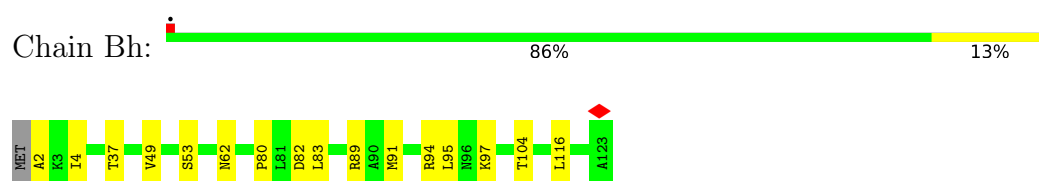
- Molecule 35: 60S ribosomal protein L35a



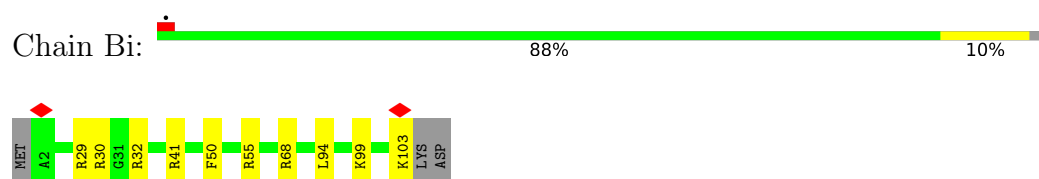
- Molecule 36: 60S ribosomal protein L34



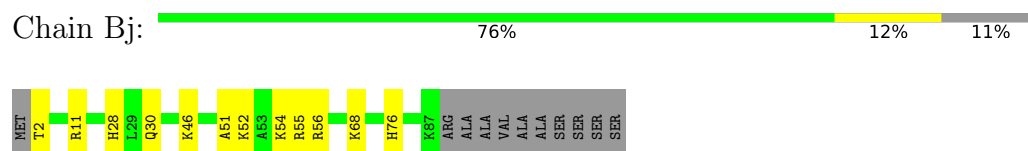
- Molecule 37: 60S ribosomal protein L35



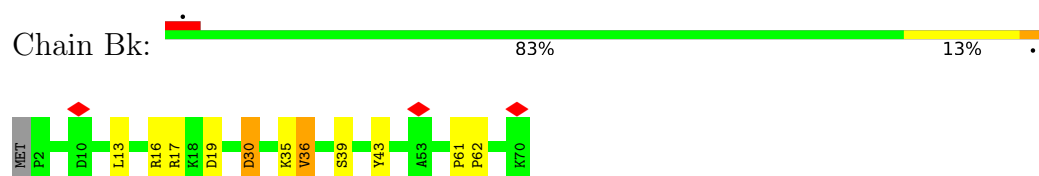
- Molecule 38: 60S ribosomal protein L36



- Molecule 39: Ribosomal protein L37



- Molecule 40: 60S ribosomal protein L38



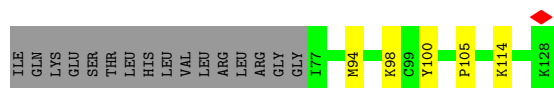
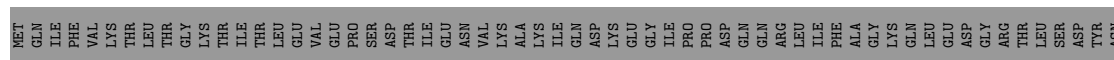
- Molecule 41: 60S ribosomal protein L39-like



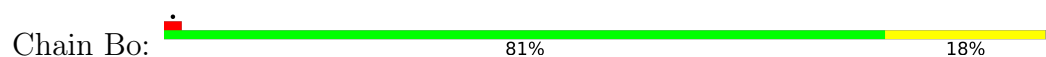




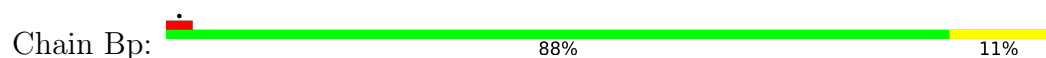
- Molecule 42: Ubiquitin-ribosomal protein eL40 fusion protein



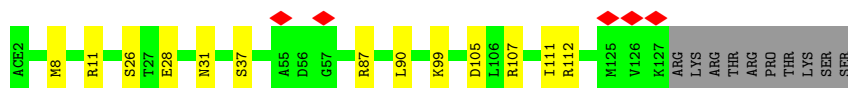
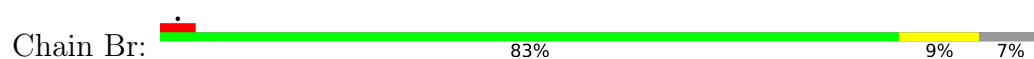
- Molecule 43: Large ribosomal subunit protein eL42



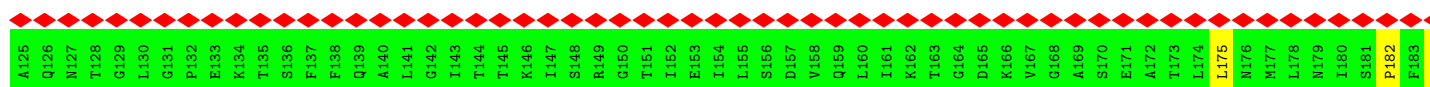
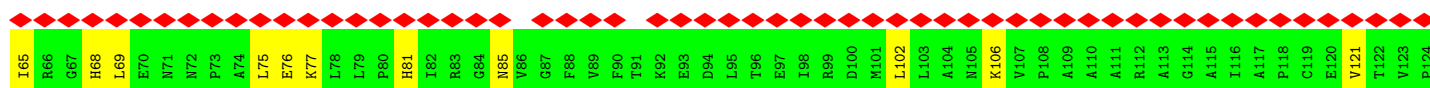
- Molecule 44: 60S ribosomal protein L37a

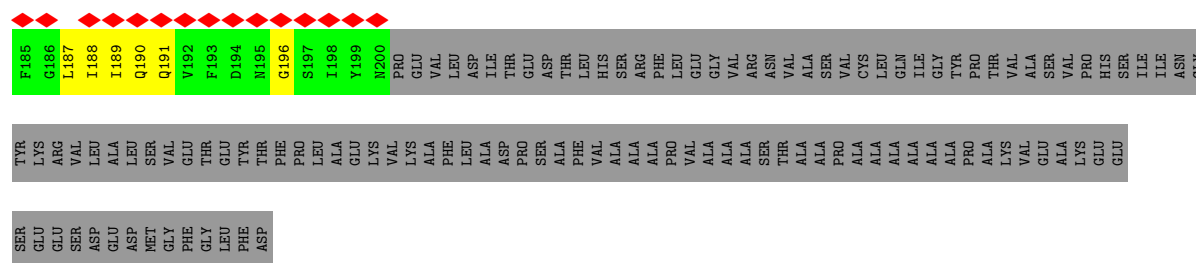


- Molecule 45: [histone H4]-N-methyl-L-lysine20 N-methyltransferase KMT5B

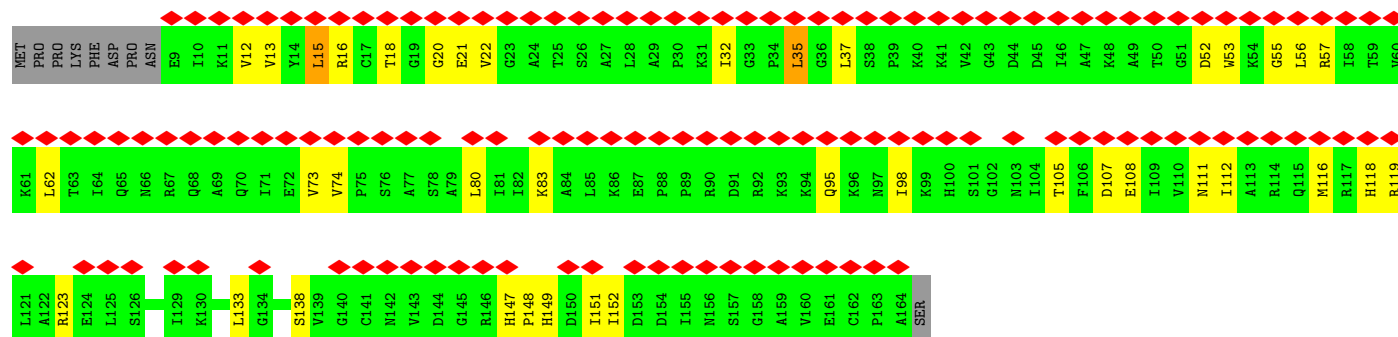
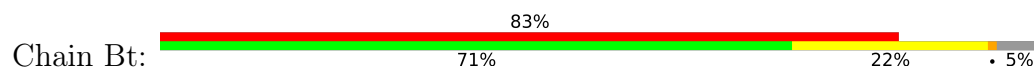


- Molecule 46: Large ribosomal subunit protein uL10

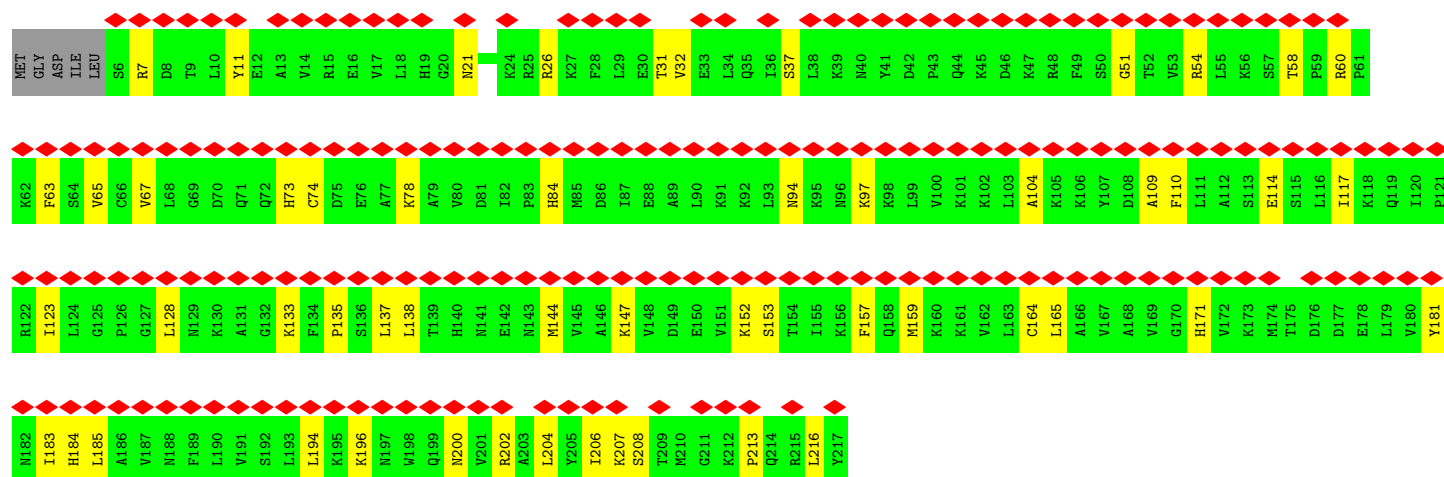
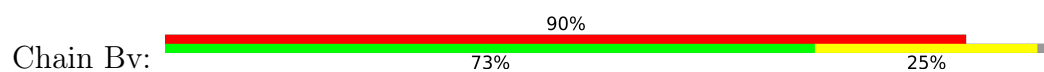




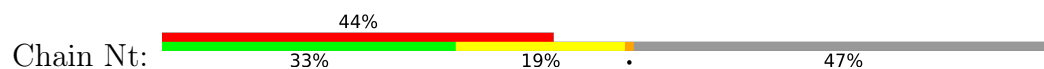
• Molecule 47: 60S ribosomal protein L12

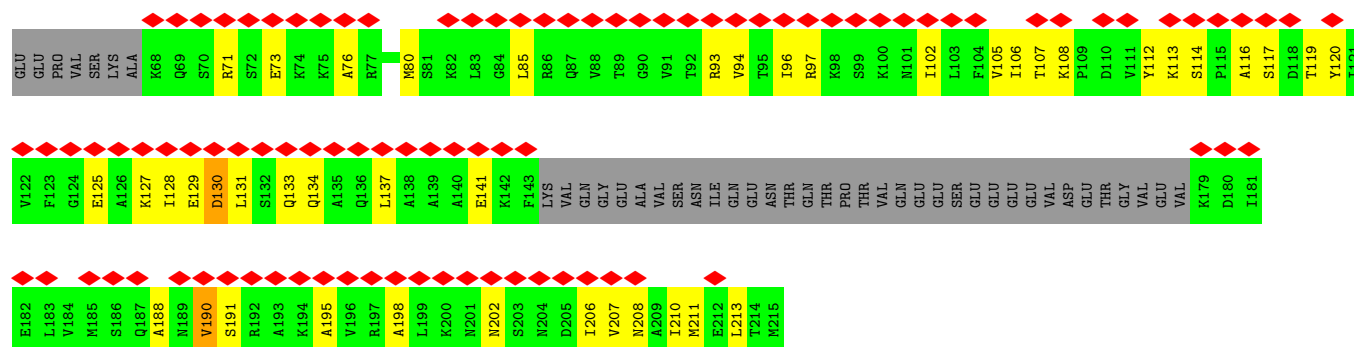


• Molecule 48: Ribosomal protein uL1

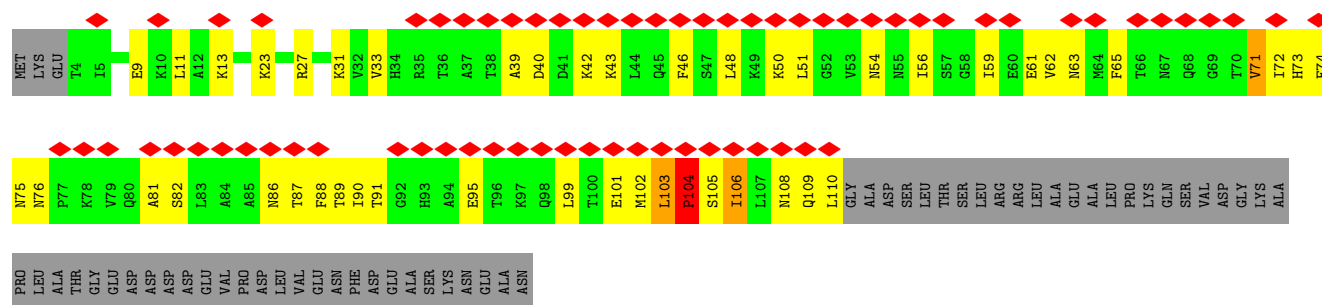
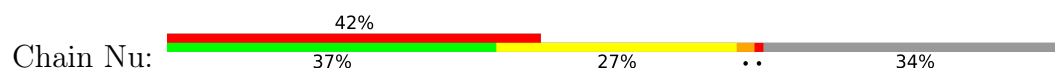


• Molecule 49: Nascent polypeptide-associated complex subunit alpha

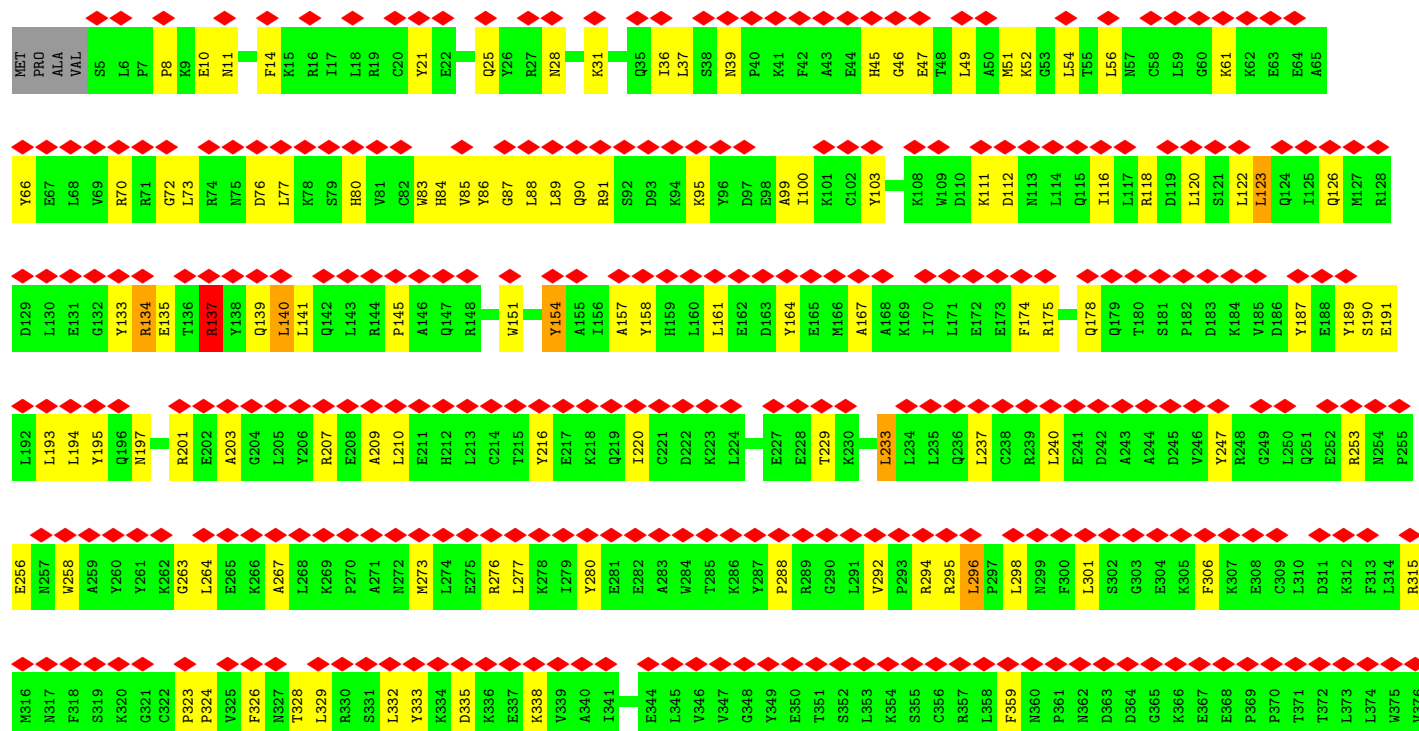
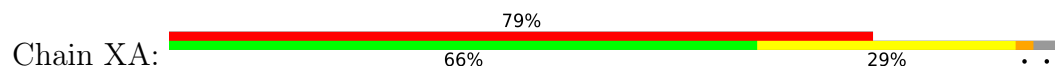




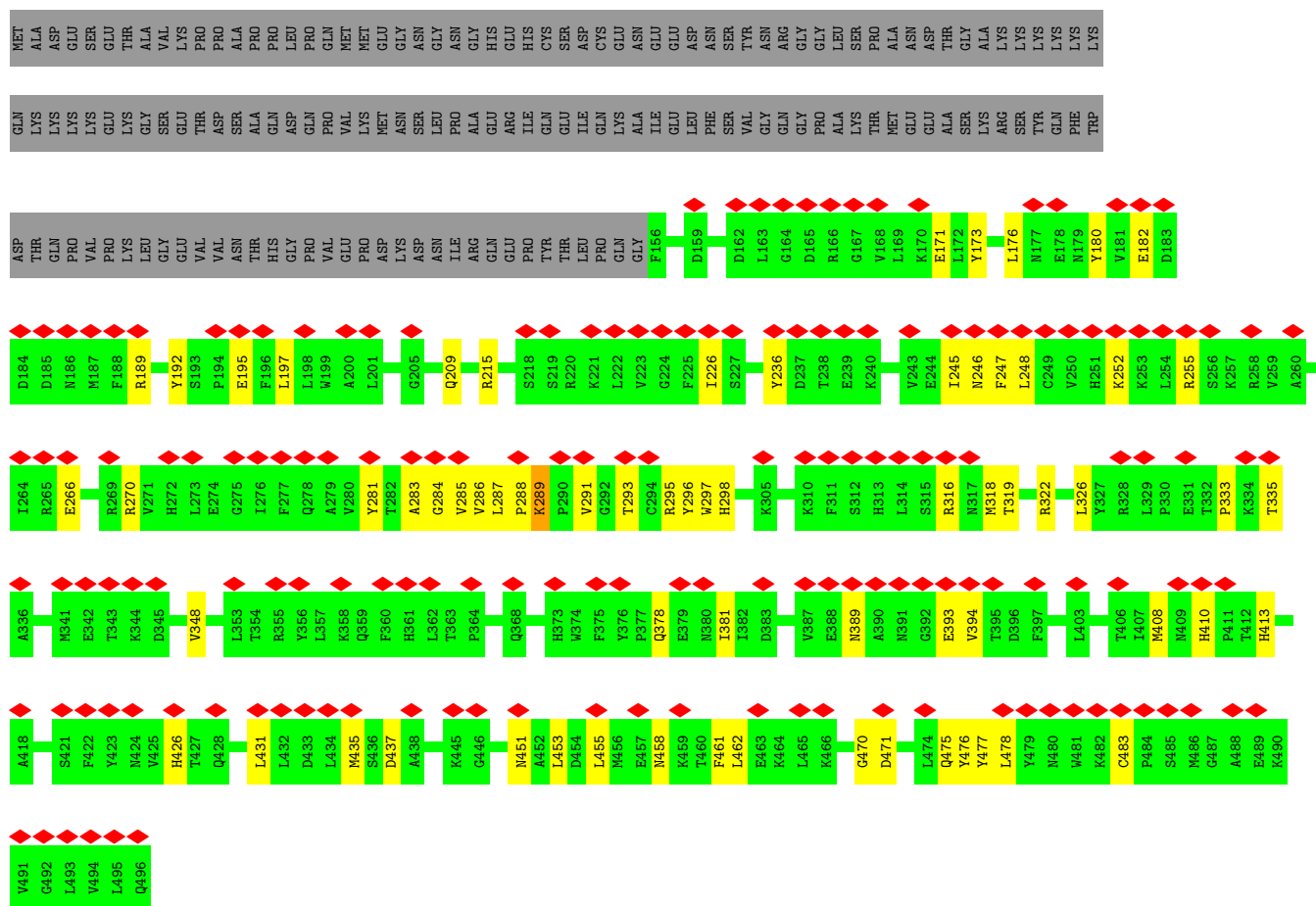
• Molecule 50: Isoform 2 of Transcription factor BTF3



• Molecule 51: N-alpha-acetyltransferase 15, NatA auxiliary subunit

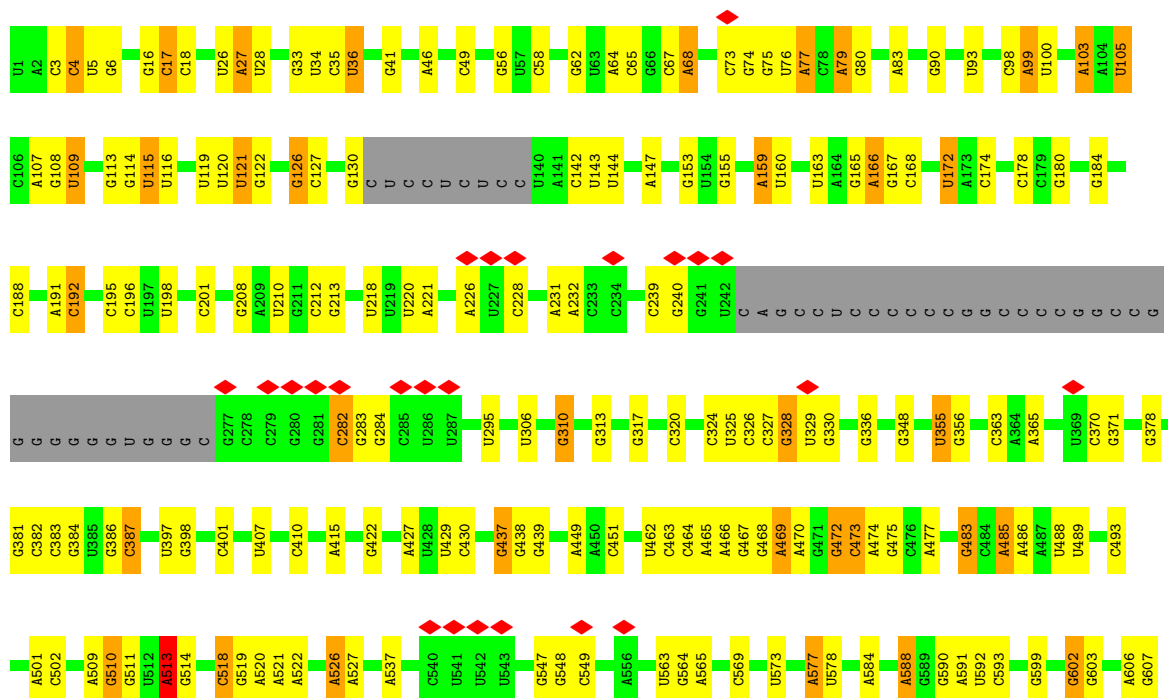


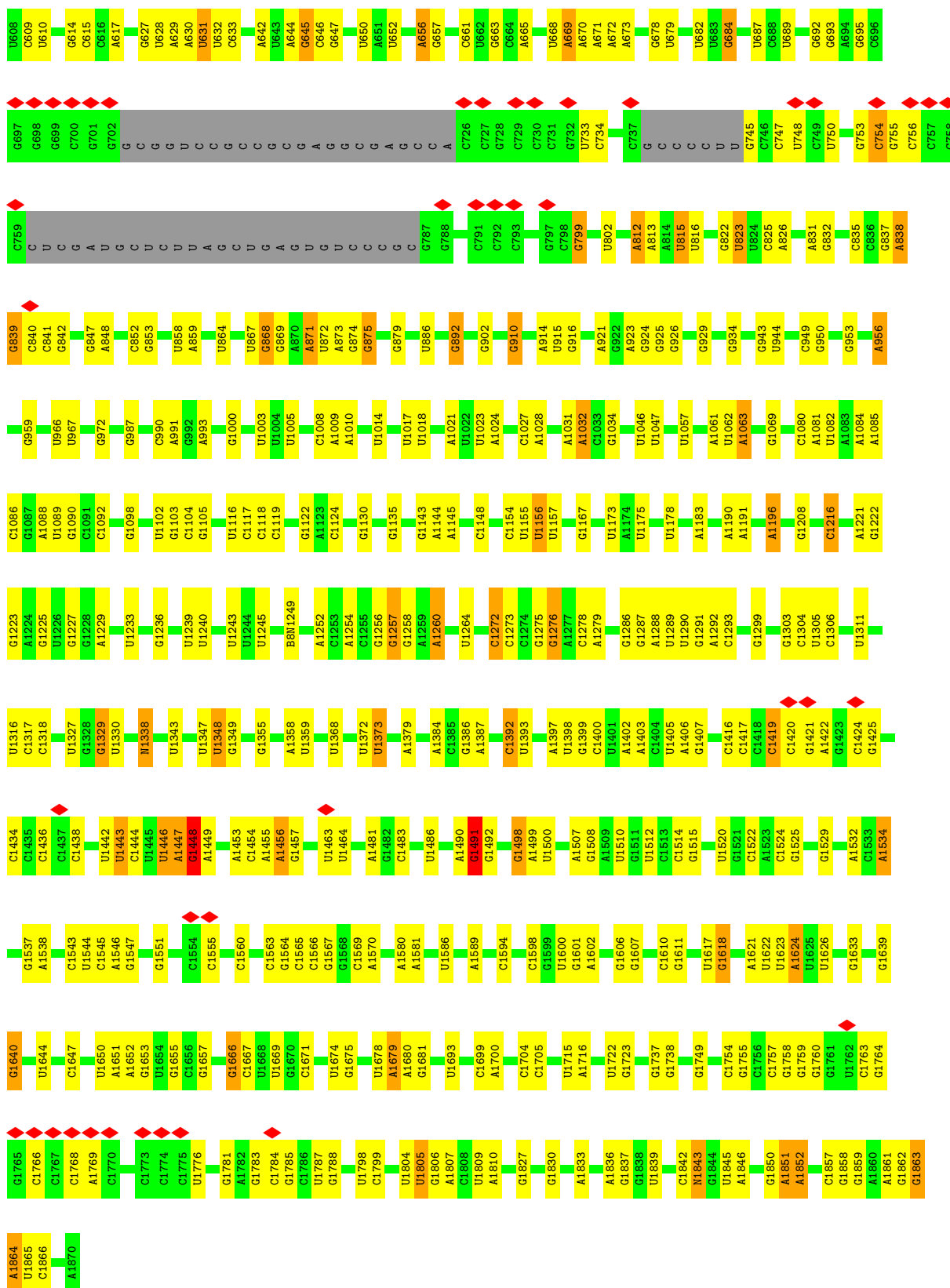




### • Molecule 54: 18S rRNA

Chain A2: 62% 28% 5% 5%



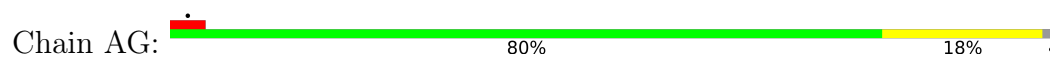


• Molecule 55: Small ribosomal subunit protein eS27

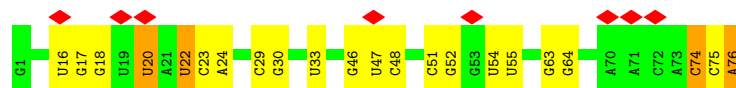
Chain AA: 86% 13%



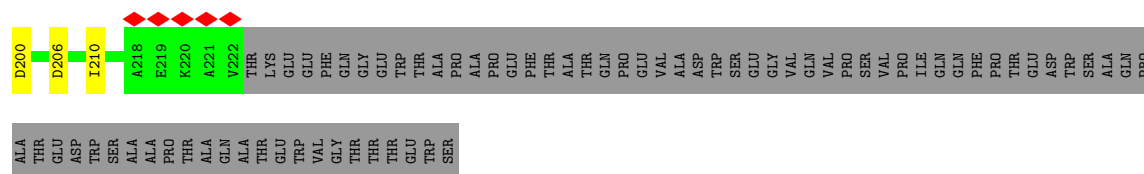
- Molecule 61: Small ribosomal subunit protein uS14



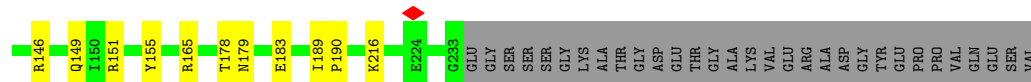
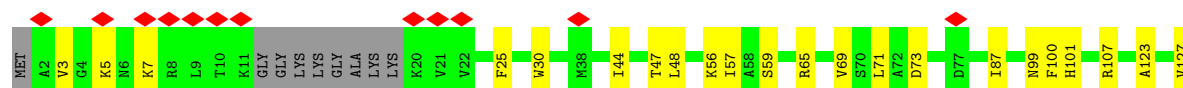
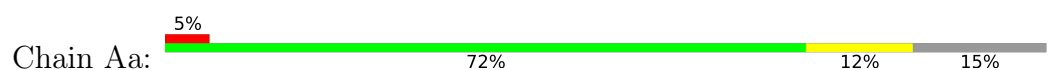
- Molecule 62: P site Phe tRNA



- Molecule 63: Small ribosomal subunit protein uS2



- Molecule 64: 40S ribosomal protein S3a

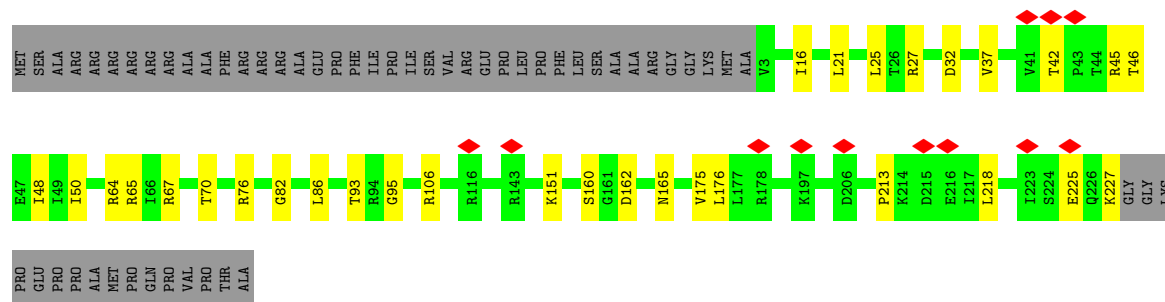


- Molecule 65: 40S ribosomal protein S2

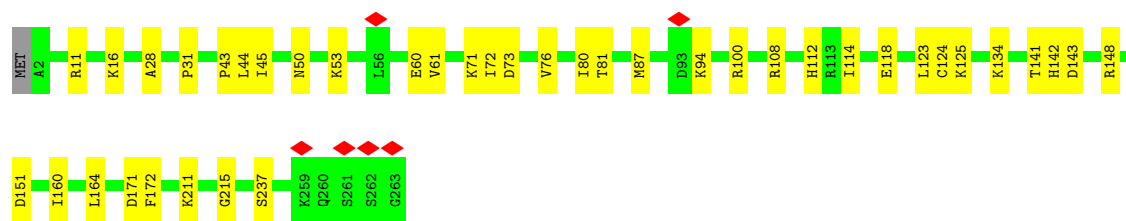
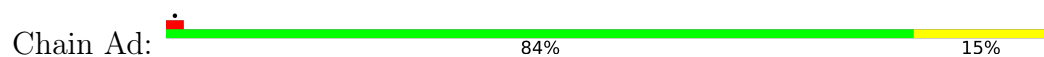




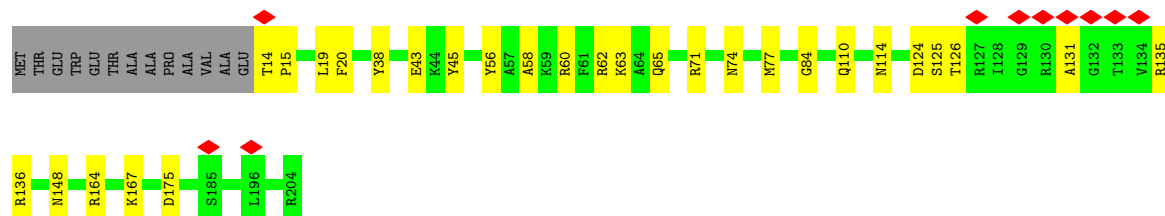
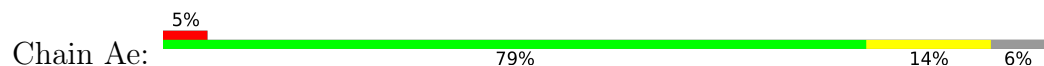
- Molecule 66: 40S ribosomal protein S3



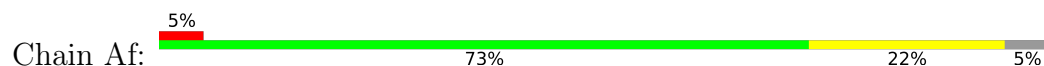
- Molecule 67: 40S ribosomal protein S4

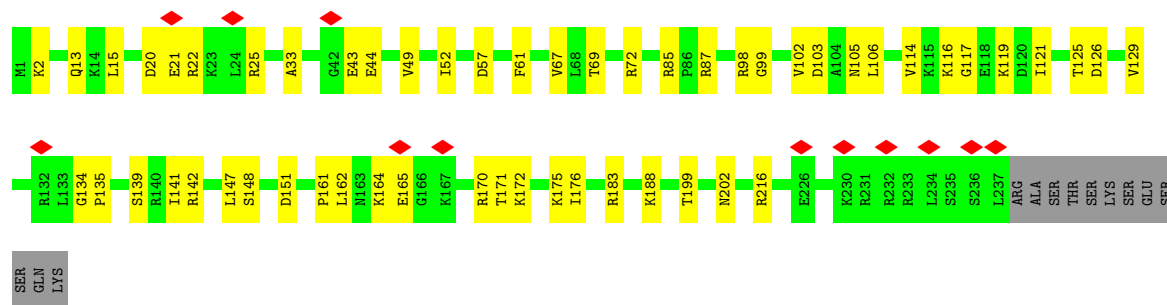


- Molecule 68: Small ribosomal subunit protein uS7

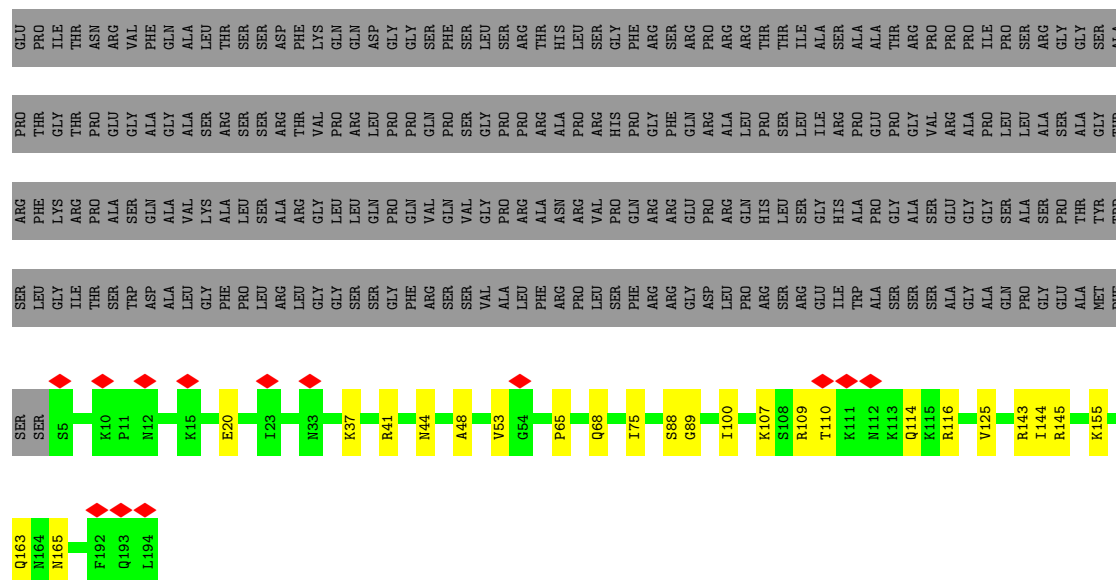
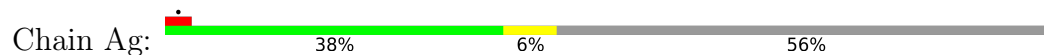


- Molecule 69: 40S ribosomal protein S6

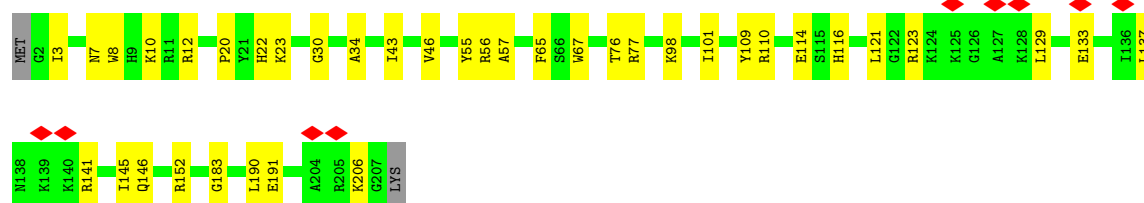
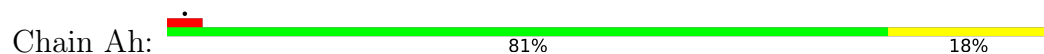




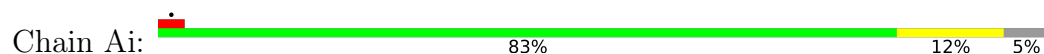
- Molecule 70: 40S ribosomal protein S7



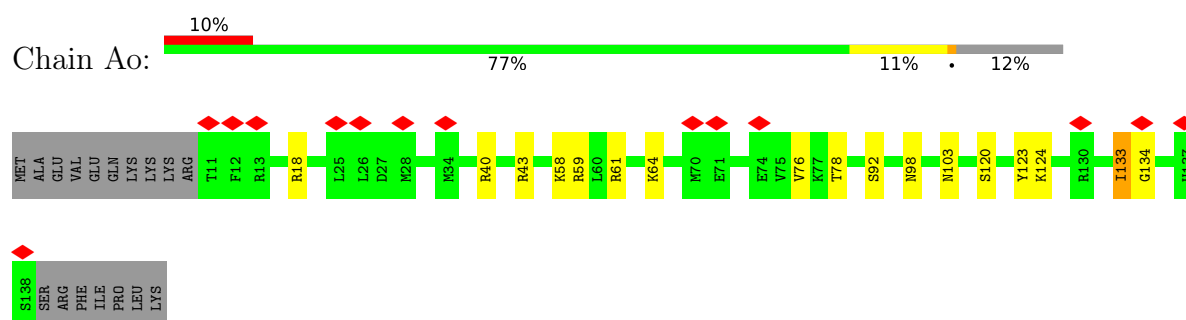
- Molecule 71: 40S ribosomal protein S8



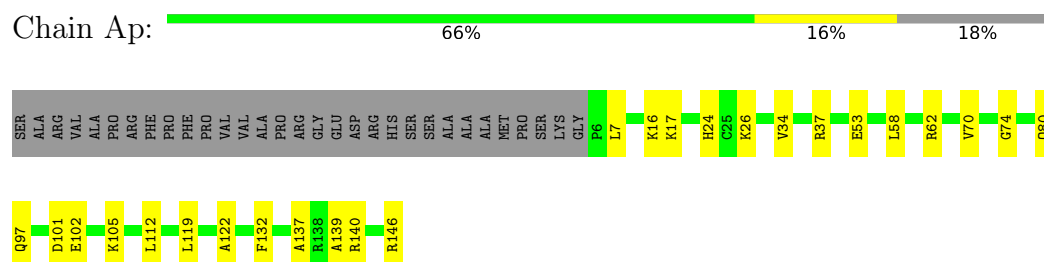
- Molecule 72: Small ribosomal subunit protein uS4



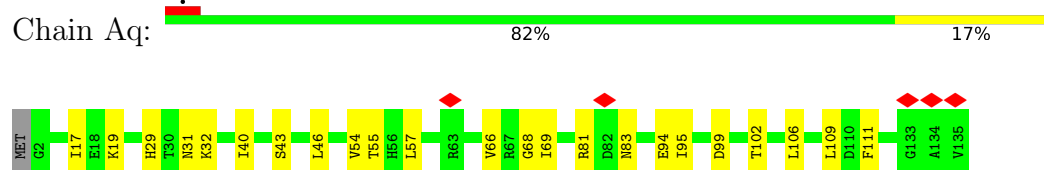




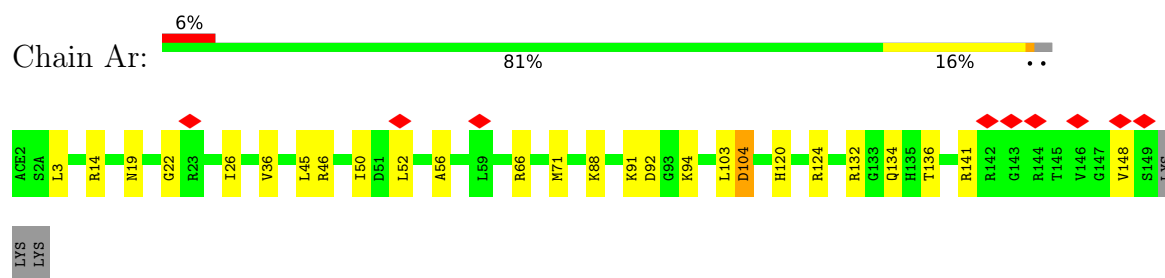
- Molecule 79: Small ribosomal subunit protein uS9



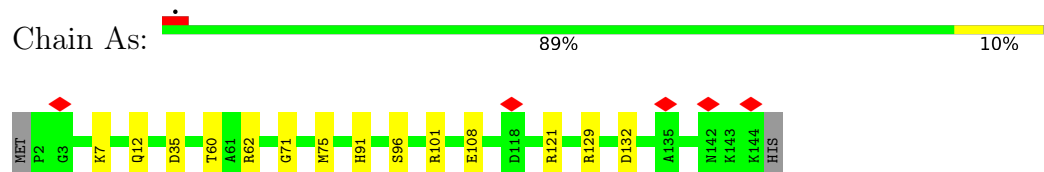
- Molecule 80: Small ribosomal subunit protein eS17



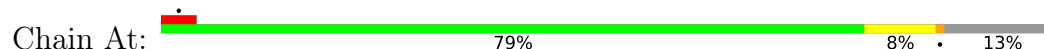
- Molecule 81: Small ribosomal subunit protein uS13

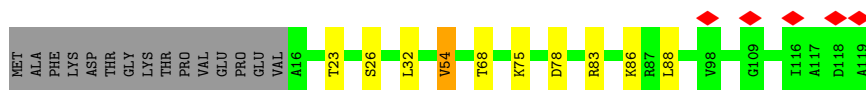


- Molecule 82: 40S ribosomal protein S19

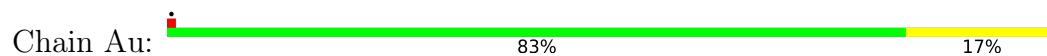


- Molecule 83: Small ribosomal subunit protein uS10





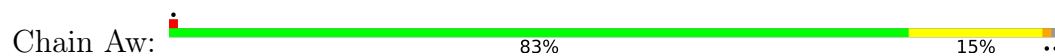
- Molecule 84: Small ribosomal subunit protein eS21



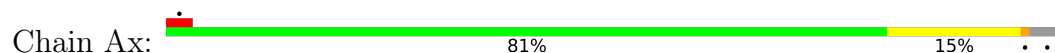
- Molecule 85: Small ribosomal subunit protein uS8



- Molecule 86: 40S ribosomal protein S23



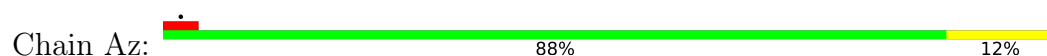
- Molecule 87: 40S ribosomal protein S24



- Molecule 88: Small ribosomal subunit protein eS25



- Molecule 89: Small ribosomal subunit protein eS32





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15709	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	0.826	Depositor
Minimum map value	-0.395	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.039	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 ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B5	0.13	1/87403 (0.0%)	0.15	0/136359
2	B7	0.13	0/2861	0.17	0/4459
3	B8	0.14	0/3635	0.17	0/5661
4	BA	0.10	0/1965	0.25	0/2633
5	BB	0.22	0/3261	0.35	1/4364 (0.0%)
6	BC	0.09	0/2938	0.21	0/3948
7	BD	0.08	0/2437	0.21	0/3264
8	BE	0.09	0/1998	0.22	0/2673
9	BF	0.09	0/1922	0.23	0/2563
10	BG	0.08	0/1908	0.22	0/2566
11	BH	0.08	0/1535	0.23	0/2063
12	BI	0.08	0/1756	0.21	0/2346
13	BJ	0.08	0/1385	0.23	0/1852
15	BL	0.09	0/1733	0.22	0/2316
16	BM	0.10	0/1158	0.22	0/1547
17	BN	0.09	0/1746	0.22	0/2338
18	BO	0.08	0/1662	0.21	0/2222
19	BP	0.08	0/1317	0.21	0/1768
20	BQ	0.09	0/1539	0.21	0/2054
21	BR	0.07	0/1524	0.18	0/2013
22	BS	0.09	0/1497	0.22	0/2008
23	BT	0.09	0/1326	0.22	0/1770
24	BU	0.08	0/820	0.23	0/1100
25	BV	0.36	0/1048	0.44	0/1402
26	BW	0.07	0/1006	0.19	0/1334
27	BX	0.08	0/984	0.22	0/1323
28	BY	0.09	0/1132	0.21	0/1504
29	BZ	0.09	0/1130	0.23	0/1507
30	Ba	0.24	0/1179	0.30	0/1572
31	Bb	0.08	0/884	0.20	0/1169
32	Bc	0.08	0/847	0.18	0/1134



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Bd	0.10	0/903	0.21	0/1216
34	Be	0.08	0/1088	0.23	0/1451
35	Bf	0.09	0/903	0.22	0/1208
36	Bg	0.08	0/916	0.23	0/1220
37	Bh	0.07	0/1021	0.19	0/1348
38	Bi	0.07	0/841	0.20	0/1112
39	Bj	0.09	0/720	0.24	0/952
40	Bk	0.09	0/575	0.19	0/761
41	Bl	0.08	0/459	0.18	0/608
42	Bm	0.08	0/426	0.28	0/564
43	Bo	0.08	0/866	0.22	0/1141
44	Bp	0.09	0/718	0.23	0/953
45	Br	0.10	0/1027	0.24	0/1376
46	Bs	0.07	0/1530	0.20	0/2064
47	Bt	0.08	0/1193	0.22	0/1609
48	Bv	0.09	0/1735	0.28	0/2328
49	Nt	0.53	1/884 (0.1%)	0.65	0/1181
50	Nu	0.61	0/836	0.77	1/1122 (0.1%)
51	XA	0.40	0/7038	0.54	1/9468 (0.0%)
52	XB	0.08	0/1404	0.23	0/1890
53	MA	0.21	0/2884	0.31	0/3912
54	A2	0.17	1/40342 (0.0%)	0.18	0/62877
55	AA	0.08	0/665	0.22	0/891
56	AB	0.07	0/497	0.19	0/666
57	AC	0.07	0/622	0.21	0/822
58	AD	0.07	0/462	0.20	0/607
59	AE	0.09	0/828	0.22	0/1109
60	AF	0.09	0/2493	0.22	0/3394
61	AG	0.07	0/470	0.26	0/623
62	AT	0.17	0/1766	0.23	0/2749
63	AZ	0.09	0/1778	0.22	0/2416
64	Aa	0.08	0/1841	0.23	0/2459
65	Ab	0.09	0/1742	0.23	0/2354
66	Ac	0.08	0/1779	0.21	0/2395
67	Ad	0.08	0/2118	0.22	0/2849
68	Ae	0.08	0/1531	0.23	0/2059
69	Af	0.07	0/1946	0.20	0/2590
70	Ag	0.08	0/1552	0.21	0/2079
71	Ah	0.08	0/1715	0.21	0/2287
72	Ai	0.08	0/1550	0.20	0/2069
73	Aj	0.27	0/834	0.37	0/1125
74	Ak	0.09	0/1284	0.22	0/1717
75	Al	0.07	0/968	0.22	0/1296

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	Am	0.10	0/1232	0.21	0/1656
77	An	0.08	0/912	0.21	0/1230
78	Ao	0.07	0/1069	0.20	0/1429
79	Ap	0.09	0/1142	0.23	0/1528
80	Aq	0.23	0/1094	0.32	0/1469
81	Ar	0.08	0/1233	0.23	0/1653
82	As	0.08	0/1119	0.20	0/1498
83	At	0.10	0/831	0.20	0/1115
84	Au	0.09	0/645	0.21	0/864
85	Av	0.09	0/1051	0.20	0/1406
86	Aw	0.08	0/1107	0.21	0/1475
87	Ax	0.08	0/1032	0.21	0/1371
88	Ay	0.08	0/691	0.20	0/922
89	Az	0.06	0/240	0.15	0/305
All	All	0.15	3/247684 (0.0%)	0.22	3/361670 (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
5	BB	0	2
25	BV	0	1
51	XA	0	4
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	Nt	130	ASP	N-CA	6.22	1.50	1.46
54	A2	577	A2M	O3'-P	5.01	1.61	1.56
1	B5	1270	A2M	O3'-P	5.00	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	XA	589	ASP	N-CA-C	-7.46	103.13	111.71
5	BB	255	GLY	CA-C-O	-5.20	118.12	122.33
50	Nu	104	PRO	CB-CA-C	5.09	119.96	111.56

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	BB	100	ARG	Sidechain
5	BB	97	ARG	Sidechain
25	BV	90	ARG	Sidechain
51	XA	134	ARG	Sidechain
51	XA	91	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	B5	80772	0	40886	622	0
2	B7	2561	0	1295	22	0
3	B8	3319	0	1684	19	0
4	BA	1940	0	2029	31	0
5	BB	3206	0	3353	48	0
6	BC	2886	0	3057	31	0
7	BD	2391	0	2424	32	0
8	BE	1960	0	2153	27	0
9	BF	1886	0	2008	15	0
10	BG	1877	0	2023	15	0
11	BH	1516	0	1597	15	0
12	BI	1717	0	1764	33	0
13	BJ	1362	0	1399	15	0
14	BK	60	0	14	3	0
15	BL	1702	0	1820	18	0
16	BM	1137	0	1211	12	0
17	BN	1701	0	1749	22	0
18	BO	1630	0	1778	15	0
19	BP	1289	0	1329	13	0
20	BQ	1515	0	1634	25	0
21	BR	1508	0	1664	16	0
22	BS	1457	0	1492	15	0
23	BT	1298	0	1366	22	0
24	BU	806	0	827	17	0
25	BV	1034	0	1097	17	0
26	BW	991	0	1048	16	0
27	BX	967	0	1040	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	BY	1115	0	1205	10	0
29	BZ	1107	0	1182	12	0
30	Ba	1163	0	1202	16	0
31	Bb	881	0	957	9	0
32	Bc	836	0	888	9	0
33	Bd	888	0	930	10	0
34	Be	1070	0	1165	8	0
35	Bf	884	0	924	7	0
36	Bg	906	0	998	15	0
37	Bh	1013	0	1147	15	0
38	Bi	830	0	916	6	0
39	Bj	705	0	737	11	0
40	Bk	569	0	637	7	0
41	Bl	447	0	480	9	0
42	Bm	432	0	470	4	0
43	Bo	863	0	929	13	0
44	Bp	708	0	756	6	0
45	Br	1014	0	1083	12	0
46	Bs	1507	0	1564	30	0
47	Bt	1178	0	1235	26	0
48	Bv	1707	0	1815	39	0
49	Nt	879	0	938	45	0
50	Nu	828	0	874	46	0
51	XA	6900	0	6944	234	0
52	XB	1375	0	1348	56	0
53	MA	2804	0	2822	54	0
54	A2	37833	0	19167	302	0
55	AA	651	0	672	7	0
56	AB	495	0	523	6	0
57	AC	610	0	634	16	0
58	AD	457	0	502	9	0
59	AE	814	0	863	10	0
60	AF	2436	0	2393	41	0
61	AG	459	0	448	10	0
62	AT	1621	0	823	19	0
63	AZ	1743	0	1748	23	0
64	Aa	1815	0	1908	26	0
65	Ab	1706	0	1796	19	0
66	Ac	1751	0	1846	24	0
67	Ad	2076	0	2177	25	0
68	Ae	1509	0	1563	19	0
69	Af	1923	0	2089	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	Ag	1529	0	1627	16	0
71	Ah	1686	0	1772	27	0
72	Ai	1525	0	1640	17	0
73	Aj	810	0	836	11	0
74	Ak	1262	0	1335	9	0
75	Al	958	0	993	12	0
76	Am	1208	0	1294	12	0
77	An	899	0	912	18	0
78	Ao	1048	0	1093	13	0
79	Ap	1124	0	1193	21	0
80	Aq	1080	0	1135	16	0
81	Ar	1217	0	1279	18	0
82	As	1113	0	1145	15	0
83	At	821	0	883	9	0
84	Au	640	0	633	10	0
85	Av	1034	0	1080	16	0
86	Aw	1099	0	1162	16	0
87	Ax	1015	0	1086	15	0
88	Ay	683	0	761	11	0
89	Az	239	0	289	3	0
90	A2	80	0	152	8	0
90	B5	210	0	399	15	0
90	BS	10	0	19	1	0
91	A2	14	0	26	2	0
91	B5	28	0	52	2	0
92	A2	108	0	0	0	0
92	Aw	1	0	0	0	0
92	B5	278	0	0	0	0
92	B7	9	0	0	0	0
92	B8	9	0	0	0	0
92	BB	2	0	0	0	0
92	BP	1	0	0	0	0
92	BR	1	0	0	0	0
92	BV	1	0	0	0	0
92	Ba	1	0	0	0	0
92	Bj	1	0	0	0	0
93	A2	29	0	0	0	0
93	Ad	1	0	0	0	0
93	Ar	1	0	0	0	0
93	B5	117	0	0	0	0
93	B7	3	0	0	0	0
93	B8	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	BA	1	0	0	0	0
93	BI	1	0	0	0	0
93	BN	1	0	0	0	0
93	BQ	2	0	0	0	0
93	BT	1	0	0	0	0
93	BY	1	0	0	0	0
93	Bb	2	0	0	0	0
93	Be	1	0	0	0	0
93	Bj	1	0	0	0	0
93	Bo	1	0	0	0	0
94	AC	1	0	0	0	0
94	AE	1	0	0	0	0
94	AG	1	0	0	0	0
94	Bg	1	0	0	0	0
94	Bj	1	0	0	0	0
94	Bm	1	0	0	0	0
94	Bo	1	0	0	0	0
94	Bp	1	0	0	0	0
95	XA	36	0	6	1	0
96	A2	529	0	0	3	0
96	AE	1	0	0	0	0
96	AT	1	0	0	0	0
96	Aa	3	0	0	0	0
96	Ad	1	0	0	0	0
96	Af	2	0	0	0	0
96	Ak	1	0	0	0	0
96	Am	1	0	0	0	0
96	Ap	2	0	0	0	0
96	As	1	0	0	0	0
96	At	1	0	0	1	0
96	Aw	5	0	0	2	0
96	B5	1379	0	0	12	0
96	B7	45	0	0	0	0
96	B8	50	0	0	0	0
96	BA	7	0	0	0	0
96	BB	6	0	0	0	0
96	BC	2	0	0	0	0
96	BF	1	0	0	0	0
96	BI	2	0	0	0	0
96	BL	2	0	0	0	0
96	BN	4	0	0	0	0
96	BO	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
96	BP	3	0	0	0	0
96	BR	4	0	0	0	0
96	BT	1	0	0	0	0
96	BV	3	0	0	0	0
96	BX	1	0	0	0	0
96	Ba	5	0	0	0	0
96	Bd	1	0	0	0	0
96	Be	3	0	0	0	0
96	Bg	2	0	0	0	0
96	Bj	3	0	0	0	0
96	Bl	1	0	0	0	0
All	All	239026	0	179841	2217	0

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

The worst 5 of 2217 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)
51:XA:73:LEU:O	51:XA:77:LEU:HD12	1.26	1.30
54:A2:1338:4AC:O2'	83:At:68:THR:HG22	1.29	1.27
51:XA:73:LEU:O	51:XA:77:LEU:CD1	1.90	1.19
51:XA:89:LEU:HD12	51:XA:90:GLN:N	1.63	1.12
65:Ab:114:LYS:HD3	65:Ab:121:ARG:HH21	1.12	1.11

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	BA	250/257 (97%)	242 (97%)	8 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BB	395/403 (98%)	387 (98%)	8 (2%)	0	100	100
6	BC	361/413 (87%)	358 (99%)	3 (1%)	0	100	100
7	BD	291/297 (98%)	285 (98%)	6 (2%)	0	100	100
8	BE	239/291 (82%)	236 (99%)	3 (1%)	0	100	100
9	BF	224/247 (91%)	217 (97%)	7 (3%)	0	100	100
10	BG	229/266 (86%)	226 (99%)	3 (1%)	0	100	100
11	BH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
12	BI	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
13	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
15	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
16	BM	136/218 (62%)	135 (99%)	1 (1%)	0	100	100
17	BN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
18	BO	197/203 (97%)	197 (100%)	0	0	100	100
19	BP	157/184 (85%)	156 (99%)	1 (1%)	0	100	100
20	BQ	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
21	BR	178/196 (91%)	178 (100%)	0	0	100	100
22	BS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
23	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
24	BU	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
25	BV	137/140 (98%)	134 (98%)	3 (2%)	0	100	100
26	BW	119/157 (76%)	119 (100%)	0	0	100	100
27	BX	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
28	BY	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
29	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
30	Ba	144/148 (97%)	136 (94%)	8 (6%)	0	100	100
31	Bb	103/245 (42%)	99 (96%)	4 (4%)	0	100	100
32	Bc	106/115 (92%)	106 (100%)	0	0	100	100
33	Bd	105/125 (84%)	105 (100%)	0	0	100	100
34	Be	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
35	Bf	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
36	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
38	Bi	100/105 (95%)	100 (100%)	0	0	100	100
39	Bj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
40	Bk	67/70 (96%)	67 (100%)	0	0	100	100
41	Bl	48/51 (94%)	48 (100%)	0	0	100	100
42	Bm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
43	Bo	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
44	Bp	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
45	Br	125/137 (91%)	123 (98%)	2 (2%)	0	100	100
46	Bs	194/318 (61%)	189 (97%)	5 (3%)	0	100	100
47	Bt	154/165 (93%)	151 (98%)	3 (2%)	0	100	100
48	Bv	210/217 (97%)	200 (95%)	10 (5%)	0	100	100
49	Nt	109/215 (51%)	102 (94%)	7 (6%)	0	100	100
50	Nu	105/162 (65%)	93 (89%)	9 (9%)	3 (3%)	3	24
51	XA	835/866 (96%)	802 (96%)	33 (4%)	0	100	100
52	XB	166/235 (71%)	163 (98%)	3 (2%)	0	100	100
53	MA	340/496 (68%)	331 (97%)	9 (3%)	0	100	100
55	AA	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
56	AB	61/69 (88%)	61 (100%)	0	0	100	100
57	AC	72/156 (46%)	69 (96%)	3 (4%)	0	100	100
58	AD	55/133 (41%)	55 (100%)	0	0	100	100
59	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
60	AF	311/317 (98%)	303 (97%)	8 (3%)	0	100	100
61	AG	53/56 (95%)	53 (100%)	0	0	100	100
63	AZ	220/295 (75%)	216 (98%)	4 (2%)	0	100	100
64	Aa	220/264 (83%)	217 (99%)	3 (1%)	0	100	100
65	Ab	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
66	Ac	223/281 (79%)	221 (99%)	2 (1%)	0	100	100
67	Ad	260/263 (99%)	258 (99%)	2 (1%)	0	100	100
68	Ae	189/204 (93%)	184 (97%)	5 (3%)	0	100	100
69	Af	235/249 (94%)	235 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	Ag	188/432 (44%)	186 (99%)	2 (1%)	0	100	100
71	Ah	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
72	Ai	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
73	Aj	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
74	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
75	Al	122/132 (92%)	121 (99%)	1 (1%)	0	100	100
76	Am	148/151 (98%)	148 (100%)	0	0	100	100
77	An	120/151 (80%)	117 (98%)	3 (2%)	0	100	100
78	Ao	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
79	Ap	139/172 (81%)	133 (96%)	6 (4%)	0	100	100
80	Aq	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
81	Ar	147/152 (97%)	144 (98%)	3 (2%)	0	100	100
82	As	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
83	At	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
84	Au	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
85	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
86	Aw	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
87	Ax	123/130 (95%)	122 (99%)	1 (1%)	0	100	100
88	Ay	83/124 (67%)	82 (99%)	1 (1%)	0	100	100
89	Az	23/25 (92%)	23 (100%)	0	0	100	100
All	All	13456/15812 (85%)	13206 (98%)	247 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
50	Nu	104	PRO
50	Nu	106	ILE
50	Nu	103	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BA	194/198 (98%)	193 (100%)	1 (0%)	86	92
5	BB	344/347 (99%)	339 (98%)	5 (2%)	60	77
6	BC	302/336 (90%)	301 (100%)	1 (0%)	91	96
7	BD	247/250 (99%)	247 (100%)	0	100	100
8	BE	216/251 (86%)	215 (100%)	1 (0%)	86	92
9	BF	197/215 (92%)	197 (100%)	0	100	100
10	BG	199/223 (89%)	197 (99%)	2 (1%)	73	84
11	BH	169/171 (99%)	169 (100%)	0	100	100
12	BI	180/181 (99%)	180 (100%)	0	100	100
13	BJ	143/149 (96%)	143 (100%)	0	100	100
15	BL	175/176 (99%)	175 (100%)	0	100	100
16	BM	117/161 (73%)	117 (100%)	0	100	100
17	BN	171/172 (99%)	171 (100%)	0	100	100
18	BO	171/173 (99%)	169 (99%)	2 (1%)	67	81
19	BP	140/163 (86%)	140 (100%)	0	100	100
20	BQ	164/165 (99%)	163 (99%)	1 (1%)	84	91
21	BR	159/175 (91%)	159 (100%)	0	100	100
22	BS	154/154 (100%)	154 (100%)	0	100	100
23	BT	139/140 (99%)	139 (100%)	0	100	100
24	BU	88/113 (78%)	88 (100%)	0	100	100
25	BV	106/107 (99%)	105 (99%)	1 (1%)	75	86
26	BW	100/126 (79%)	98 (98%)	2 (2%)	50	72
27	BX	106/134 (79%)	106 (100%)	0	100	100
28	BY	124/135 (92%)	124 (100%)	0	100	100
29	BZ	117/118 (99%)	117 (100%)	0	100	100
30	Ba	118/119 (99%)	118 (100%)	0	100	100
31	Bb	87/183 (48%)	87 (100%)	0	100	100
32	Bc	92/98 (94%)	91 (99%)	1 (1%)	70	82
33	Bd	98/110 (89%)	98 (100%)	0	100	100
34	Be	116/121 (96%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	Bf	89/89 (100%)	89 (100%)	0	100	100
36	Bg	98/100 (98%)	97 (99%)	1 (1%)	73	84
37	Bh	109/110 (99%)	109 (100%)	0	100	100
38	Bi	86/89 (97%)	85 (99%)	1 (1%)	67	81
39	Bj	73/80 (91%)	73 (100%)	0	100	100
40	Bk	64/65 (98%)	62 (97%)	2 (3%)	35	63
41	Bl	47/48 (98%)	47 (100%)	0	100	100
42	Bm	47/115 (41%)	47 (100%)	0	100	100
43	Bo	92/93 (99%)	92 (100%)	0	100	100
44	Bp	74/75 (99%)	73 (99%)	1 (1%)	62	79
45	Br	110/120 (92%)	110 (100%)	0	100	100
46	Bs	164/258 (64%)	164 (100%)	0	100	100
47	Bt	128/137 (93%)	122 (95%)	6 (5%)	22	51
48	Bv	191/195 (98%)	191 (100%)	0	100	100
49	Nt	97/183 (53%)	95 (98%)	2 (2%)	48	71
50	Nu	91/136 (67%)	85 (93%)	6 (7%)	14	41
51	XA	746/769 (97%)	719 (96%)	27 (4%)	30	58
52	XB	147/202 (73%)	142 (97%)	5 (3%)	32	60
53	MA	311/443 (70%)	307 (99%)	4 (1%)	65	80
55	AA	75/76 (99%)	75 (100%)	0	100	100
56	AB	56/62 (90%)	56 (100%)	0	100	100
57	AC	67/140 (48%)	67 (100%)	0	100	100
58	AD	47/106 (44%)	47 (100%)	0	100	100
59	AE	88/98 (90%)	86 (98%)	2 (2%)	45	69
60	AF	272/275 (99%)	270 (99%)	2 (1%)	81	89
61	AG	48/49 (98%)	48 (100%)	0	100	100
63	AZ	183/243 (75%)	181 (99%)	2 (1%)	70	82
64	Aa	203/231 (88%)	201 (99%)	2 (1%)	73	84
65	Ab	185/223 (83%)	185 (100%)	0	100	100
66	Ac	189/232 (82%)	188 (100%)	1 (0%)	86	92
67	Ad	224/225 (100%)	224 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Ae	161/170 (95%)	161 (100%)	0	100	100
69	Af	207/218 (95%)	207 (100%)	0	100	100
70	Ag	170/360 (47%)	168 (99%)	2 (1%)	67	81
71	Ah	178/180 (99%)	177 (99%)	1 (1%)	84	91
72	Ai	161/168 (96%)	160 (99%)	1 (1%)	84	91
73	Aj	87/136 (64%)	86 (99%)	1 (1%)	70	82
74	Ak	139/142 (98%)	139 (100%)	0	100	100
75	Al	104/108 (96%)	101 (97%)	3 (3%)	37	64
76	Am	130/131 (99%)	130 (100%)	0	100	100
77	An	95/119 (80%)	93 (98%)	2 (2%)	48	71
78	Ao	114/130 (88%)	113 (99%)	1 (1%)	75	86
79	Ap	117/140 (84%)	117 (100%)	0	100	100
80	Aq	120/121 (99%)	119 (99%)	1 (1%)	79	88
81	Ar	128/131 (98%)	125 (98%)	3 (2%)	45	69
82	As	112/114 (98%)	112 (100%)	0	100	100
83	At	94/107 (88%)	93 (99%)	1 (1%)	70	82
84	Au	68/68 (100%)	66 (97%)	2 (3%)	37	64
85	Av	112/113 (99%)	112 (100%)	0	100	100
86	Aw	112/114 (98%)	110 (98%)	2 (2%)	54	74
87	Ax	107/112 (96%)	106 (99%)	1 (1%)	75	86
88	Ay	75/102 (74%)	75 (100%)	0	100	100
89	Az	24/24 (100%)	24 (100%)	0	100	100
All	All	11749/13439 (87%)	11647 (99%)	102 (1%)	74	86

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	XA	631	ASP
53	MA	455	LEU
86	Aw	105	PHE
51	XA	634	GLU
52	XB	28	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 178 such sidechains are listed below:

Mol	Chain	Res	Type
53	MA	410	HIS
69	Af	177	GLN
53	MA	475	GLN
64	Aa	40	ASN
74	Ak	39	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B5	3752/4808 (78%)	462 (12%)	3 (0%)
2	B7	119/120 (99%)	6 (5%)	0
3	B8	155/158 (98%)	20 (12%)	0
54	A2	1764/1870 (94%)	228 (12%)	0
62	AT	75/76 (98%)	11 (14%)	0
All	All	5865/7032 (83%)	727 (12%)	3 (0%)

5 of 727 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B5	3	C
1	B5	39	A
1	B5	42	A
1	B5	58	G
1	B5	59	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B5	1588	G
1	B5	4372	A
1	B5	4445	U

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

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
54	PSU	A2	1178	54	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	B5	400	1	18,25,26	1.02	1 (5%)	18,36,39	1.20	2 (11%)
1	OMU	B5	3973	1	19,22,23	1.23	3 (15%)	26,31,34	1.69	4 (15%)
1	PSU	B5	4246	1	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
1	PSU	B5	1721	1	18,21,22	1.32	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	2208	1,92	19,22,23	0.81	0	26,31,34	0.84	0
1	A2M	B5	4269	1,92	18,25,26	0.61	0	18,36,39	0.84	1 (5%)
54	PSU	A2	1368	54	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	B5	3462	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
54	OMC	A2	463	54	19,22,23	0.82	0	26,31,34	0.83	0
54	A2M	A2	485	54	18,25,26	1.02	1 (5%)	18,36,39	1.25	2 (11%)
1	OMG	B5	4364	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
1	A2M	B5	1479	1	18,25,26	1.01	1 (5%)	18,36,39	1.24	2 (11%)
1	OMG	B5	1260	1	18,26,27	0.95	1 (5%)	19,38,41	1.10	2 (10%)
1	A2M	B5	2244	1,92	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
1	1MA	B5	1266	1,92	16,25,26	1.58	2 (12%)	18,37,40	1.05	3 (16%)
1	5MC	B5	4193	1	18,22,23	0.94	2 (11%)	26,32,35	1.21	3 (11%)
54	PSU	A2	687	54	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
54	PSU	A2	1693	54	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
54	OMC	A2	1392	54	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
54	6MZ	A2	1833	54,92	18,25,26	0.91	1 (5%)	16,36,39	1.94	4 (25%)
1	OMC	B5	2667	1	19,22,23	0.80	0	26,31,34	0.77	0
1	PSU	B5	1720	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
54	PSU	A2	407	54	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	2475	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
54	A2M	A2	166	54	18,25,26	1.05	1 (5%)	18,36,39	1.27	2 (11%)
62	5MU	AT	54	62	19,22,23	1.40	5 (26%)	28,32,35	2.03	6 (21%)
62	PSU	AT	55	62	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
54	OMU	A2	1805	54	19,22,23	1.23	3 (15%)	26,31,34	1.70	5 (19%)
3	OMG	B8	75	3	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	PSU	B5	3496	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4099	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	1489	1,92	18,25,26	0.99	1 (5%)	18,36,39	1.39	2 (11%)
1	OMC	B5	1820	1,92	19,22,23	0.80	0	26,31,34	0.80	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	A2M	B5	2658	1,92	18,25,26	1.02	1 (5%)	18,36,39	1.18	2 (11%)
1	OMG	B5	4369	1	18,26,27	1.00	2 (11%)	19,38,41	0.74	0
3	PSU	B8	69	3	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
54	OMC	A2	1704	54	19,22,23	0.80	0	26,31,34	0.77	0
86	HY3	Aw	62	86	6,8,9	6.44	4 (66%)	5,10,12	0.96	0
1	PSU	B5	3427	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1638	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
5	HIC	BB	245	5	8,11,12	0.88	0	6,14,16	0.85	0
54	A2M	A2	27	54,92	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
1	PSU	B5	1683	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	B5	4435	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
1	OMG	B5	4240	1	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
1	PSU	B5	4267	1	18,21,22	0.85	1 (5%)	22,30,33	0.69	0
54	PSU	A2	650	54	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
54	OMG	A2	684	54	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
54	B8N	A2	1249	54	24,29,30	1.31	3 (12%)	29,42,45	1.26	3 (10%)
1	PSU	B5	3554	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	3585	1,92	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
54	A2M	A2	577	54	18,25,26	1.01	1 (5%)	18,36,39	1.21	2 (11%)
54	PSU	A2	1644	54,92	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	B5	2630	1,92	18,25,26	0.99	1 (5%)	18,36,39	1.37	2 (11%)
1	PSU	B5	4711	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
54	PSU	A2	1245	54	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1537	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4298	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
54	PSU	A2	823	54	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
54	PSU	A2	1626	54	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
54	4AC	A2	1338	54	21,24,25	1.07	1 (4%)	29,34,37	1.18	3 (10%)
1	PSU	B5	3616	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	3652	1,92	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	1477	1	18,26,27	0.94	1 (5%)	19,38,41	1.10	2 (10%)
1	A2M	B5	3492	1,54	18,25,26	1.00	1 (5%)	18,36,39	1.36	2 (11%)
1	PSU	B5	1491	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	OMC	B5	1284	1	19,22,23	0.81	0	26,31,34	0.81	0
1	PSU	B5	1799	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	OMG	A2	437	54	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	B5	4045	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
54	MA6	A2	1852	54	18,26,27	1.10	2 (11%)	19,38,41	1.93	3 (15%)
1	OMG	B5	2207	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
1	OMG	B5	3631	1,92	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
42	M3L	Bm	98	42	10,11,12	0.83	0	9,14,16	0.59	0
1	PSU	B5	3576	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	1632	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	4 (18%)
54	PSU	A2	864	54	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	3447	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4166	1	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
1	OMG	B5	4383	1	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
1	OMG	B5	2719	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
54	OMC	A2	174	54,92	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
54	OMU	A2	355	54	19,22,23	1.22	2 (10%)	26,31,34	1.72	4 (15%)
1	A2M	B5	398	1	18,25,26	1.02	1 (5%)	18,36,39	1.24	2 (11%)
54	PSU	A2	967	54	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
54	G7M	A2	1640	54,62	20,26,27	2.99	7 (35%)	17,39,42	0.97	1 (5%)
31	MLZ	Bb	5	31	8,9,10	0.48	0	4,9,11	0.17	0
1	OMG	B5	3676	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
54	PSU	A2	573	54	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	2351	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	3359	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
30	V5N	Ba	39	30	4,11,12	0.76	0	5,14,16	1.48	1 (20%)
1	OMG	B5	4245	1	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
54	PSU	A2	119	54	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
54	PSU	A2	109	54	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
54	PSU	A2	1239	54	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	1718	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	3974	1	18,26,27	0.90	1 (5%)	19,38,41	1.12	2 (10%)
1	PSU	B5	4042	1	18,21,22	1.33	2 (11%)	22,30,33	1.92	4 (18%)
54	MA6	A2	1851	54	18,26,27	1.09	2 (11%)	19,38,41	2.00	3 (15%)
1	5MC	B5	3514	1,92	18,22,23	0.97	2 (11%)	26,32,35	1.16	3 (11%)
54	OMU	A2	429	54	19,22,23	1.20	3 (15%)	26,31,34	1.68	4 (15%)
1	PSU	B5	3494	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	OMU	A2	121	54	19,22,23	1.22	3 (15%)	26,31,34	1.71	4 (15%)
54	A2M	A2	669	54,92	18,25,26	0.99	1 (5%)	18,36,39	1.32	2 (11%)
1	PSU	B5	4039	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
54	A2M	A2	1384	54	18,25,26	1.04	1 (5%)	18,36,39	1.21	2 (11%)
1	OMG	B5	4116	1	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
1	PSU	B5	4740	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	B5	4202	1	19,22,23	0.82	0	26,31,34	0.85	0
1	OMG	B5	2267	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
54	PSU	A2	36	54	18,21,22	1.33	2 (11%)	22,30,33	1.92	3 (13%)
54	PSU	A2	652	54	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
54	PSU	A2	34	54	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4177	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	OMU	B5	4244	1	19,22,23	1.21	2 (10%)	26,31,34	1.69	5 (19%)
1	6MZ	B5	3966	1	18,25,26	0.89	1 (5%)	16,36,39	1.98	4 (25%)
54	PSU	A2	1446	54	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	B5	3466	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
54	PSU	A2	210	54	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	OMU	B5	2680	1	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
1	PSU	B5	4169	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	UR3	B5	4276	1	19,22,23	0.28	0	26,32,35	0.70	0
1	OMC	B5	3433	1	19,22,23	0.79	0	26,31,34	0.77	0
54	OMG	A2	868	54	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
1	OMG	B5	4138	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	B5	4278	1	18,21,22	0.86	1 (5%)	22,30,33	0.61	0
54	OMG	A2	1491	54,92	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
1	OMC	B5	2265	1,92	19,22,23	0.83	0	26,31,34	0.86	1 (3%)
54	PSU	A2	815	54	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4419	1	18,21,22	0.88	1 (5%)	22,30,33	0.67	0
1	OMG	B5	1580	1,92	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
1	OMC	B5	4282	1,92	19,22,23	0.83	0	26,31,34	0.86	1 (3%)
54	A2M	A2	99	54,92	18,25,26	1.04	1 (5%)	18,36,39	1.20	2 (11%)
54	OMG	A2	1448	54	18,26,27	1.00	2 (11%)	19,38,41	0.85	0
1	A2M	B5	1270	1	18,25,26	0.99	1 (5%)	18,36,39	1.23	2 (11%)
54	PSU	A2	105	54	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
54	OMU	A2	172	54	19,22,23	1.20	3 (15%)	26,31,34	1.72	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMC	B5	2704	1	19,22,23	0.81	0	26,31,34	0.84	1 (3%)
1	OMC	B5	3601	1	19,22,23	0.81	0	26,31,34	0.80	0
1	PSU	B5	4374	1	18,21,22	0.84	1 (5%)	22,30,33	0.57	0
54	PSU	A2	816	54	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
54	PSU	A2	1046	54	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
54	OMU	A2	1327	54,92	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
54	PSU	A2	1348	54	18,21,22	1.32	2 (11%)	22,30,33	1.89	3 (13%)
54	OMG	A2	510	54,92	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	B5	4058	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	3490	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	B5	1810	1,92	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
54	OMU	A2	116	54	19,22,23	1.19	2 (10%)	26,31,34	1.70	4 (15%)
54	PSU	A2	867	54	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
54	PSU	A2	1047	54	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
54	PSU	A2	802	54	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
54	PSU	A2	1082	54	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	B5	3573	1	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
1	OMG	B5	3476	1	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	PSU	B5	3369	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	2647	1	19,22,23	0.81	0	26,31,34	0.82	0
1	OMU	B5	4366	1	19,22,23	1.21	2 (10%)	26,31,34	1.72	5 (19%)
1	A2M	B5	3450	1	18,25,26	1.03	1 (5%)	18,36,39	1.16	2 (11%)
54	A2M	A2	1679	54	18,25,26	1.02	1 (5%)	18,36,39	1.29	2 (11%)
1	A2M	B5	4336	1	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	B5	1801	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
1	OMG	B5	3524	1	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
54	OMG	A2	1329	54	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
1	PSU	B5	4107	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
54	A2M	A2	591	54	18,25,26	1.03	1 (5%)	18,36,39	1.25	2 (11%)
54	PSU	A2	1233	54	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
1	PSU	B5	4382	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	UY1	B5	3550	1	19,22,23	1.39	3 (15%)	22,31,34	1.87	5 (22%)
1	A2M	B5	3456	1	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
54	PSU	A2	93	54	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
54	A2M	A2	1032	54	18,25,26	1.01	1 (5%)	18,36,39	1.20	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	A2M	B5	3599	1	18,25,26	1.00	1 (5%)	18,36,39	1.25	2 (11%)
82	NMM	As	67	82	9,11,12	0.59	0	6,12,14	0.34	0
1	OMU	B5	4052	1	19,22,23	1.22	3 (15%)	26,31,34	1.72	4 (15%)
1	OMG	B5	3942	1,62	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
1	A2M	B5	4317	1	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
54	PSU	A2	1175	54	18,21,22	1.32	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4203	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
54	OMG	A2	602	54	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
3	PSU	B8	55	3	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
54	PSU	A2	1005	54	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	B5	2206	1,92	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	B5	3500	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
54	4AC	A2	1843	54	21,24,25	1.11	2 (9%)	29,34,37	1.28	3 (10%)
54	PSU	A2	218	54	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	B5	3557	1	18,25,26	1.01	1 (5%)	18,36,39	1.21	2 (11%)
54	A2M	A2	513	54	18,25,26	1.04	1 (5%)	18,36,39	1.20	2 (11%)
1	PSU	B5	4322	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	1731	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
54	OMU	A2	1443	54,92	19,22,23	1.25	3 (15%)	26,31,34	1.70	5 (19%)
1	PSU	B5	4149	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	B5	2194	1,92	19,22,23	0.82	0	26,31,34	0.89	1 (3%)
1	A2M	B5	3562	1	18,25,26	1.03	1 (5%)	18,36,39	1.19	2 (11%)
1	PSU	B5	4188	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	3583	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4217	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
54	A2M	A2	159	54	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
54	OMU	A2	628	54	19,22,23	1.17	2 (10%)	26,31,34	1.71	5 (19%)
1	A2M	B5	3517	1	18,25,26	0.97	1 (5%)	18,36,39	1.32	2 (11%)
43	MLZ	Bo	53	43	8,9,10	0.49	0	4,9,11	0.11	0
54	A2M	A2	469	54	18,25,26	1.05	1 (5%)	18,36,39	1.24	2 (11%)
4	V5N	BA	216	4	4,11,12	0.77	0	5,14,16	1.53	1 (20%)
1	PSU	B5	4749	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
54	OMC	A2	518	54	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
1	OMU	B5	2258	1	19,22,23	1.23	3 (15%)	26,31,34	1.68	4 (15%)
1	PSU	B5	4325	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	B5	3502	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	B5	3540	1	19,22,23	0.81	0	26,31,34	0.80	0
54	PSU	A2	1057	54	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
54	OMG	A2	645	54	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
1	OMU	B5	3657	1	19,22,23	1.21	2 (10%)	26,31,34	1.73	5 (19%)
54	PSU	A2	682	54	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
54	OMU	A2	1289	54	19,22,23	0.20	0	26,31,34	0.35	0
54	PSU	A2	610	54	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	3371	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	B5	3619	1	19,22,23	0.81	0	26,31,34	0.82	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
54	PSU	A2	1178	54	-	0/7/25/26	0/2/2/2
1	A2M	B5	400	1	-	0/5/27/28	0/3/3/3
1	OMU	B5	3973	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4246	1	-	3/7/25/26	0/2/2/2
1	PSU	B5	1721	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2208	1,92	-	0/9/27/28	0/2/2/2
1	A2M	B5	4269	1,92	-	0/5/27/28	0/3/3/3
54	PSU	A2	1368	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	3462	1	-	0/7/25/26	0/2/2/2
54	OMC	A2	463	54	-	0/9/27/28	0/2/2/2
54	A2M	A2	485	54	-	0/5/27/28	0/3/3/3
1	OMG	B5	4364	1	-	0/5/27/28	0/3/3/3
1	A2M	B5	1479	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	1260	1	-	0/5/27/28	0/3/3/3
1	A2M	B5	2244	1,92	-	0/5/27/28	0/3/3/3
1	1MA	B5	1266	1,92	-	0/3/25/26	0/3/3/3
1	5MC	B5	4193	1	-	4/7/25/26	0/2/2/2
54	PSU	A2	687	54	-	0/7/25/26	0/2/2/2
54	PSU	A2	1693	54	-	0/7/25/26	0/2/2/2
54	OMC	A2	1392	54	-	0/9/27/28	0/2/2/2
54	6MZ	A2	1833	54,92	-	0/5/27/28	0/3/3/3
1	OMC	B5	2667	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	1720	1	-	0/7/25/26	0/2/2/2
54	PSU	A2	407	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	2475	1	-	0/7/25/26	0/2/2/2
54	A2M	A2	166	54	-	0/5/27/28	0/3/3/3
62	5MU	AT	54	62	-	0/7/25/26	0/2/2/2
62	PSU	AT	55	62	-	0/7/25/26	0/2/2/2
54	OMU	A2	1805	54	-	0/9/27/28	0/2/2/2
3	OMG	B8	75	3	-	0/5/27/28	0/3/3/3
1	PSU	B5	3496	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4099	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	1489	1,92	-	2/5/27/28	0/3/3/3
1	OMC	B5	1820	1,92	-	1/9/27/28	0/2/2/2
1	A2M	B5	2658	1,92	-	0/5/27/28	0/3/3/3
1	OMG	B5	4369	1	-	0/5/27/28	0/3/3/3
3	PSU	B8	69	3	-	0/7/25/26	0/2/2/2
54	OMC	A2	1704	54	-	1/9/27/28	0/2/2/2
86	HY3	Aw	62	86	-	1/1/12/14	0/1/1/1
1	PSU	B5	3427	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1638	1	-	0/7/25/26	0/2/2/2
5	HIC	BB	245	5	-	2/5/6/8	0/1/1/1
54	A2M	A2	27	54,92	-	1/5/27/28	0/3/3/3
1	PSU	B5	1683	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4435	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4240	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4267	1	-	0/7/25/26	0/2/2/2
54	PSU	A2	650	54	-	0/7/25/26	0/2/2/2
54	OMG	A2	684	54	-	2/5/27/28	0/3/3/3
54	B8N	A2	1249	54	-	4/16/34/35	0/2/2/2
1	PSU	B5	3554	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3585	1,92	-	0/7/25/26	0/2/2/2
54	A2M	A2	577	54	-	0/5/27/28	0/3/3/3
54	PSU	A2	1644	54,92	-	0/7/25/26	0/2/2/2
1	A2M	B5	2630	1,92	-	0/5/27/28	0/3/3/3
1	PSU	B5	4711	1	-	0/7/25/26	0/2/2/2
54	PSU	A2	1245	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	1537	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4298	1	-	0/7/25/26	0/2/2/2
54	PSU	A2	823	54	-	0/7/25/26	0/2/2/2
54	PSU	A2	1626	54	-	0/7/25/26	0/2/2/2
54	4AC	A2	1338	54	-	4/11/29/30	0/2/2/2
1	PSU	B5	3616	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3652	1,92	-	0/7/25/26	0/2/2/2
1	OMG	B5	1477	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	B5	3492	1,54	-	1/5/27/28	0/3/3/3
1	PSU	B5	1491	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	1284	1	-	2/9/27/28	0/2/2/2
1	PSU	B5	1799	1	-	0/7/25/26	0/2/2/2
54	OMG	A2	437	54	-	0/5/27/28	0/3/3/3
1	PSU	B5	4045	1	-	0/7/25/26	0/2/2/2
54	MA6	A2	1852	54	-	3/7/29/30	0/3/3/3
1	OMG	B5	2207	1	-	2/5/27/28	0/3/3/3
1	OMG	B5	3631	1,92	-	2/5/27/28	0/3/3/3
42	M3L	Bm	98	42	-	0/9/10/12	-
1	PSU	B5	3576	1	-	1/7/25/26	0/2/2/2
1	PSU	B5	1632	1	-	0/7/25/26	0/2/2/2
54	PSU	A2	864	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	3447	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4166	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4383	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	2719	1	-	0/5/27/28	0/3/3/3
54	OMC	A2	174	54,92	-	0/9/27/28	0/2/2/2
54	OMU	A2	355	54	-	1/9/27/28	0/2/2/2
1	A2M	B5	398	1	-	4/5/27/28	0/3/3/3
54	PSU	A2	967	54	-	0/7/25/26	0/2/2/2
54	G7M	A2	1640	54,62	-	0/3/25/26	0/3/3/3
31	MLZ	Bb	5	31	-	2/7/8/10	-
1	OMG	B5	3676	1	-	0/5/27/28	0/3/3/3
54	PSU	A2	573	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	2351	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3359	1	-	0/5/27/28	0/3/3/3
30	V5N	Ba	39	30	-	0/5/10/12	0/1/1/1
1	OMG	B5	4245	1	-	0/5/27/28	0/3/3/3
54	PSU	A2	119	54	-	0/7/25/26	0/2/2/2
54	PSU	A2	109	54	-	0/7/25/26	0/2/2/2
54	PSU	A2	1239	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	1718	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3974	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4042	1	-	0/7/25/26	0/2/2/2
54	MA6	A2	1851	54	-	0/7/29/30	0/3/3/3
1	5MC	B5	3514	1,92	-	0/7/25/26	0/2/2/2
54	OMU	A2	429	54	-	4/9/27/28	0/2/2/2
1	PSU	B5	3494	1	-	1/7/25/26	0/2/2/2
54	OMU	A2	121	54	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	A2M	A2	669	54,92	-	2/5/27/28	0/3/3/3
1	PSU	B5	4039	1	-	0/7/25/26	0/2/2/2
54	A2M	A2	1384	54	-	0/5/27/28	0/3/3/3
1	OMG	B5	4116	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4740	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	4202	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	2267	1	-	1/5/27/28	0/3/3/3
54	PSU	A2	36	54	-	0/7/25/26	0/2/2/2
54	PSU	A2	652	54	-	0/7/25/26	0/2/2/2
54	PSU	A2	34	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	4177	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	4244	1	-	0/9/27/28	0/2/2/2
1	6MZ	B5	3966	1	-	0/5/27/28	0/3/3/3
54	PSU	A2	1446	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	3466	1	-	0/7/25/26	0/2/2/2
54	PSU	A2	210	54	-	0/7/25/26	0/2/2/2
1	OMU	B5	2680	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4169	1	-	0/7/25/26	0/2/2/2
1	UR3	B5	4276	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3433	1	-	4/9/27/28	0/2/2/2
54	OMG	A2	868	54	-	1/5/27/28	0/3/3/3
1	OMG	B5	4138	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4278	1	-	0/7/25/26	0/2/2/2
54	OMG	A2	1491	54,92	-	0/5/27/28	0/3/3/3
1	OMC	B5	2265	1,92	-	0/9/27/28	0/2/2/2
54	PSU	A2	815	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	4419	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	1580	1,92	-	0/5/27/28	0/3/3/3
1	OMC	B5	4282	1,92	-	0/9/27/28	0/2/2/2
54	A2M	A2	99	54,92	-	0/5/27/28	0/3/3/3
54	OMG	A2	1448	54	-	2/5/27/28	0/3/3/3
1	A2M	B5	1270	1	-	0/5/27/28	0/3/3/3
54	PSU	A2	105	54	-	0/7/25/26	0/2/2/2
54	OMU	A2	172	54	-	0/9/27/28	0/2/2/2
1	OMC	B5	2704	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	3601	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4374	1	-	0/7/25/26	0/2/2/2
54	PSU	A2	816	54	-	0/7/25/26	0/2/2/2
54	PSU	A2	1046	54	-	0/7/25/26	0/2/2/2
54	OMU	A2	1327	54,92	-	0/9/27/28	0/2/2/2
54	PSU	A2	1348	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	OMG	A2	510	54,92	-	2/5/27/28	0/3/3/3
1	PSU	B5	4058	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3490	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	1810	1,92	-	1/5/27/28	0/3/3/3
54	OMU	A2	116	54	-	0/9/27/28	0/2/2/2
54	PSU	A2	867	54	-	0/7/25/26	0/2/2/2
54	PSU	A2	1047	54	-	0/7/25/26	0/2/2/2
54	PSU	A2	802	54	-	0/7/25/26	0/2/2/2
54	PSU	A2	1082	54	-	1/7/25/26	0/2/2/2
1	OMC	B5	3573	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	3476	1	-	1/5/27/28	0/3/3/3
1	PSU	B5	3369	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2647	1	-	0/9/27/28	0/2/2/2
1	OMU	B5	4366	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	3450	1	-	0/5/27/28	0/3/3/3
54	A2M	A2	1679	54	-	0/5/27/28	0/3/3/3
1	A2M	B5	4336	1	-	1/5/27/28	0/3/3/3
1	PSU	B5	1801	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3524	1	-	0/5/27/28	0/3/3/3
54	OMG	A2	1329	54	-	0/5/27/28	0/3/3/3
1	PSU	B5	4107	1	-	0/7/25/26	0/2/2/2
54	A2M	A2	591	54	-	0/5/27/28	0/3/3/3
54	PSU	A2	1233	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	4382	1	-	4/7/25/26	0/2/2/2
1	UY1	B5	3550	1	-	1/9/27/28	0/2/2/2
1	A2M	B5	3456	1	-	0/5/27/28	0/3/3/3
54	PSU	A2	93	54	-	0/7/25/26	0/2/2/2
54	A2M	A2	1032	54	-	1/5/27/28	0/3/3/3
1	A2M	B5	3599	1	-	0/5/27/28	0/3/3/3
82	NMM	As	67	82	-	0/9/11/13	-
1	OMU	B5	4052	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	3942	1,62	-	0/5/27/28	0/3/3/3
1	A2M	B5	4317	1	-	0/5/27/28	0/3/3/3
54	PSU	A2	1175	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	4203	1	-	0/7/25/26	0/2/2/2
54	OMG	A2	602	54	-	0/5/27/28	0/3/3/3
3	PSU	B8	55	3	-	0/7/25/26	0/2/2/2
54	PSU	A2	1005	54	-	0/7/25/26	0/2/2/2
1	A2M	B5	2206	1,92	-	0/5/27/28	0/3/3/3
1	PSU	B5	3500	1	-	0/7/25/26	0/2/2/2
54	4AC	A2	1843	54	-	2/11/29/30	0/2/2/2
54	PSU	A2	218	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	B5	3557	1	-	0/5/27/28	0/3/3/3
54	A2M	A2	513	54	-	2/5/27/28	0/3/3/3
1	PSU	B5	4322	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1731	1	-	0/7/25/26	0/2/2/2
54	OMU	A2	1443	54,92	-	1/9/27/28	0/2/2/2
1	PSU	B5	4149	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2194	1,92	-	1/9/27/28	0/2/2/2
1	A2M	B5	3562	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4188	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3583	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4217	1	-	0/7/25/26	0/2/2/2
54	A2M	A2	159	54	-	1/5/27/28	0/3/3/3
54	OMU	A2	628	54	-	4/9/27/28	0/2/2/2
1	A2M	B5	3517	1	-	2/5/27/28	0/3/3/3
43	MLZ	Bo	53	43	-	0/7/8/10	-
54	A2M	A2	469	54	-	0/5/27/28	0/3/3/3
4	V5N	BA	216	4	-	1/5/10/12	0/1/1/1
1	PSU	B5	4749	1	-	0/7/25/26	0/2/2/2
54	OMC	A2	518	54	-	0/9/27/28	0/2/2/2
1	OMU	B5	2258	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4325	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3502	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3540	1	-	0/9/27/28	0/2/2/2
54	PSU	A2	1057	54	-	0/7/25/26	0/2/2/2
54	OMG	A2	645	54	-	3/5/27/28	0/3/3/3
1	OMU	B5	3657	1	-	1/9/27/28	0/2/2/2
54	PSU	A2	682	54	-	0/7/25/26	0/2/2/2
54	OMU	A2	1289	54	-	1/9/27/28	0/2/2/2
54	PSU	A2	610	54	-	0/7/25/26	0/2/2/2
1	PSU	B5	3371	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3619	1	-	2/9/27/28	0/2/2/2

The worst 5 of 331 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	Aw	62	HY3	C4-C3	-11.18	1.33	1.52
86	Aw	62	HY3	C3-CA	10.32	1.65	1.55
54	A2	1640	G7M	C5-C4	7.43	1.54	1.39
54	A2	1640	G7M	O6-C6	7.27	1.38	1.23
1	B5	1266	1MA	C2-N3	4.88	1.34	1.29

The worst 5 of 530 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A2	1233	PSU	N1-C2-N3	6.09	122.03	115.13
54	A2	1368	PSU	N1-C2-N3	6.08	122.02	115.13
1	B5	1683	PSU	N1-C2-N3	6.07	122.01	115.13
1	B5	1799	PSU	N1-C2-N3	6.06	122.00	115.13
54	A2	36	PSU	N1-C2-N3	6.05	121.99	115.13

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B5	2207	OMG	O4'-C4'-C5'-O5'
1	B5	3433	OMC	C2'-C1'-N1-C2
1	B5	3433	OMC	C2'-C1'-N1-C6
1	B5	4193	5MC	O4'-C1'-N1-C2
1	B5	4193	5MC	O4'-C1'-N1-C6

There are no ring outliers.

97 monomers are involved in 114 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	400	A2M	1	0
1	B5	2208	OMC	2	0
1	B5	3462	PSU	1	0
54	A2	463	OMC	3	0
54	A2	485	A2M	1	0
1	B5	4364	OMG	1	0
1	B5	1479	A2M	1	0
1	B5	1260	OMG	1	0
54	A2	1392	OMC	1	0
1	B5	2667	OMC	1	0
54	A2	166	A2M	2	0
54	A2	1805	OMU	2	0
3	B8	75	OMG	1	0
1	B5	4099	PSU	1	0
1	B5	1489	A2M	1	0
1	B5	2658	A2M	2	0
54	A2	1704	OMC	1	0
5	BB	245	HIC	1	0
54	A2	27	A2M	1	0
54	A2	684	OMG	1	0
54	A2	577	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	2630	A2M	1	0
54	A2	1338	4AC	2	0
1	B5	3652	PSU	1	0
1	B5	1284	OMC	1	0
54	A2	437	OMG	2	0
1	B5	2207	OMG	1	0
1	B5	3631	OMG	1	0
42	Bm	98	M3L	1	0
1	B5	4166	PSU	1	0
1	B5	4383	OMG	1	0
54	A2	355	OMU	1	0
1	B5	398	A2M	1	0
54	A2	1640	G7M	1	0
1	B5	3676	OMG	1	0
30	Ba	39	V5N	1	0
54	A2	109	PSU	1	0
1	B5	1718	PSU	2	0
54	A2	1851	MA6	1	0
54	A2	121	OMU	2	0
1	B5	4039	PSU	1	0
1	B5	4202	OMC	1	0
1	B5	2267	OMG	1	0
54	A2	36	PSU	1	0
1	B5	4244	OMU	1	0
54	A2	1446	PSU	1	0
54	A2	868	OMG	1	0
1	B5	4138	OMG	1	0
54	A2	1491	OMG	1	0
54	A2	815	PSU	1	0
1	B5	4282	OMC	2	0
54	A2	99	A2M	1	0
54	A2	1448	OMG	1	0
1	B5	1270	A2M	1	0
54	A2	105	PSU	1	0
54	A2	172	OMU	1	0
1	B5	2704	OMC	1	0
54	A2	1348	PSU	1	0
54	A2	510	OMG	1	0
1	B5	4058	PSU	1	0
1	B5	1810	A2M	2	0
1	B5	3573	OMC	1	0
1	B5	3476	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	2647	OMC	1	0
1	B5	4366	OMU	2	0
1	B5	3450	A2M	2	0
54	A2	1679	A2M	1	0
1	B5	4336	A2M	1	0
1	B5	3524	OMG	1	0
54	A2	1329	OMG	1	0
1	B5	4382	PSU	1	0
1	B5	3550	UY1	2	0
1	B5	3456	A2M	1	0
54	A2	1032	A2M	1	0
1	B5	4052	OMU	1	0
1	B5	4317	A2M	1	0
1	B5	4203	PSU	1	0
54	A2	602	OMG	1	0
1	B5	2206	A2M	1	0
54	A2	1843	4AC	1	0
1	B5	3557	A2M	1	0
54	A2	513	A2M	1	0
54	A2	1443	OMU	1	0
1	B5	2194	OMC	1	0
1	B5	3562	A2M	2	0
54	A2	159	A2M	2	0
1	B5	3517	A2M	1	0
54	A2	469	A2M	1	0
4	BA	216	V5N	1	0
54	A2	518	OMC	1	0
1	B5	2258	OMU	2	0
1	B5	4325	PSU	1	0
1	B5	3502	PSU	2	0
1	B5	3540	OMC	1	0
1	B5	3657	OMU	1	0
54	A2	1289	OMU	1	0
1	B5	3619	OMC	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 622 ligands modelled in this entry, 420 are monoatomic and 168 are unknown - leaving 34 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	$\# Z  > 2$
90	SPD	A2	1903	-	9,9,9	0.15	0	8,8,8	0.21	0
91	SPM	B5	4914	-	13,13,13	0.15	0	12,12,12	0.14	0
90	SPD	B5	4904	-	9,9,9	0.16	0	8,8,8	0.17	0
90	SPD	B5	4909	-	9,9,9	0.15	0	8,8,8	0.19	0
90	SPD	B5	4908	-	9,9,9	0.16	0	8,8,8	0.17	0
91	SPM	B5	4911	-	13,13,13	0.15	0	12,12,12	0.23	0
90	SPD	A2	1904	-	9,9,9	0.16	0	8,8,8	0.18	0
90	SPD	B5	4916	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	B5	4917	-	9,9,9	0.16	0	8,8,8	0.18	0
90	SPD	B5	4903	-	9,9,9	0.16	0	8,8,8	0.19	0
90	SPD	A2	1906	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	B5	4922	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	B5	4901	-	9,9,9	0.15	0	8,8,8	0.15	0
90	SPD	B5	4920	-	9,9,9	0.15	0	8,8,8	0.17	0
90	SPD	A2	1905	-	9,9,9	0.16	0	8,8,8	0.18	0
90	SPD	B5	4902	-	9,9,9	0.16	0	8,8,8	0.18	0
90	SPD	B5	4910	-	9,9,9	0.15	0	8,8,8	0.17	0
91	SPM	A2	1909	-	13,13,13	0.14	0	12,12,12	0.14	0
90	SPD	B5	4906	-	9,9,9	0.15	0	8,8,8	0.19	0
90	SPD	A2	1902	-	9,9,9	0.15	0	8,8,8	0.17	0
90	SPD	B5	4918	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	B5	4919	-	9,9,9	0.16	0	8,8,8	0.20	0
90	SPD	B5	4912	-	9,9,9	0.15	0	8,8,8	0.19	0
90	SPD	B5	4923	-	9,9,9	0.15	0	8,8,8	0.16	0
95	IHP	XA	901	-	36,36,36	1.52	6 (16%)	54,60,60	0.92	3 (5%)
90	SPD	B5	4915	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.18	0
90	SPD	B5	4921	-	9,9,9	0.16	0	8,8,8	0.19	0
90	SPD	A2	1908	-	9,9,9	0.16	0	8,8,8	0.18	0
90	SPD	B5	4907	-	9,9,9	0.15	0	8,8,8	0.17	0
90	SPD	B5	4913	-	9,9,9	0.15	0	8,8,8	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
90	SPD	BS	201	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.17	0
90	SPD	B5	4905	-	9,9,9	0.16	0	8,8,8	0.18	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
90	SPD	A2	1903	-	-	0/7/7/7	-
91	SPM	B5	4914	-	-	0/11/11/11	-
90	SPD	B5	4904	-	-	0/7/7/7	-
90	SPD	B5	4909	-	-	1/7/7/7	-
90	SPD	B5	4908	-	-	0/7/7/7	-
91	SPM	B5	4911	-	-	1/11/11/11	-
90	SPD	A2	1904	-	-	0/7/7/7	-
90	SPD	B5	4916	-	-	0/7/7/7	-
90	SPD	B5	4917	-	-	0/7/7/7	-
90	SPD	B5	4903	-	-	1/7/7/7	-
90	SPD	A2	1906	-	-	0/7/7/7	-
90	SPD	B5	4922	-	-	0/7/7/7	-
90	SPD	B5	4901	-	-	1/7/7/7	-
90	SPD	B5	4920	-	-	0/7/7/7	-
90	SPD	A2	1905	-	-	0/7/7/7	-
90	SPD	B5	4902	-	-	1/7/7/7	-
90	SPD	B5	4910	-	-	0/7/7/7	-
91	SPM	A2	1909	-	-	1/11/11/11	-
90	SPD	B5	4906	-	-	0/7/7/7	-
90	SPD	A2	1902	-	-	0/7/7/7	-
90	SPD	B5	4918	-	-	0/7/7/7	-
90	SPD	B5	4919	-	-	0/7/7/7	-
90	SPD	B5	4912	-	-	0/7/7/7	-
90	SPD	B5	4923	-	-	1/7/7/7	-
95	IHP	XA	901	-	-	6/30/54/54	0/1/1/1
90	SPD	B5	4915	-	-	0/7/7/7	-
90	SPD	A2	1901	-	-	1/7/7/7	-
90	SPD	B5	4921	-	-	1/7/7/7	-
90	SPD	A2	1908	-	-	0/7/7/7	-
90	SPD	B5	4907	-	-	0/7/7/7	-
90	SPD	B5	4913	-	-	0/7/7/7	-
90	SPD	BS	201	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	SPD	A2	1907	-	-	1/7/7/7	-
90	SPD	B5	4905	-	-	1/7/7/7	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
95	XA	901	IHP	P4-O14	3.54	1.66	1.59
95	XA	901	IHP	P3-O13	3.22	1.65	1.59
95	XA	901	IHP	P5-O15	3.20	1.65	1.59
95	XA	901	IHP	P2-O12	3.20	1.65	1.59
95	XA	901	IHP	P6-O16	3.17	1.65	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
95	XA	901	IHP	C4-C3-C2	3.55	118.19	110.41
95	XA	901	IHP	C5-C4-C3	3.51	118.10	110.41
95	XA	901	IHP	C3-C2-C1	2.39	115.65	110.41

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
95	XA	901	IHP	C5-C4-O14-P4
95	XA	901	IHP	C5-O15-P5-O35
91	A2	1909	SPM	C8-C9-N10-C11
95	XA	901	IHP	C4-O14-P4-O44
95	XA	901	IHP	C4-C5-O15-P5

There are no ring outliers.

22 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	A2	1903	SPD	1	0
90	B5	4904	SPD	1	0
90	B5	4908	SPD	1	0
91	B5	4911	SPM	2	0
90	A2	1904	SPD	1	0
90	B5	4903	SPD	1	0
90	A2	1906	SPD	1	0
90	B5	4922	SPD	1	0

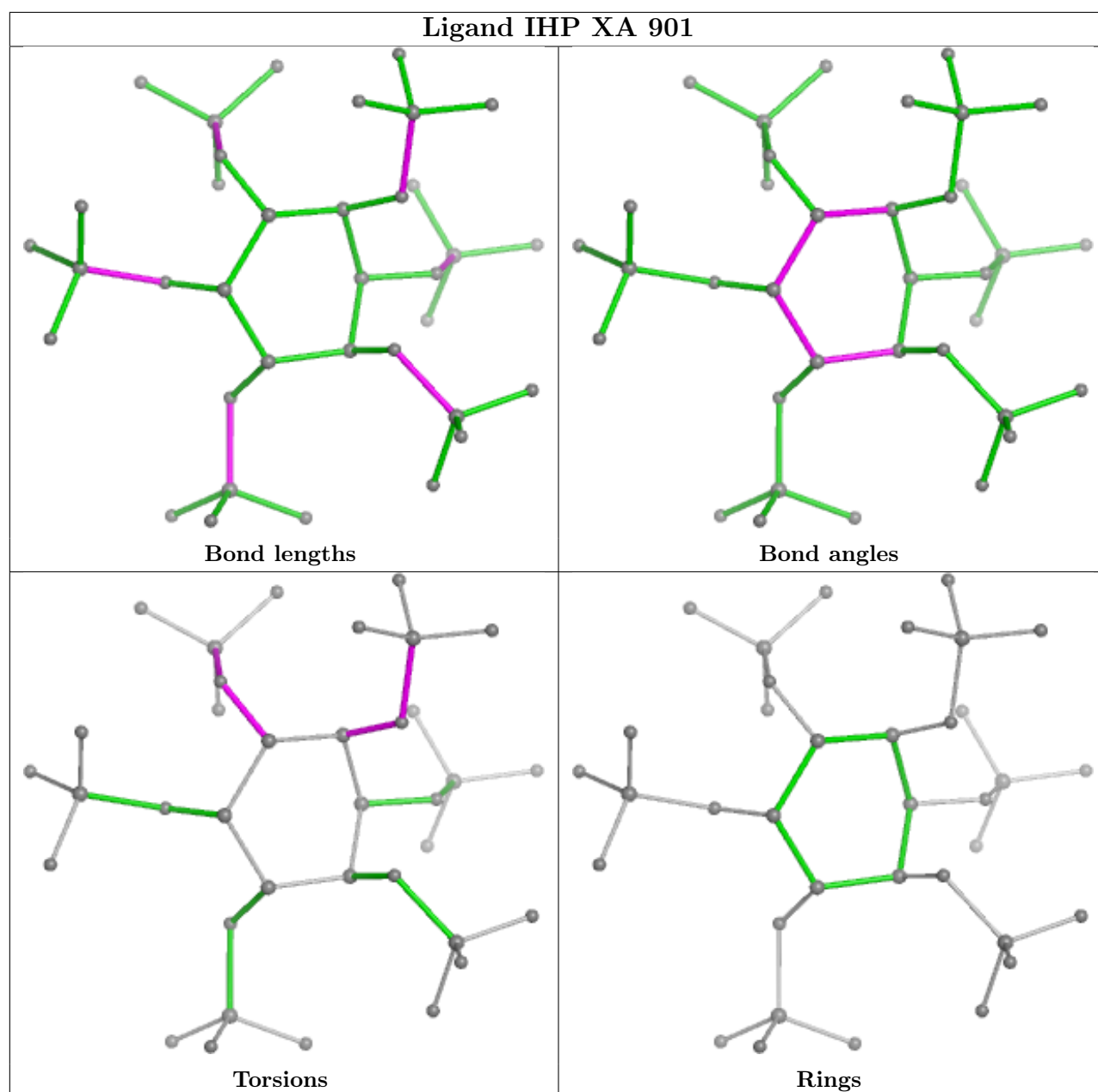
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	A2	1905	SPD	2	0
90	B5	4910	SPD	1	0
91	A2	1909	SPM	2	0
90	B5	4918	SPD	3	0
90	B5	4923	SPD	1	0
95	XA	901	IHP	1	0
90	B5	4915	SPD	1	0
90	A2	1901	SPD	1	0
90	B5	4921	SPD	1	0
90	A2	1908	SPD	1	0
90	B5	4907	SPD	3	0
90	BS	201	SPD	1	0
90	A2	1907	SPD	1	0
90	B5	4905	SPD	1	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

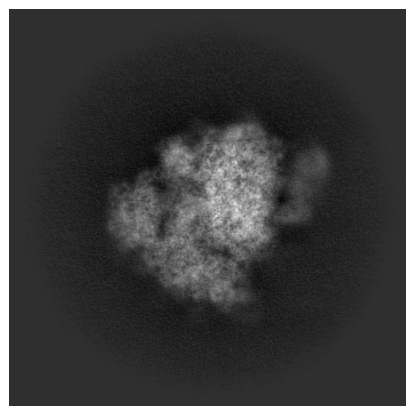
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53296. These allow visual inspection of the internal detail of the map and identification of artifacts.

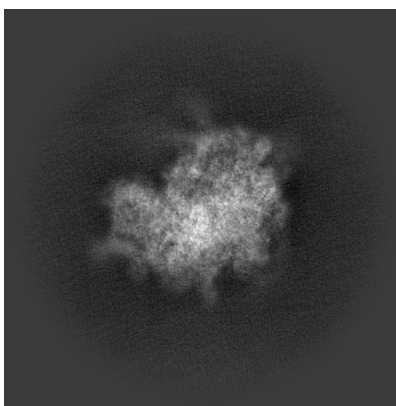
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

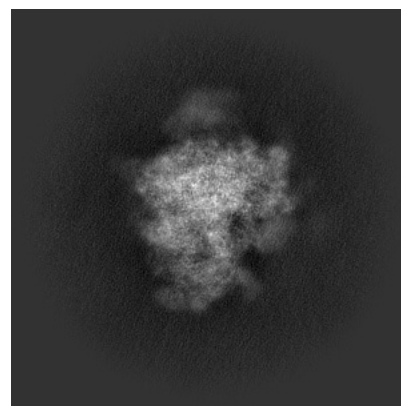
#### 6.1.1 Primary map



X

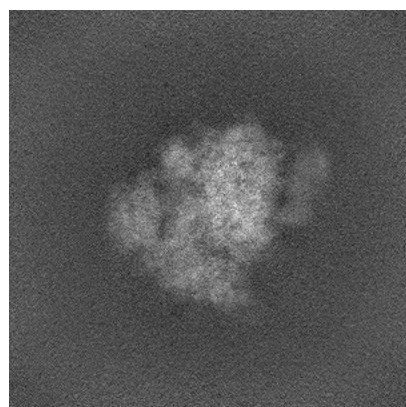


Y

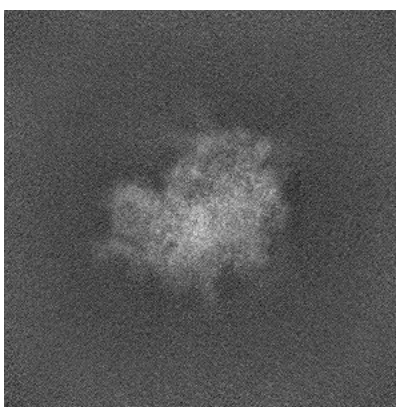


Z

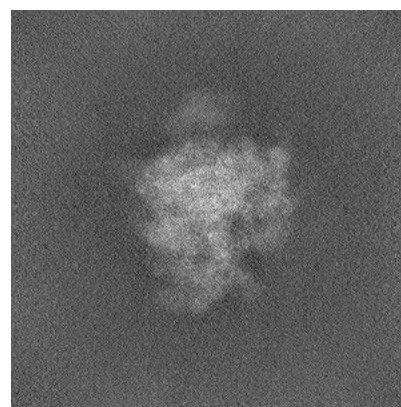
#### 6.1.2 Raw map



X



Y

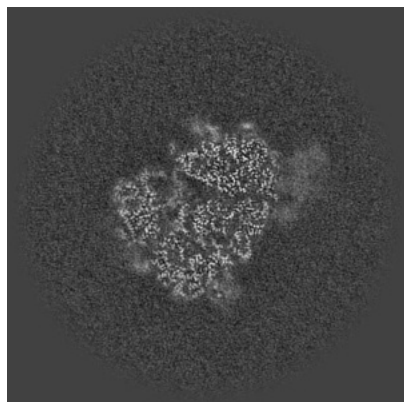


Z

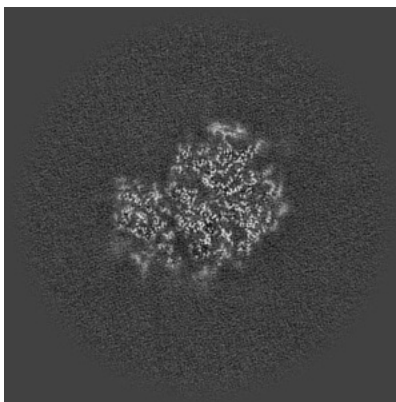
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

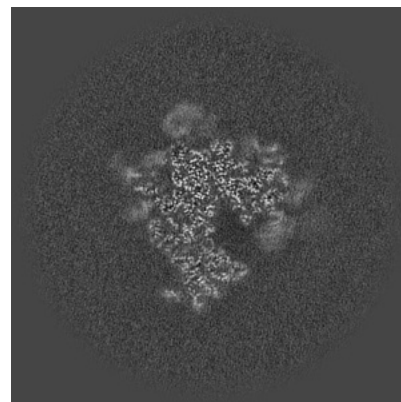
### 6.2.1 Primary map



X Index: 280

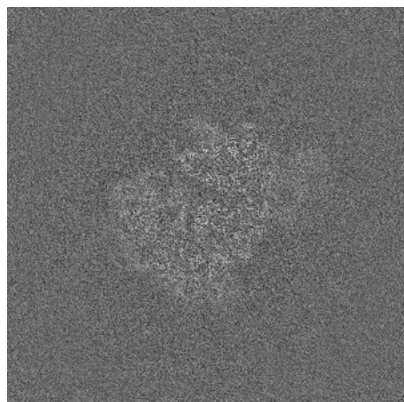


Y Index: 280

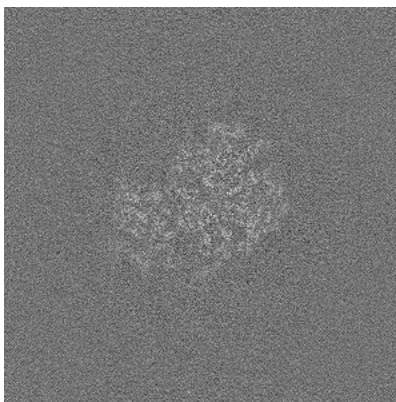


Z Index: 280

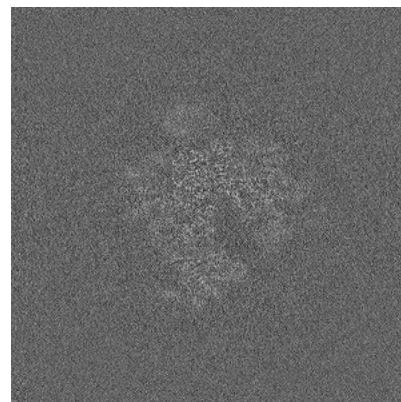
### 6.2.2 Raw map



X Index: 280



Y Index: 280



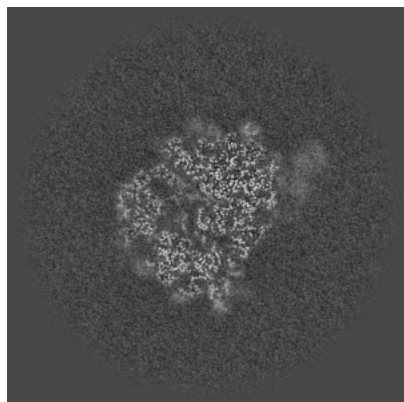
Z Index: 280

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

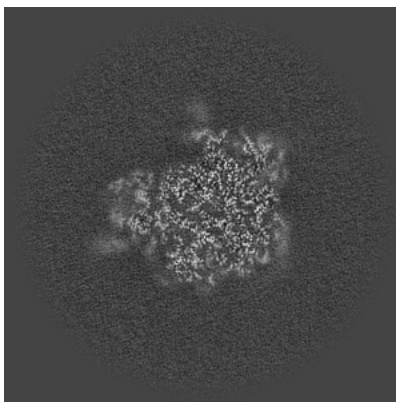


## 6.3 Largest variance slices [i](#)

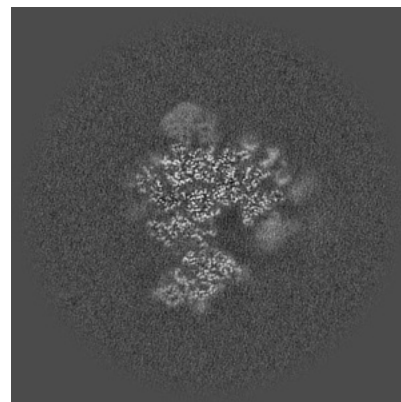
### 6.3.1 Primary map



X Index: 287

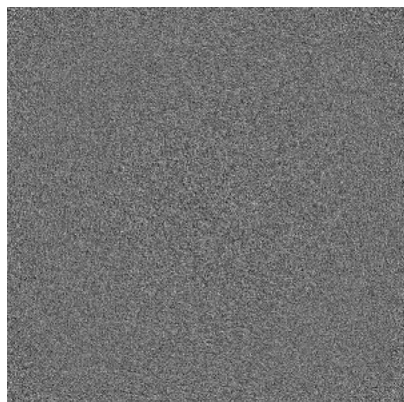


Y Index: 314

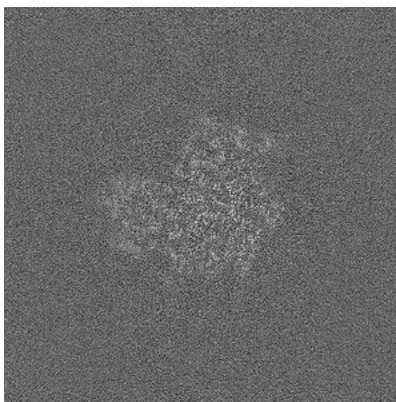


Z Index: 272

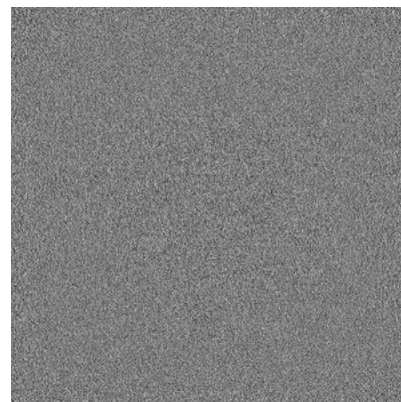
### 6.3.2 Raw map



X Index: 0



Y Index: 295

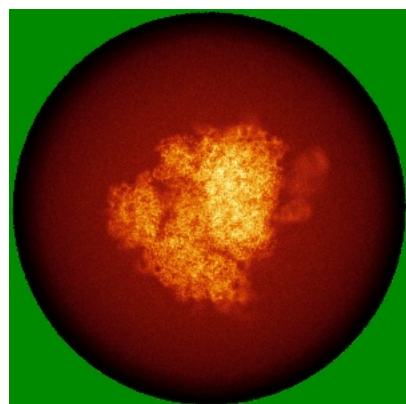


Z Index: 0

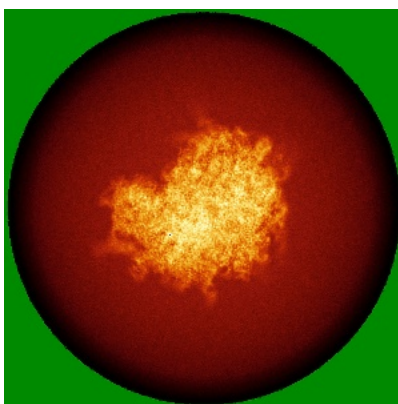
The images above show the largest variance slices of the map in three orthogonal directions.

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

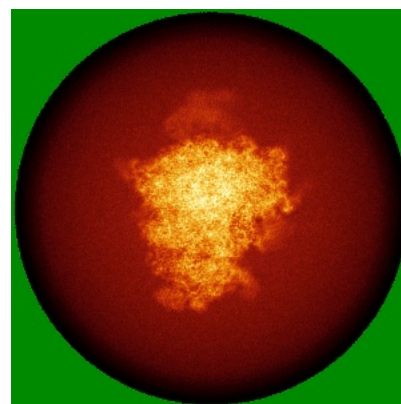
### 6.4.1 Primary map



X

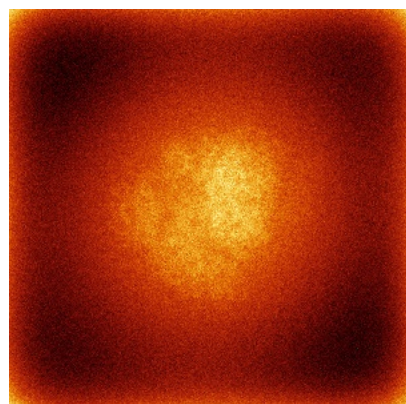


Y

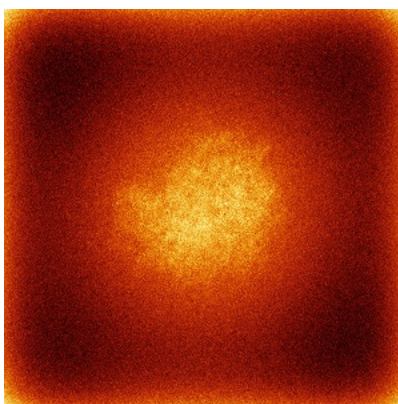


Z

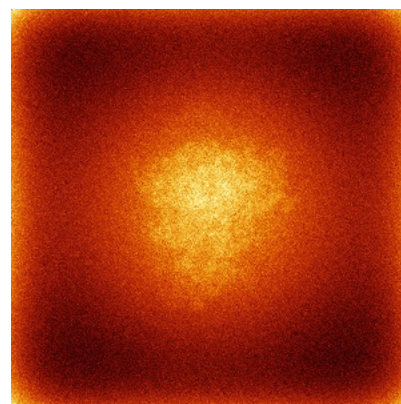
### 6.4.2 Raw map



X



Y

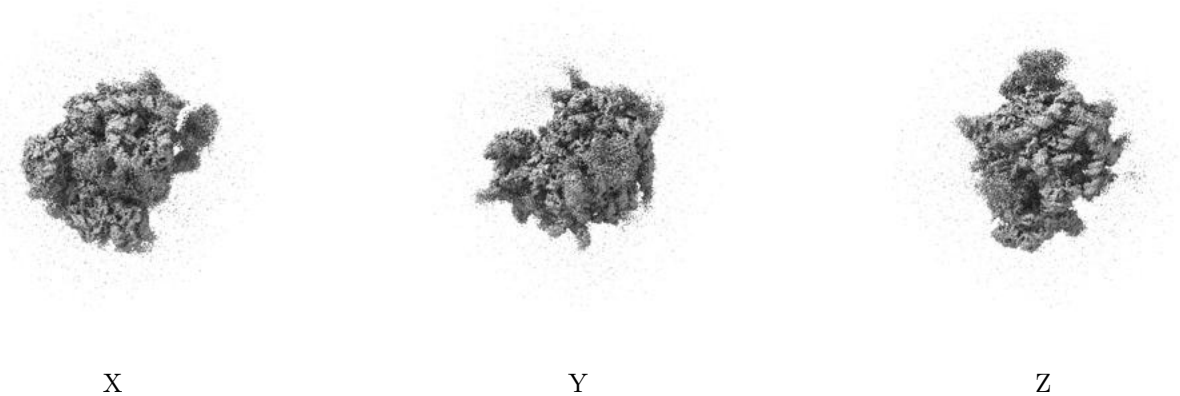


Z

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

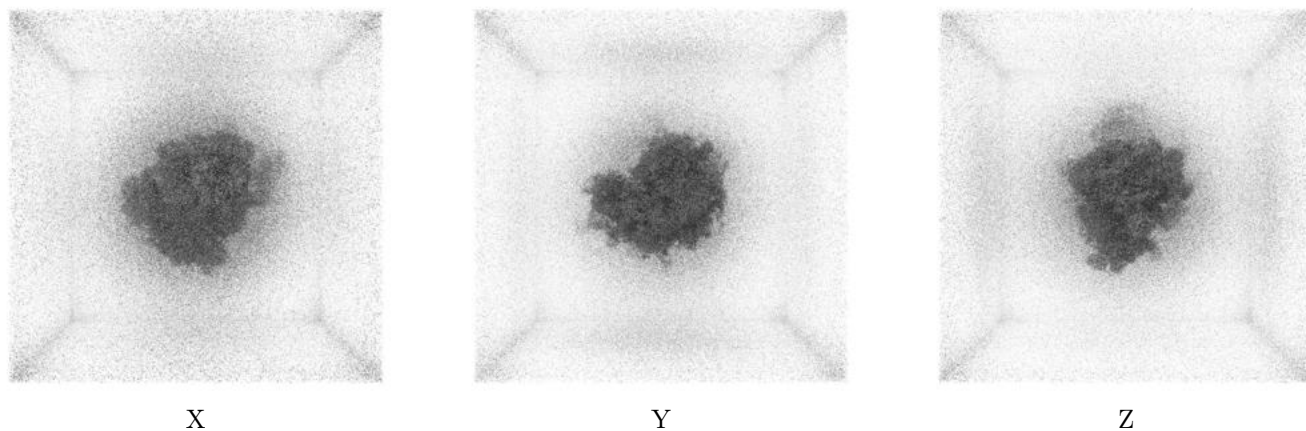
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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



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.

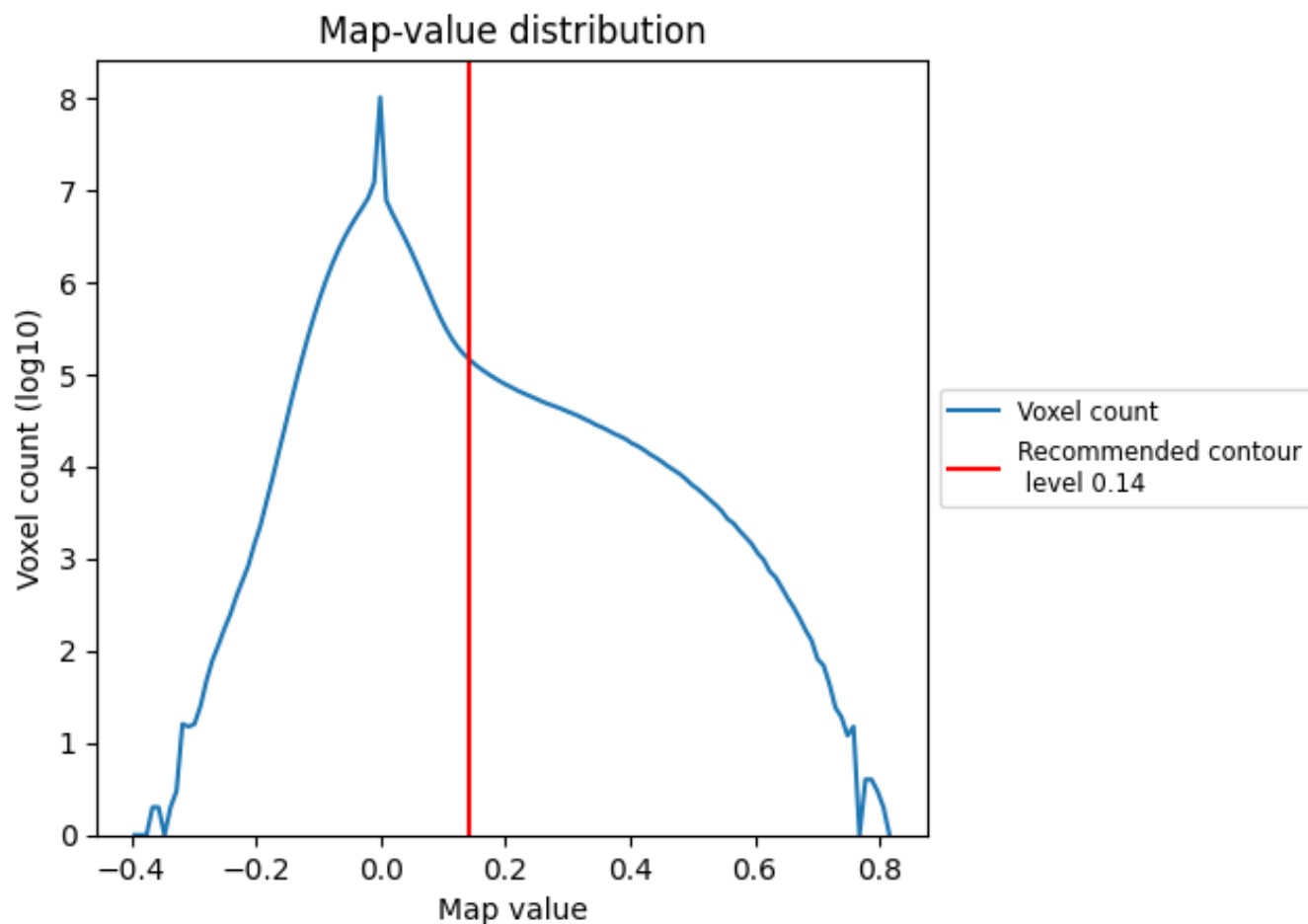
## 6.6 Mask visualisation [i](#)

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.

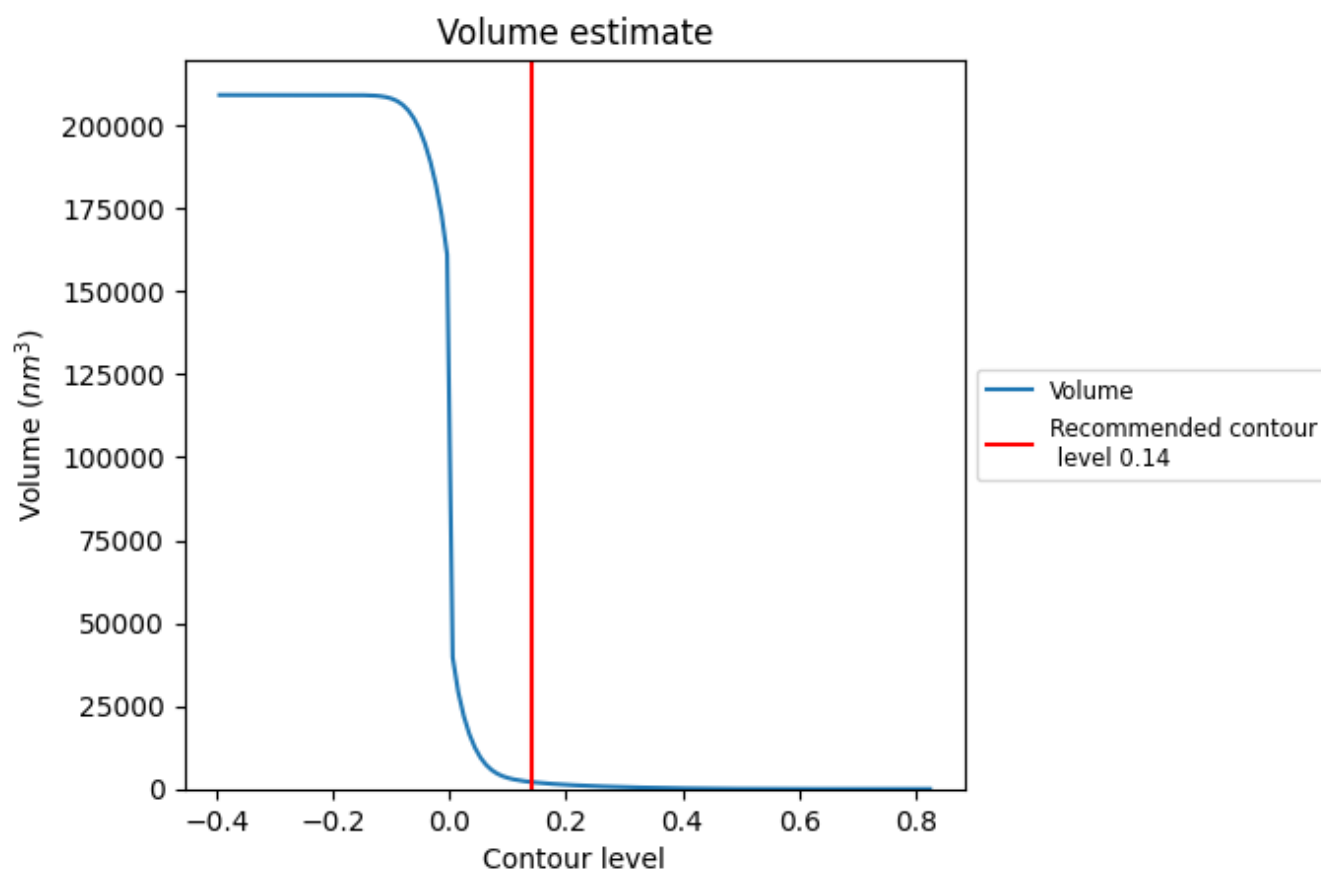
### 7.1 Map-value distribution [i](#)



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.



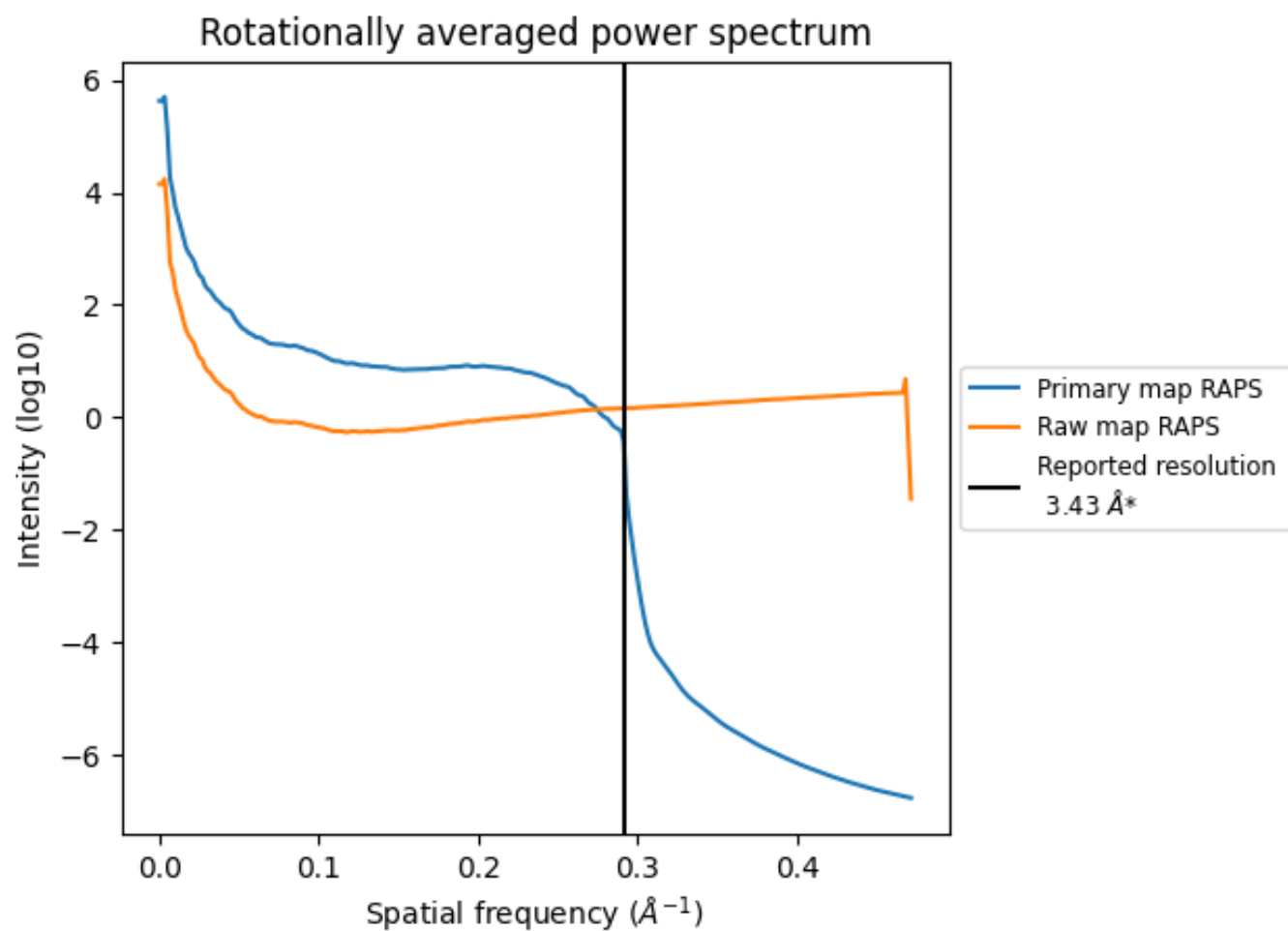
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2097  $\text{nm}^3$ ; this corresponds to an approximate mass of 1894 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

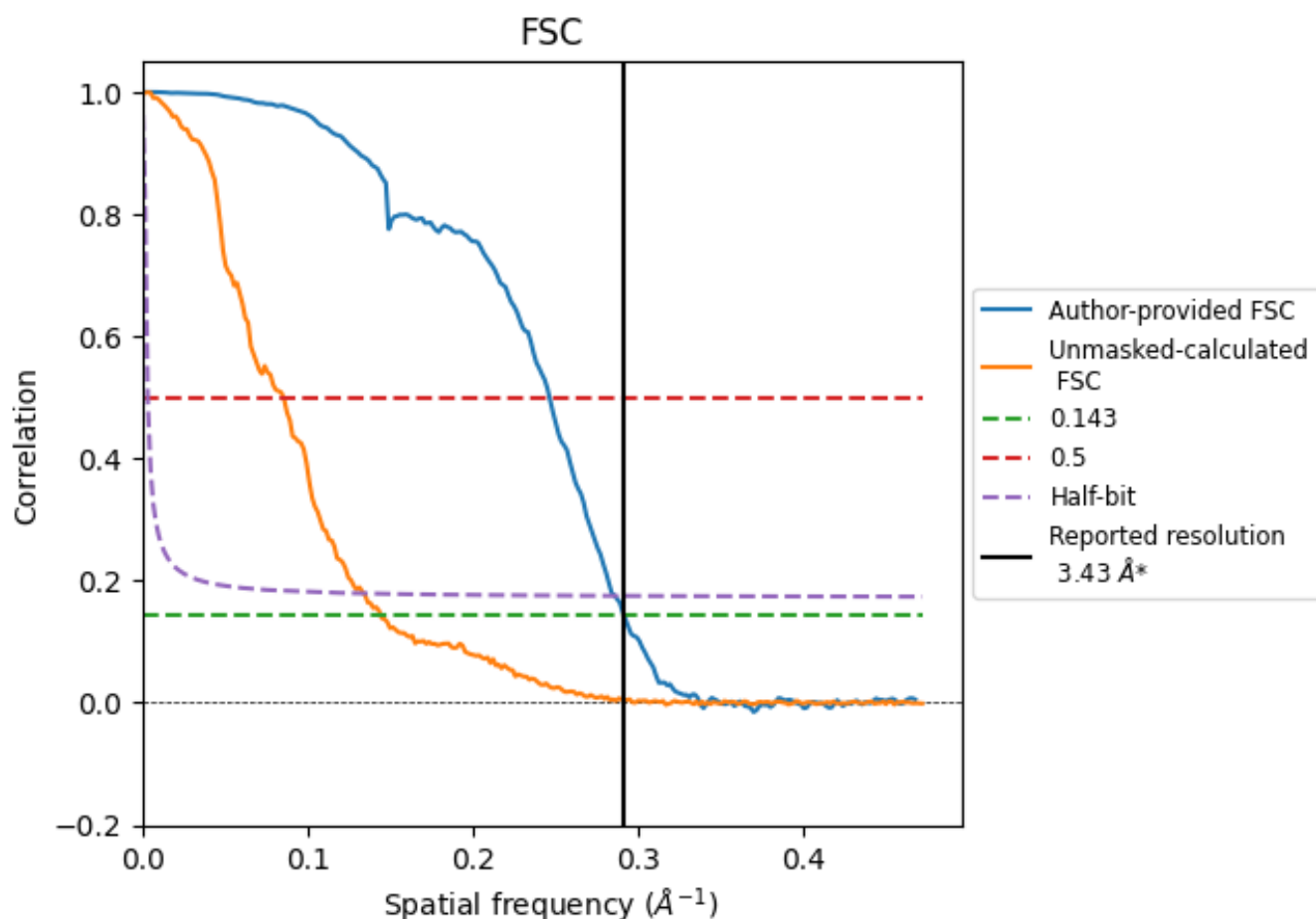


\*Reported resolution corresponds to spatial frequency of 0.292  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.292 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

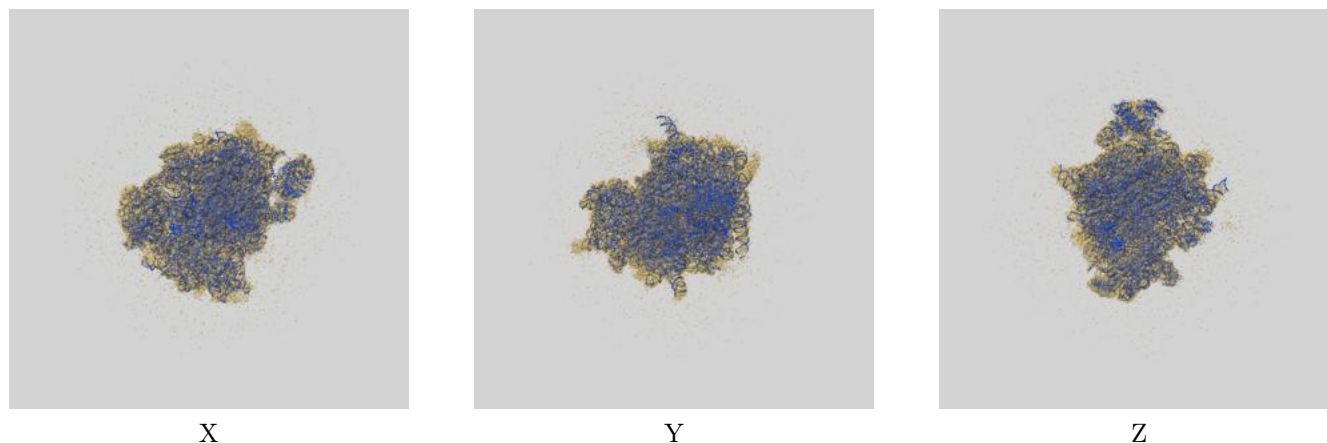
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	3.43	4.06	3.50
Unmasked-calculated*	6.93	11.72	7.47

\*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 6.93 differs from the reported value 3.43 by more than 10 %

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

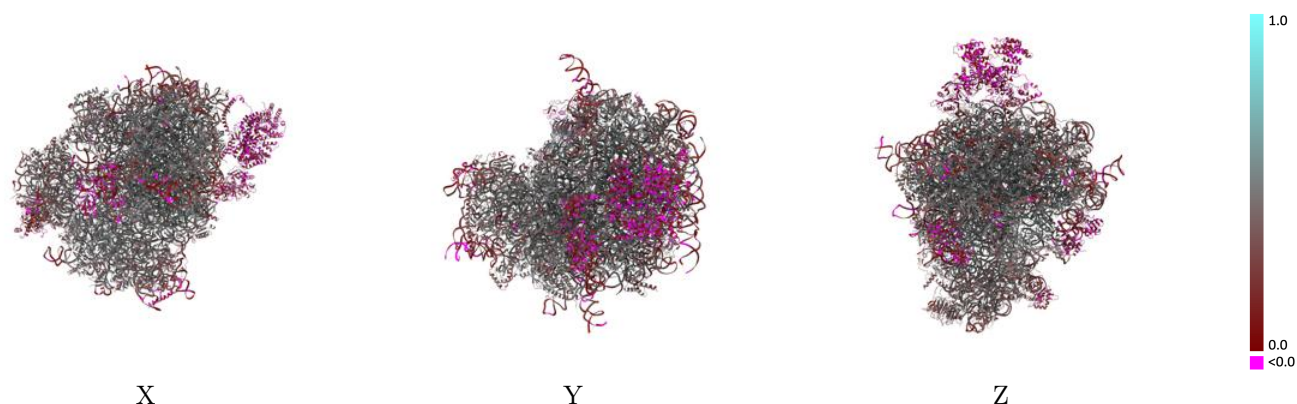
This section contains information regarding the fit between EMDB map EMD-53296 and PDB model 9QQB. Per-residue inclusion information can be found in section [3](#) on page [30](#).

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



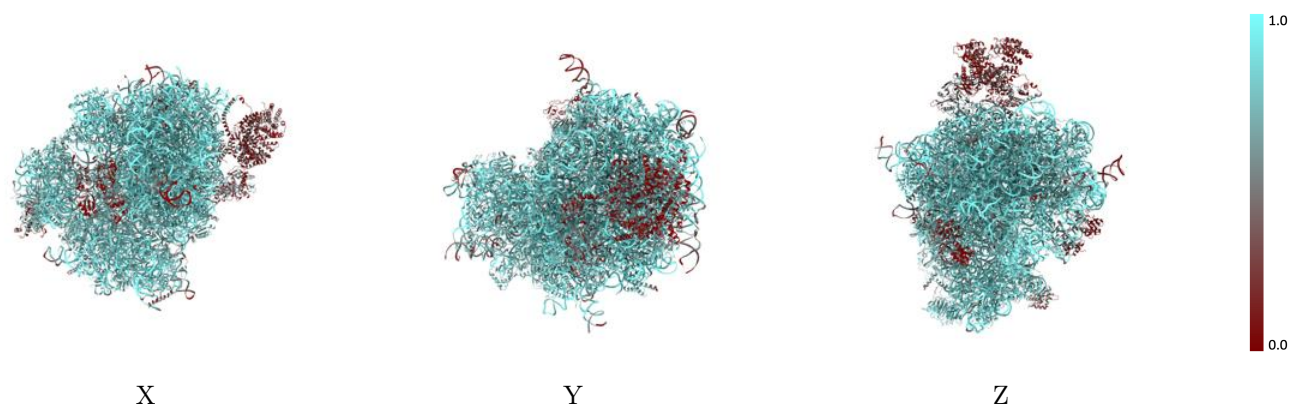
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



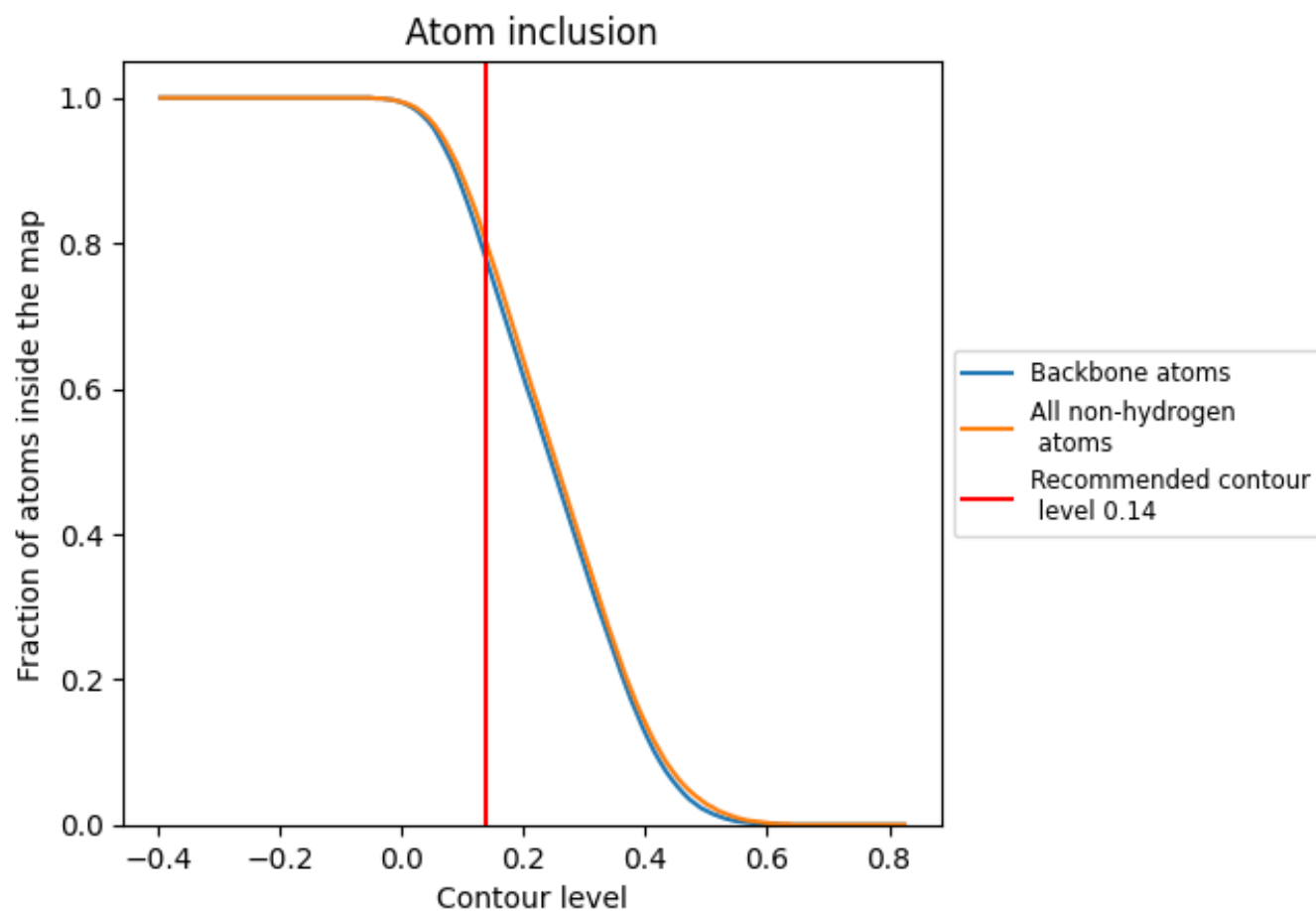
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 80% 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	 0.7990	 0.3920
A2	 0.9050	 0.4020
AA	 0.7840	 0.4090
AB	 0.6960	 0.4110
AC	 0.3130	 0.1190
AD	 0.6840	 0.3950
AE	 0.8150	 0.4490
AF	 0.7530	 0.3270
AG	 0.8030	 0.4080
AT	 0.6590	 0.3300
AZ	 0.8120	 0.4230
Aa	 0.7580	 0.4170
Ab	 0.7970	 0.4460
Ac	 0.7300	 0.3720
Ad	 0.8190	 0.4360
Ae	 0.7400	 0.4010
Af	 0.7430	 0.3410
Ag	 0.7480	 0.3750
Ah	 0.7710	 0.4340
Ai	 0.8120	 0.4310
Aj	 0.7570	 0.3430
Ak	 0.7260	 0.4320
Al	 0.3820	 0.1540
Am	 0.7890	 0.4380
An	 0.7630	 0.4280
Ao	 0.7210	 0.3370
Ap	 0.8050	 0.4200
Aq	 0.7540	 0.3840
Ar	 0.7650	 0.3740
As	 0.8070	 0.3930
At	 0.7410	 0.3810
Au	 0.8100	 0.4390
Av	 0.8000	 0.4750
Aw	 0.8050	 0.4680
Ax	 0.8090	 0.4050



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Chain	Atom inclusion	Q-score
Ay	 0.6730	 0.3460
Az	 0.7890	 0.4760
B5	 0.8930	 0.4090
B7	 0.9750	 0.4620
B8	 0.9340	 0.4360
BA	 0.7910	 0.4850
BB	 0.8210	 0.4780
BC	 0.8280	 0.4760
BD	 0.8370	 0.4400
BE	 0.7810	 0.4100
BF	 0.8150	 0.4730
BG	 0.7680	 0.4180
BH	 0.8110	 0.4590
BI	 0.7830	 0.4580
BJ	 0.7980	 0.4300
BK	 0.3330	 0.2880
BL	 0.8040	 0.4470
BM	 0.8280	 0.4470
BN	 0.8500	 0.4980
BO	 0.8280	 0.4760
BP	 0.7900	 0.4710
BQ	 0.8310	 0.4900
BR	 0.7960	 0.4330
BS	 0.8350	 0.4780
BT	 0.7980	 0.4660
BU	 0.7750	 0.3960
BV	 0.7390	 0.4560
BW	 0.6200	 0.3080
BX	 0.7910	 0.4540
BY	 0.7870	 0.4580
BZ	 0.8260	 0.4460
Ba	 0.8710	 0.4900
Bb	 0.7230	 0.3860
Bc	 0.7360	 0.4080
Bd	 0.7930	 0.4610
Be	 0.8130	 0.4820
Bf	 0.8320	 0.4880
Bg	 0.7900	 0.4500
Bh	 0.8120	 0.4430
Bi	 0.7780	 0.4250
Bj	 0.8860	 0.4960
Bk	 0.7680	 0.3970

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Chain	Atom inclusion	Q-score
Bl	 0.7960	 0.4690
Bm	 0.7920	 0.4640
Bo	 0.8060	 0.4670
Bp	 0.7720	 0.4630
Br	 0.8280	 0.4670
Bs	 0.1180	 0.0830
Bt	 0.1250	 0.0630
Bv	 0.1120	 0.0800
MA	 0.4410	 0.1180
Nt	 0.1820	 0.0790
Nu	 0.3500	 0.1910
XA	 0.2050	 0.0750
XB	 0.1720	 0.0640