



wwPDB EM Validation Summary Report ⓘ

Jun 19, 2026 – 06:32 am BST

PDB ID : 8BTK / pdb_00008btk
EMDB ID : EMD-16232
Title : Structure of the TRAP complex with the Sec translocon and a translating ribosome
Authors : Jaskolowski, M.; Jomaa, A.; Gamberdinger, M.; Shrestha, S.; Leibundgut, M.; Deuerling, E.; Ban, N.
Deposited on : 2022-11-29
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

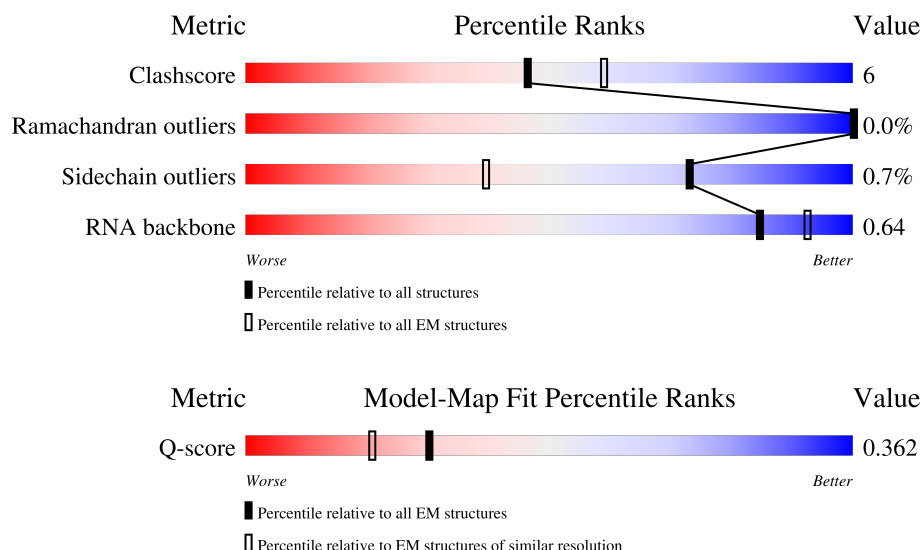
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



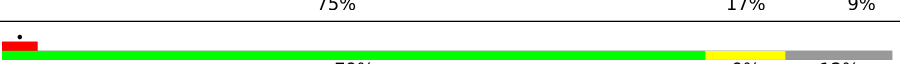
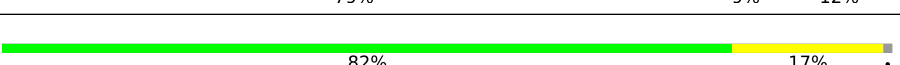
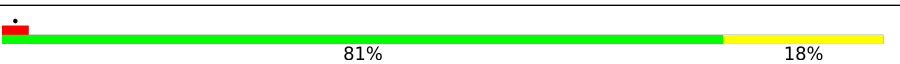
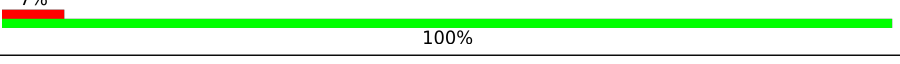
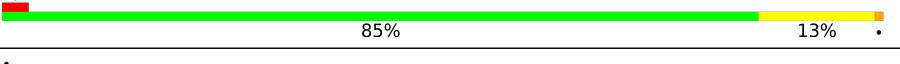
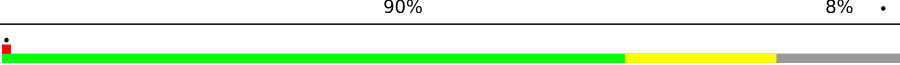
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B5	4808	
2	B7	120	
3	B8	158	

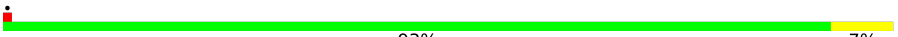
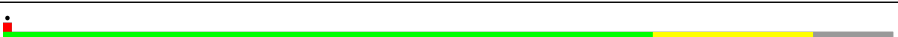
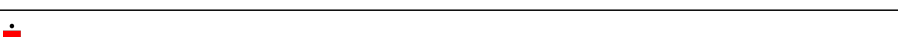
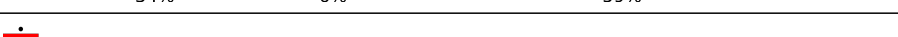
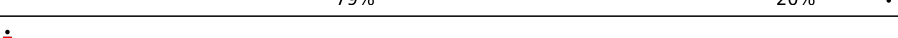
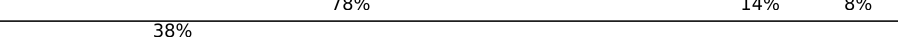
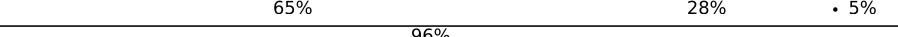
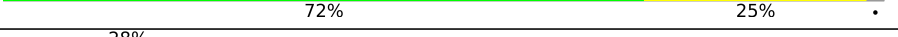
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Mol	Chain	Length	Quality of chain
4	BA	257	
5	BB	403	
6	BC	413	
7	BD	297	
8	BE	291	
9	BF	247	
10	BG	266	
11	BH	192	
12	BI	214	
13	BJ	178	
14	BK	29	
15	BL	211	
16	BM	218	
17	BN	204	
18	BO	203	
19	BP	184	
20	BQ	188	
21	BR	196	
22	BS	176	
23	BT	160	
24	BU	128	
25	BV	140	
26	BW	157	
27	BX	156	
28	BY	145	

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Mol	Chain	Length	Quality of chain
29	BZ	136	
30	Ba	148	
31	Bb	245	
32	Bc	115	
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	SX	476	
50	SY	68	
51	SZ	96	
52	A2	1870	
53	AA	84	

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Mol	Chain	Length	Quality of chain
54	AB	69	
55	AC	156	
56	AD	133	
57	AE	115	
58	AF	317	
59	AG	56	
60	AH	4	
61	AT	75	
62	AZ	295	
63	Aa	264	
64	Ab	293	
65	Ac	281	
66	Ad	263	
67	Ae	204	
68	Af	249	
69	Ag	432	
70	Ah	208	
71	Ai	194	
72	Aj	165	
73	Ak	158	
74	Al	132	
75	Am	151	
76	An	151	
77	Ao	145	
78	Ap	172	

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Mol	Chain	Length	Quality of chain
79	Aq	135	
80	Ar	152	
81	As	145	
82	At	119	
83	Au	83	
84	Av	130	
85	Aw	143	
86	Ax	130	
87	Ay	124	
88	Az	25	
89	TA	286	
90	TB	183	
91	TC	185	
92	TD	173	

2 Entry composition

There are 98 unique types of molecules in this entry. The entry contains 233722 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	119	Total	C	N	O	P	0	0
			2538	1131	451	837	119		

- 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 60S ribosomal protein L8.

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 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BC	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 7 is a protein called Ribosomal_L18_c domain-containing protein.

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 uL30,60S ribosomal protein L7.

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

- 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 are 2 discrepancies between the modelled and reference sequences:

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

- 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 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 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	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 15 is a protein called L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BL	210	Total	C	N	O	S	0	0
			1701	1065	354	278	4		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 16 is a protein called 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 60S ribosomal protein L13a.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	174	LEU	ILE	conflict	UNP A0A0N8ETI8
BO	194	ASP	GLU	conflict	UNP A0A0N8ETI8

- Molecule 19 is a protein called 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 60S ribosomal protein L19.

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

- Molecule 22 is a protein called 60S ribosomal protein L18a.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BS	1	MET	THR	conflict	UNP G1TTY7

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Chain	Residue	Modelled	Actual	Comment	Reference
BS	18	PRO	-	insertion	UNP G1TTY7
BS	19	THR	-	insertion	UNP G1TTY7
BS	20	PRO	SER	conflict	UNP G1TTY7
BS	49	SER	LEU	conflict	UNP G1TTY7
BS	50	GLN	GLU	conflict	UNP G1TTY7
BS	95	ARG	HIS	conflict	UNP G1TTY7
BS	101	THR	ILE	conflict	UNP G1TTY7
BS	102	THR	MET	conflict	UNP G1TTY7
BS	104	GLY	SER	conflict	UNP G1TTY7
BS	138	ARG	PRO	conflict	UNP G1TTY7
BS	168	SER	TYR	conflict	UNP G1TTY7

- 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	conflict	UNP G1TSG1
BU	36	ALA	GLU	conflict	UNP G1TSG1
BU	39	PHE	SER	conflict	UNP G1TSG1
BU	54	GLY	ARG	conflict	UNP G1TSG1
BU	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 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 Ribosomal_L23eN domain-containing protein.

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 eL30.

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 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 eL32.

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	88	Total	C	N	O	S	0	0
			721	443	160	113	5		

- Molecule 40 is a protein called eL38.

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	conflict	UNP G1U001

- Molecule 41 is a protein called eL39.

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.

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 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 eL43.

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 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Br	126	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	103	ARG	HIS	conflict	UNP G1U7L1

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

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 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 Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SX	425	Total	C	N	O	S	0	0
			3317	2186	534	576	21		

- Molecule 50 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SY	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 51 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SZ	29	Total	C	N	O	S	0	0
			229	157	36	34	2		

- Molecule 52 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	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 53 is a protein called 40S ribosomal protein S27.

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

- Molecule 54 is a protein called Ribosomal protein S28.

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

- Molecule 55 is a protein called Ribosomal protein S27a.

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

- Molecule 56 is a protein called 40S ribosomal protein S30.

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

- Molecule 57 is a protein called eS26.

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

- Molecule 58 is a protein called RACK1.

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

- Molecule 59 is a protein called uS14.

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

- Molecule 60 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AH	4	Total	C	N	O	P	0	0
			66	28	11	23	4		

- Molecule 61 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AT	75	Total	C	N	O	P	0	0
			1597	713	279	530	75		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AZ	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 63 is a protein called 40S ribosomal protein S3a.

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

- Molecule 64 is a protein called Ribosomal_S5_C domain-containing protein,40S ribosomal protein S2.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	2	ALA	VAL	conflict	UNP A0A5F9D8I1
Ab	36	ARG	CYS	conflict	UNP A0A5F9D8I1
Ab	38	ARG	GLY	conflict	UNP A0A5F9D8I1
Ab	39	GLY	LYS	conflict	UNP A0A5F9D8I1
Ab	40	ARG	ALA	conflict	UNP A0A5F9D8I1

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Chain	Residue	Modelled	Actual	Comment	Reference
Ab	42	ARG	ASP	conflict	UNP A0A5F9D8I1
Ab	73	MET	VAL	conflict	UNP G1TUT9
Ab	119	GLY	ALA	conflict	UNP G1TUT9
Ab	194	ARG	HIS	conflict	UNP G1TUT9
Ab	215	MET	LEU	conflict	UNP G1TUT9
Ab	227	ARG	TRP	conflict	UNP G1TUT9
Ab	228	GLY	SER	conflict	UNP G1TUT9

- Molecule 65 is a protein called 40S ribosomal protein S3.

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

- Molecule 66 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	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	conflict	UNP G1TK17
Ad	51	ARG	LYS	conflict	UNP G1TK17
Ad	78	THR	ALA	conflict	UNP G1TK17
Ad	156	VAL	MET	conflict	UNP G1TK17

- Molecule 67 is a protein called Ribosomal protein S5.

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

- Molecule 68 is a protein called 40S ribosomal protein S6.

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

- Molecule 69 is a protein called 40S ribosomal protein S7.

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

- Molecule 70 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	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	conflict	UNP G1TJW1

- Molecule 71 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 72 is a protein called Ribosomal protein eS10.

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

- Molecule 73 is a protein called 40S ribosomal protein S11.

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

- Molecule 74 is a protein called 40S ribosomal protein S12.

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

- Molecule 75 is a protein called uS15.

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

- Molecule 76 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	136	Total	C	N	O	S	0	0
			1017	622	199	190	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	5F0	ASP	conflict	UNP G1U472

- Molecule 77 is a protein called 40S ribosomal protein uS19.

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

- Molecule 78 is a protein called uS9.

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

- Molecule 79 is a protein called 40S ribosomal protein eS17.

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

- Molecule 80 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ar	148	Total	C	N	O	S	0	0
			1217	763	245	208	1		

- Molecule 81 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	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	conflict	UNP G1TN62
As	142	ASN	LYS	conflict	UNP G1TN62

- Molecule 82 is a protein called 40S ribosomal protein uS10.

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

- Molecule 83 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Au	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Au	3	ASN	SER	conflict	UNP G1TM82
Au	4	ASP	ASN	conflict	UNP G1TM82
Au	33	GLN	PRO	conflict	UNP G1TM82
Au	50	PHE	SER	conflict	UNP G1TM82

- Molecule 84 is a protein called Ribosomal protein S15a.

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

- Molecule 85 is a protein called 40S ribosomal protein S23.

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

- Molecule 86 is a protein called 40S ribosomal protein S24.

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

- Molecule 87 is a protein called 40S ribosomal protein S25.

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

- Molecule 88 is a protein called 60S ribosomal protein L41.

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

- Molecule 89 is a protein called Translocon-associated protein subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	TA	172	Total	C	N	O	S	0	0
			1372	888	219	261	4		

- Molecule 90 is a protein called Translocon-associated protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	TB	161	Total	C	N	O	S	0	0
			1254	807	210	235	2		

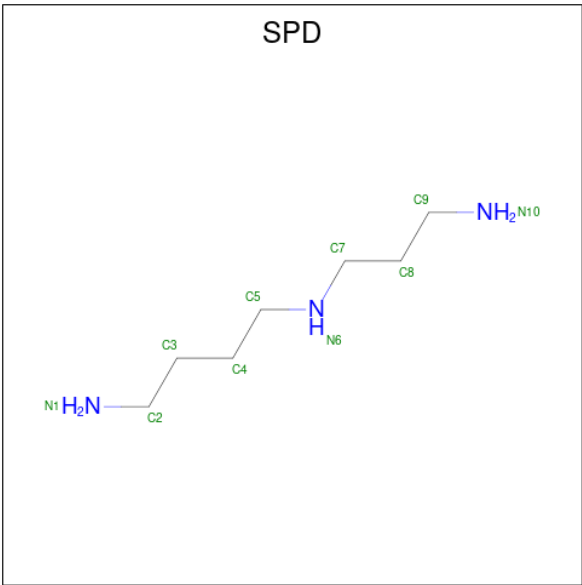
- Molecule 91 is a protein called Signal sequence receptor subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	TC	160	Total	C	N	O	S	0	0
			1295	853	212	227	3		

- Molecule 92 is a protein called Translocon-associated protein subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	TD	150	Total	C	N	O	S	0	0
			1185	755	199	228	3		

- Molecule 93 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



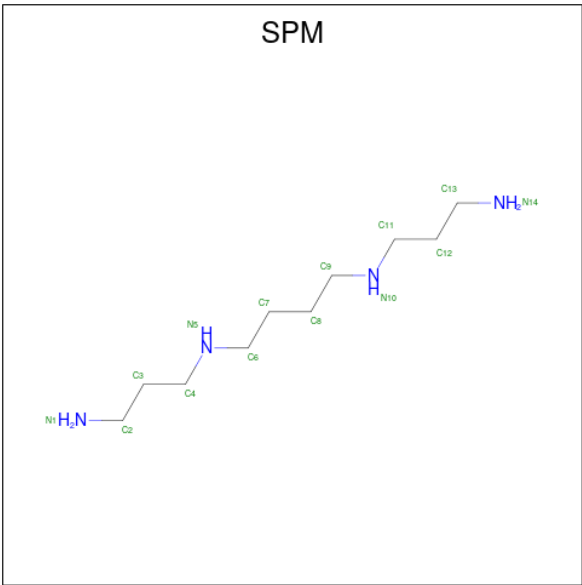
Mol	Chain	Residues	Atoms			AltConf
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N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

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Mol	Chain	Residues	Atoms			AltConf
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	B5	1	Total	C	N	0
			10	7	3	
93	BN	1	Total	C	N	0
			10	7	3	
93	A2	1	Total	C	N	0
			10	7	3	
93	A2	1	Total	C	N	0
			10	7	3	
93	A2	1	Total	C	N	0
			10	7	3	
93	A2	1	Total	C	N	0
			10	7	3	
93	A2	1	Total	C	N	0
			10	7	3	
93	A2	1	Total	C	N	0
			10	7	3	
93	A2	1	Total	C	N	0
			10	7	3	

- Molecule 94 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



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

- Molecule 95 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
95	B5	510	Total	Mg	0
			510	510	
95	B7	15	Total	Mg	0
			15	15	
95	B8	16	Total	Mg	0
			16	16	
95	BA	4	Total	Mg	0
			4	4	
95	BB	3	Total	Mg	0
			3	3	
95	BC	1	Total	Mg	0
			1	1	
95	BH	1	Total	Mg	0
			1	1	
95	BI	2	Total	Mg	0
			2	2	
95	BL	1	Total	Mg	0
			1	1	

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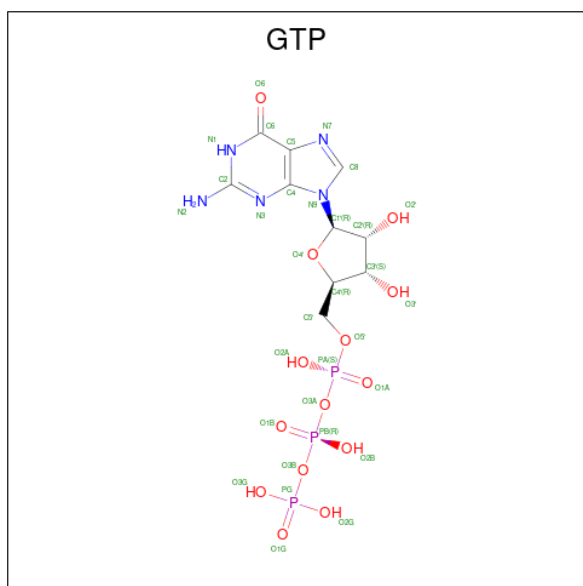
Mol	Chain	Residues	Atoms		AltConf
95	BN	1	Total 1	Mg 1	0
95	BP	1	Total 1	Mg 1	0
95	BQ	2	Total 2	Mg 2	0
95	BR	1	Total 1	Mg 1	0
95	BT	2	Total 2	Mg 2	0
95	BV	1	Total 1	Mg 1	0
95	Ba	1	Total 1	Mg 1	0
95	Bb	1	Total 1	Mg 1	0
95	Be	2	Total 2	Mg 2	0
95	Bf	1	Total 1	Mg 1	0
95	Bj	1	Total 1	Mg 1	0
95	Bl	1	Total 1	Mg 1	0
95	Bo	1	Total 1	Mg 1	0
95	A2	167	Total 167	Mg 167	0
95	AH	1	Total 1	Mg 1	0
95	AT	7	Total 7	Mg 7	0
95	Ad	1	Total 1	Mg 1	0
95	Ae	1	Total 1	Mg 1	0
95	Ak	1	Total 1	Mg 1	0
95	An	1	Total 1	Mg 1	0
95	Ar	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
95	As	1	Total	Mg	0
			1	1	

- Molecule 96 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms				AltConf
97	BD	1	Total	C	N	O	0
			7	4	1	2	

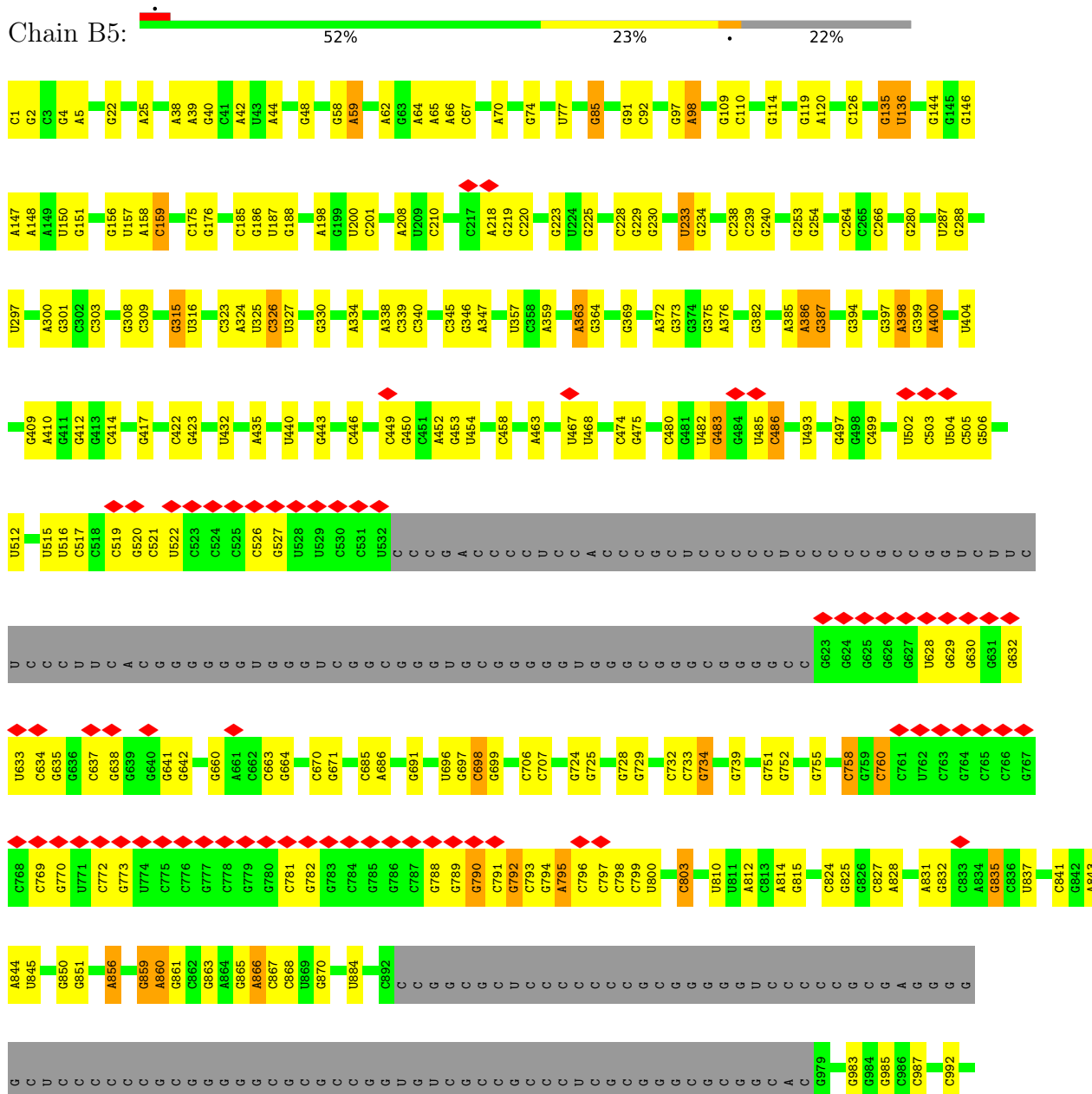
- Molecule 98 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

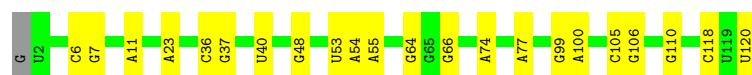
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 28S rRNA



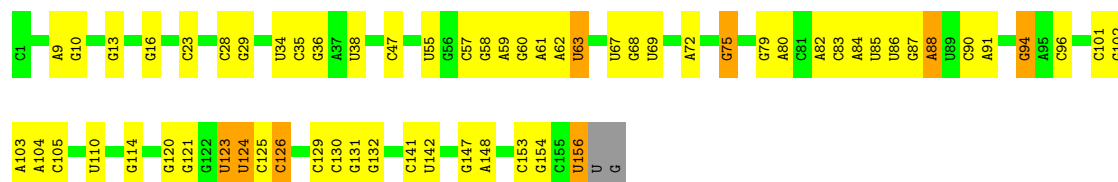






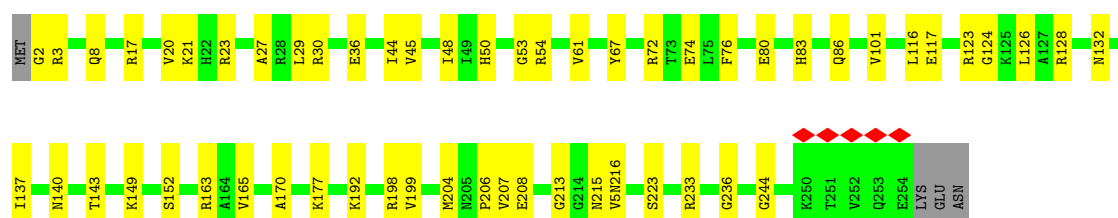
- Molecule 3: 5.8S rRNA

Chain B8: 



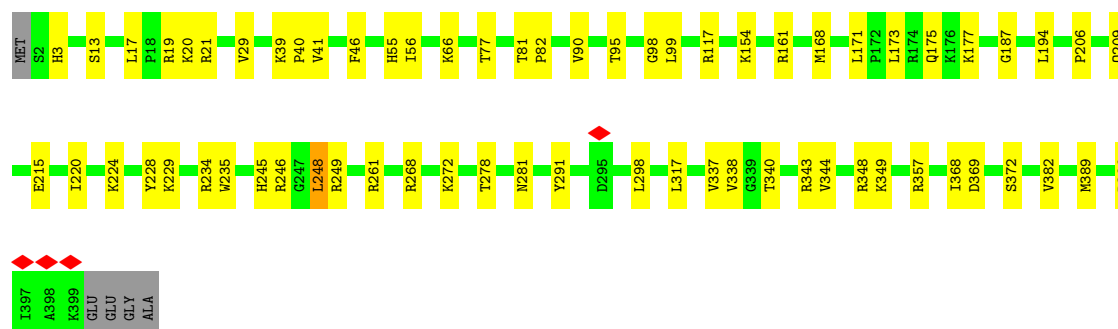
- Molecule 4: 60S ribosomal protein L8

Chain BA: 



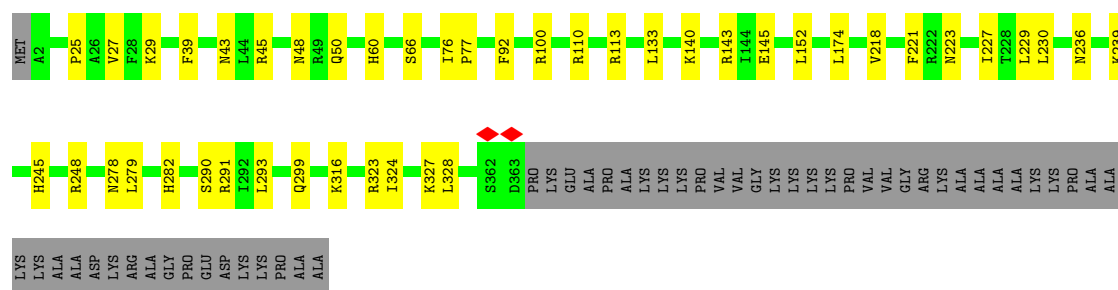
- Molecule 5: Ribosomal protein L3

Chain BB: 



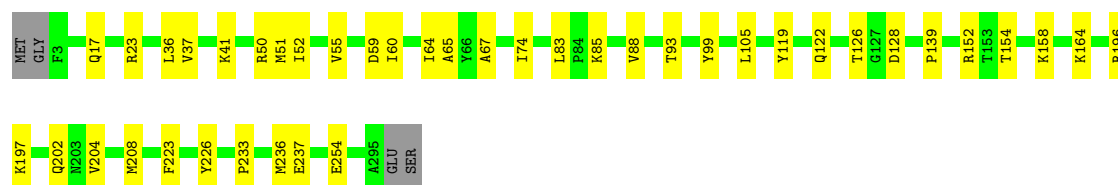
- Molecule 6: 60S ribosomal protein L4

Chain BC: 



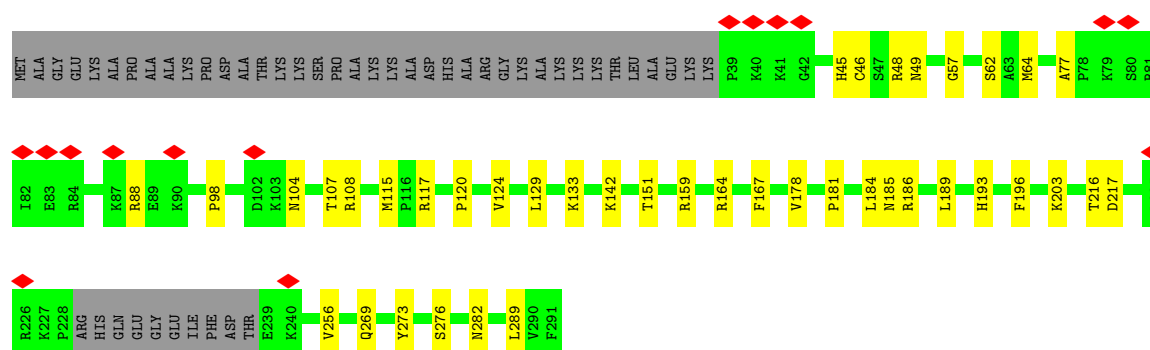
- Molecule 7: Ribosomal_L18_c domain-containing protein

Chain BD:  85% 14%



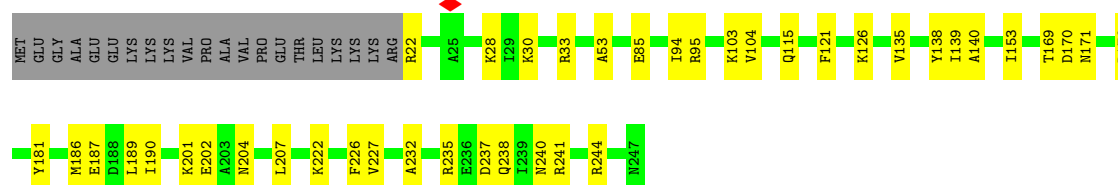
• Molecule 8: 60S ribosomal protein L6

Chain BE:  5% 69% 14% 16%



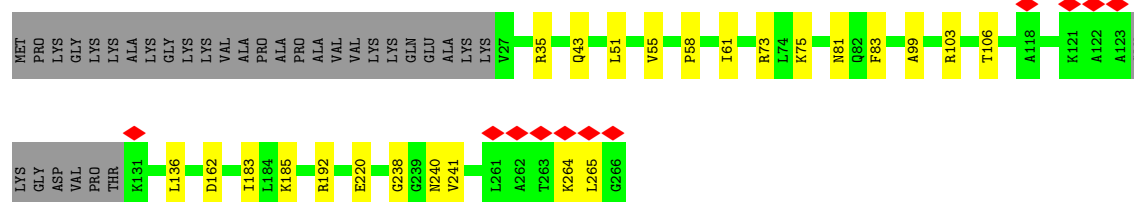
• Molecule 9: uL30,60S ribosomal protein L7

Chain BF:  75% 17% 9%



• Molecule 10: 60S ribosomal protein L7a

Chain BG:  79% 9% 12%

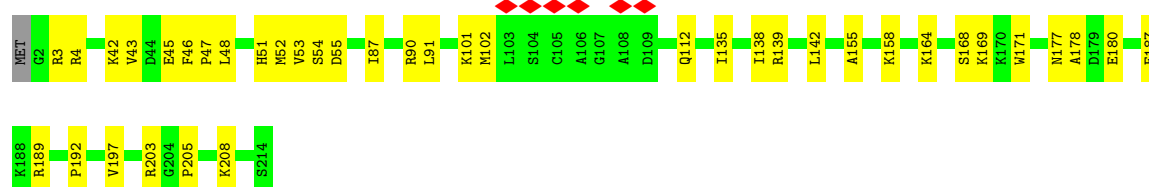
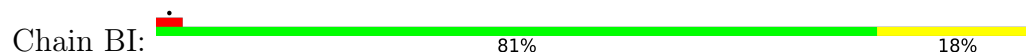


• Molecule 11: 60S ribosomal protein L9

Chain BH:  82% 17%



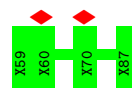
- Molecule 12: Ribosomal protein L10



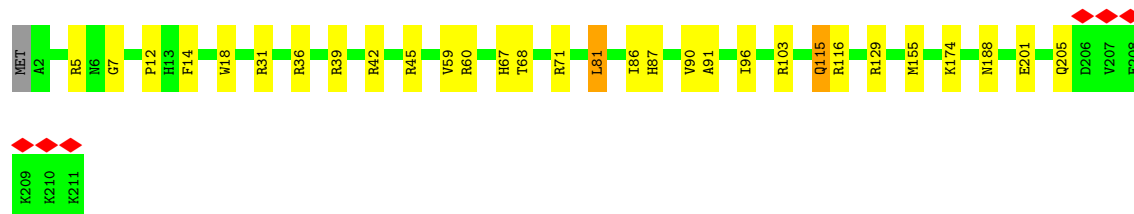
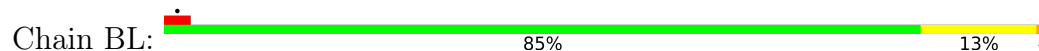
- Molecule 13: Ribosomal protein L11



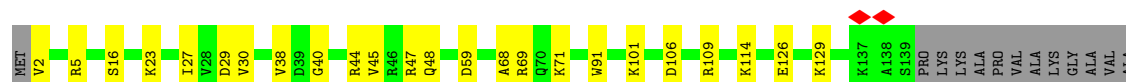
- Molecule 14: Nascent chain



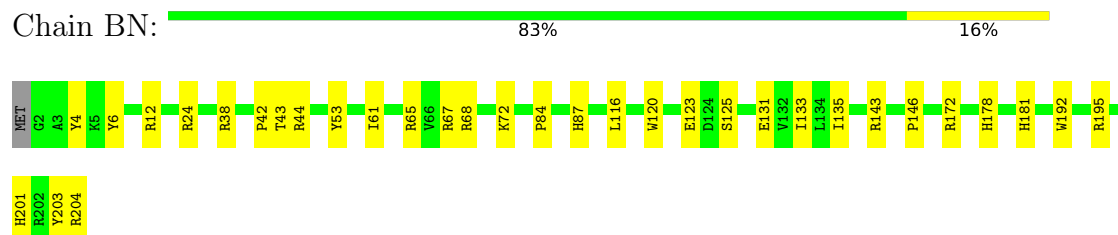
- Molecule 15: L13



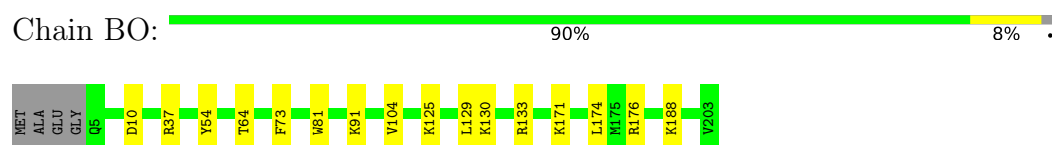
- Molecule 16: Ribosomal protein L14



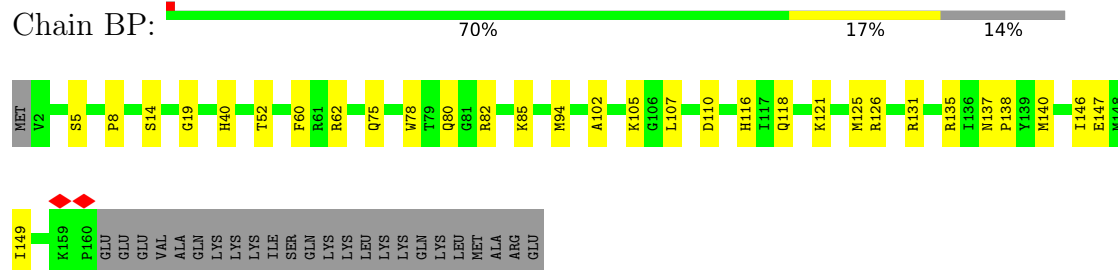
- Molecule 17: Ribosomal protein L15



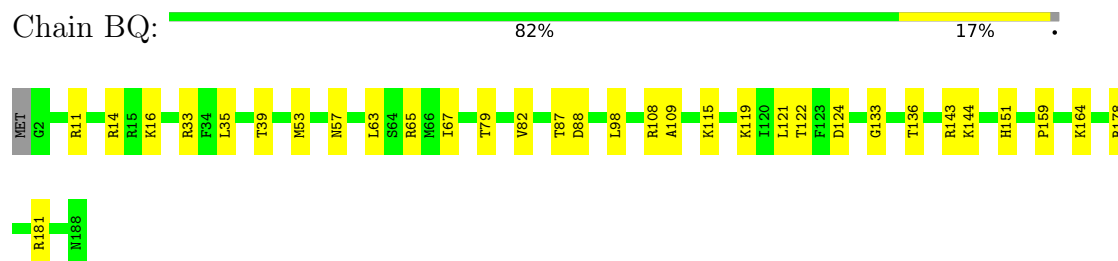
- Molecule 18: 60S ribosomal protein L13a



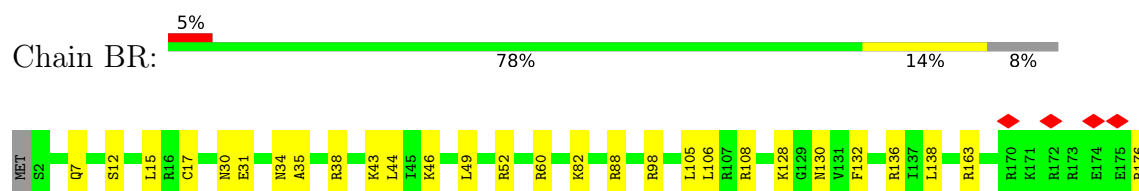
- Molecule 19: uL22

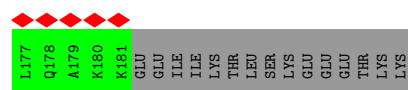


- Molecule 20: eL18



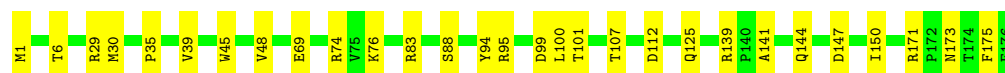
- Molecule 21: 60S ribosomal protein L19





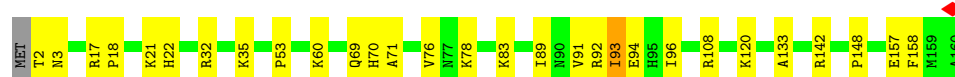
- Molecule 22: 60S ribosomal protein L18a

Chain BS: 84% 16%



- Molecule 23: 60S ribosomal protein L21

Chain BT: 81% 18%



- Molecule 24: 60S ribosomal protein L22

Chain BU: 68% 9% 23%



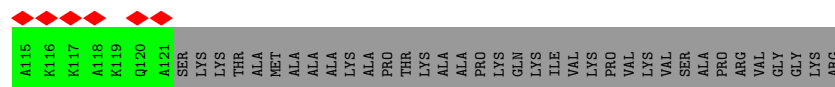
- Molecule 25: Ribosomal protein L23

Chain BV: 82% 17%



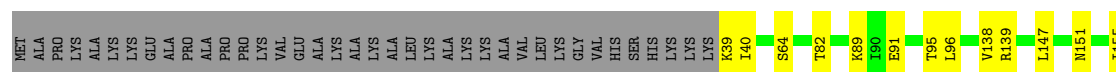
- Molecule 26: Ribosomal protein L24

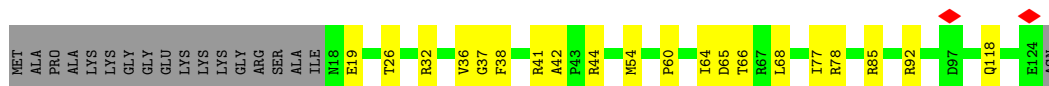
Chain BW: 31% 66% 11% 23%



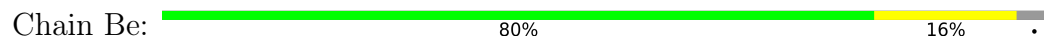
- Molecule 27: Ribosomal_L23eN domain-containing protein

Chain BX: 67% 9% 24%





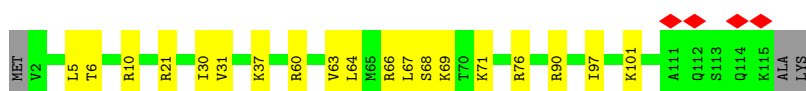
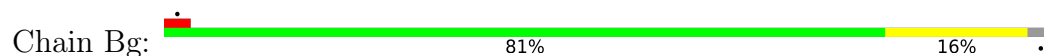
• Molecule 34: eL32



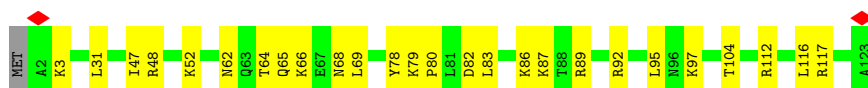
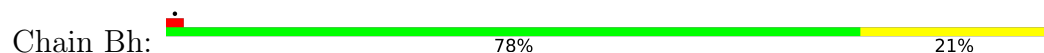
• Molecule 35: 60S ribosomal protein L35a



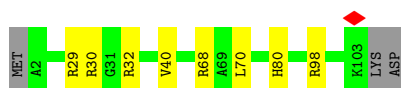
• Molecule 36: 60S ribosomal protein L34



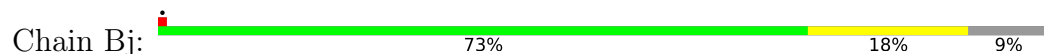
• Molecule 37: 60S ribosomal protein L35



• Molecule 38: 60S ribosomal protein L36

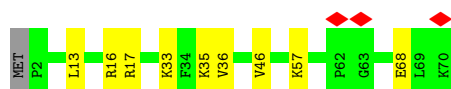


• Molecule 39: Ribosomal protein L37



• Molecule 40: eL38

Chain Bk:  86% 13%



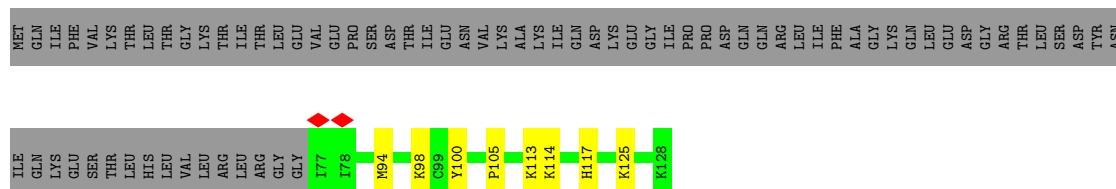
- Molecule 41: eL39

Chain Bl:  86% 12%



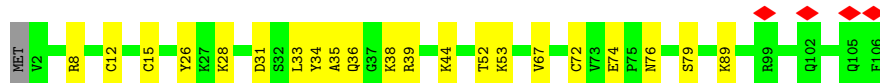
- Molecule 42: Ubiquitin

Chain Bm:  34% 6% 59%

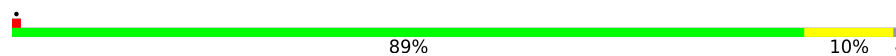


- Molecule 43: eL42

Chain Bo:  79% 20%



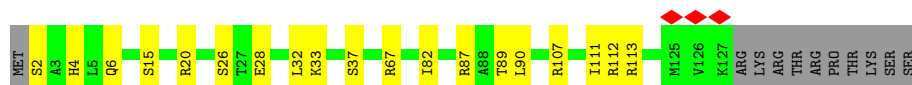
- Molecule 44: eL43

Chain Bp:  89% 10%

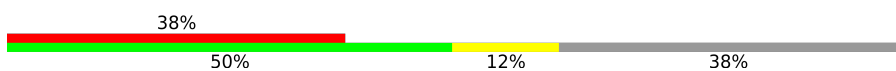


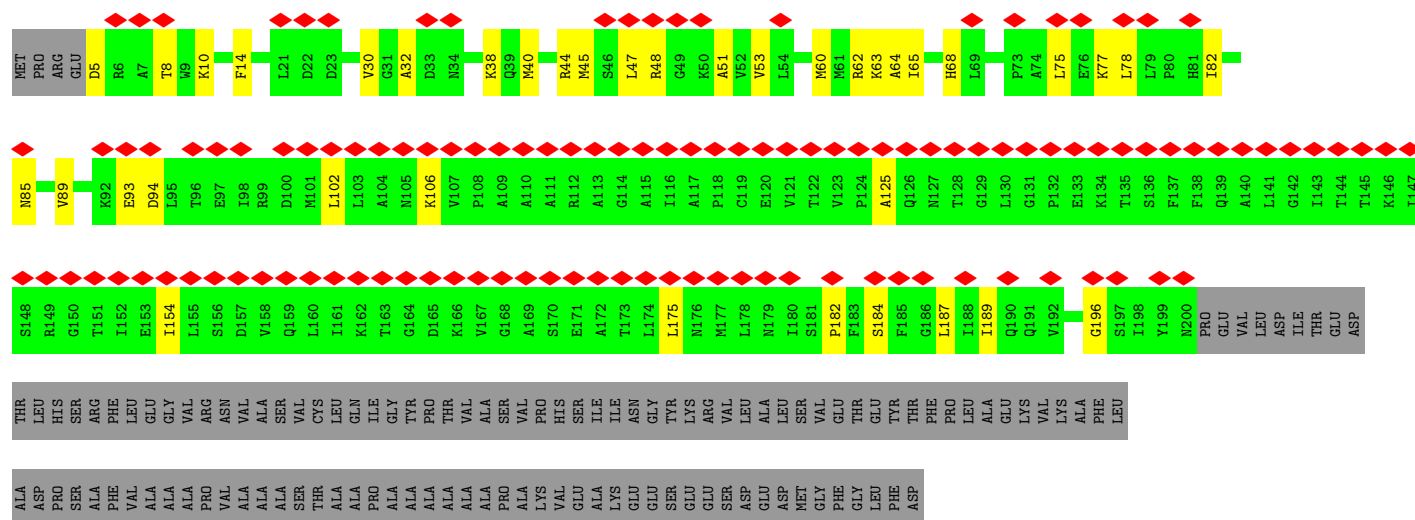
- Molecule 45: 60S ribosomal protein L28

Chain Br:  78% 14% 8%

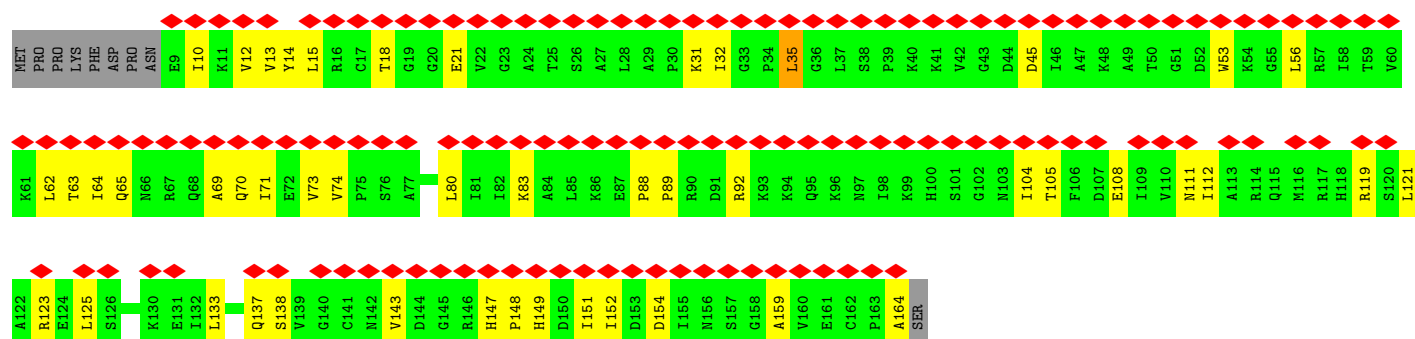
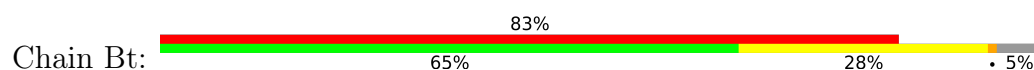


- Molecule 46: 60S acidic ribosomal protein P0

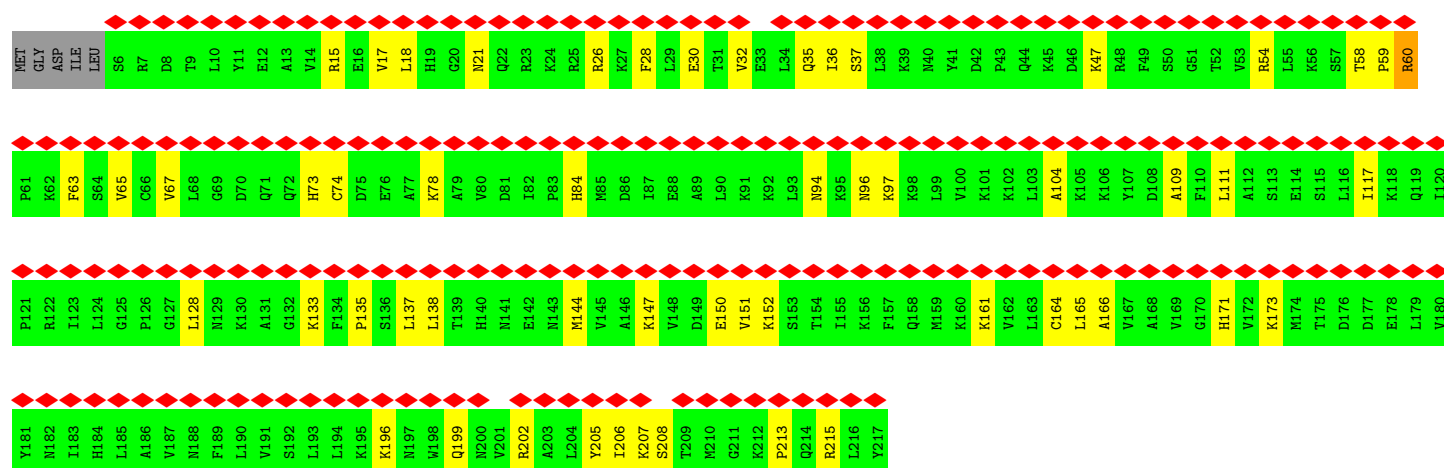
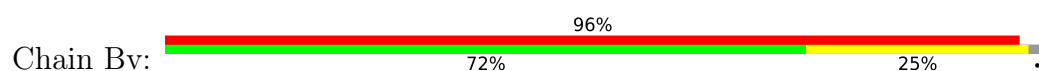
Chain Bs:  38% 50% 12% 38%



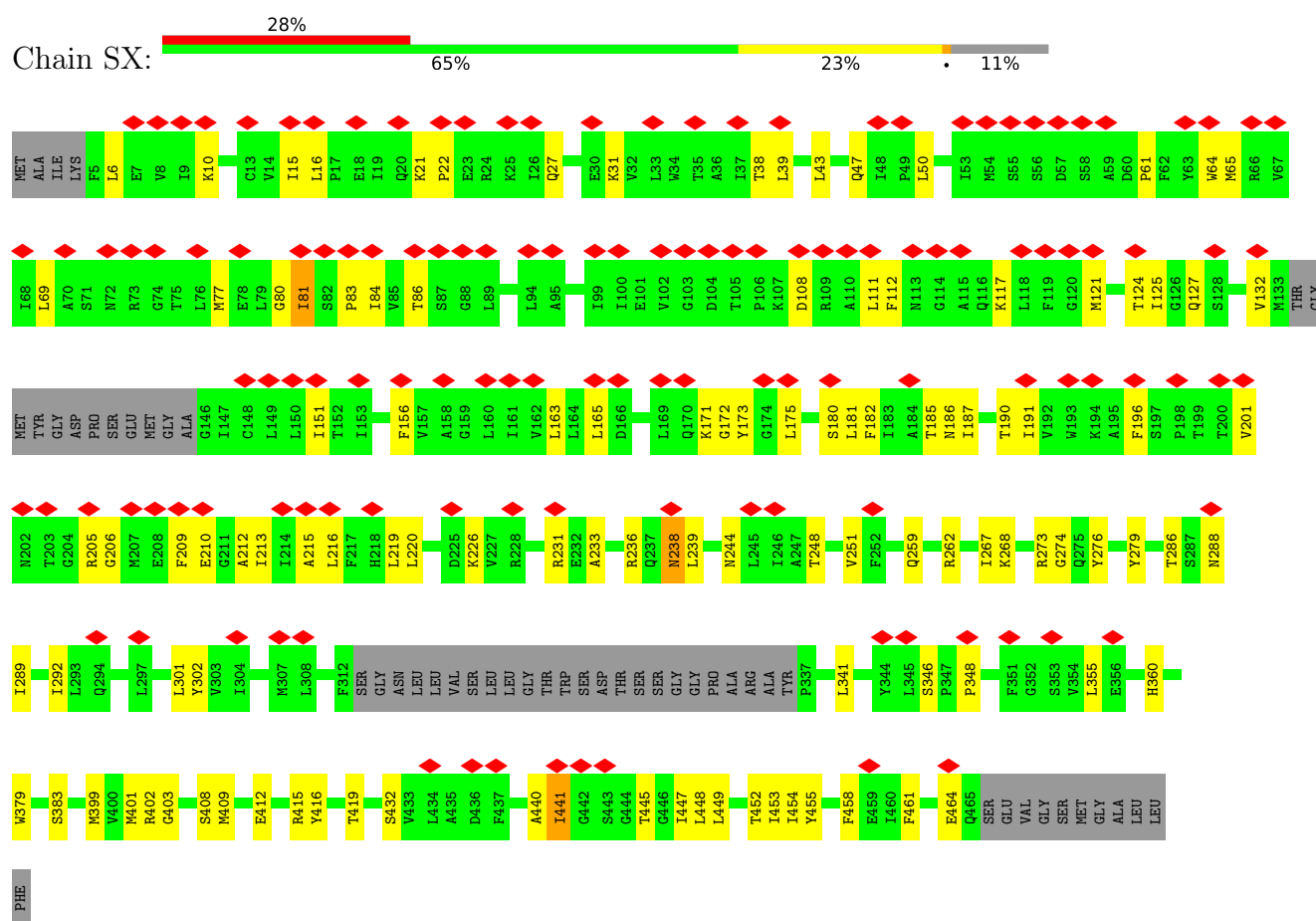
• Molecule 47: Ribosomal protein L12



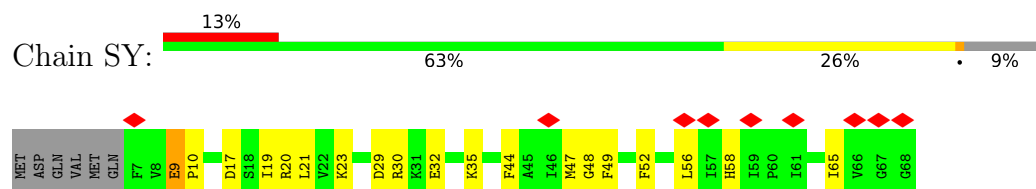
• Molecule 48: Ribosomal protein uL1



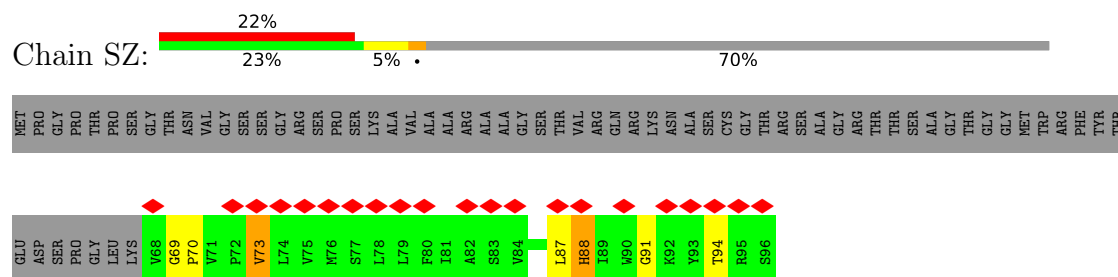
• Molecule 49: Protein transport protein Sec61 subunit alpha isoform 1



- Molecule 50: Protein transport protein Sec61 subunit gamma



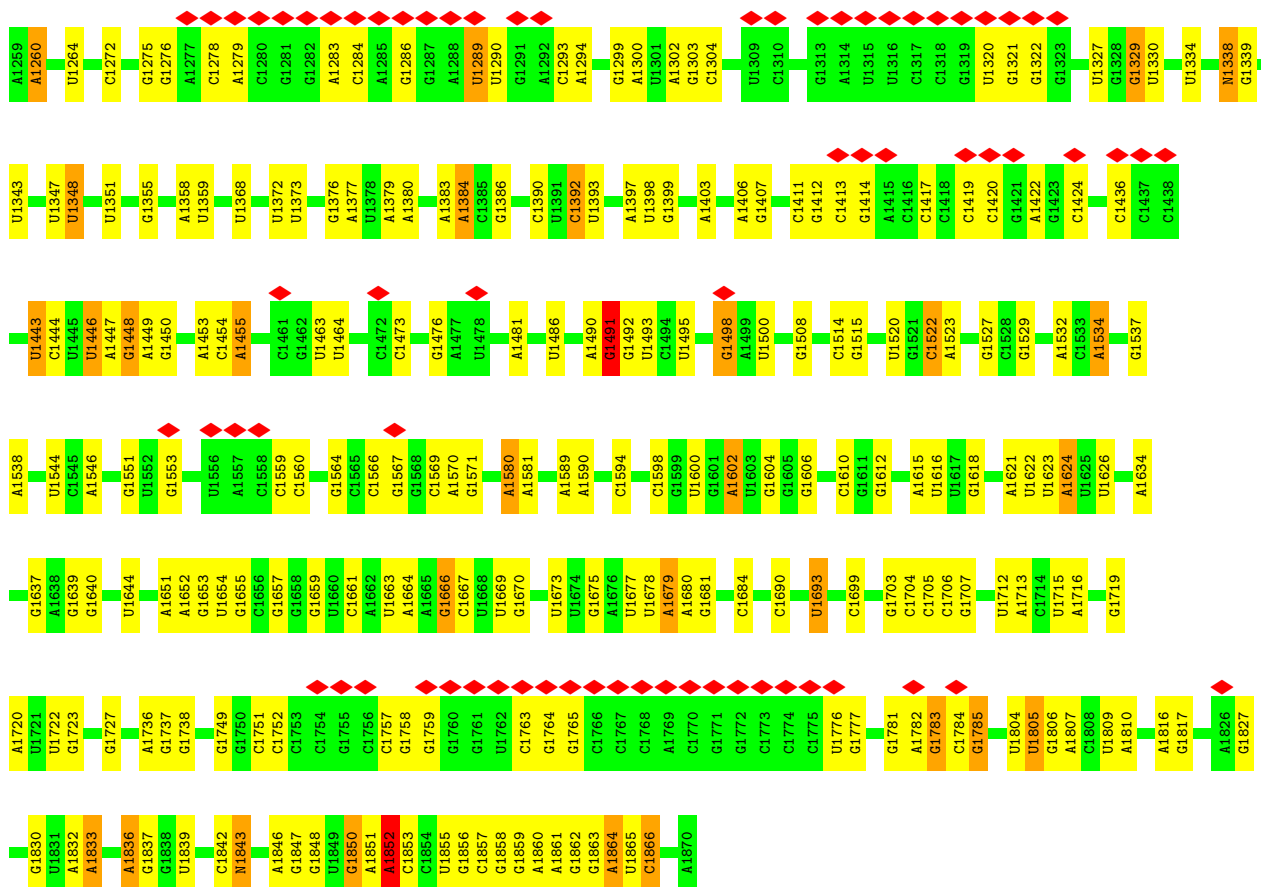
- Molecule 51: Protein transport protein Sec61 subunit beta



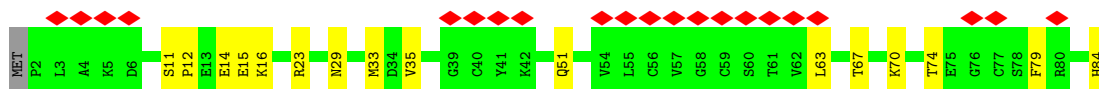
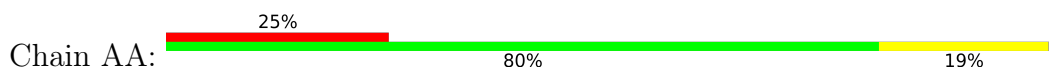
- Molecule 52: 18S rRNA



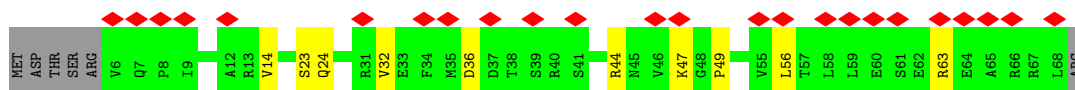
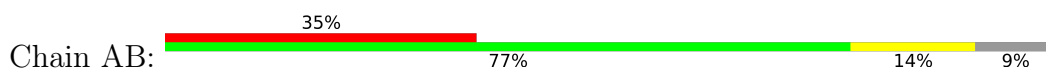




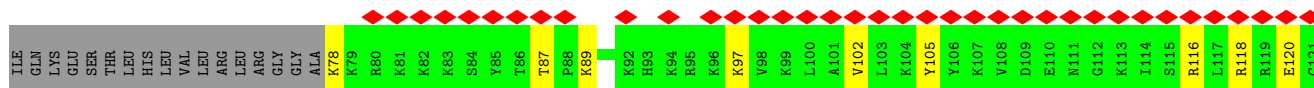
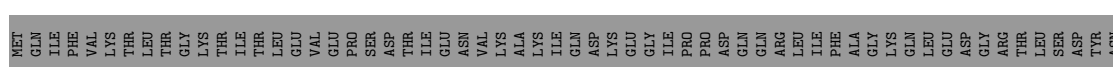
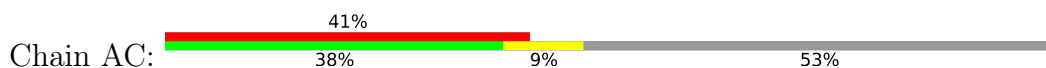
• Molecule 53: 40S ribosomal protein S27

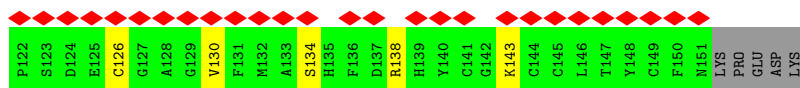


• Molecule 54: Ribosomal protein S28

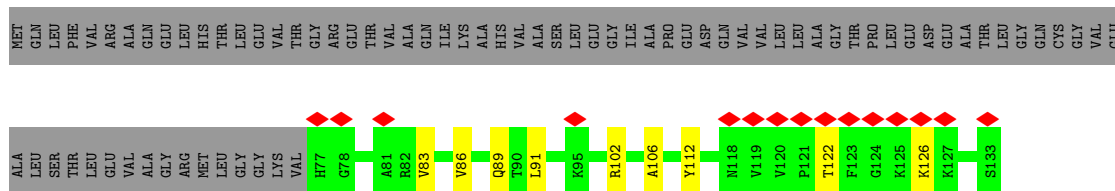
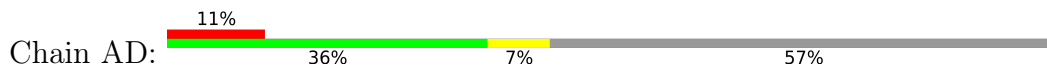


• Molecule 55: Ribosomal protein S27a

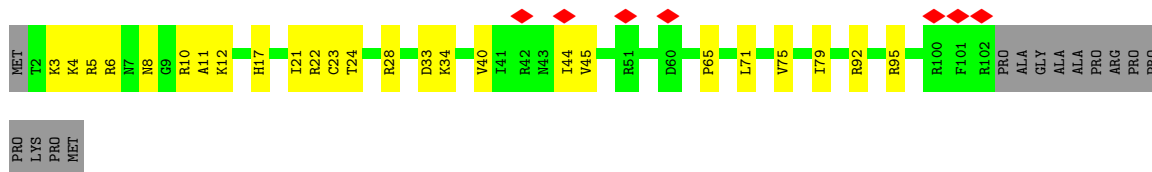




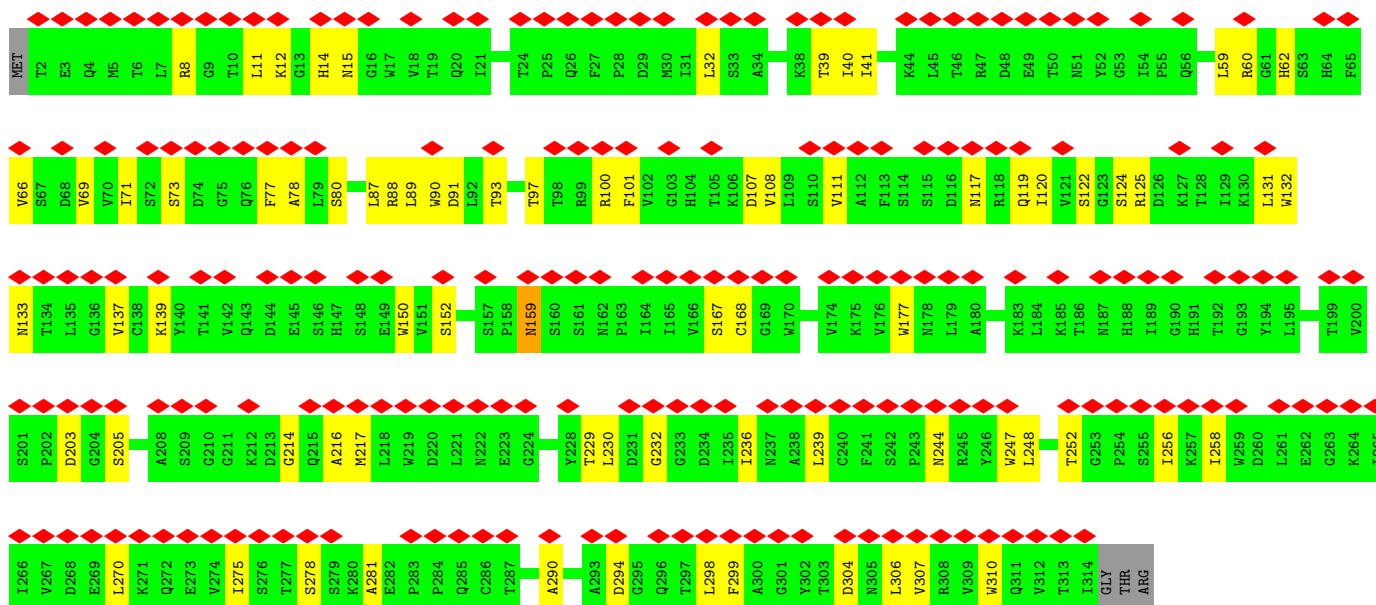
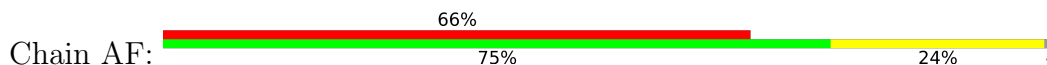
• Molecule 56: 40S ribosomal protein S30



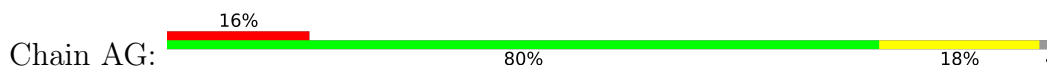
• Molecule 57: eS26



• Molecule 58: RACK1



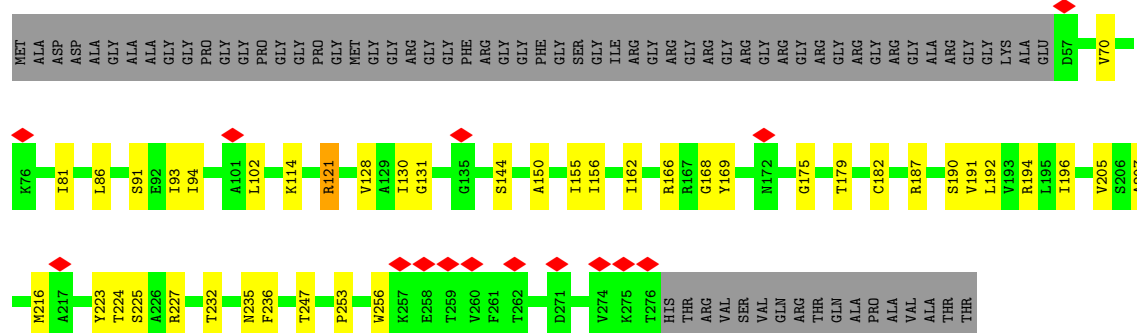
• Molecule 59: uS14



LYS
ALA
THR
GLY
ASP
GLU
GLY
THR
GLY
ALA
LYS
VAL
PRO
GLY
ARG
ALA
GLY
ASP
GLY
TYR
PRO
PRO
VAL
GLN
GLU
SER
VAL

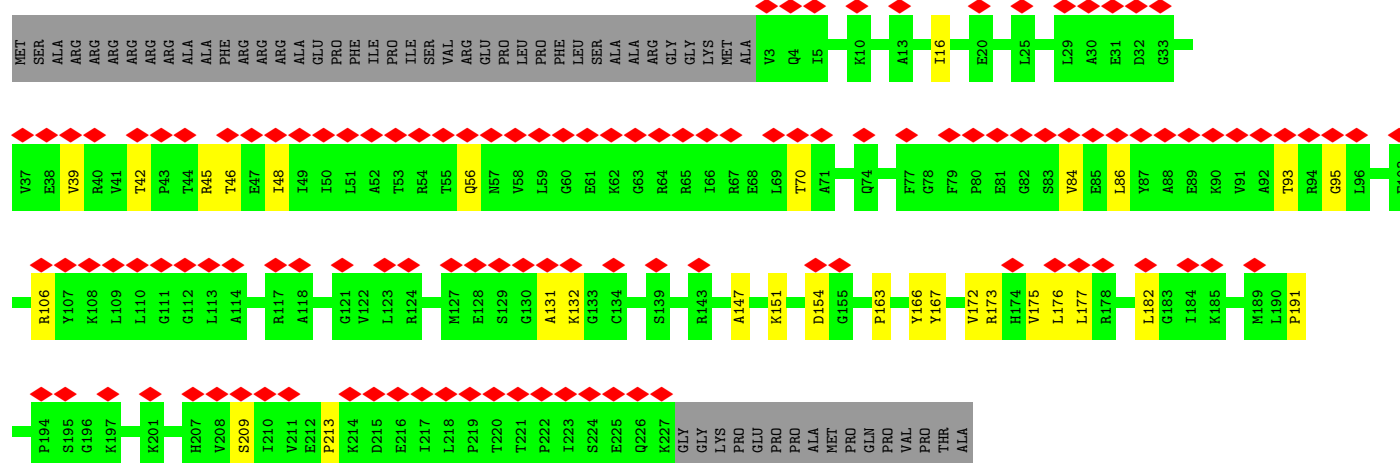
- Molecule 64: Ribosomal_S5_C domain-containing protein, 40S ribosomal protein S2

Chain Ab: 



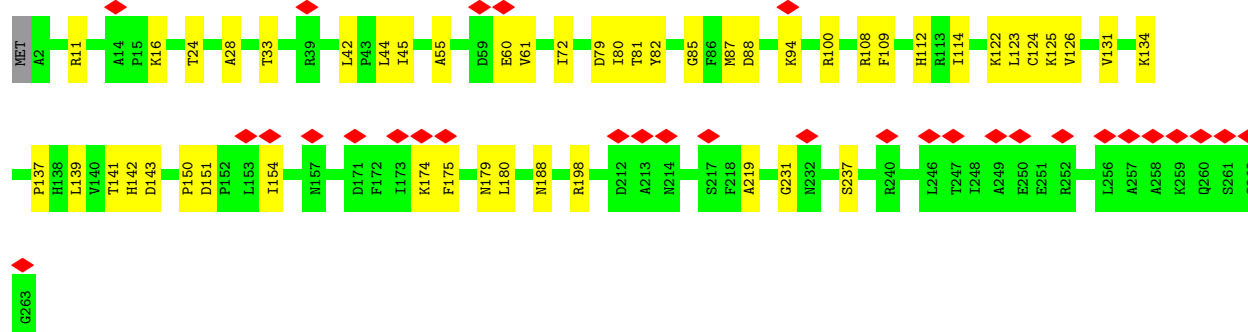
- Molecule 65: 40S ribosomal protein S3

Chain Ac: 

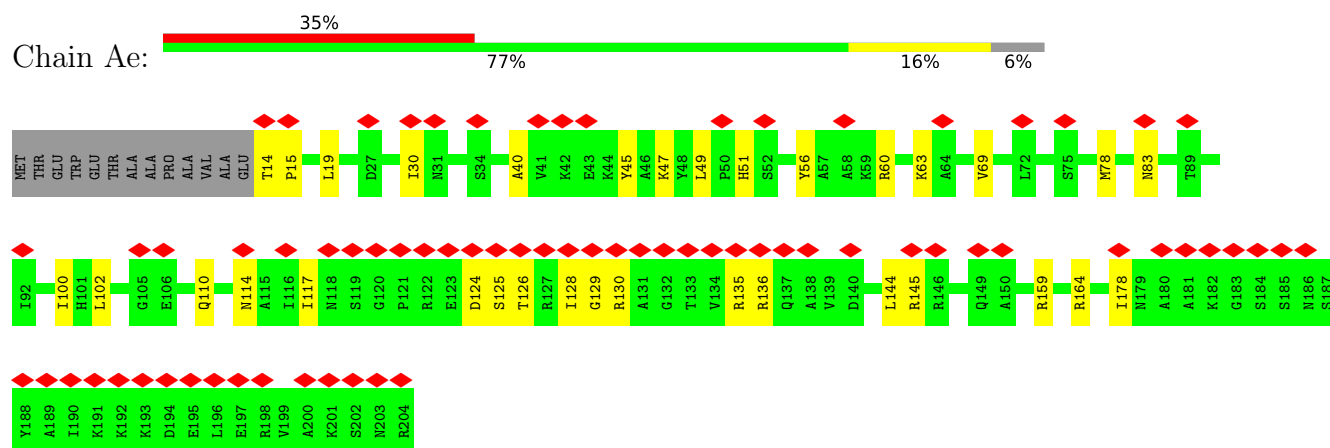


- Molecule 66: 40S ribosomal protein S4

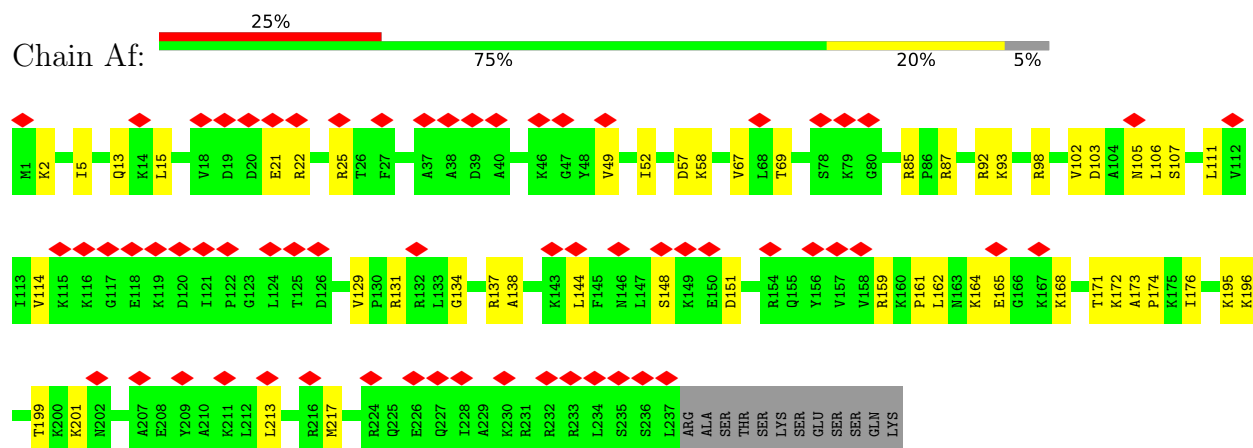
Chain Ad: 



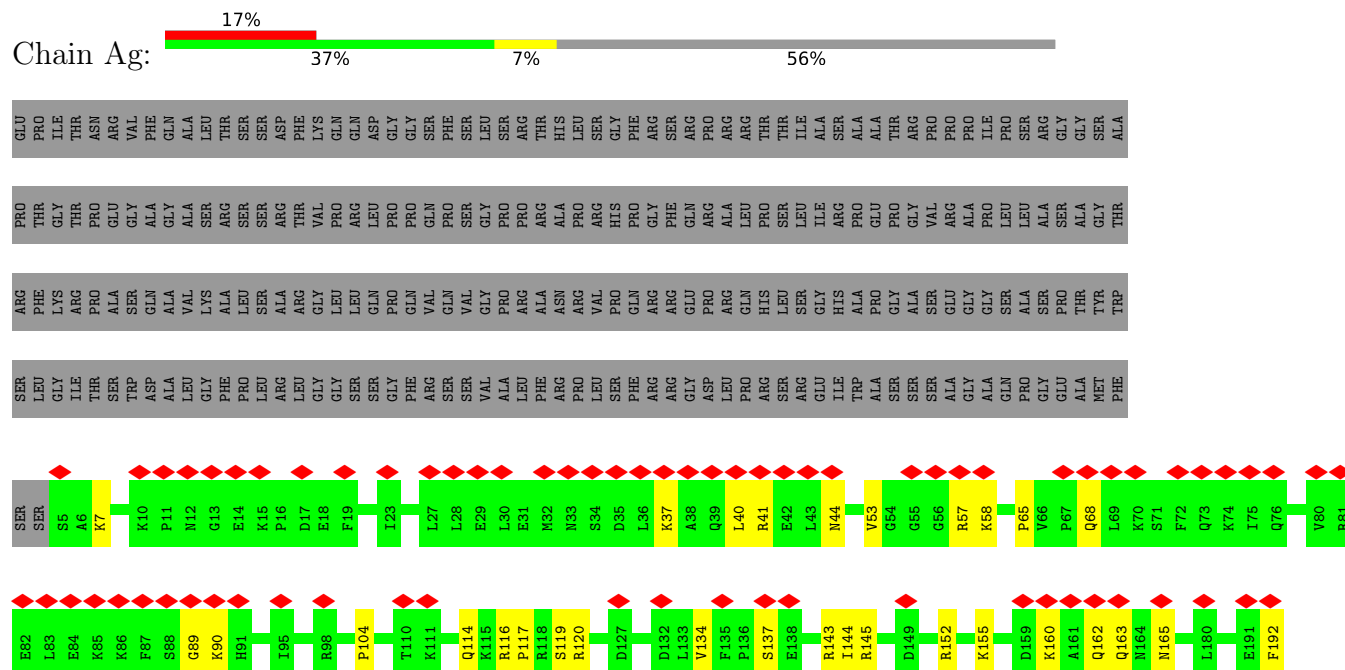
Chain Ae:

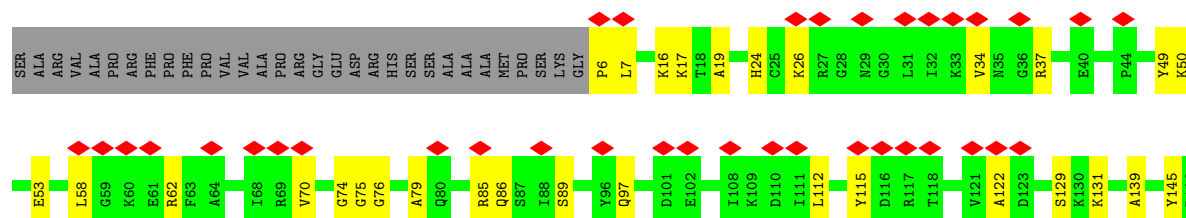


Chain Af:

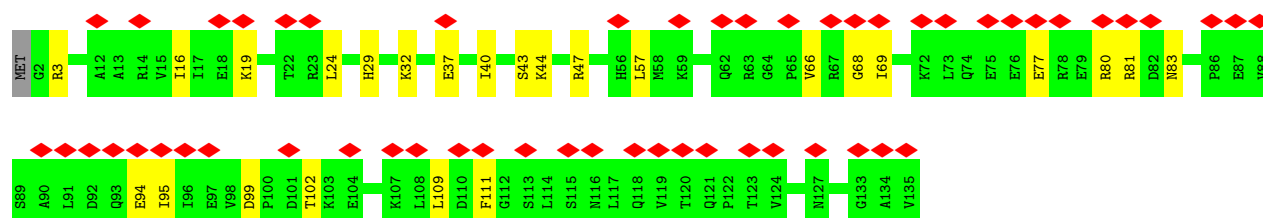
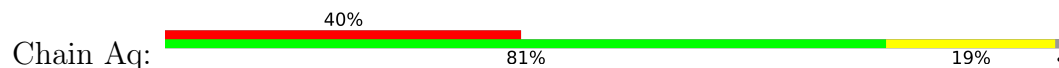


Chain Ag:

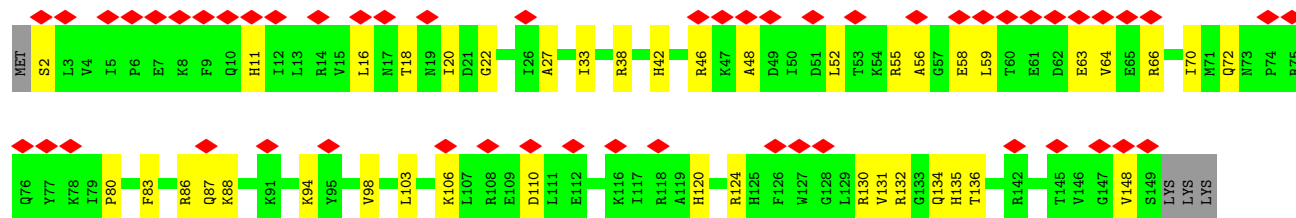




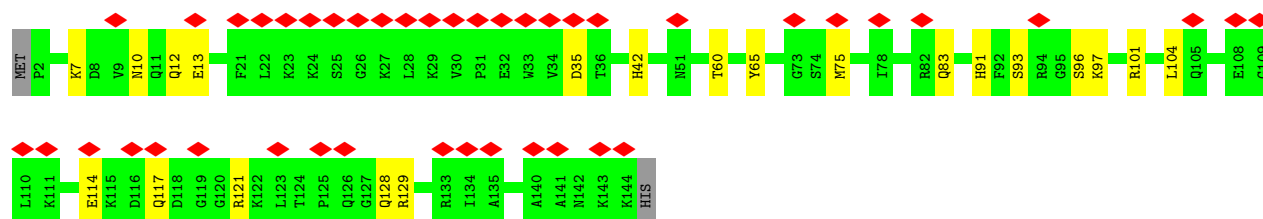
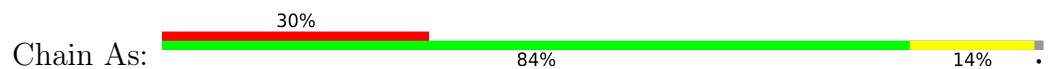
• Molecule 79: 40S ribosomal protein eS17



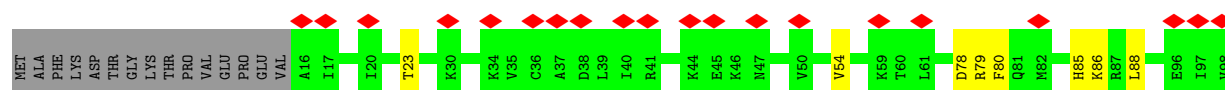
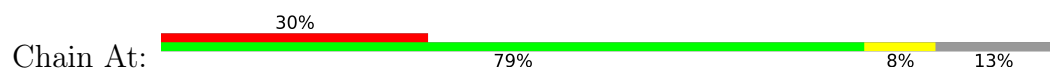
• Molecule 80: 40S ribosomal protein S18

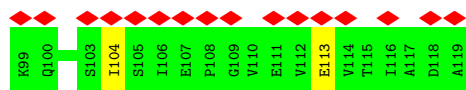


• Molecule 81: 40S ribosomal protein S19

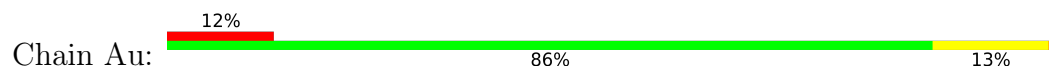


• Molecule 82: 40S ribosomal protein uS10

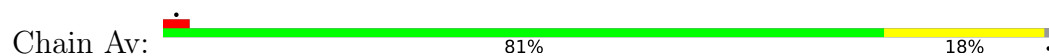




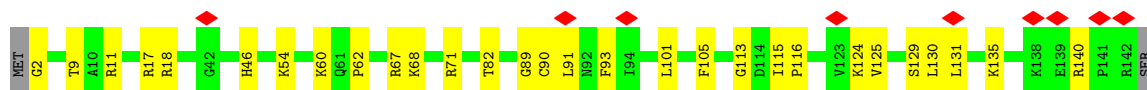
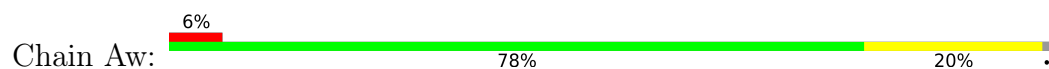
- Molecule 83: 40S ribosomal protein S21



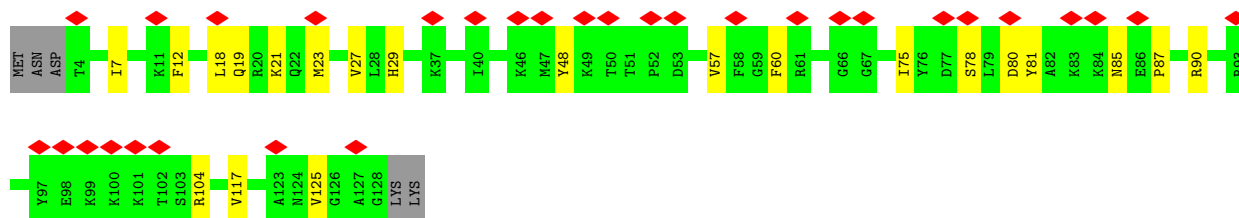
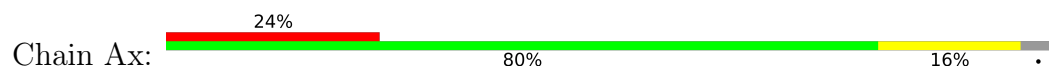
- Molecule 84: Ribosomal protein S15a



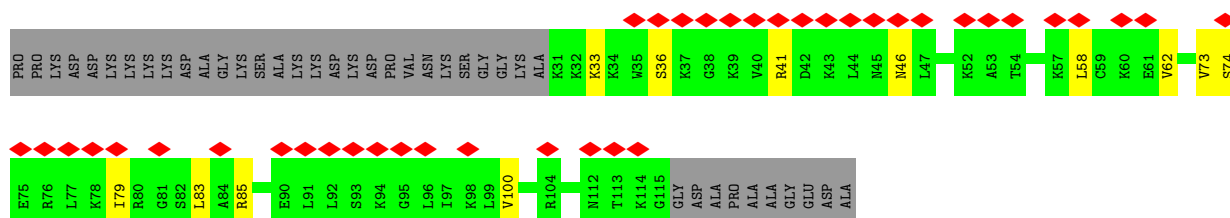
- Molecule 85: 40S ribosomal protein S23



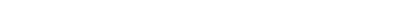
- Molecule 86: 40S ribosomal protein S24

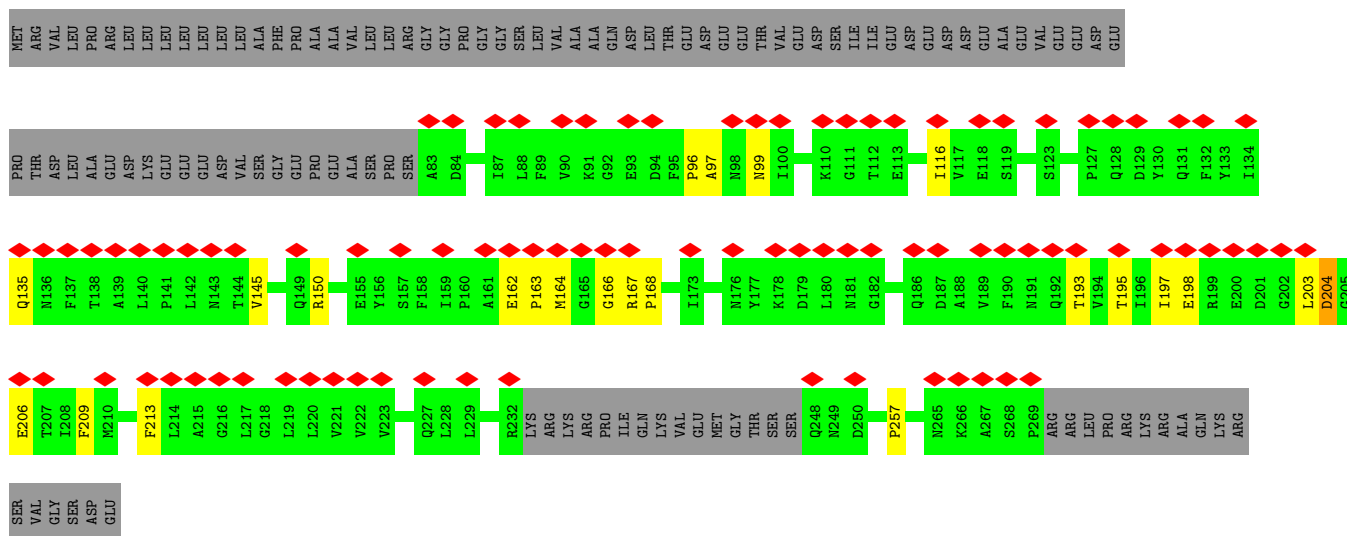


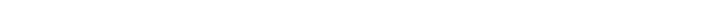
- Molecule 87: 40S ribosomal protein S25

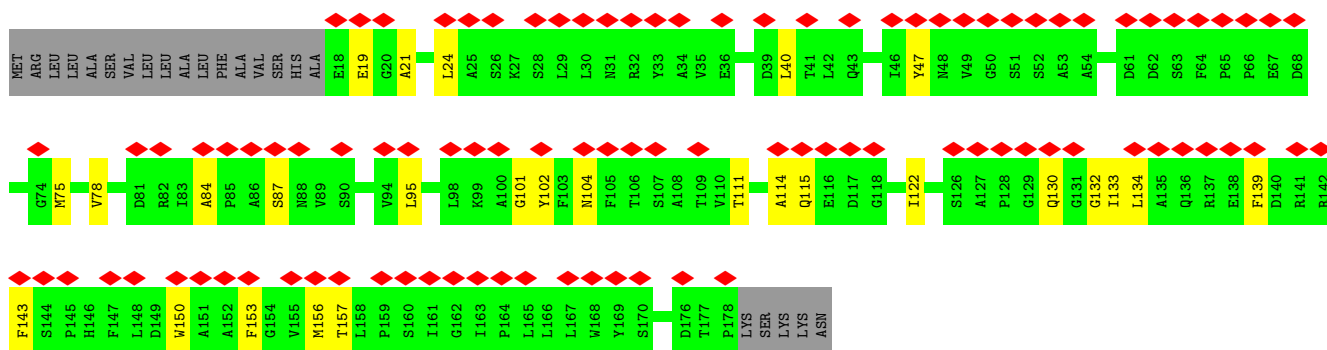


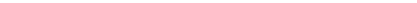
- Molecule 88: 60S ribosomal protein L41

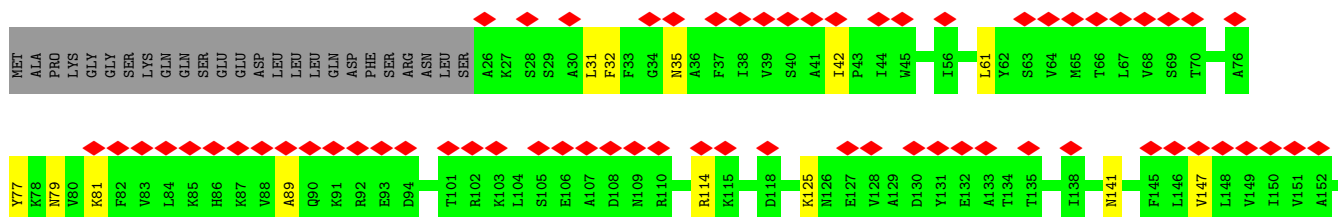
- Chain TA: 

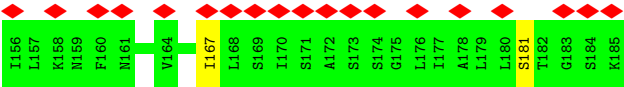


- Chain TB:  54% 73% 15% 12%

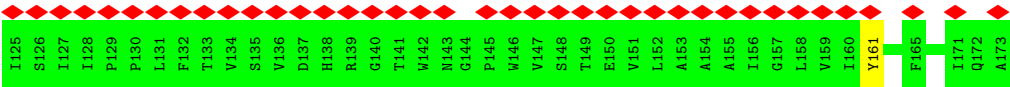
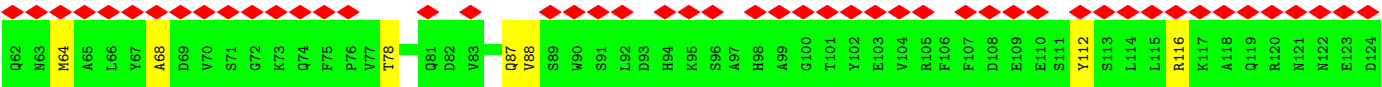
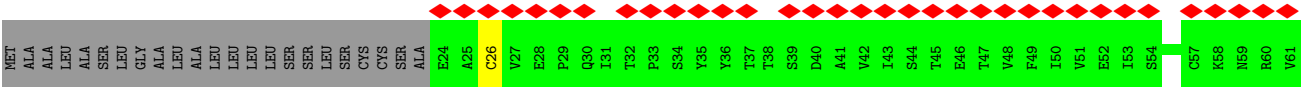
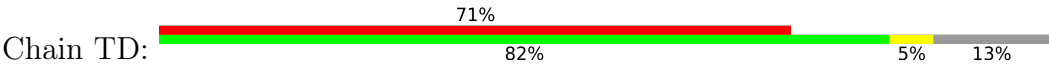


- Chain TC: 





• Molecule 92: Translocon-associated protein subunit delta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22643	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	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: OMG, 5F0, AAC, OMC, V5N, UR3, MG, B8N, 6MZ, SPD, GTP, SPM, AYA, MA6, SAC, NMM, M3L, A2M, 5MU, 4AC, AME, PSU, UY1, HIC, 1MA, 5MC, HY3, MLZ, G7M, OMU, ZN

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	0.10	2/87403 (0.0%)	0.11	0/136359
2	B7	0.05	0/2835	0.08	0/4418
3	B8	0.06	0/3635	0.13	0/5661
4	BA	0.08	0/1965	0.22	0/2633
5	BB	0.07	0/3261	0.19	0/4364
6	BC	0.07	0/2932	0.19	0/3939
7	BD	0.06	0/2437	0.19	0/3264
8	BE	0.08	0/1998	0.20	0/2673
9	BF	0.07	0/1922	0.19	0/2563
10	BG	0.07	0/1908	0.18	0/2566
11	BH	0.06	0/1535	0.19	0/2063
12	BI	0.08	0/1756	0.21	0/2346
13	BJ	0.06	0/1385	0.19	0/1852
15	BL	0.07	0/1732	0.20	0/2316
16	BM	0.06	0/1158	0.18	0/1547
17	BN	0.07	0/1746	0.19	0/2338
18	BO	0.06	0/1662	0.18	0/2222
19	BP	0.07	0/1317	0.21	0/1768
20	BQ	0.07	0/1539	0.20	0/2054
21	BR	0.05	0/1524	0.16	0/2013
22	BS	0.08	0/1497	0.19	0/2008
23	BT	0.07	0/1326	0.20	0/1770
24	BU	0.06	0/820	0.19	0/1100
25	BV	0.08	0/1048	0.20	0/1402
26	BW	0.06	0/1006	0.19	0/1334
27	BX	0.07	0/984	0.19	0/1323
28	BY	0.06	0/1132	0.21	0/1504
29	BZ	0.07	0/1130	0.17	0/1507
30	Ba	0.07	0/1179	0.21	0/1572
31	Bb	0.08	0/884	0.20	0/1169
32	Bc	0.06	0/847	0.17	0/1134

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Bd	0.08	0/903	0.20	0/1216
34	Be	0.06	0/1088	0.20	0/1451
35	Bf	0.08	0/903	0.19	0/1208
36	Bg	0.06	0/916	0.19	0/1220
37	Bh	0.05	0/1021	0.16	0/1348
38	Bi	0.07	0/841	0.21	0/1112
39	Bj	0.07	0/736	0.21	0/973
40	Bk	0.06	0/575	0.17	0/761
41	Bl	0.06	0/459	0.18	0/608
42	Bm	0.06	0/426	0.20	0/564
43	Bo	0.08	0/866	0.21	0/1141
44	Bp	0.06	0/718	0.20	0/953
45	Br	0.07	0/1020	0.20	0/1366
46	Bs	0.08	0/1530	0.20	0/2064
47	Bt	0.07	0/1193	0.21	0/1609
48	Bv	0.08	0/1735	0.25	0/2328
49	SX	0.09	0/3388	0.24	0/4590
50	SY	0.09	0/504	0.24	0/673
51	SZ	0.10	0/236	0.23	0/321
52	A2	0.13	3/40342 (0.0%)	0.11	0/62877
53	AA	0.06	0/665	0.20	0/891
54	AB	0.05	0/497	0.18	0/666
55	AC	0.07	0/622	0.22	0/822
56	AD	0.06	0/462	0.20	0/607
57	AE	0.07	0/828	0.20	0/1109
58	AF	0.07	0/2493	0.21	0/3394
59	AG	0.06	0/470	0.19	0/623
60	AH	0.04	0/72	0.10	0/110
61	AT	0.04	0/1714	0.09	0/2668
62	AZ	0.07	0/1771	0.19	0/2406
63	Aa	0.07	0/1841	0.21	0/2459
64	Ab	0.07	0/1742	0.20	0/2354
65	Ac	0.07	0/1779	0.19	0/2395
66	Ad	0.07	0/2118	0.20	0/2849
67	Ae	0.08	0/1531	0.25	0/2059
68	Af	0.07	0/1946	0.19	0/2590
69	Ag	0.06	0/1552	0.18	0/2079
70	Ah	0.06	0/1715	0.19	0/2287
71	Ai	0.06	0/1550	0.18	0/2069
72	Aj	0.07	0/834	0.20	0/1125
73	Ak	0.07	0/1284	0.20	0/1717
74	Al	0.07	0/968	0.22	0/1296
75	Am	0.07	0/1232	0.19	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	An	0.07	0/1020	0.19	0/1366
77	Ao	0.07	0/1069	0.19	0/1429
78	Ap	0.08	0/1142	0.24	0/1528
79	Aq	0.06	0/1094	0.18	0/1469
80	Ar	0.07	0/1226	0.19	0/1643
81	As	0.06	0/1119	0.18	0/1498
82	At	0.06	0/831	0.19	0/1115
83	Au	0.05	0/636	0.17	0/852
84	Av	0.07	0/1051	0.19	0/1406
85	Aw	0.06	0/1107	0.20	0/1475
86	Ax	0.06	0/1032	0.18	0/1371
87	Ay	0.07	0/691	0.21	0/922
88	Az	0.05	0/240	0.14	0/305
89	TA	0.09	0/1404	0.22	0/1910
90	TB	0.07	0/1287	0.20	0/1753
91	TC	0.06	0/1324	0.16	0/1791
92	TD	0.06	0/1214	0.21	0/1656
All	All	0.09	5/244076 (0.0%)	0.15	0/356885

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
43	Bo	0	1
76	An	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1327	OMU	O3'-P	5.08	1.61	1.56
1	B5	4269	A2M	O3'-P	5.08	1.61	1.56
52	A2	159	A2M	O3'-P	5.07	1.61	1.56
52	A2	1679	A2M	O3'-P	5.04	1.61	1.56
1	B5	3562	A2M	O3'-P	5.02	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
76	An	138	5F0	Mainchain,Peptide
43	Bo	53	MLZ	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B5	80772	0	40880	726	0
2	B7	2538	0	1284	12	0
3	B8	3319	0	1684	39	0
4	BA	1940	0	2029	43	0
5	BB	3206	0	3352	50	0
6	BC	2886	0	3057	30	0
7	BD	2391	0	2424	30	0
8	BE	1960	0	2153	29	0
9	BF	1886	0	2008	28	0
10	BG	1877	0	2023	15	0
11	BH	1516	0	1597	21	0
12	BI	1717	0	1764	25	0
13	BJ	1362	0	1399	13	0
14	BK	145	0	33	0	0
15	BL	1701	0	1820	24	0
16	BM	1137	0	1211	19	0
17	BN	1701	0	1749	26	0
18	BO	1630	0	1778	13	0
19	BP	1289	0	1329	20	0
20	BQ	1515	0	1634	21	0
21	BR	1508	0	1664	20	0
22	BS	1457	0	1492	18	0
23	BT	1298	0	1366	26	0
24	BU	806	0	827	7	0
25	BV	1034	0	1097	21	0
26	BW	991	0	1048	16	0
27	BX	967	0	1040	10	0
28	BY	1115	0	1205	12	0
29	BZ	1107	0	1182	20	0
30	Ba	1163	0	1202	22	0
31	Bb	881	0	957	7	0
32	Bc	836	0	888	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Bd	888	0	930	11	0
34	Be	1070	0	1165	15	0
35	Bf	884	0	924	7	0
36	Bg	906	0	998	14	0
37	Bh	1013	0	1147	24	0
38	Bi	830	0	916	6	0
39	Bj	721	0	755	17	0
40	Bk	569	0	637	6	0
41	Bl	447	0	479	5	0
42	Bm	432	0	470	7	0
43	Bo	863	0	929	13	0
44	Bp	708	0	756	7	0
45	Br	1014	0	1083	14	0
46	Bs	1507	0	1564	25	0
47	Bt	1178	0	1235	28	0
48	Bv	1707	0	1815	34	0
49	SX	3317	0	3447	76	0
50	SY	494	0	527	12	0
51	SZ	229	0	245	6	0
52	A2	37833	0	19167	377	0
53	AA	651	0	672	10	0
54	AB	495	0	523	7	0
55	AC	610	0	634	12	0
56	AD	457	0	502	11	0
57	AE	814	0	863	19	0
58	AF	2436	0	2393	49	0
59	AG	459	0	448	9	0
60	AH	66	0	33	0	0
61	AT	1597	0	811	23	0
62	AZ	1743	0	1748	28	0
63	Aa	1815	0	1908	21	0
64	Ab	1706	0	1796	29	0
65	Ac	1751	0	1846	19	0
66	Ad	2076	0	2177	29	0
67	Ae	1509	0	1563	27	0
68	Af	1923	0	2089	39	0
69	Ag	1529	0	1627	20	0
70	Ah	1686	0	1772	27	0
71	Ai	1525	0	1640	23	0
72	Aj	810	0	836	8	0
73	Ak	1262	0	1335	14	0
74	Al	958	0	993	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	Am	1208	0	1294	21	0
76	An	1017	0	1035	23	0
77	Ao	1048	0	1093	14	0
78	Ap	1124	0	1193	21	0
79	Aq	1080	0	1135	17	0
80	Ar	1217	0	1279	27	0
81	As	1113	0	1145	17	0
82	At	821	0	883	7	0
83	Au	640	0	633	9	0
84	Av	1034	0	1080	18	0
85	Aw	1099	0	1162	21	0
86	Ax	1015	0	1086	14	0
87	Ay	683	0	761	11	0
88	Az	239	0	289	2	0
89	TA	1372	0	1332	17	0
90	TB	1254	0	1230	17	0
91	TC	1295	0	1340	9	0
92	TD	1185	0	1148	6	0
93	A2	80	0	152	9	0
93	B5	210	0	399	13	0
93	BN	10	0	19	0	0
94	A2	14	0	26	1	0
94	B5	28	0	52	3	0
95	A2	167	0	0	0	0
95	AH	1	0	0	0	0
95	AT	7	0	0	0	0
95	Ad	1	0	0	0	0
95	Ae	1	0	0	0	0
95	Ak	1	0	0	0	0
95	An	1	0	0	0	0
95	Ar	1	0	0	0	0
95	As	1	0	0	0	0
95	B5	510	0	0	0	0
95	B7	15	0	0	0	0
95	B8	16	0	0	0	0
95	BA	4	0	0	0	0
95	BB	3	0	0	0	0
95	BC	1	0	0	0	0
95	BH	1	0	0	0	0
95	BI	2	0	0	0	0
95	BL	1	0	0	0	0
95	BN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
95	BP	1	0	0	0	0
95	BQ	2	0	0	0	0
95	BR	1	0	0	0	0
95	BT	2	0	0	0	0
95	BV	1	0	0	0	0
95	Ba	1	0	0	0	0
95	Bb	1	0	0	0	0
95	Be	2	0	0	0	0
95	Bf	1	0	0	0	0
95	Bj	1	0	0	0	0
95	Bl	1	0	0	0	0
95	Bo	1	0	0	0	0
96	B7	32	0	11	0	0
97	BD	7	0	6	0	0
98	AC	1	0	0	0	0
98	AE	1	0	0	0	0
98	AG	1	0	0	0	0
98	Bg	1	0	0	0	0
98	Bj	1	0	0	0	0
98	Bm	1	0	0	0	0
98	Bo	1	0	0	0	0
98	Bp	1	0	0	0	0
All	All	233722	0	176357	2204	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 2204 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)
52:A2:1092:C:HO2'	84:Av:2:VAL:N	1.66	0.94
1:B5:2277:G:H5'	49:SX:403:GLY:HA2	1.70	0.74
1:B5:4361:C:H5''	5:BB:357:ARG:HE	1.53	0.73
52:A2:929:G:H1	52:A2:1014:U:H3	1.36	0.73
52:A2:1397:A:O2'	52:A2:1399:G:N7	2.21	0.73

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	BA	250/257 (97%)	241 (96%)	9 (4%)	0	100	100
5	BB	395/403 (98%)	391 (99%)	4 (1%)	0	100	100
6	BC	360/413 (87%)	356 (99%)	4 (1%)	0	100	100
7	BD	291/297 (98%)	288 (99%)	3 (1%)	0	100	100
8	BE	239/291 (82%)	236 (99%)	3 (1%)	0	100	100
9	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
10	BG	229/266 (86%)	229 (100%)	0	0	100	100
11	BH	188/192 (98%)	188 (100%)	0	0	100	100
12	BI	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
13	BJ	168/178 (94%)	168 (100%)	0	0	100	100
15	BL	208/211 (99%)	206 (99%)	2 (1%)	0	100	100
16	BM	136/218 (62%)	135 (99%)	1 (1%)	0	100	100
17	BN	201/204 (98%)	200 (100%)	1 (0%)	0	100	100
18	BO	197/203 (97%)	196 (100%)	1 (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%)	171 (98%)	3 (2%)	0	100	100
23	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
24	BU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
25	BV	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
26	BW	119/157 (76%)	119 (100%)	0	0	100	100
27	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
28	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
29	BZ	133/136 (98%)	133 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	Ba	144/148 (97%)	139 (96%)	4 (3%)	1 (1%)	18	51
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
37	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
38	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
39	Bj	86/97 (89%)	86 (100%)	0	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%)	49 (100%)	0	0	100	100
43	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
44	Bp	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
45	Br	124/137 (90%)	124 (100%)	0	0	100	100
46	Bs	194/318 (61%)	188 (97%)	6 (3%)	0	100	100
47	Bt	154/165 (93%)	151 (98%)	3 (2%)	0	100	100
48	Bv	210/217 (97%)	205 (98%)	5 (2%)	0	100	100
49	SX	419/476 (88%)	404 (96%)	15 (4%)	0	100	100
50	SY	60/68 (88%)	60 (100%)	0	0	100	100
51	SZ	27/96 (28%)	27 (100%)	0	0	100	100
53	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
54	AB	61/69 (88%)	61 (100%)	0	0	100	100
55	AC	72/156 (46%)	71 (99%)	1 (1%)	0	100	100
56	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
57	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
58	AF	311/317 (98%)	307 (99%)	4 (1%)	0	100	100
59	AG	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
62	AZ	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
63	Aa	220/264 (83%)	219 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	Ab	218/293 (74%)	218 (100%)	0	0	100	100
65	Ac	223/281 (79%)	221 (99%)	2 (1%)	0	100	100
66	Ad	260/263 (99%)	260 (100%)	0	0	100	100
67	Ae	189/204 (93%)	186 (98%)	3 (2%)	0	100	100
68	Af	235/249 (94%)	235 (100%)	0	0	100	100
69	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
70	Ah	204/208 (98%)	202 (99%)	2 (1%)	0	100	100
71	Ai	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
72	Aj	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
73	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
74	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
75	Am	148/151 (98%)	148 (100%)	0	0	100	100
76	An	133/151 (88%)	132 (99%)	1 (1%)	0	100	100
77	Ao	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
78	Ap	139/172 (81%)	138 (99%)	1 (1%)	0	100	100
79	Aq	132/135 (98%)	132 (100%)	0	0	100	100
80	Ar	146/152 (96%)	143 (98%)	3 (2%)	0	100	100
81	As	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
82	At	102/119 (86%)	101 (99%)	1 (1%)	0	100	100
83	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
84	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
85	Aw	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
86	Ax	123/130 (95%)	123 (100%)	0	0	100	100
87	Ay	83/124 (67%)	83 (100%)	0	0	100	100
88	Az	23/25 (92%)	23 (100%)	0	0	100	100
89	TA	168/286 (59%)	165 (98%)	3 (2%)	0	100	100
90	TB	159/183 (87%)	159 (100%)	0	0	100	100
91	TC	158/185 (85%)	158 (100%)	0	0	100	100
92	TD	148/173 (86%)	148 (100%)	0	0	100	100
All	All	13050/15304 (85%)	12903 (99%)	146 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	Ba	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BA	194/198 (98%)	193 (100%)	1 (0%)	81	80
5	BB	344/347 (99%)	342 (99%)	2 (1%)	78	79
6	BC	302/337 (90%)	302 (100%)	0	100	100
7	BD	247/250 (99%)	247 (100%)	0	100	100
8	BE	216/251 (86%)	216 (100%)	0	100	100
9	BF	197/215 (92%)	196 (100%)	1 (0%)	81	80
10	BG	199/223 (89%)	197 (99%)	2 (1%)	68	75
11	BH	169/171 (99%)	169 (100%)	0	100	100
12	BI	180/181 (99%)	179 (99%)	1 (1%)	78	79
13	BJ	143/149 (96%)	143 (100%)	0	100	100
15	BL	175/176 (99%)	173 (99%)	2 (1%)	65	74
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%)	170 (99%)	1 (1%)	78	79
19	BP	140/163 (86%)	140 (100%)	0	100	100
20	BQ	164/165 (99%)	162 (99%)	2 (1%)	63	73
21	BR	159/175 (91%)	158 (99%)	1 (1%)	78	79
22	BS	154/154 (100%)	154 (100%)	0	100	100
23	BT	139/140 (99%)	137 (99%)	2 (1%)	59	71
24	BU	88/113 (78%)	88 (100%)	0	100	100
25	BV	106/107 (99%)	106 (100%)	0	100	100
26	BW	100/126 (79%)	100 (100%)	0	100	100
27	BX	106/134 (79%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	92 (100%)	0	100	100
33	Bd	98/110 (89%)	98 (100%)	0	100	100
34	Be	116/121 (96%)	116 (100%)	0	100	100
35	Bf	89/89 (100%)	89 (100%)	0	100	100
36	Bg	98/100 (98%)	98 (100%)	0	100	100
37	Bh	109/110 (99%)	109 (100%)	0	100	100
38	Bi	86/89 (97%)	86 (100%)	0	100	100
39	Bj	74/80 (92%)	74 (100%)	0	100	100
40	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	70
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%)	59	71
45	Br	109/120 (91%)	109 (100%)	0	100	100
46	Bs	164/258 (64%)	161 (98%)	3 (2%)	51	69
47	Bt	128/137 (93%)	123 (96%)	5 (4%)	28	54
48	Bv	191/195 (98%)	188 (98%)	3 (2%)	55	70
49	SX	361/398 (91%)	352 (98%)	9 (2%)	42	63
50	SY	53/59 (90%)	51 (96%)	2 (4%)	29	55
51	SZ	26/74 (35%)	24 (92%)	2 (8%)	12	37
53	AA	75/76 (99%)	74 (99%)	1 (1%)	61	72
54	AB	56/62 (90%)	55 (98%)	1 (2%)	51	69
55	AC	67/140 (48%)	67 (100%)	0	100	100
56	AD	47/106 (44%)	47 (100%)	0	100	100
57	AE	88/98 (90%)	85 (97%)	3 (3%)	32	57
58	AF	272/275 (99%)	270 (99%)	2 (1%)	76	78
59	AG	48/49 (98%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	AZ	182/243 (75%)	179 (98%)	3 (2%)	55	70
63	Aa	203/231 (88%)	201 (99%)	2 (1%)	68	75
64	Ab	185/223 (83%)	184 (100%)	1 (0%)	81	80
65	Ac	189/232 (82%)	187 (99%)	2 (1%)	65	74
66	Ad	224/225 (100%)	224 (100%)	0	100	100
67	Ae	161/170 (95%)	161 (100%)	0	100	100
68	Af	207/218 (95%)	207 (100%)	0	100	100
69	Ag	170/360 (47%)	169 (99%)	1 (1%)	78	79
70	Ah	178/180 (99%)	178 (100%)	0	100	100
71	Ai	161/168 (96%)	160 (99%)	1 (1%)	78	79
72	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	74
73	Ak	139/142 (98%)	138 (99%)	1 (1%)	76	78
74	Al	104/108 (96%)	103 (99%)	1 (1%)	68	75
75	Am	130/131 (99%)	130 (100%)	0	100	100
76	An	105/118 (89%)	103 (98%)	2 (2%)	50	68
77	Ao	114/130 (88%)	112 (98%)	2 (2%)	51	69
78	Ap	117/140 (84%)	117 (100%)	0	100	100
79	Aq	120/121 (99%)	120 (100%)	0	100	100
80	Ar	127/131 (97%)	125 (98%)	2 (2%)	55	70
81	As	112/114 (98%)	111 (99%)	1 (1%)	70	76
82	At	94/107 (88%)	93 (99%)	1 (1%)	65	74
83	Au	67/67 (100%)	65 (97%)	2 (3%)	36	60
84	Av	112/113 (99%)	111 (99%)	1 (1%)	70	76
85	Aw	112/114 (98%)	110 (98%)	2 (2%)	51	69
86	Ax	107/112 (96%)	107 (100%)	0	100	100
87	Ay	75/102 (74%)	75 (100%)	0	100	100
88	Az	24/24 (100%)	24 (100%)	0	100	100
89	TA	151/249 (61%)	150 (99%)	1 (1%)	76	78
90	TB	134/152 (88%)	133 (99%)	1 (1%)	76	78
91	TC	142/164 (87%)	142 (100%)	0	100	100
92	TD	130/146 (89%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	11361/12947 (88%)	11285 (99%)	76 (1%)	73 78

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
71	Ai	55	LYS
84	Av	105	THR
73	Ak	24	LEU
80	Ar	94	LYS
90	TB	143	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
68	Af	56	ASN
70	Ah	7	ASN
78	Ap	114	GLN
19	BP	120	ASN
19	BP	75	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B5	3752/4808 (78%)	424 (11%)	2 (0%)
2	B7	118/120 (98%)	6 (5%)	0
3	B8	155/158 (98%)	20 (12%)	0
52	A2	1764/1870 (94%)	199 (11%)	0
60	AH	2/4 (50%)	0	0
61	AT	74/75 (98%)	8 (10%)	0
All	All	5865/7035 (83%)	657 (11%)	2 (0%)

5 of 657 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B5	39	A
1	B5	42	A
1	B5	59	A
1	B5	64	A
1	B5	65	A

All (2) RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PSU	B5	1720	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4099	95,1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	G7M	A2	1640	52,61	23,26,27	3.14	9 (39%)	35,39,42	3.31	13 (37%)
52	PSU	A2	1693	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
61	5MC	AT	48	61	18,22,23	0.95	2 (11%)	26,32,35	1.11	2 (7%)
1	OMG	B5	3524	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	OMC	B5	3573	1	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
1	PSU	B5	4177	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	OMG	A2	1491	52,95	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
52	6MZ	A2	1833	52,95	22,25,26	1.44	4 (18%)	30,36,39	2.16	9 (30%)
1	PSU	B5	4149	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
52	PSU	A2	1626	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	OMC	B5	2208	95,1	19,22,23	0.81	0	26,31,34	0.81	0
52	PSU	A2	109	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	A2M	A2	591	52	22,25,26	1.48	4 (18%)	31,36,39	2.21	7 (22%)
3	PSU	B8	55	3	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1368	52	18,21,22	1.33	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	PSU	B5	4042	1	18,21,22	1.32	2 (11%)	22,30,33	1.90	3 (13%)
52	OMU	A2	116	52	19,22,23	1.20	2 (10%)	26,31,34	1.68	4 (15%)
52	PSU	A2	407	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	M3L	Bm	98	42	10,11,12	0.82	0	9,14,16	0.48	0
1	PSU	B5	3371	1	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	B5	4166	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
61	PSU	AT	54	61	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	1046	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4419	95,1	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	0.85	0
1	PSU	B5	3466	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	6MZ	B5	3966	1	22,25,26	1.44	4 (18%)	30,36,39	2.20	9 (30%)
1	PSU	B5	4188	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	OMU	A2	121	52	19,22,23	1.21	3 (15%)	26,31,34	1.66	4 (15%)
1	PSU	B5	1801	95,1	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3447	1	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
43	MLZ	Bo	53	43	8,9,10	0.49	0	4,9,11	0.11	0
52	OMU	A2	1327	52,95	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
1	A2M	B5	3562	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
52	OMC	A2	1704	52	19,22,23	0.82	0	26,31,34	0.81	0
52	OMU	A2	429	52	19,22,23	1.20	3 (15%)	26,31,34	1.68	4 (15%)
52	PSU	A2	1233	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	OMU	A2	172	52	19,22,23	1.19	3 (15%)	26,31,34	1.70	5 (19%)
1	PSU	B5	3652	95,1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	687	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	823	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1245	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	610	52	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
1	OMC	B5	2704	1	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
52	PSU	A2	652	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1799	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	4AC	A2	1338	52	21,24,25	1.03	1 (4%)	29,34,37	1.26	3 (10%)
52	PSU	A2	1348	52	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
52	A2M	A2	1679	52	22,25,26	1.47	4 (18%)	31,36,39	2.23	10 (32%)
1	PSU	B5	3585	95,1	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	34	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	A2M	A2	469	52	22,25,26	1.48	4 (18%)	31,36,39	2.09	9 (29%)
1	PSU	B5	4217	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	AME	Au	1	83	9,10,11	0.48	0	9,11,13	0.86	1 (11%)
1	5MC	B5	3514	95,1	18,22,23	0.97	2 (11%)	26,32,35	1.19	3 (11%)
52	MA6	A2	1852	52	23,26,27	2.25	5 (21%)	34,38,41	3.69	14 (41%)
1	OMG	B5	1260	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	B5	4740	95,1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	B5	3599	1	22,25,26	1.46	4 (18%)	31,36,39	2.08	9 (29%)
52	PSU	A2	1175	52,95	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1721	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	119	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	OMU	A2	355	52,95	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
1	OMU	B5	4244	95,1	19,22,23	1.19	2 (10%)	26,31,34	1.69	5 (19%)
1	A2M	B5	3492	52,95,1	22,25,26	1.46	4 (18%)	31,36,39	2.17	10 (32%)
1	A2M	B5	2206	95,1	22,25,26	1.46	4 (18%)	31,36,39	2.14	9 (29%)
1	PSU	B5	3494	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	1638	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	OMU	A2	628	52	19,22,23	1.18	2 (10%)	26,31,34	1.70	5 (19%)
1	OMG	B5	2719	1	23,26,27	1.20	3 (13%)	33,38,41	1.97	6 (18%)
52	PSU	A2	1082	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	MA6	A2	1851	52	23,26,27	2.28	5 (21%)	34,38,41	3.71	13 (38%)
1	PSU	B5	1537	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
52	OMU	A2	1443	52,95	19,22,23	1.23	3 (15%)	26,31,34	1.69	5 (19%)
80	SAC	Ar	2	80	7,8,9	0.53	0	8,9,11	0.92	1 (12%)
1	OMC	B5	3433	95,1	19,22,23	0.79	0	26,31,34	0.75	0
52	PSU	A2	1057	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	3496	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	B5	4138	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
52	A2M	A2	99	52,95	22,25,26	1.48	4 (18%)	31,36,39	2.13	10 (32%)
1	PSU	B5	3616	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
62	SAC	AZ	2	62	7,8,9	0.54	0	8,9,11	0.86	1 (12%)
1	A2M	B5	2658	95,1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
1	OMC	B5	4202	1	19,22,23	0.82	0	26,31,34	0.82	0
52	PSU	A2	816	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	815	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	1731	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4107	95,1	18,21,22	1.35	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
52	PSU	A2	1047	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
3	OMG	B8	75	3	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
31	MLZ	Bb	5	31,95	8,9,10	0.49	0	4,9,11	0.16	0
52	OMC	A2	174	52,95	19,22,23	0.81	0	26,31,34	0.78	0
52	A2M	A2	485	52	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
1	PSU	B5	3369	95,1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	2351	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	OMC	A2	518	52	19,22,23	0.82	0	26,31,34	0.83	0
52	PSU	A2	650	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	A2M	A2	159	52	22,25,26	1.47	4 (18%)	31,36,39	2.16	10 (32%)
1	OMG	B5	1477	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	4749	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	B8N	A2	1249	52	24,29,30	1.29	3 (12%)	29,42,45	1.27	3 (10%)
1	PSU	B5	4278	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
52	OMU	A2	1805	52,95	19,22,23	1.22	3 (15%)	26,31,34	1.68	5 (19%)
52	PSU	A2	1239	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	3601	1	19,22,23	0.81	0	26,31,34	0.83	0
52	A2M	A2	669	52,95	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
1	PSU	B5	3554	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	4317	1	22,25,26	1.47	4 (18%)	31,36,39	2.13	9 (29%)
1	A2M	B5	2630	95,1	22,25,26	1.46	4 (18%)	31,36,39	2.17	9 (29%)
52	OMU	A2	1289	52	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
1	PSU	B5	3427	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	B5	3476	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	B5	3974	1	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
76	5F0	An	138	76	8,8,9	1.49	2 (25%)	7,9,11	1.70	1 (14%)
1	PSU	B5	1491	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	A2M	A2	166	52	22,25,26	1.48	4 (18%)	31,36,39	2.13	9 (29%)
1	OMG	B5	4364	95,1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	B5	3583	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4711	95,1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	2667	1	19,22,23	0.81	0	26,31,34	0.86	1 (3%)
1	PSU	B5	4045	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	93	52	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4058	1	18,21,22	1.34	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	A2M	B5	3450	1	22,25,26	1.47	4 (18%)	31,36,39	2.08	9 (29%)
5	HIC	BB	245	5	10,11,12	0.62	0	8,14,16	0.38	0
52	PSU	A2	802	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	B5	1810	95,1	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
1	PSU	B5	4246	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
3	PSU	B8	69	3	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	4269	95,1	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
52	OMG	A2	1329	52,95	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
81	NMM	As	67	81	9,11,12	0.60	0	6,12,14	0.39	0
52	PSU	A2	1644	52,95	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	PSU	A2	36	52	18,21,22	1.33	2 (11%)	22,30,33	1.84	3 (13%)
1	OMG	B5	3359	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	B5	3502	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	1MA	B5	1266	95,1	21,25,26	1.38	4 (19%)	31,37,40	1.69	5 (16%)
1	OMG	B5	4245	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
52	OMG	A2	602	52	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
52	OMG	A2	868	52	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
61	5MU	AT	53	61	19,22,23	1.42	5 (26%)	28,32,35	2.00	5 (17%)
1	A2M	B5	4336	1	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
52	OMC	A2	1392	52	19,22,23	0.83	0	26,31,34	0.85	1 (3%)
52	PSU	A2	967	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	B5	2244	95,1	22,25,26	1.48	4 (18%)	31,36,39	2.12	10 (32%)
52	OMG	A2	437	52	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	OMC	B5	1820	95,1	19,22,23	0.79	0	26,31,34	0.79	0
1	OMG	B5	2207	1	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
1	PSU	B5	3500	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	B5	3657	1	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
52	PSU	A2	573	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	B5	2258	1	19,22,23	1.23	4 (21%)	26,31,34	1.68	4 (15%)
52	OMG	A2	510	52,95	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
52	OMG	A2	1448	52	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	B5	1580	95,1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	B5	3576	1	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	B5	2475	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	1446	52	18,21,22	1.35	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
1	OMG	B5	4383	95,1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
52	PSU	A2	867	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4298	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	1270	1	22,25,26	1.46	4 (18%)	31,36,39	2.08	9 (29%)
52	A2M	A2	1384	52	22,25,26	1.46	4 (18%)	31,36,39	2.15	10 (32%)
4	V5N	BA	216	4	9,11,12	2.10	2 (22%)	9,14,16	1.71	2 (22%)
1	PSU	B5	4435	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	4369	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	4374	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	4116	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	A2M	B5	3456	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
1	PSU	B5	4039	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMU	B5	2680	95,1	19,22,23	1.22	2 (10%)	26,31,34	1.72	4 (15%)
1	PSU	B5	4325	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
45	SAC	Br	2	45	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
52	4AC	A2	1843	52,95	21,24,25	1.09	2 (9%)	29,34,37	1.24	3 (10%)
1	PSU	B5	4382	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	OMG	A2	645	52	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMU	B5	4052	1	19,22,23	1.22	3 (15%)	26,31,34	1.69	5 (19%)
1	PSU	B5	1632	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
1	PSU	B5	1683	95,1	18,21,22	1.32	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4169	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
6	AYA	BC	2	6	6,7,8	0.72	0	5,8,10	0.33	0
1	OMU	B5	4366	1	19,22,23	1.22	3 (15%)	26,31,34	1.73	4 (15%)
52	A2M	A2	513	52	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
1	OMC	B5	2265	95,1	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
1	OMC	B5	2647	1	19,22,23	0.81	0	26,31,34	0.85	1 (3%)
30	V5N	Ba	39	30	9,11,12	2.07	2 (22%)	9,14,16	1.68	2 (22%)
1	A2M	B5	1479	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
1	OMG	B5	2267	1	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
52	A2M	A2	577	52	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
1	A2M	B5	3517	1	22,25,26	1.44	4 (18%)	31,36,39	2.18	11 (35%)
85	HY3	Aw	62	85	6,8,9	2.00	1 (16%)	5,10,12	1.11	1 (20%)
52	PSU	A2	1178	52,95	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1718	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	B5	398	1	22,25,26	1.47	4 (18%)	31,36,39	2.15	9 (29%)
52	PSU	A2	218	52	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	UR3	B5	4276	1	19,22,23	0.99	1 (5%)	26,32,35	1.42	1 (3%)
1	OMU	B5	3973	1	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
1	OMC	B5	3540	1	19,22,23	0.82	0	26,31,34	0.81	0
1	5MC	B5	4193	95,1	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
1	PSU	B5	3462	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	4322	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	4267	95,1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
52	OMC	A2	463	52	19,22,23	0.82	0	26,31,34	0.79	0
52	PSU	A2	864	52	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	3942	61,1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	OMC	B5	1284	1	19,22,23	0.81	0	26,31,34	0.78	0
52	PSU	A2	105	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	OMG	A2	684	52	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
1	OMC	B5	2194	95,1	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
1	A2M	B5	400	1	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
1	OMG	B5	3676	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
52	A2M	A2	27	52,95	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
1	A2M	B5	1489	95,1	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
1	OMG	B5	4240	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	4203	1	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	210	52	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	1005	52	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
52	A2M	A2	1032	52	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
1	OMG	B5	3631	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	UY1	B5	3550	95,1	19,22,23	1.40	3 (15%)	22,31,34	1.87	5 (22%)
1	OMC	B5	4282	95,1	19,22,23	0.82	0	26,31,34	0.84	0
1	A2M	B5	3557	1	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
52	PSU	A2	682	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	1720	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4099	95,1	-	0/7/25/26	0/2/2/2
52	G7M	A2	1640	52,61	-	2/7/25/26	0/3/3/3
52	PSU	A2	1693	52	-	0/7/25/26	0/2/2/2
61	5MC	AT	48	61	-	0/7/25/26	0/2/2/2
1	OMG	B5	3524	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	3573	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4177	1	-	0/7/25/26	0/2/2/2
52	OMG	A2	1491	52,95	-	0/9/27/28	0/3/3/3
52	6MZ	A2	1833	52,95	-	0/9/27/28	0/3/3/3
1	PSU	B5	4149	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1626	52	-	0/7/25/26	0/2/2/2
1	OMC	B5	2208	95,1	-	0/9/27/28	0/2/2/2
52	PSU	A2	109	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	591	52	-	3/9/27/28	0/3/3/3
3	PSU	B8	55	3	-	0/7/25/26	0/2/2/2
52	PSU	A2	1368	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3490	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4042	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	116	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	407	52	-	0/7/25/26	0/2/2/2
42	M3L	Bm	98	42	-	0/9/10/12	-
1	PSU	B5	3371	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4166	1	-	0/7/25/26	0/2/2/2
61	PSU	AT	54	61	-	0/7/25/26	0/2/2/2
52	PSU	A2	1046	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4419	95,1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3619	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	3466	1	-	0/7/25/26	0/2/2/2
1	6MZ	B5	3966	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4188	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	121	52	-	0/9/27/28	0/2/2/2
1	PSU	B5	1801	95,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3447	1	-	0/7/25/26	0/2/2/2
43	MLZ	Bo	53	43	-	0/7/8/10	-
52	OMU	A2	1327	52,95	-	0/9/27/28	0/2/2/2
1	A2M	B5	3562	1	-	0/9/27/28	0/3/3/3
52	OMC	A2	1704	52	-	1/9/27/28	0/2/2/2
52	OMU	A2	429	52	-	4/9/27/28	0/2/2/2
52	PSU	A2	1233	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	172	52	-	0/9/27/28	0/2/2/2
1	PSU	B5	3652	95,1	-	0/7/25/26	0/2/2/2
52	PSU	A2	687	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	A2	823	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1245	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	610	52	-	0/7/25/26	0/2/2/2
1	OMC	B5	2704	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	652	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	1799	1	-	0/7/25/26	0/2/2/2
52	4AC	A2	1338	52	-	4/11/29/30	0/2/2/2
52	PSU	A2	1348	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	1679	52	-	1/9/27/28	0/3/3/3
1	PSU	B5	3585	95,1	-	0/7/25/26	0/2/2/2
52	PSU	A2	34	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	469	52	-	2/9/27/28	0/3/3/3
1	PSU	B5	4217	1	-	0/7/25/26	0/2/2/2
83	AME	Au	1	83	-	2/9/10/12	-
1	5MC	B5	3514	95,1	-	0/7/25/26	0/2/2/2
52	MA6	A2	1852	52	-	4/11/29/30	0/3/3/3
1	OMG	B5	1260	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4740	95,1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3599	1	-	1/9/27/28	0/3/3/3
52	PSU	A2	1175	52,95	-	0/7/25/26	0/2/2/2
1	PSU	B5	1721	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	119	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	355	52,95	-	0/9/27/28	0/2/2/2
1	OMU	B5	4244	95,1	-	0/9/27/28	0/2/2/2
1	A2M	B5	3492	52,95,1	-	1/9/27/28	0/3/3/3
1	A2M	B5	2206	95,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3494	1	-	1/7/25/26	0/2/2/2
1	PSU	B5	1638	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	628	52	-	4/9/27/28	0/2/2/2
1	OMG	B5	2719	1	-	0/9/27/28	0/3/3/3
52	PSU	A2	1082	52	-	0/7/25/26	0/2/2/2
52	MA6	A2	1851	52	-	0/11/29/30	0/3/3/3
1	PSU	B5	1537	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	1443	52,95	-	1/9/27/28	0/2/2/2
80	SAC	Ar	2	80	-	0/7/8/10	-
1	OMC	B5	3433	95,1	-	4/9/27/28	0/2/2/2
52	PSU	A2	1057	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3496	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4138	1	-	0/9/27/28	0/3/3/3
52	A2M	A2	99	52,95	-	2/9/27/28	0/3/3/3
1	PSU	B5	3616	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	SAC	AZ	2	62	-	2/7/8/10	-
1	A2M	B5	2658	95,1	-	0/9/27/28	0/3/3/3
1	OMC	B5	4202	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	816	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	815	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	1731	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4107	95,1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1047	52	-	0/7/25/26	0/2/2/2
3	OMG	B8	75	3	-	0/9/27/28	0/3/3/3
31	MLZ	Bb	5	31,95	-	2/7/8/10	-
52	OMC	A2	174	52,95	-	0/9/27/28	0/2/2/2
52	A2M	A2	485	52	-	0/9/27/28	0/3/3/3
1	PSU	B5	3369	95,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	2351	1	-	0/7/25/26	0/2/2/2
52	OMC	A2	518	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	650	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	159	52	-	0/9/27/28	0/3/3/3
1	OMG	B5	1477	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4749	1	-	0/7/25/26	0/2/2/2
52	B8N	A2	1249	52	-	4/16/34/35	0/2/2/2
1	PSU	B5	4278	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	1805	52,95	-	0/9/27/28	0/2/2/2
52	PSU	A2	1239	52	-	0/7/25/26	0/2/2/2
1	OMC	B5	3601	1	-	0/9/27/28	0/2/2/2
52	A2M	A2	669	52,95	-	2/9/27/28	0/3/3/3
1	PSU	B5	3554	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	4317	1	-	1/9/27/28	0/3/3/3
1	A2M	B5	2630	95,1	-	2/9/27/28	0/3/3/3
52	OMU	A2	1289	52	-	0/9/27/28	0/2/2/2
1	PSU	B5	3427	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3476	1	-	1/9/27/28	0/3/3/3
1	OMG	B5	3974	1	-	0/9/27/28	0/3/3/3
76	5F0	An	138	76	-	4/9/9/10	-
1	PSU	B5	1491	1	-	0/7/25/26	0/2/2/2
52	A2M	A2	166	52	-	0/9/27/28	0/3/3/3
1	OMG	B5	4364	95,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3583	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4711	95,1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2667	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4045	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	93	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	4058	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3450	1	-	0/9/27/28	0/3/3/3
5	HIC	BB	245	5	-	2/5/6/8	0/1/1/1
52	PSU	A2	802	52	-	2/7/25/26	0/2/2/2
1	A2M	B5	1810	95,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4246	1	-	1/7/25/26	0/2/2/2
3	PSU	B8	69	3	-	0/7/25/26	0/2/2/2
1	A2M	B5	4269	95,1	-	0/9/27/28	0/3/3/3
52	OMG	A2	1329	52,95	-	0/9/27/28	0/3/3/3
81	NMM	As	67	81	-	0/9/11/13	-
52	PSU	A2	1644	52,95	-	0/7/25/26	0/2/2/2
52	PSU	A2	36	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	3359	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3502	1	-	0/7/25/26	0/2/2/2
1	1MA	B5	1266	95,1	-	0/7/25/26	0/3/3/3
1	OMG	B5	4245	1	-	0/9/27/28	0/3/3/3
52	OMG	A2	602	52	-	0/9/27/28	0/3/3/3
52	OMG	A2	868	52	-	1/9/27/28	0/3/3/3
61	5MU	AT	53	61	-	0/7/25/26	0/2/2/2
1	A2M	B5	4336	1	-	1/9/27/28	0/3/3/3
52	OMC	A2	1392	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	967	52	-	0/7/25/26	0/2/2/2
1	A2M	B5	2244	95,1	-	0/9/27/28	0/3/3/3
52	OMG	A2	437	52	-	0/9/27/28	0/3/3/3
1	OMC	B5	1820	95,1	-	1/9/27/28	0/2/2/2
1	OMG	B5	2207	1	-	2/9/27/28	0/3/3/3
1	PSU	B5	3500	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	3657	1	-	1/9/27/28	0/2/2/2
52	PSU	A2	573	52	-	0/7/25/26	0/2/2/2
1	OMU	B5	2258	1	-	0/9/27/28	0/2/2/2
52	OMG	A2	510	52,95	-	1/9/27/28	0/3/3/3
52	OMG	A2	1448	52	-	2/9/27/28	0/3/3/3
1	OMG	B5	1580	95,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3576	1	-	1/7/25/26	0/2/2/2
1	PSU	B5	2475	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1446	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	4383	95,1	-	0/9/27/28	0/3/3/3
52	PSU	A2	867	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4298	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	1270	1	-	0/9/27/28	0/3/3/3
52	A2M	A2	1384	52	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	V5N	BA	216	4	-	2/9/10/12	0/1/1/1
1	PSU	B5	4435	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4369	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4374	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4116	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	3456	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4039	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	2680	95,1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4325	1	-	0/7/25/26	0/2/2/2
45	SAC	Br	2	45	-	0/7/8/10	-
52	4AC	A2	1843	52,95	-	4/11/29/30	0/2/2/2
1	PSU	B5	4382	1	-	4/7/25/26	0/2/2/2
52	OMG	A2	645	52	-	3/9/27/28	0/3/3/3
1	OMU	B5	4052	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	1632	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1683	95,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4169	1	-	0/7/25/26	0/2/2/2
6	AYA	BC	2	6	-	3/4/6/8	-
1	OMU	B5	4366	1	-	1/9/27/28	0/2/2/2
52	A2M	A2	513	52	-	2/9/27/28	0/3/3/3
1	OMC	B5	2265	95,1	-	0/9/27/28	0/2/2/2
1	OMC	B5	2647	1	-	0/9/27/28	0/2/2/2
30	V5N	Ba	39	30	-	0/9/10/12	0/1/1/1
1	A2M	B5	1479	1	-	0/9/27/28	0/3/3/3
1	OMG	B5	2267	1	-	1/9/27/28	0/3/3/3
52	A2M	A2	577	52	-	2/9/27/28	0/3/3/3
1	A2M	B5	3517	1	-	2/9/27/28	0/3/3/3
85	HY3	Aw	62	85	-	1/1/12/14	0/1/1/1
52	PSU	A2	1178	52,95	-	0/7/25/26	0/2/2/2
1	PSU	B5	1718	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	398	1	-	4/9/27/28	0/3/3/3
52	PSU	A2	218	52	-	0/7/25/26	0/2/2/2
1	UR3	B5	4276	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	3973	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	3540	1	-	0/9/27/28	0/2/2/2
1	5MC	B5	4193	95,1	-	4/7/25/26	0/2/2/2
1	PSU	B5	3462	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4322	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4267	95,1	-	0/7/25/26	0/2/2/2
52	OMC	A2	463	52	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	A2	864	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	3942	61,1	-	0/9/27/28	0/3/3/3
1	OMC	B5	1284	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	105	52	-	0/7/25/26	0/2/2/2
52	OMG	A2	684	52	-	1/9/27/28	0/3/3/3
1	OMC	B5	2194	95,1	-	2/9/27/28	0/2/2/2
1	A2M	B5	400	1	-	0/9/27/28	0/3/3/3
1	OMG	B5	3676	1	-	0/9/27/28	0/3/3/3
52	A2M	A2	27	52,95	-	2/9/27/28	0/3/3/3
1	A2M	B5	1489	95,1	-	2/9/27/28	0/3/3/3
1	OMG	B5	4240	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4203	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	210	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1005	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	1032	52	-	0/9/27/28	0/3/3/3
1	OMG	B5	3631	1	-	1/9/27/28	0/3/3/3
1	UY1	B5	3550	95,1	-	1/9/27/28	0/2/2/2
1	OMC	B5	4282	95,1	-	1/9/27/28	0/2/2/2
1	A2M	B5	3557	1	-	0/9/27/28	0/3/3/3
52	PSU	A2	682	52	-	0/7/25/26	0/2/2/2

The worst 5 of 521 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1640	G7M	C4-N9	7.81	1.58	1.38
52	A2	1640	G7M	O6-C6	7.69	1.38	1.23
52	A2	1851	MA6	C5-N7	6.90	1.52	1.39
52	A2	1852	MA6	C5-N7	6.80	1.51	1.39
52	A2	1640	G7M	C5-C4	6.25	1.54	1.38

The worst 5 of 966 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	1851	MA6	C4-N9-C8	14.65	121.61	105.73
52	A2	1852	MA6	C4-N9-C8	14.47	121.41	105.73
52	A2	1640	G7M	C8-N7-C5	11.37	122.00	107.78
52	A2	591	A2M	C5-C4-N3	-7.05	117.55	126.75
52	A2	1852	MA6	N3-C4-N9	6.98	138.59	127.08

There are no chirality outliers.

5 of 117 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	C2'-C1'-N1-C6
1	B5	4382	PSU	O4'-C1'-C5-C4

There are no ring outliers.

113 monomers are involved in 147 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A2	1693	PSU	1	0
61	AT	48	5MC	2	0
1	B5	3524	OMG	1	0
1	B5	4177	PSU	1	0
52	A2	1491	OMG	1	0
52	A2	1833	6MZ	1	0
1	B5	4149	PSU	1	0
1	B5	2208	OMC	2	0
1	B5	4042	PSU	1	0
52	A2	116	OMU	1	0
42	Bm	98	M3L	1	0
1	B5	3371	PSU	1	0
1	B5	4166	PSU	1	0
1	B5	3619	OMC	1	0
52	A2	121	OMU	2	0
1	B5	3562	A2M	2	0
52	A2	1704	OMC	2	0
52	A2	1233	PSU	1	0
52	A2	172	OMU	1	0
52	A2	1245	PSU	1	0
52	A2	610	PSU	1	0
1	B5	2704	OMC	1	0
52	A2	1338	4AC	2	0
52	A2	1348	PSU	1	0
52	A2	1679	A2M	2	0
1	B5	3585	PSU	1	0
52	A2	469	A2M	1	0
83	Au	1	AME	1	0
52	A2	1852	MA6	1	0
1	B5	1260	OMG	1	0
52	A2	119	PSU	1	0
52	A2	355	OMU	1	0
1	B5	3492	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	2206	A2M	1	0
1	B5	1638	PSU	2	0
52	A2	1082	PSU	1	0
52	A2	1443	OMU	1	0
1	B5	3433	OMC	1	0
1	B5	4138	OMG	2	0
52	A2	99	A2M	2	0
1	B5	2658	A2M	2	0
1	B5	4202	OMC	1	0
3	B8	75	OMG	1	0
52	A2	485	A2M	2	0
1	B5	3369	PSU	1	0
52	A2	518	OMC	1	0
52	A2	650	PSU	1	0
52	A2	1249	B8N	1	0
1	B5	4278	PSU	1	0
52	A2	1805	OMU	2	0
1	B5	4317	A2M	1	0
1	B5	2630	A2M	1	0
52	A2	1289	OMU	2	0
1	B5	3476	OMG	1	0
1	B5	3974	OMG	1	0
52	A2	166	A2M	2	0
1	B5	4364	OMG	2	0
1	B5	2667	OMC	1	0
1	B5	4058	PSU	1	0
1	B5	3450	A2M	2	0
5	BB	245	HIC	1	0
1	B5	1810	A2M	2	0
1	B5	4269	A2M	1	0
52	A2	1329	OMG	1	0
52	A2	36	PSU	2	0
52	A2	602	OMG	1	0
1	B5	4336	A2M	1	0
52	A2	1392	OMC	1	0
1	B5	2244	A2M	1	0
52	A2	437	OMG	1	0
1	B5	2207	OMG	1	0
1	B5	2258	OMU	1	0
52	A2	510	OMG	1	0
52	A2	1448	OMG	2	0
52	A2	1446	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	4383	OMG	1	0
1	B5	4298	PSU	1	0
1	B5	1270	A2M	2	0
52	A2	1384	A2M	1	0
1	B5	3456	A2M	2	0
1	B5	4039	PSU	1	0
52	A2	1843	4AC	2	0
1	B5	4382	PSU	1	0
52	A2	645	OMG	1	0
1	B5	4052	OMU	2	0
1	B5	4366	OMU	3	0
52	A2	513	A2M	2	0
1	B5	2265	OMC	1	0
1	B5	2647	OMC	2	0
30	Ba	39	V5N	1	0
1	B5	2267	OMG	1	0
52	A2	577	A2M	2	0
1	B5	3517	A2M	1	0
1	B5	1718	PSU	2	0
1	B5	398	A2M	1	0
1	B5	3973	OMU	1	0
1	B5	3540	OMC	1	0
1	B5	4193	5MC	1	0
52	A2	864	PSU	1	0
1	B5	3942	OMG	2	0
1	B5	1284	OMC	2	0
1	B5	2194	OMC	1	0
1	B5	400	A2M	1	0
1	B5	3676	OMG	2	0
52	A2	27	A2M	2	0
1	B5	1489	A2M	1	0
1	B5	4203	PSU	1	0
52	A2	1032	A2M	2	0
1	B5	3631	OMG	1	0
1	B5	3550	UY1	1	0
1	B5	4282	OMC	2	0
1	B5	3557	A2M	1	0
52	A2	682	PSU	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 793 ligands modelled in this entry, 758 are monoatomic - leaving 35 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
93	SPD	B5	4922	-	9,9,9	0.16	0	8,8,8	0.19	0
93	SPD	B5	4917	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.19	0
93	SPD	B5	4903	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPM	B5	4911	-	13,13,13	0.15	0	12,12,12	0.18	0
93	SPD	BN	301	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1906	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4915	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	B5	4910	-	9,9,9	0.15	0	8,8,8	0.16	0
93	SPD	B5	4920	-	9,9,9	0.16	0	8,8,8	0.19	0
97	AAC	BD	301	7	6,6,7	0.89	0	6,6,8	1.11	1 (16%)
93	SPD	B5	4919	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4907	-	9,9,9	0.16	0	8,8,8	0.16	0
93	SPD	B5	4918	-	9,9,9	0.15	0	8,8,8	0.21	0
93	SPD	A2	1908	-	9,9,9	0.16	0	8,8,8	0.19	0
93	SPD	B5	4906	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPM	A2	1909	-	13,13,13	0.14	0	12,12,12	0.16	0
93	SPD	B5	4912	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1904	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4923	-	9,9,9	0.16	0	8,8,8	0.15	0
93	SPD	A2	1901	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	A2	1903	-	9,9,9	0.16	0	8,8,8	0.16	0
93	SPD	B5	4902	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1902	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	B5	4909	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	A2	1905	-	9,9,9	0.15	0	8,8,8	0.17	0
93	SPD	B5	4904	-	9,9,9	0.16	0	8,8,8	0.18	0
96	GTP	B7	201	2	30,34,34	0.49	0	46,54,54	0.57	0
93	SPD	B5	4916	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	B5	4921	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPM	B5	4914	-	13,13,13	0.15	0	12,12,12	0.15	0
93	SPD	B5	4908	-	9,9,9	0.16	0	8,8,8	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
93	SPD	B5	4901	-	9,9,9	0.15	0	8,8,8	0.14	0
93	SPD	B5	4913	-	9,9,9	0.15	0	8,8,8	0.18	0
93	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
93	SPD	B5	4922	-	-	0/7/7/7	-
93	SPD	B5	4917	-	-	0/7/7/7	-
93	SPD	A2	1907	-	-	1/7/7/7	-
93	SPD	B5	4903	-	-	1/7/7/7	-
94	SPM	B5	4911	-	-	1/11/11/11	-
93	SPD	BN	301	-	-	1/7/7/7	-
93	SPD	A2	1906	-	-	0/7/7/7	-
93	SPD	B5	4915	-	-	0/7/7/7	-
93	SPD	B5	4910	-	-	0/7/7/7	-
93	SPD	B5	4920	-	-	0/7/7/7	-
97	AAC	BD	301	7	-	0/3/4/5	-
93	SPD	B5	4919	-	-	1/7/7/7	-
93	SPD	B5	4907	-	-	0/7/7/7	-
93	SPD	B5	4918	-	-	0/7/7/7	-
93	SPD	A2	1908	-	-	0/7/7/7	-
93	SPD	B5	4906	-	-	0/7/7/7	-
94	SPM	A2	1909	-	-	1/11/11/11	-
93	SPD	B5	4912	-	-	0/7/7/7	-
93	SPD	A2	1904	-	-	0/7/7/7	-
93	SPD	B5	4923	-	-	1/7/7/7	-
93	SPD	A2	1901	-	-	1/7/7/7	-
93	SPD	A2	1903	-	-	0/7/7/7	-
93	SPD	B5	4902	-	-	2/7/7/7	-
93	SPD	A2	1902	-	-	0/7/7/7	-
93	SPD	B5	4909	-	-	1/7/7/7	-
93	SPD	A2	1905	-	-	0/7/7/7	-
93	SPD	B5	4904	-	-	0/7/7/7	-
96	GTP	B7	201	2	-	0/22/38/38	0/3/3/3
93	SPD	B5	4916	-	-	0/7/7/7	-
93	SPD	B5	4921	-	-	1/7/7/7	-
94	SPM	B5	4914	-	-	0/11/11/11	-
93	SPD	B5	4908	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	SPD	B5	4901	-	-	2/7/7/7	-
93	SPD	B5	4913	-	-	0/7/7/7	-
93	SPD	B5	4905	-	-	1/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	BD	301	AAC	O2-C1-C2	-2.27	118.86	125.42

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
94	A2	1909	SPM	C8-C9-N10-C11
93	B5	4902	SPD	C2-C3-C4-C5
93	B5	4921	SPD	C2-C3-C4-C5
94	B5	4911	SPM	C6-C7-C8-C9
93	A2	1901	SPD	C2-C3-C4-C5

There are no ring outliers.

18 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
93	A2	1907	SPD	2	0
93	B5	4903	SPD	2	0
94	B5	4911	SPM	2	0
93	A2	1906	SPD	1	0
93	B5	4915	SPD	2	0
93	B5	4919	SPD	1	0
93	B5	4907	SPD	1	0
93	B5	4918	SPD	1	0
93	B5	4906	SPD	1	0
94	A2	1909	SPM	1	0
93	A2	1904	SPD	2	0
93	B5	4923	SPD	3	0
93	A2	1901	SPD	1	0
93	A2	1903	SPD	1	0
93	A2	1902	SPD	1	0
93	A2	1905	SPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
93	B5	4916	SPD	2	0
94	B5	4914	SPM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

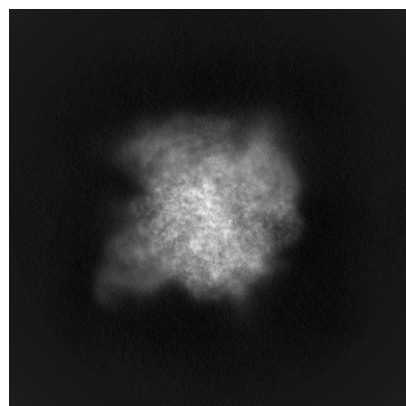
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16232. These allow visual inspection of the internal detail of the map and identification of artifacts.

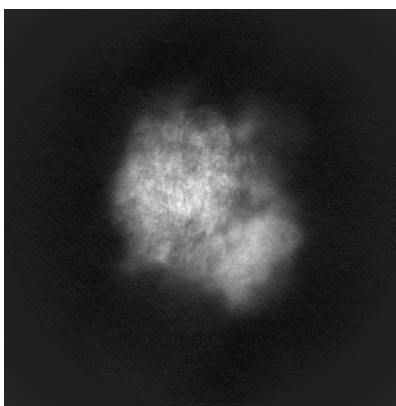
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

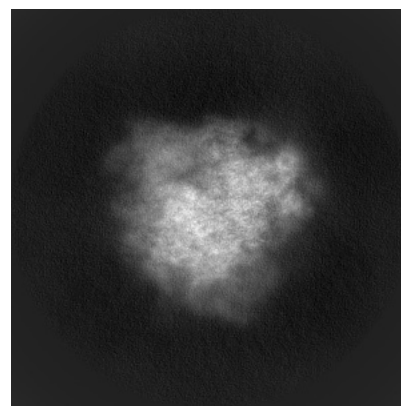
6.1.1 Primary map



X

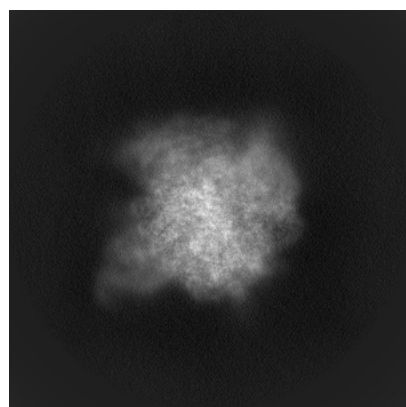


Y

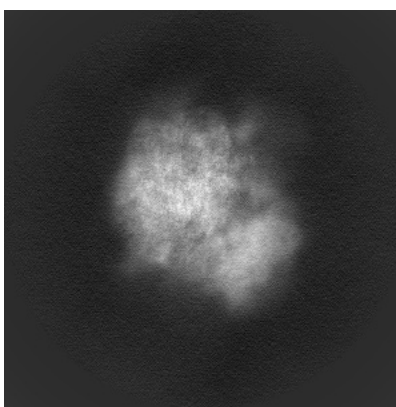


Z

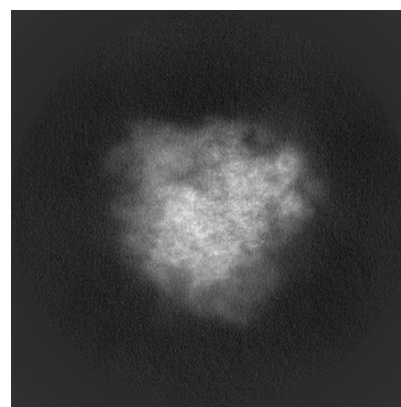
6.1.2 Raw map



X



Y

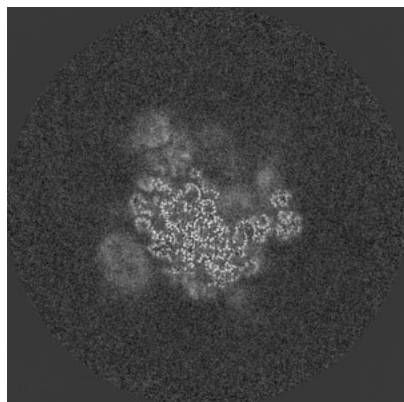


Z

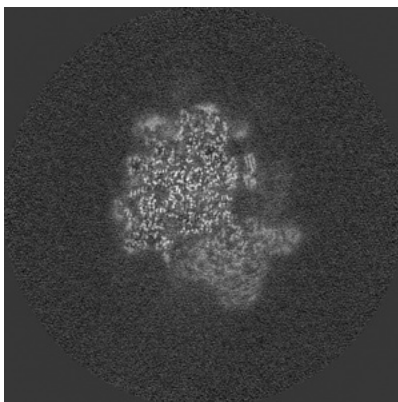
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

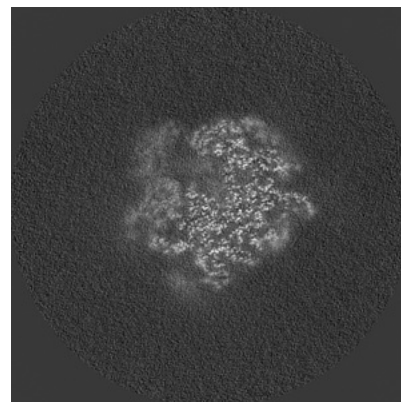
6.2.1 Primary map



X Index: 256

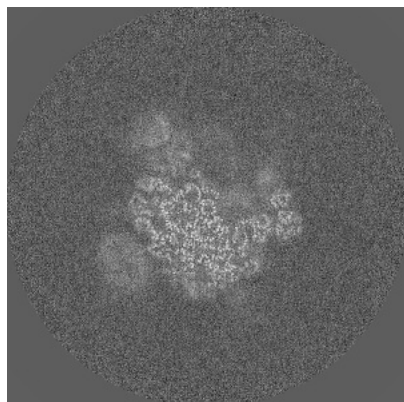


Y Index: 256

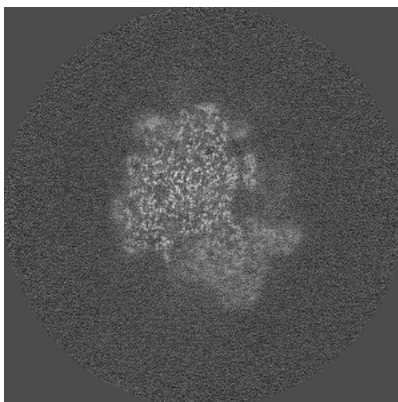


Z Index: 256

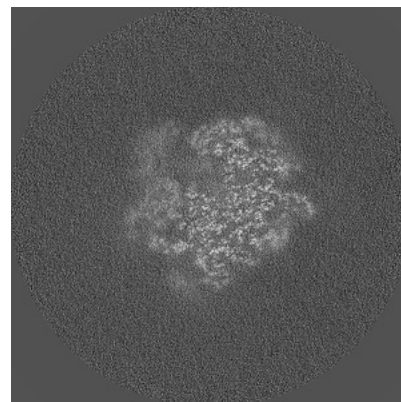
6.2.2 Raw map



X Index: 256



Y Index: 256

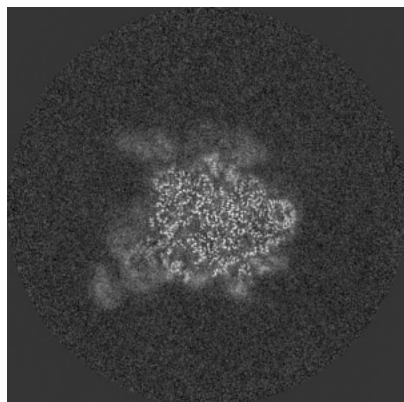


Z Index: 256

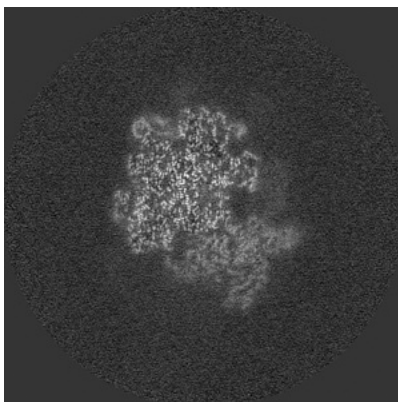
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

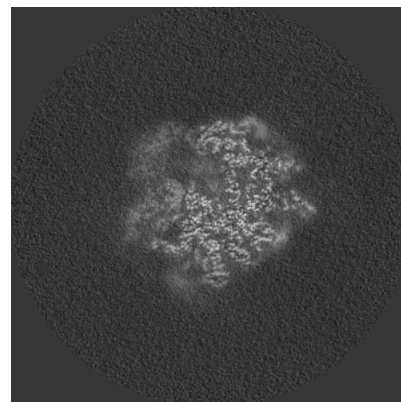
6.3.1 Primary map



X Index: 283

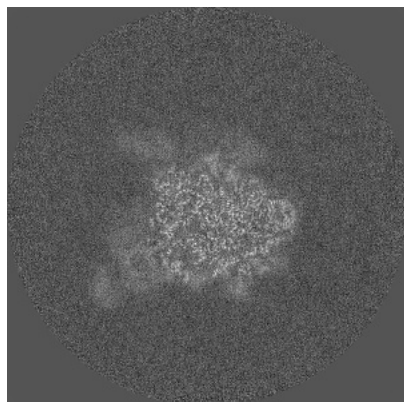


Y Index: 261

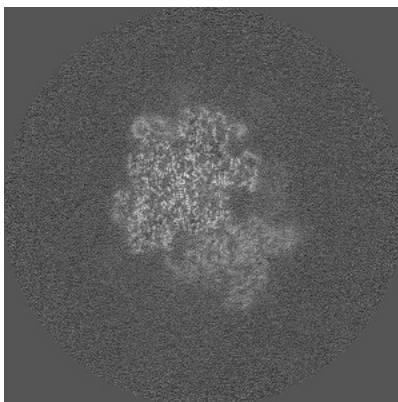


Z Index: 259

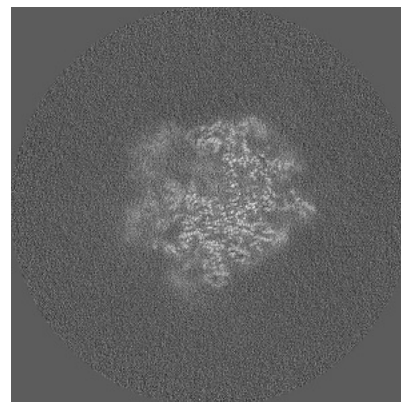
6.3.2 Raw map



X Index: 283



Y Index: 261

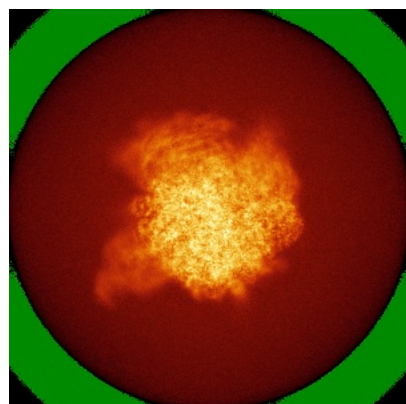


Z Index: 260

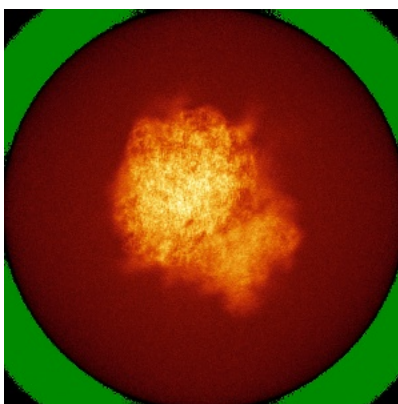
The images above show the largest variance slices of the map in three orthogonal directions.

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

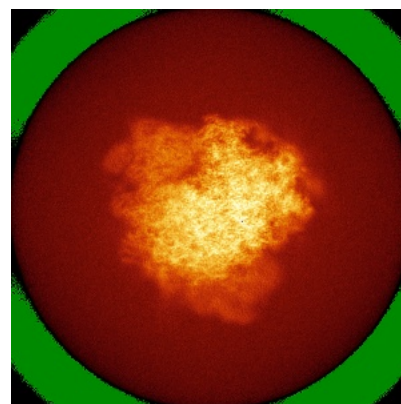
6.4.1 Primary map



X

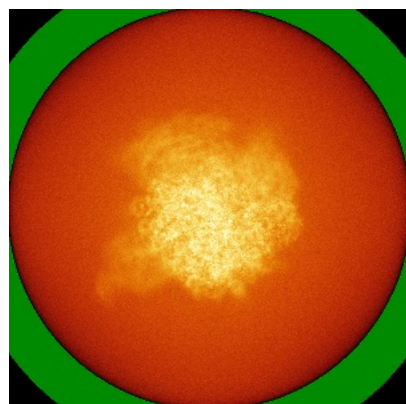


Y

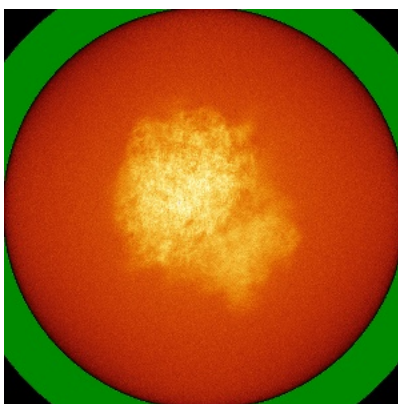


Z

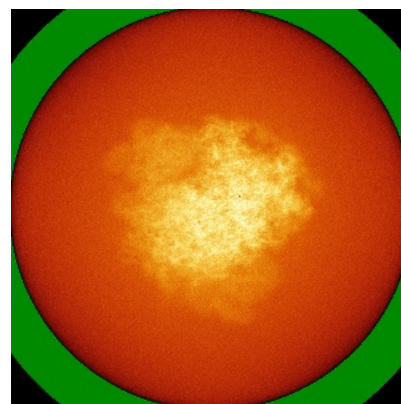
6.4.2 Raw map



X



Y

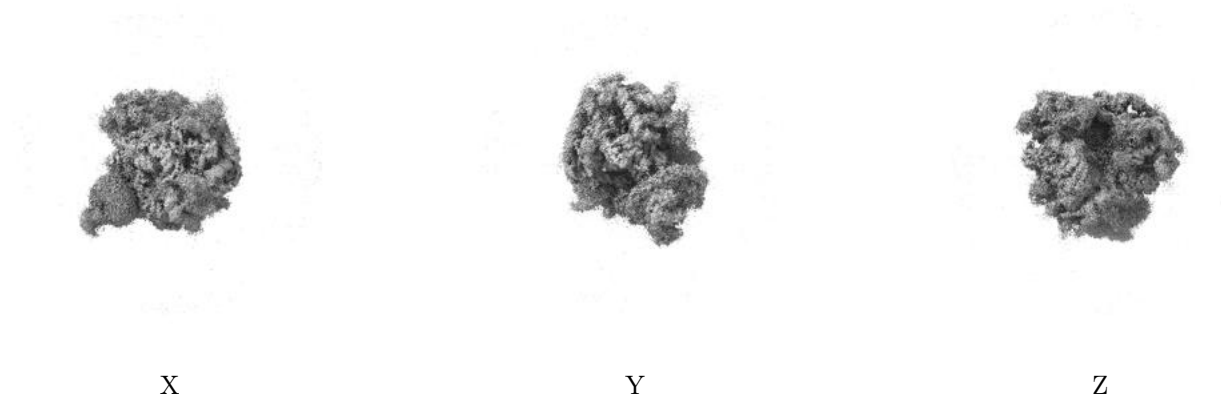


Z

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.

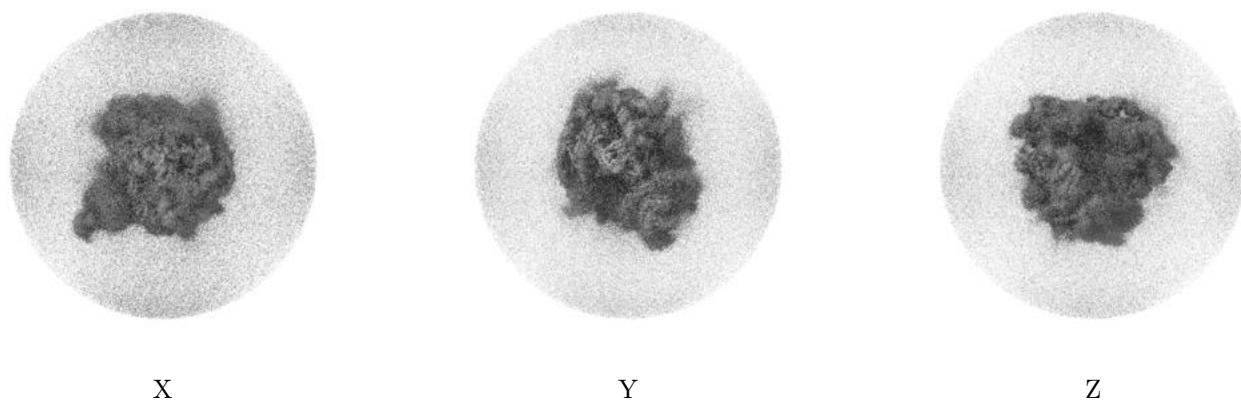
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

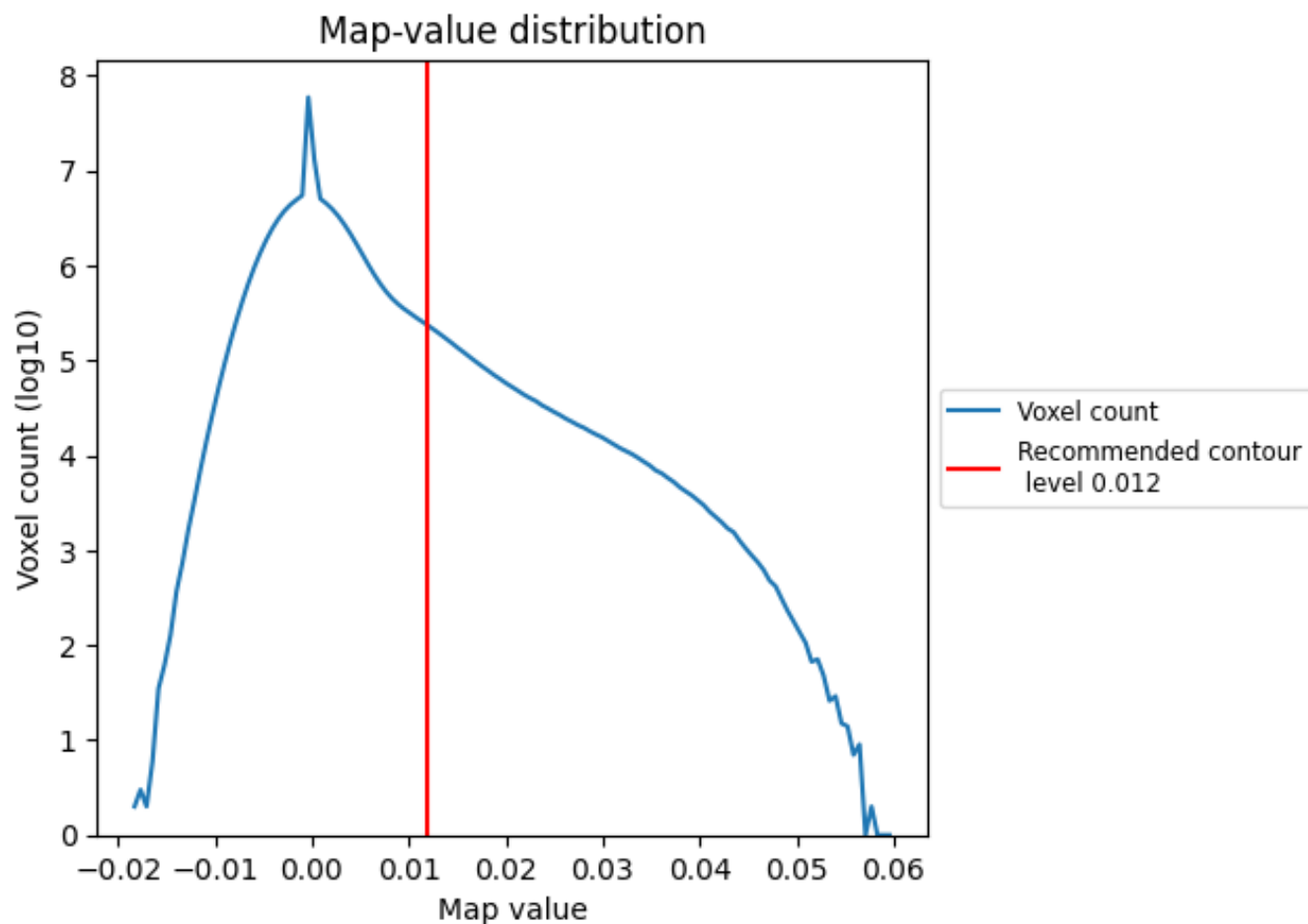
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

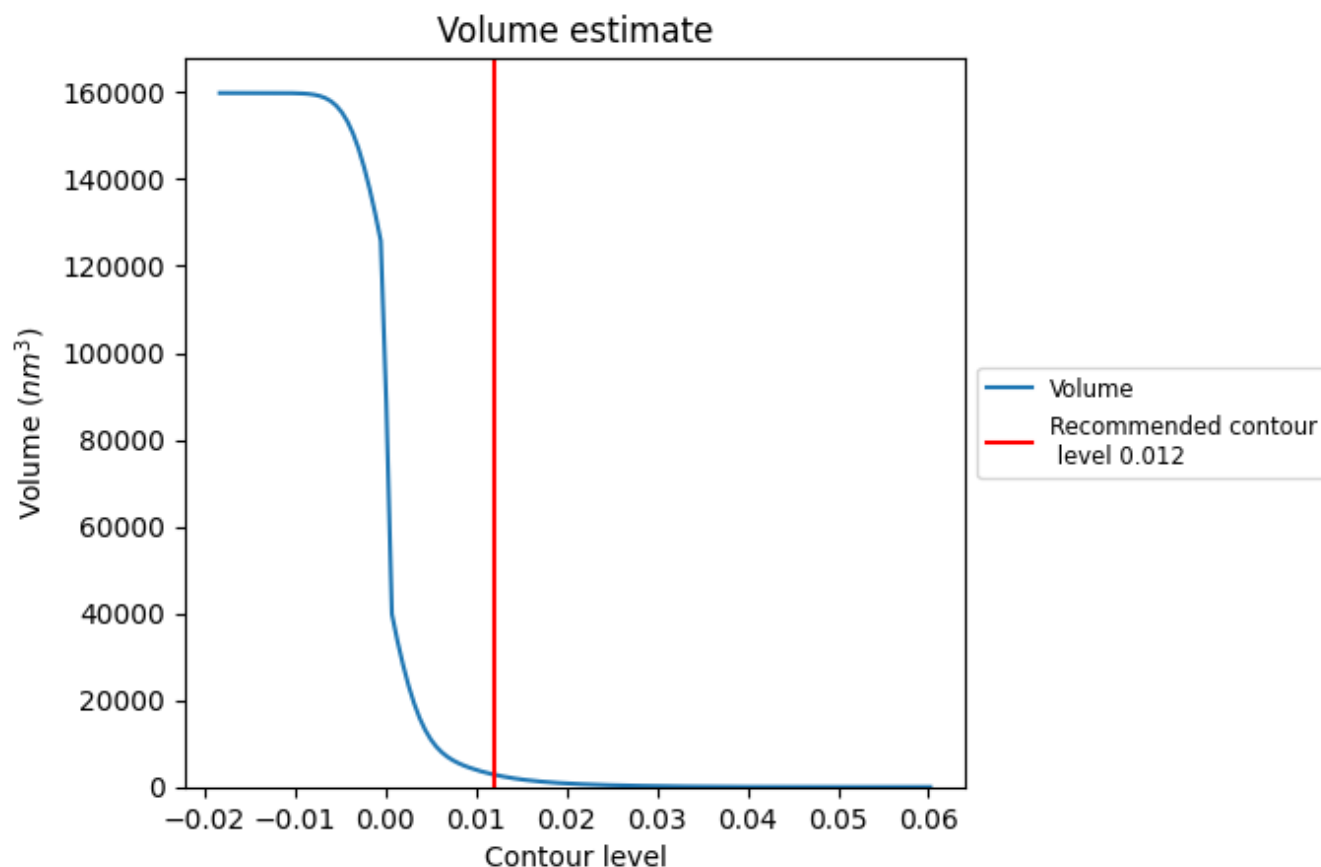
This section contains the results of statistical analysis of the map.

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.

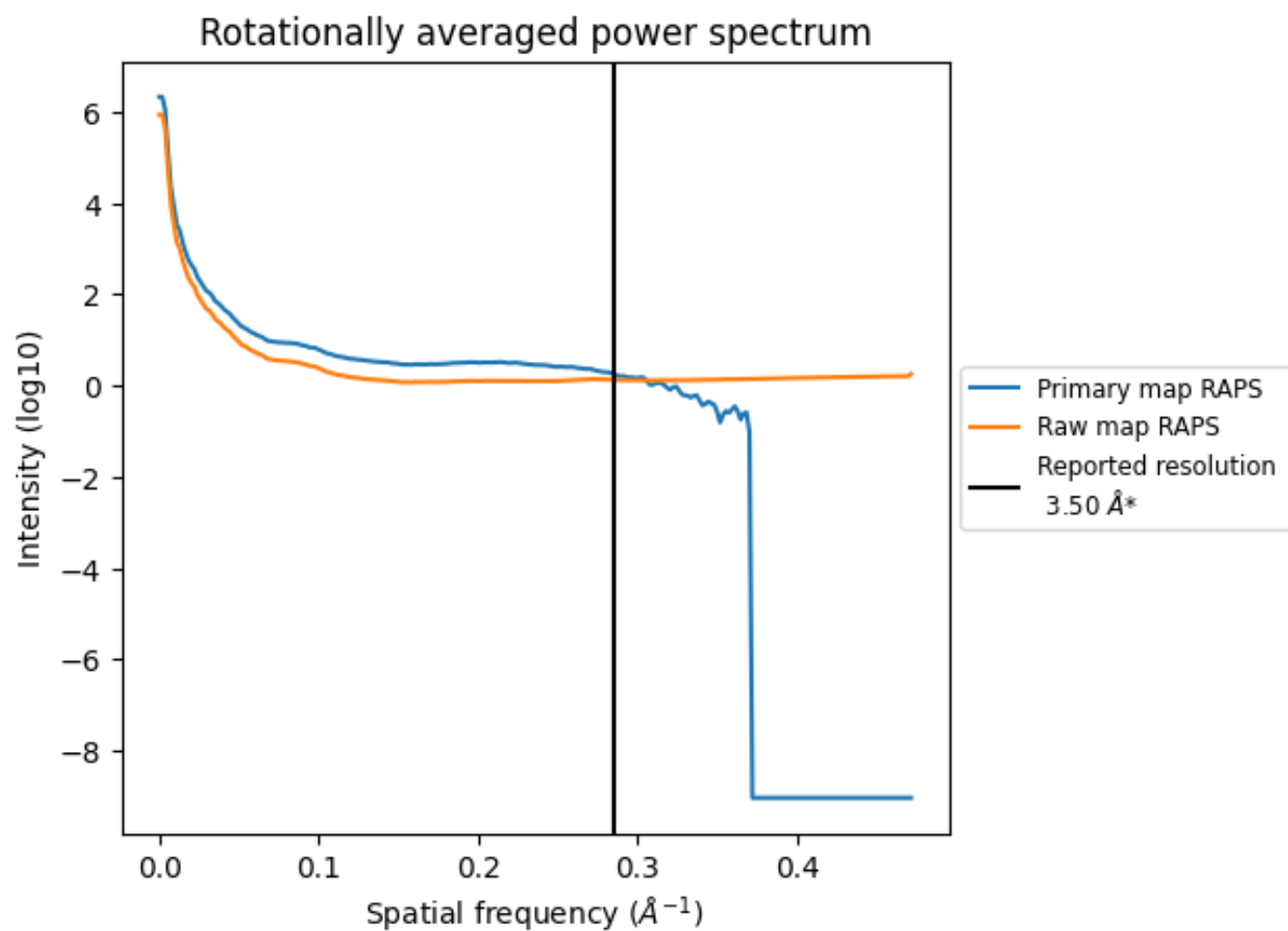
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2852 nm³; this corresponds to an approximate mass of 2576 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 ⓘ

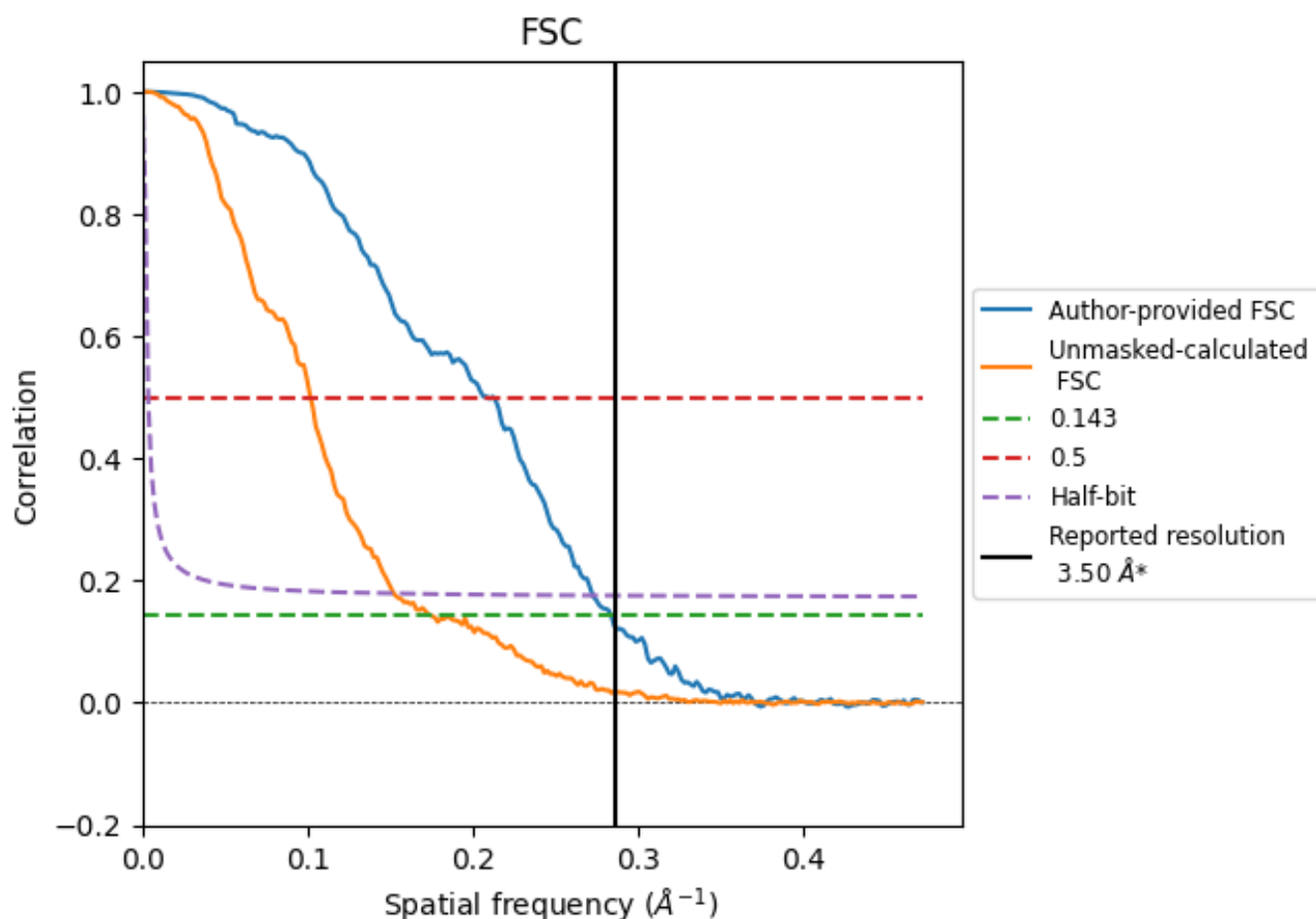


*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

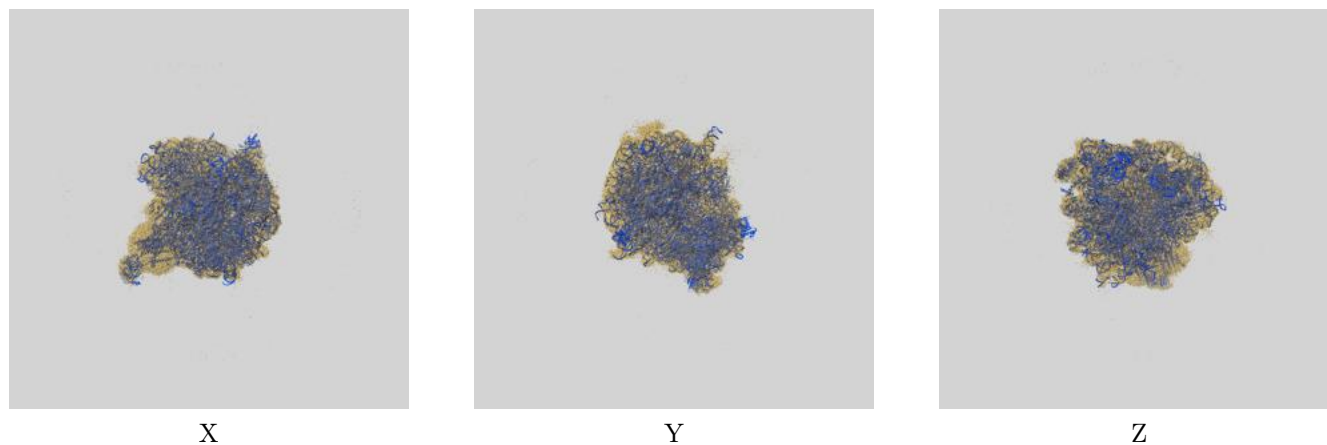
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.53	4.79	3.67
Unmasked-calculated*	5.74	9.82	6.57

*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 5.74 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

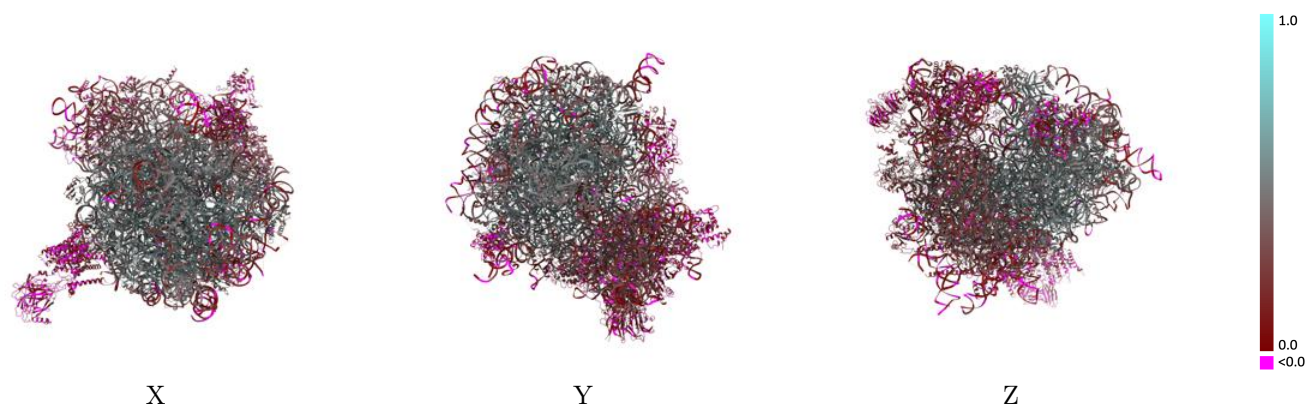
This section contains information regarding the fit between EMDB map EMD-16232 and PDB model 8BTK. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



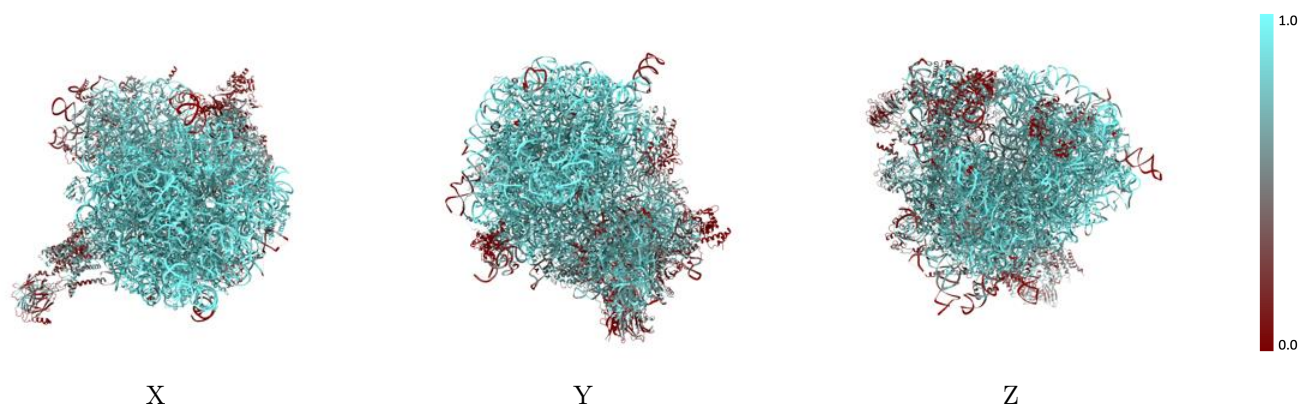
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



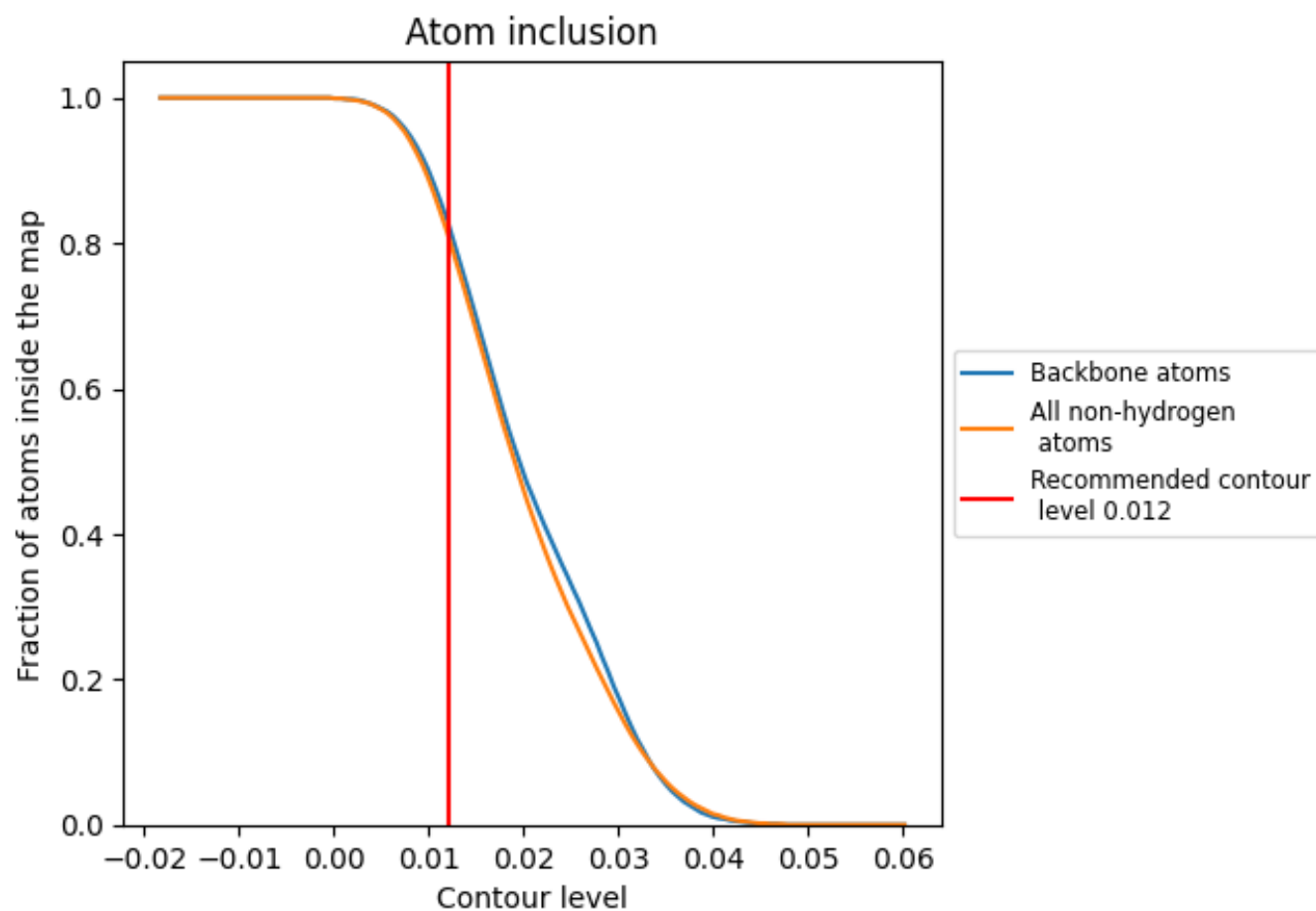
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 81% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8130	 0.3620
A2	 0.8260	 0.2850
AA	 0.6120	 0.2480
AB	 0.4950	 0.1730
AC	 0.1480	 0.0390
AD	 0.5960	 0.2210
AE	 0.7810	 0.3420
AF	 0.3110	 0.1180
AG	 0.6240	 0.2030
AH	 0.1940	 0.0250
AT	 0.4880	 0.1690
AZ	 0.6640	 0.2980
Aa	 0.6470	 0.3000
Ab	 0.7530	 0.3250
Ac	 0.4050	 0.1730
Ad	 0.7170	 0.2710
Ae	 0.5430	 0.2010
Af	 0.5790	 0.2120
Ag	 0.4930	 0.2280
Ah	 0.6090	 0.2620
Ai	 0.6870	 0.2630
Aj	 0.3700	 0.1210
Ak	 0.6280	 0.2850
Al	 0.0140	 0.0620
Am	 0.7240	 0.3290
An	 0.6940	 0.3100
Ao	 0.5050	 0.1730
Ap	 0.6240	 0.2030
Aq	 0.5170	 0.2240
Ar	 0.5520	 0.1950
As	 0.5560	 0.1870
At	 0.5550	 0.1670
Au	 0.6760	 0.2890
Av	 0.7850	 0.3410
Aw	 0.7720	 0.3290



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Chain	Atom inclusion	Q-score
Ax	 0.5930	 0.1760
Ay	 0.4210	 0.1720
Az	 0.8530	 0.4140
B5	 0.9300	 0.4300
B7	 0.9940	 0.5030
B8	 0.9850	 0.4620
BA	 0.9370	 0.5160
BB	 0.9340	 0.5000
BC	 0.9580	 0.5070
BD	 0.9010	 0.4540
BE	 0.8570	 0.4000
BF	 0.9400	 0.4960
BG	 0.8680	 0.4280
BH	 0.8950	 0.4450
BI	 0.8900	 0.4670
BJ	 0.8390	 0.3870
BK	 0.9170	 0.3470
BL	 0.8980	 0.4610
BM	 0.8980	 0.4480
BN	 0.9720	 0.5310
BO	 0.9470	 0.5050
BP	 0.9230	 0.5120
BQ	 0.9660	 0.5220
BR	 0.8590	 0.4220
BS	 0.9550	 0.5090
BT	 0.9190	 0.4980
BU	 0.8520	 0.3690
BV	 0.9090	 0.4810
BW	 0.5920	 0.2990
BX	 0.9110	 0.4800
BY	 0.9090	 0.4810
BZ	 0.9080	 0.4500
Ba	 0.9610	 0.5210
Bb	 0.8180	 0.3850
Bc	 0.8330	 0.3990
Bd	 0.9050	 0.4880
Be	 0.9530	 0.5190
Bf	 0.9500	 0.5340
Bg	 0.9150	 0.4650
Bh	 0.9000	 0.4670
Bi	 0.9070	 0.4390
Bj	 0.9620	 0.5270

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Chain	Atom inclusion	Q-score
Bk	 0.7900	 0.4050
Bl	 0.9490	 0.5040
Bm	 0.8160	 0.4060
Bo	 0.8840	 0.4750
Bp	 0.9200	 0.4980
Br	 0.9480	 0.4990
Bs	 0.3620	 0.1160
Bt	 0.1570	 0.0760
Bv	 0.0600	 0.0630
SX	 0.5620	 0.1520
SY	 0.6650	 0.2130
SZ	 0.2760	 0.0800
TA	 0.3920	 0.0740
TB	 0.3550	 0.0590
TC	 0.3960	 0.0780
TD	 0.2000	 0.0470