



wwPDB EM Validation Summary Report ⓘ

Jun 22, 2026 – 10:32 PM EDT

PDB ID : 9C3H / pdb_00009c3h
EMDB ID : EMD-45170
Title : Structure of the CNOT3-bound human 80S ribosome with tRNA-ARG in the P-site.
Authors : Erzberger, J.P.; Cruz, V.E.
Deposited on : 2024-06-01
Resolution : 2.00 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:

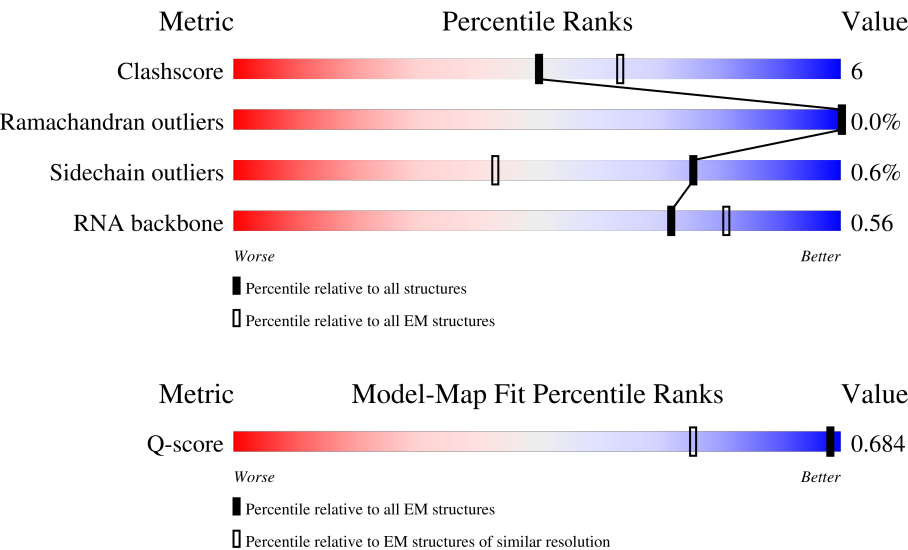
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 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.



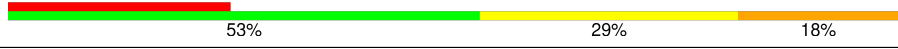
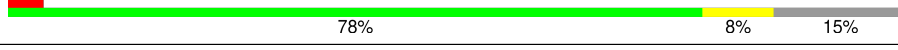
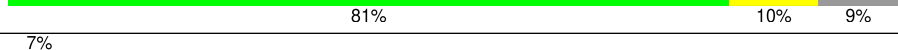
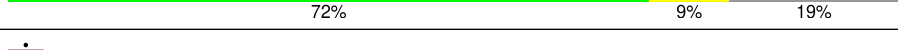
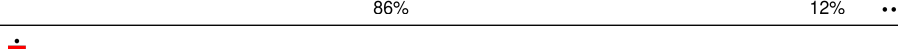
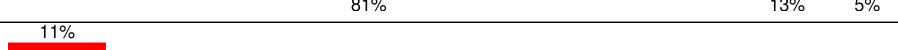
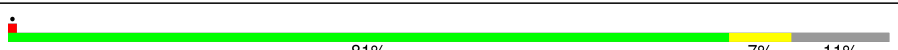
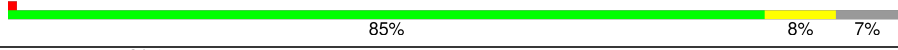
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1659 (1.50 - 2.50)

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	L1	157	11% 57% 36% 6%
2	L5	5069	9% 45% 22% 30%
3	L8	297	9% 85% 14%

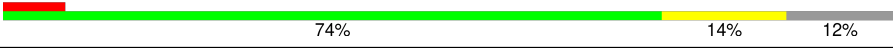
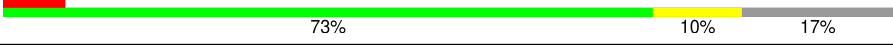
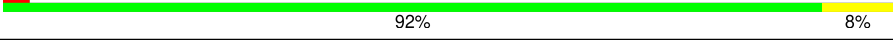
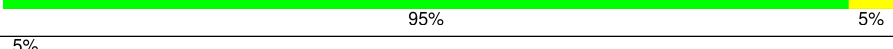
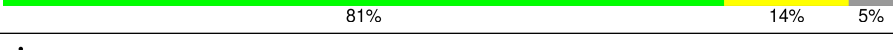
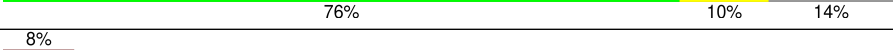
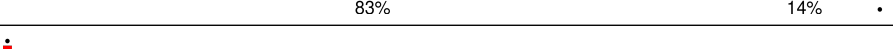
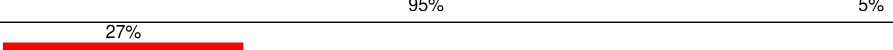
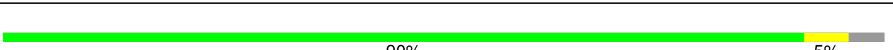
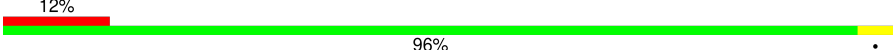
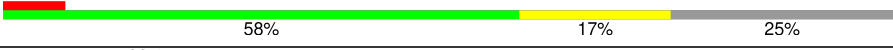
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Mol	Chain	Length	Quality of chain
4	L9	121	
5	LB	403	
6	S4	76	
7	LC	427	
8	LD	257	
9	LE	145	
10	LF	248	
11	LG	266	
12	LH	192	
13	LI	135	
14	LJ	178	
15	LK	288	
16	LM	215	
17	LN	204	
18	LO	123	
19	LP	97	
20	LQ	211	
21	LR	196	
22	LS	176	
23	LT	160	
24	LU	51	
25	LV	140	
26	LW	157	
27	LY	203	
28	LZ	136	

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Mol	Chain	Length	Quality of chain
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	106	
34	Lf	110	
35	Lg	117	
36	Lh	184	
37	Li	105	
38	Lj	188	
39	Lk	70	
40	Ll	137	
41	Lm	128	
42	Ln	156	
43	Lo	99	
44	Lp	92	
45	Lz	214	
46	NC	25	
47	S1	264	
48	S2	1869	
49	S5	9	
50	SA	295	
51	SB	609	
52	SC	293	
53	SD	204	

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Mol	Chain	Length	Quality of chain
54	SE	263	
55	SG	249	
56	SH	194	
57	SI	208	
58	SJ	194	
59	SK	243	
60	SL	158	
61	SM	165	
62	SN	151	
63	SO	151	
64	SP	145	
65	SQ	146	
66	SS	135	
67	ST	152	
68	SU	145	
69	SV	83	
70	SW	130	
71	SX	143	
72	SY	132	
73	SZ	119	
74	Sa	115	
75	Sb	84	
76	Sc	125	
77	Sd	69	
78	Se	133	

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Mol	Chain	Length	Quality of chain
79	Sf	56	9%84%12%••
80	Sg	317	70%63%32%•
81	So	25	•96%•
82	Sy	132	92%65%26%•8%
83	Sz	156	47%28%18%•53%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 222228 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 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	148	Total	C	N	O	P	0	0
			3153	1408	563	1035	147		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L5	3531	Total	C	N	O	P	0	0
			75768	33782	13851	24605	3530		

- Molecule 3 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L8	293	Total	C	N	O	S	0	0
			2386	1510	435	427	14		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L9	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	401	Total	C	N	O	S	0	0
			3234	2058	607	555	14		

- Molecule 6 is a RNA chain called tRNA-ARG,CCG-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S4	76	Total	C	N	O	P	0	0
			1634	732	290	536	76		

- Molecule 7 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LC	365	Total	C	N	O	S	0	0
			2908	1829	580	486	13		

- Molecule 8 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL24.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LF	173	SER	ALA	conflict	UNP P18124

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LG	216	Total	C	N	O	S	0	0
			1752	1117	337	294	4		

- Molecule 12 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 13 is a protein called Large ribosomal subunit protein eL32.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LJ	167	Total	C	N	O	S	0	0
			1340	848	250	236	6		

- Molecule 15 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LK	222	Total	C	N	O	S	0	0
			1780	1147	337	292	4		

- Molecule 16 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LM	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 17 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LO	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 19 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 20 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LQ	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 21 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LR	186	Total	C	N	O	S	0	0
			1558	965	335	249	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LS	176	Total	C	N	O	S	0	0
			1460	930	284	235	11		

- Molecule 23 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LT	157	Total	C	N	O	S	0	0
			1284	815	250	214	5		

- Molecule 24 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 25 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LV	130	Total	C	N	O	S	0	0
			972	615	183	169	5		

- Molecule 26 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LW	110	Total	C	N	O	S	0	0
			893	560	180	150	3		

- Molecule 27 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	198	Total	C	N	O	S	0	0
			1624	1048	317	254	5		

- Molecule 28 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	0	0
			1106	714	208	181	3		

- Molecule 29 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	104	Total	C	N	O	S	0	0
			848	526	186	132	4		

- Molecule 31 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	101	Total	C	N	O	S	0	0
			785	498	138	142	7		

- Molecule 32 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ld	104	Total	C	N	O	S	0	0
			862	546	167	147	2		

- Molecule 33 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 34 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lf	109	Total	C	N	O	S	0	0
			875	555	174	143	3		

- Molecule 35 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lg	111	Total	C	N	O	S	0	0
			882	552	182	142	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lh	159	Total	C	N	O	S	0	0
			1289	808	249	223	9		

- Molecule 37 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 38 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lj	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 39 is a protein called Large ribosomal subunit protein eL38.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ll	124	Total	C	N	O	S	0	0
			990	614	205	167	4		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 41 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	100	Total	C	N	O	S	0	0
			816	524	142	148	2		

- Molecule 42 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	116	Total	C	N	O	S	0	0
			949	606	178	164	1		

- Molecule 43 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	52	Total	C	N	O	S	1	0
			436	272	91	67	6		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lo	?	-	GLY	deletion	UNP P62987
Lo	?	-	ILE	deletion	UNP P62987
Lo	?	-	PRO	deletion	UNP P62987
Lo	?	-	PRO	deletion	UNP P62987
Lo	?	-	ASP	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	ARG	deletion	UNP P62987
Lo	?	-	LEU	deletion	UNP P62987
Lo	?	-	ILE	deletion	UNP P62987
Lo	?	-	PHE	deletion	UNP P62987
Lo	?	-	ALA	deletion	UNP P62987
Lo	?	-	GLY	deletion	UNP P62987
Lo	?	-	LYS	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	LEU	deletion	UNP P62987
Lo	?	-	GLU	deletion	UNP P62987
Lo	?	-	ASP	deletion	UNP P62987
Lo	?	-	GLY	deletion	UNP P62987
Lo	?	-	ARG	deletion	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
Lo	?	-	THR	deletion	UNP P62987
Lo	?	-	LEU	deletion	UNP P62987
Lo	?	-	SER	deletion	UNP P62987
Lo	?	-	ASP	deletion	UNP P62987
Lo	?	-	TYR	deletion	UNP P62987
Lo	?	-	ASN	deletion	UNP P62987
Lo	?	-	ILE	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	LYS	deletion	UNP P62987

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

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lz	211	Total	C	N	O	S	0	0
			1705	1081	329	281	14		

- Molecule 46 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	NC	25	Total	C	N	O	0	0
			227	134	52	41		

- Molecule 47 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S1	221	Total	C	N	O	S	0	0
			1790	1135	323	318	14		

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	1660	Total	C	N	O	P	0	0
			35485	15869	6358	11599	1659		

- Molecule 49 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S5	9	Total	C	N	O	P	0	0
			191	85	33	64	9		

- Molecule 50 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SA	220	Total	C	N	O	S	0	0
			1731	1099	303	321	8		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 51 is a protein called CCR4-NOT transcription complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SB	232	Total	C	N	O	S	0	0
			1937	1204	344	383	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SB	608	PRO	-	expression tag	UNP O75175
SB	609	ARG	-	expression tag	UNP O75175

- Molecule 52 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SC	219	Total	C	N	O	S	0	0
			1700	1100	292	298	10		

- Molecule 53 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SD	184	Total	C	N	O	S	0	0
			1463	917	276	263	7		

- Molecule 54 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SE	262	Total	C	N	O	S	0	0
			2075	1324	386	357	8		

- Molecule 55 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SG	229	Total	C	N	O	S	0	0
			1853	1158	369	319	7		

- Molecule 56 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SH	187	Total	C	N	O	S	0	0
			1509	963	277	268	1		

- Molecule 57 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SI	207	Total	C	N	O	S	0	0
			1695	1064	334	292	5		

- Molecule 58 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 59 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SK	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 60 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SL	143	Total	C	N	O	S	0	0
			1180	754	223	197	6		

- Molecule 61 is a protein called Small ribosomal subunit protein eS10.

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

- Molecule 62 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SN	150	Total	C	N	O	S	0	0
			1207	773	229	204	1		

- Molecule 63 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SO	127	Total	C	N	O	S	0	0
			956	585	189	176	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SO	138	IAS	ASP	conflict	UNP P62263

- Molecule 64 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SP	125	Total	C	N	O	S	0	0
			1021	647	192	175	7		

- Molecule 65 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SQ	139	Total	C	N	O	S	0	0
			1108	704	210	191	3		

- Molecule 66 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SS	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 67 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	ST	147	Total	C	N	O	S	0	0
			1208	758	244	205	1		

- Molecule 68 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SU	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

- Molecule 69 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 70 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SW	129	Total	C	N	O	S	0	0
			1033	659	193	175	6		

- Molecule 71 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SX	140	Total	C	N	O	S	0	0
			1088	687	215	183	3		

- Molecule 72 is a protein called Isoform 3 of Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SY	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 73 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SZ	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 74 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sa	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 75 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 76 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sc	83	Total	C	N	O	S	0	0
			670	431	125	113	1		

- Molecule 77 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sd	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 78 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Se	55	Total	C	N	O	S	0	0
			437	271	95	70	1		

- Molecule 79 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 80 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sg	303	Total	C	N	O	S	0	0
			2364	1492	412	448	12		

- Molecule 81 is a protein called Small ribosomal subunit protein eS32.

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

- Molecule 82 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sy	121	Total	C	N	O	S	0	0
			939	590	166	174	9		

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sz	74	Total	C	N	O	S	0	0
			607	384	116	100	7		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	L1	4	Total	Mg	0
			4	4	
84	L5	204	Total	Mg	0
			204	204	
84	L9	3	Total	Mg	0
			3	3	
84	S4	6	Total	Mg	0
			6	6	
84	LD	1	Total	Mg	0
			1	1	
84	LI	2	Total	Mg	0
			2	2	
84	LN	1	Total	Mg	0
			1	1	
84	LR	2	Total	Mg	0
			2	2	
84	LV	1	Total	Mg	0
			1	1	
84	La	1	Total	Mg	0
			1	1	
84	Lh	1	Total	Mg	0
			1	1	
84	S2	97	Total	Mg	0
			97	97	

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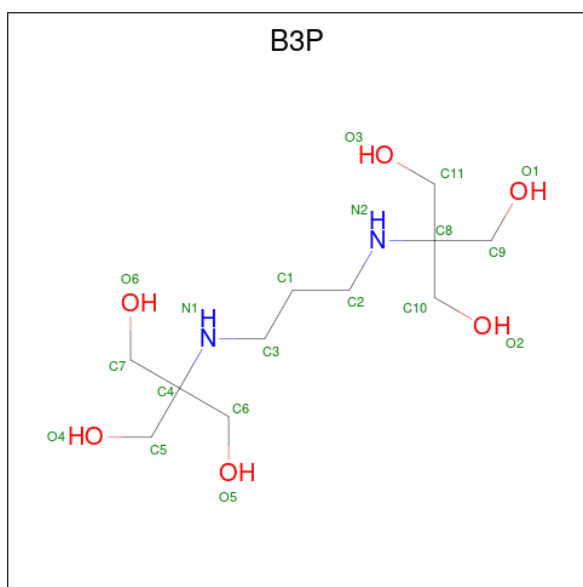
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Mol	Chain	Residues	Atoms		AltConf
84	SG	1	Total 1	Mg 1	0
84	ST	1	Total 1	Mg 1	0
84	SX	1	Total 1	Mg 1	0

- Molecule 85 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
85	L1	3	Total 3	K 3	0
85	L5	42	Total 42	K 42	0
85	L9	1	Total 1	K 1	0
85	LC	1	Total 1	K 1	0
85	LD	2	Total 2	K 2	0
85	LV	1	Total 1	K 1	0
85	Lz	1	Total 1	K 1	0
85	S2	39	Total 39	K 39	0
85	SE	1	Total 1	K 1	0
85	SO	1	Total 1	K 1	0
85	ST	1	Total 1	K 1	0
85	Sf	1	Total 1	K 1	0

- Molecule 86 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				AltConf
86	L5	1	Total	C	N	O	0
			19	11	2	6	

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

Mol	Chain	Residues	Atoms		AltConf
87	LP	1	Total	Zn	0
			1	1	
87	Le	1	Total	Zn	0
			1	1	
87	Lg	1	Total	Zn	0
			1	1	
87	Lo	1	Total	Zn	0
			1	1	
87	Lp	1	Total	Zn	0
			1	1	
87	Sa	1	Total	Zn	0
			1	1	
87	Sf	1	Total	Zn	0
			1	1	
87	Sz	1	Total	Zn	0
			1	1	

- Molecule 88 is water.

Mol	Chain	Residues	Atoms		AltConf
88	L1	153	Total 153	O 153	0
88	L5	4961	Total 4961	O 4961	0
88	L8	25	Total 25	O 25	0
88	L9	93	Total 93	O 93	0
88	LB	85	Total 85	O 85	0
88	S4	52	Total 52	O 52	0
88	LC	104	Total 104	O 104	0
88	LD	91	Total 91	O 91	0
88	LE	10	Total 10	O 10	0
88	LF	52	Total 52	O 52	0
88	LG	16	Total 16	O 16	0
88	LH	18	Total 18	O 18	0
88	LI	64	Total 64	O 64	0
88	LJ	3	Total 3	O 3	0
88	LK	12	Total 12	O 12	0
88	LM	7	Total 7	O 7	0
88	LN	89	Total 89	O 89	0
88	LO	13	Total 13	O 13	0
88	LP	33	Total 33	O 33	0
88	LQ	45	Total 45	O 45	0
88	LR	23	Total 23	O 23	0
88	LS	39	Total 39	O 39	0

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Mol	Chain	Residues	Atoms		AltConf
88	LT	41	Total 41	O 41	0
88	LU	10	Total 10	O 10	0
88	LV	27	Total 27	O 27	0
88	LW	7	Total 7	O 7	0
88	LY	42	Total 42	O 42	0
88	LZ	10	Total 10	O 10	0
88	La	46	Total 46	O 46	0
88	Lb	15	Total 15	O 15	0
88	Lc	8	Total 8	O 8	0
88	Ld	15	Total 15	O 15	0
88	Le	19	Total 19	O 19	0
88	Lf	33	Total 33	O 33	0
88	Lg	30	Total 30	O 30	0
88	Lh	42	Total 42	O 42	0
88	Li	4	Total 4	O 4	0
88	Lj	69	Total 69	O 69	0
88	Lk	4	Total 4	O 4	0
88	Ll	27	Total 27	O 27	0
88	Lm	1	Total 1	O 1	0
88	Ln	18	Total 18	O 18	0
88	Lo	3	Total 3	O 3	0

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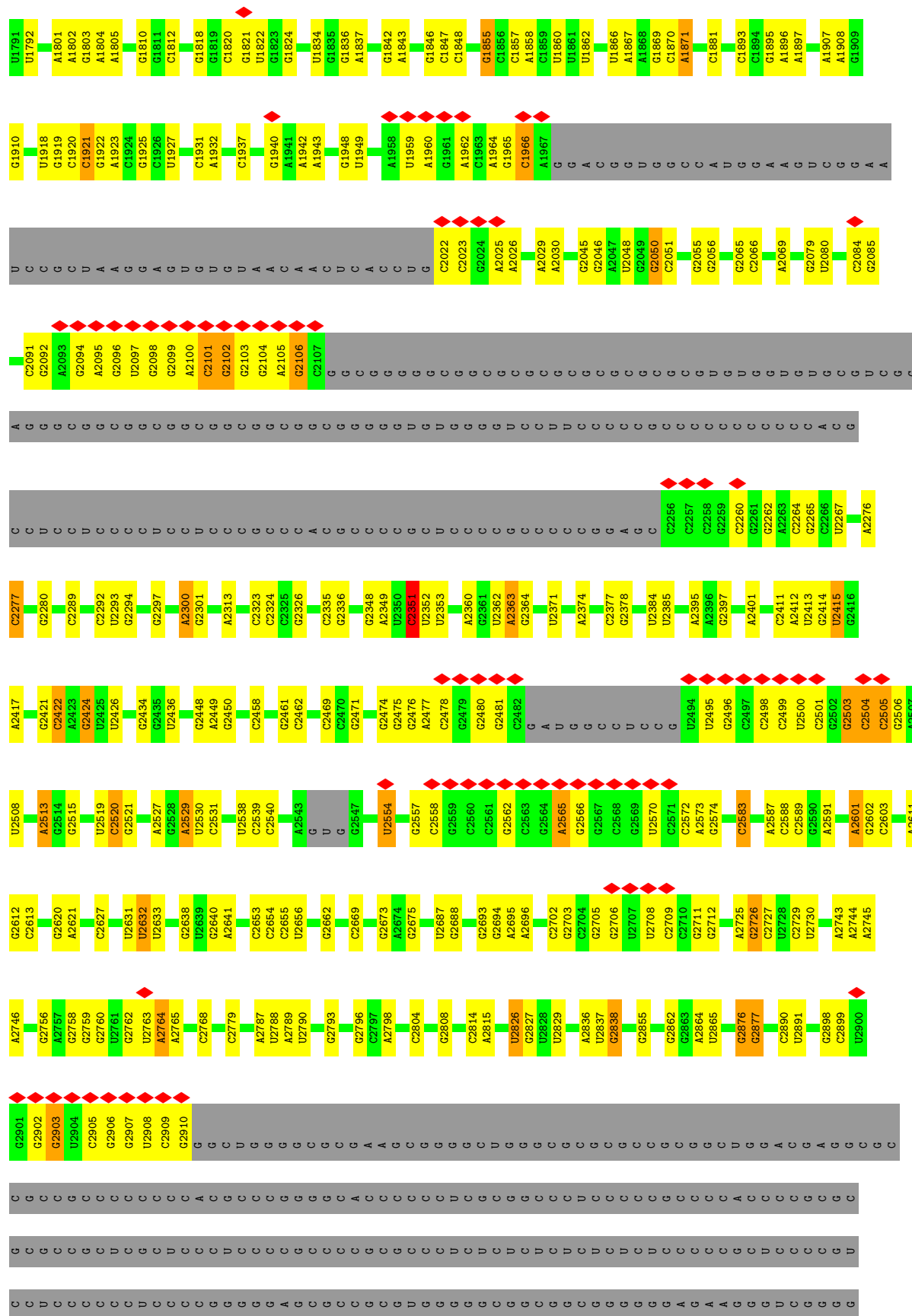
Mol	Chain	Residues	Atoms		AltConf
88	Lp	25	Total 25	O 25	0
88	Lz	16	Total 16	O 16	0
88	S1	25	Total 25	O 25	0
88	S2	2334	Total 2334	O 2334	0
88	S5	11	Total 11	O 11	0
88	SA	9	Total 9	O 9	0
88	SB	9	Total 9	O 9	0
88	SC	36	Total 36	O 36	0
88	SD	25	Total 25	O 25	0
88	SE	45	Total 45	O 45	0
88	SG	16	Total 16	O 16	0
88	SH	6	Total 6	O 6	0
88	SI	31	Total 31	O 31	0
88	SJ	34	Total 34	O 34	0
88	SK	6	Total 6	O 6	0
88	SL	43	Total 43	O 43	0
88	SM	4	Total 4	O 4	0
88	SN	32	Total 32	O 32	0
88	SO	33	Total 33	O 33	0
88	SP	14	Total 14	O 14	0
88	SQ	32	Total 32	O 32	0

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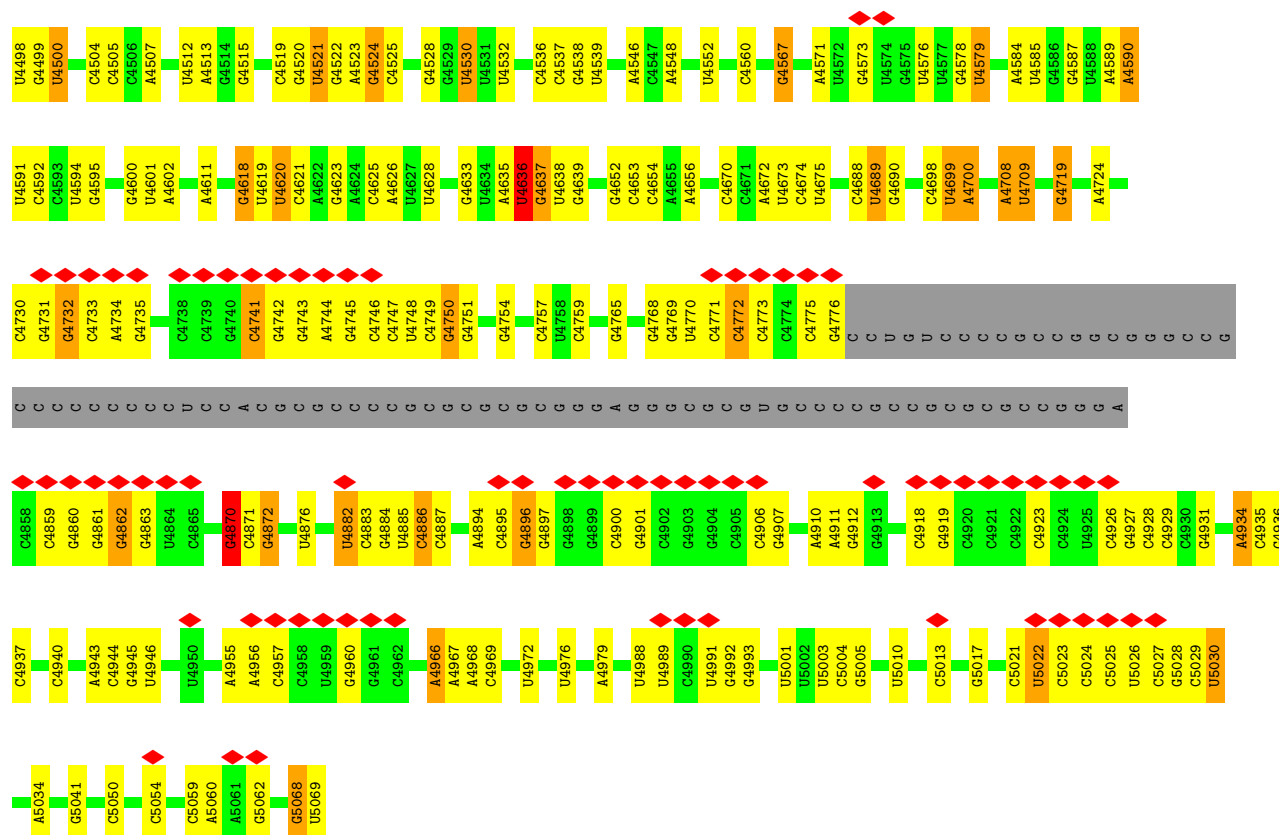
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88	SS	5	Total 5	O 5	0
88	ST	23	Total 23	O 23	0
88	SU	20	Total 20	O 20	0
88	SV	8	Total 8	O 8	0
88	SW	39	Total 39	O 39	0
88	SX	47	Total 47	O 47	0
88	SY	10	Total 10	O 10	0
88	SZ	12	Total 12	O 12	0
88	Sa	38	Total 38	O 38	0
88	Sb	11	Total 11	O 11	0
88	Sc	3	Total 3	O 3	0
88	Sd	2	Total 2	O 2	0
88	Se	10	Total 10	O 10	0
88	Sf	8	Total 8	O 8	0
88	Sg	1	Total 1	O 1	0
88	So	3	Total 3	O 3	0

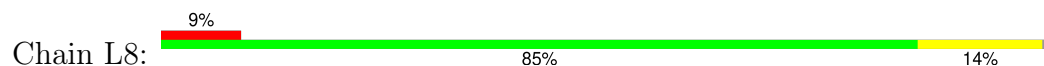




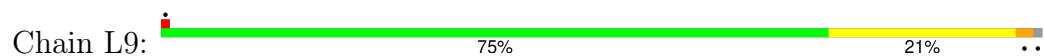




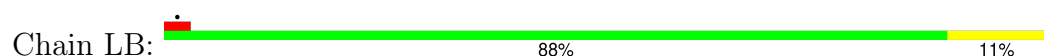
• Molecule 3: Large ribosomal subunit protein uL18



• Molecule 4: 5S rRNA



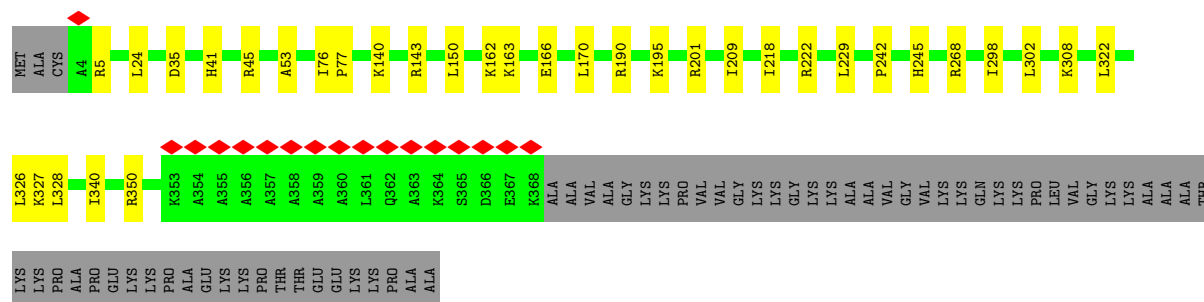
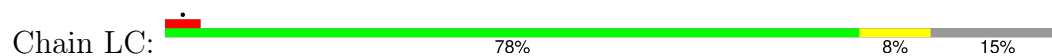
• Molecule 5: Large ribosomal subunit protein uL3



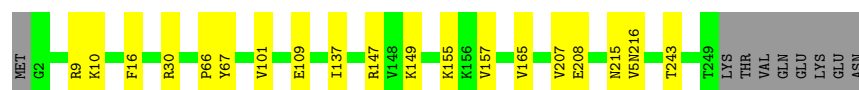
- Molecule 6: tRNA-ARG,CCG-1



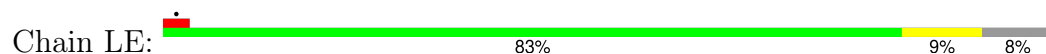
- Molecule 7: Large ribosomal subunit protein uL4



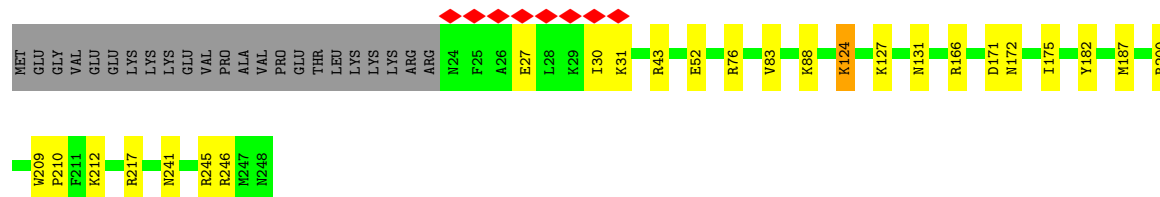
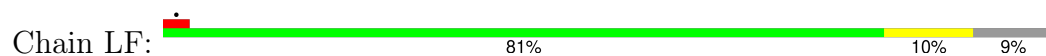
- Molecule 8: Large ribosomal subunit protein uL2



- Molecule 9: Large ribosomal subunit protein uL24

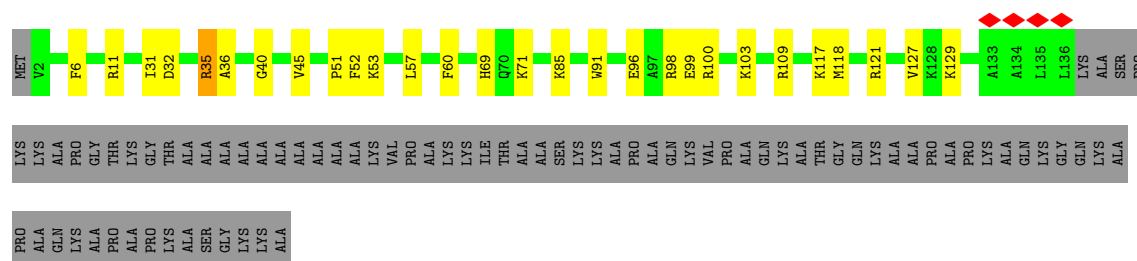


- Molecule 10: Large ribosomal subunit protein uL30



- [illegible]

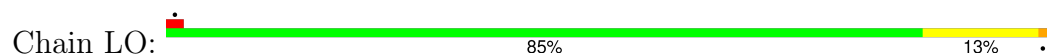
- Molecule 16: Large ribosomal subunit protein eL14



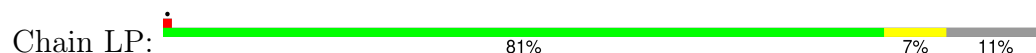
- Molecule 17: Large ribosomal subunit protein eL15



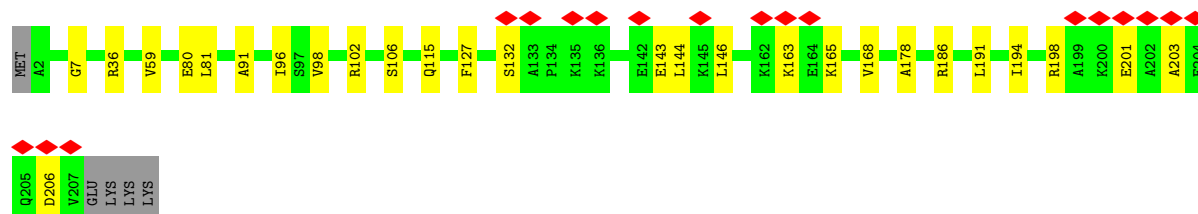
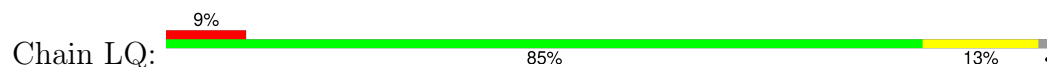
- Molecule 18: Large ribosomal subunit protein uL29



- Molecule 19: Large ribosomal subunit protein eL37

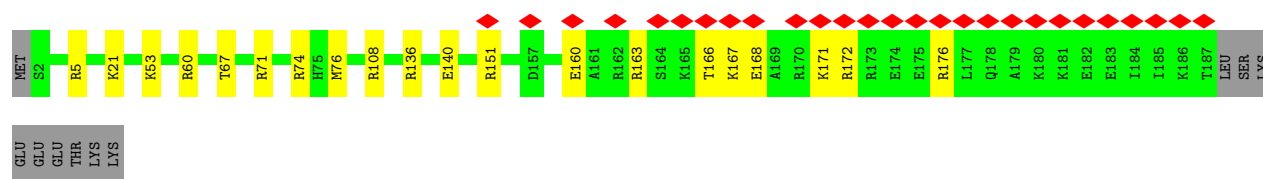


- Molecule 20: Large ribosomal subunit protein eL13

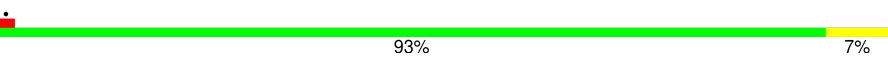


- Molecule 21: Large ribosomal subunit protein eL19

Chain LR: 

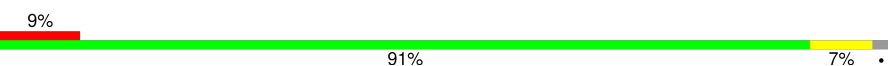


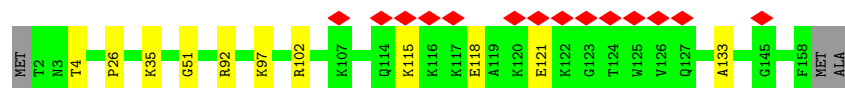
- Molecule 22: Large ribosomal subunit protein eL20

Chain LS: 



- Molecule 23: Large ribosomal subunit protein eL21

Chain LT: 



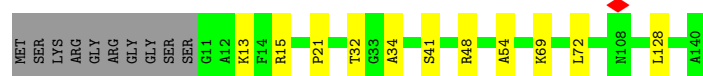
- Molecule 24: Large ribosomal subunit protein eL39

Chain LU: 



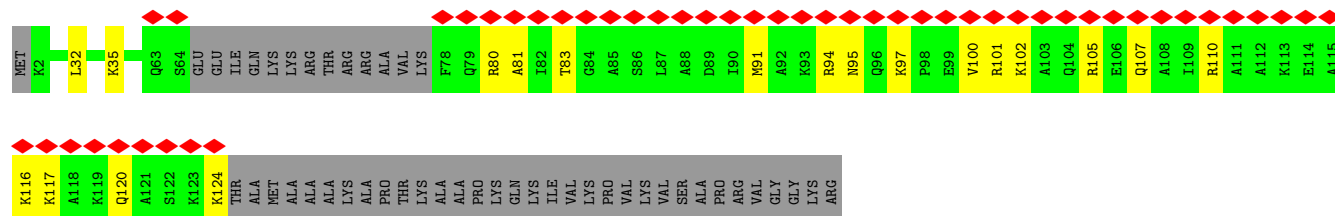
- Molecule 25: Large ribosomal subunit protein uL14

Chain LV: 



- Molecule 26: Large ribosomal subunit protein eL24

Chain LW: 



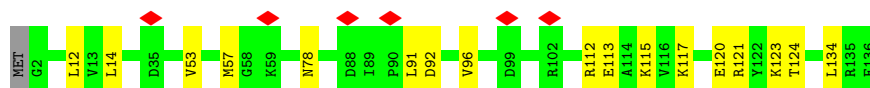
- Molecule 27: Large ribosomal subunit protein uL13

Chain LY:  90% 8%



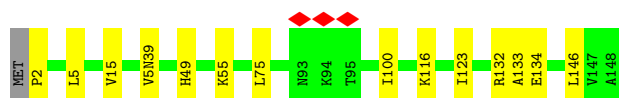
- Molecule 28: Large ribosomal subunit protein eL27

Chain LZ:  87% 12%



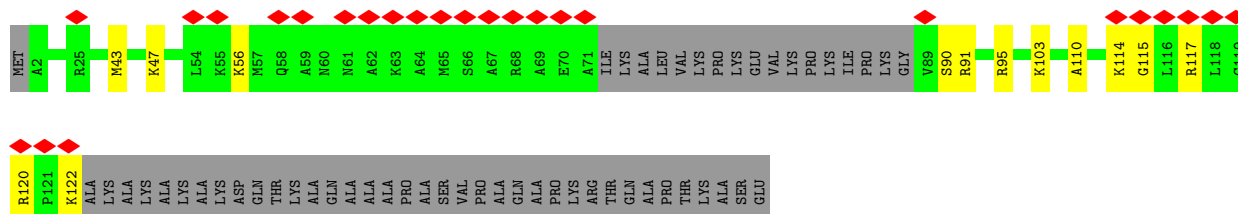
- Molecule 29: Large ribosomal subunit protein uL15

Chain La:  90% 9%



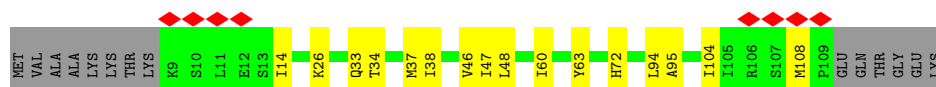
- Molecule 30: Large ribosomal subunit protein eL29

Chain Lb:  16% 57% 8% 35%



- Molecule 31: Large ribosomal subunit protein eL30

Chain Lc:  7% 74% 14% 12%



- Molecule 32: Large ribosomal subunit protein eL31

Chain Ld:  7% 73% 10% 17%



- Molecule 33: Large ribosomal subunit protein eL42

Chain Le:  92% 8%



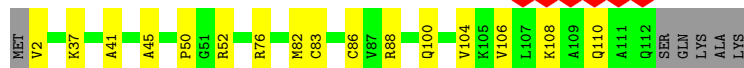
- Molecule 34: Large ribosomal subunit protein eL33

Chain Lf:  95% 5%



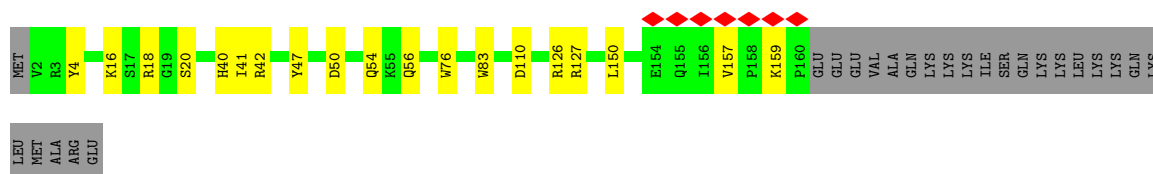
- Molecule 35: Large ribosomal subunit protein eL34

Chain Lg:  5% 81% 14% 5%



- Molecule 36: Large ribosomal subunit protein uL22

Chain Lh:  76% 10% 14%

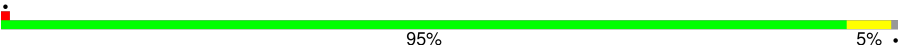


- Molecule 37: Large ribosomal subunit protein eL36

Chain Li:  8% 83% 14%



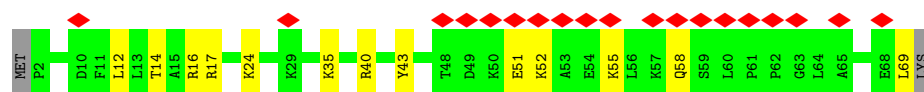
- Molecule 38: Large ribosomal subunit protein eL18

Chain Lj:  95% 5%

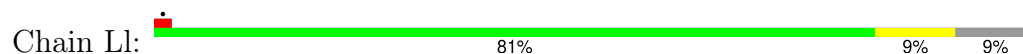


- Molecule 39: Large ribosomal subunit protein eL38

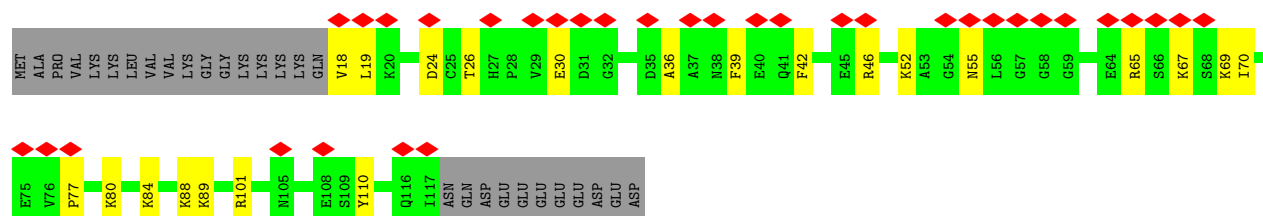
Chain Lk:  27% 79% 19%



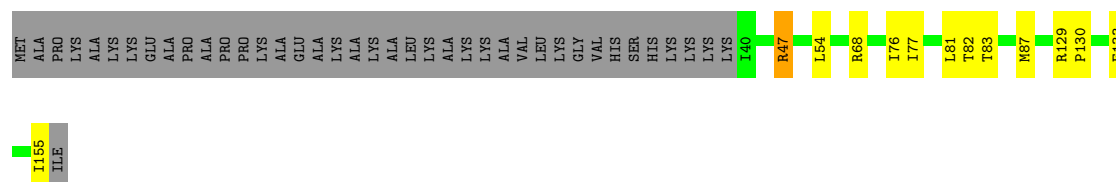
- Molecule 40: Large ribosomal subunit protein eL28



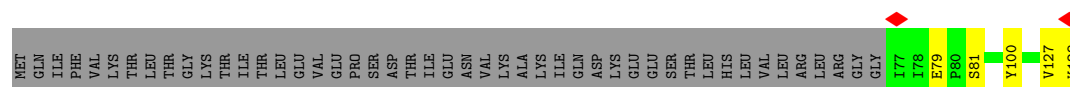
- Molecule 41: Large ribosomal subunit protein eL22



- Molecule 42: Large ribosomal subunit protein uL23



- Molecule 43: Large ribosomal subunit protein eL40



- Molecule 44: Large ribosomal subunit protein eL43



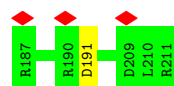
- Molecule 45: Large ribosomal subunit protein uL16

Chain Lz:  88% 10%



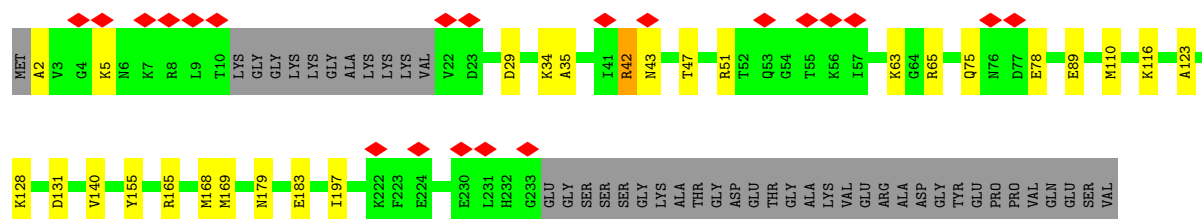
- Molecule 46: Nascent chain

Chain NC:  12% 96%

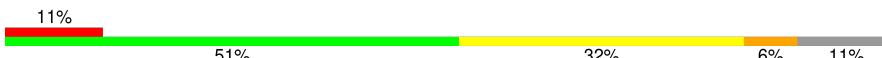


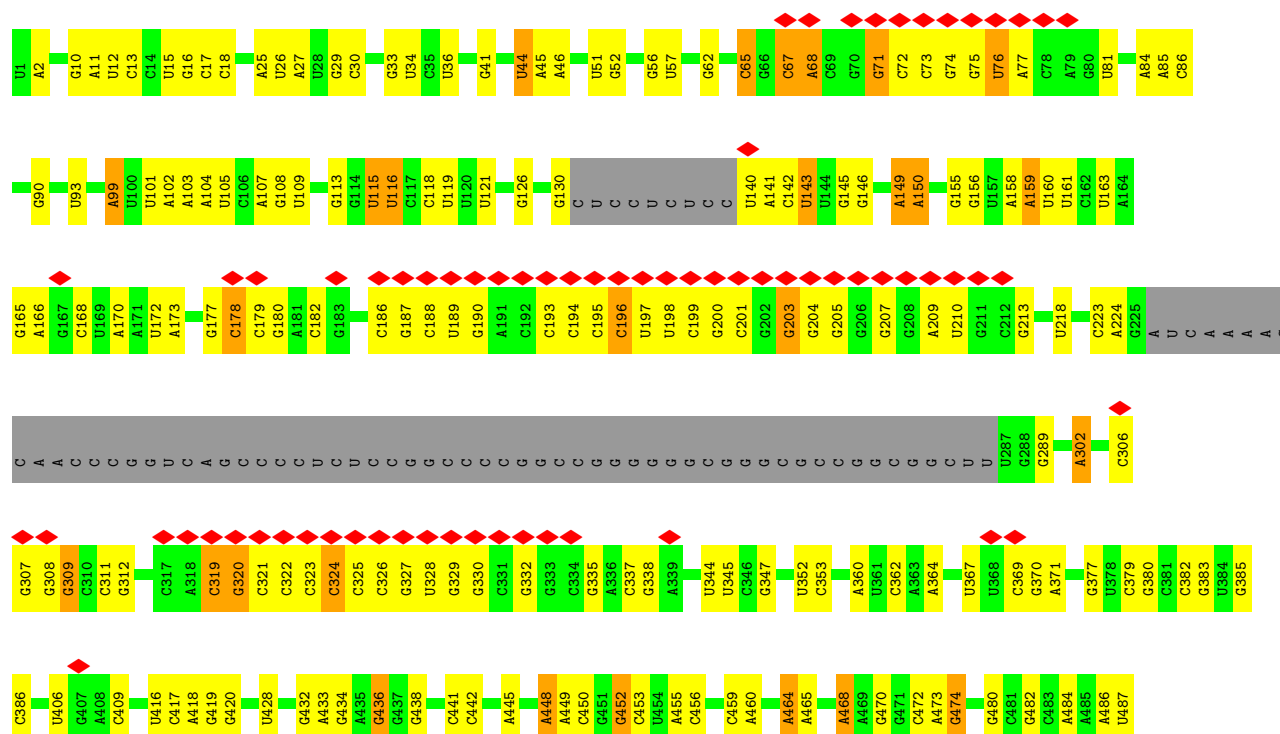
- Molecule 47: Small ribosomal subunit protein eS1

Chain S1:  8% 73% 10% 16%



- Molecule 48: 18S rRNA

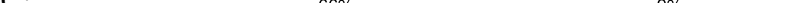
Chain S2:  11% 51% 32% 6% 11%

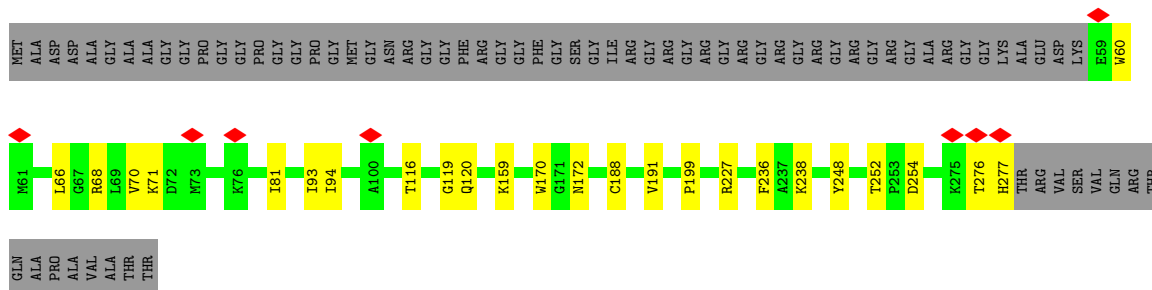




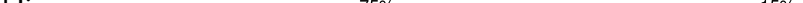
[illegible]

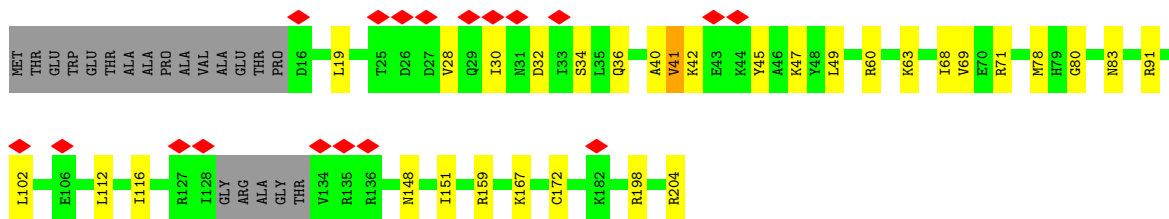
- Molecule 52: Small ribosomal subunit protein uS5

Chain SC: 

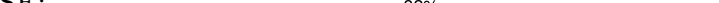


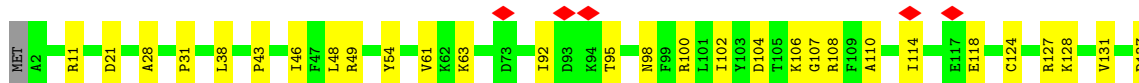
- Molecule 53: Small ribosomal subunit protein uS7

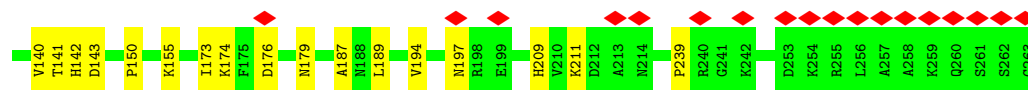
Chain SD: 



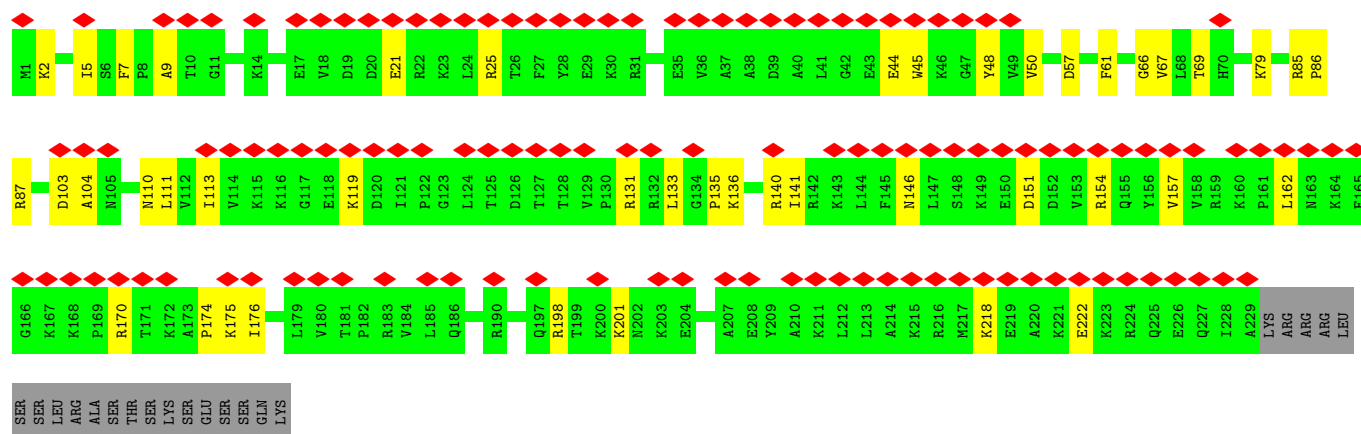
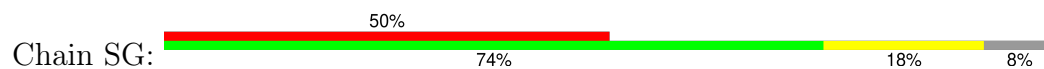
- Molecule 54: Small ribosomal subunit protein eS4, X isoform

Chain SE: 

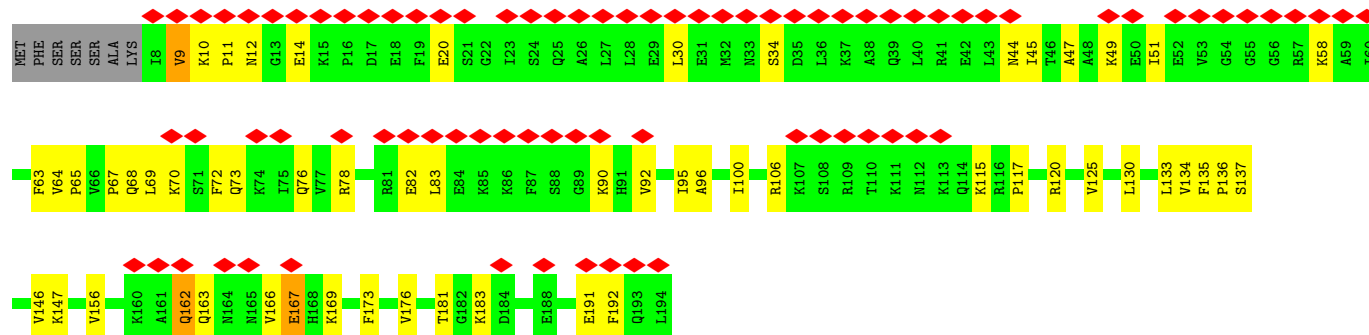
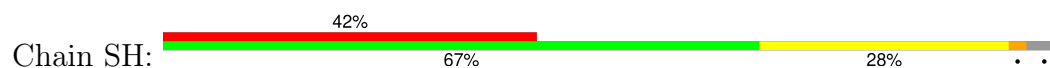




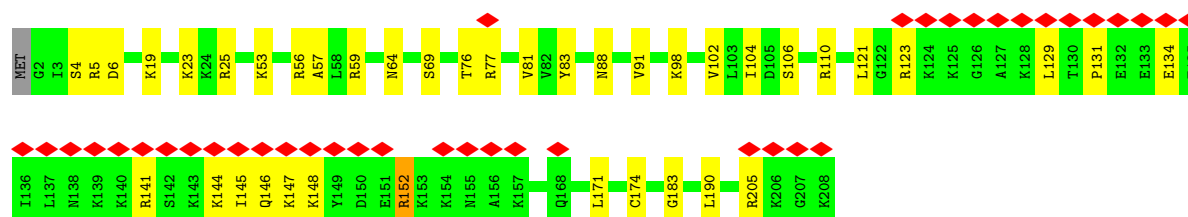
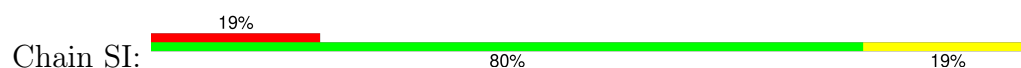
• Molecule 55: Small ribosomal subunit protein eS6



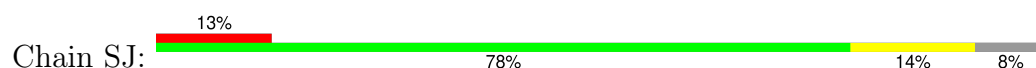
• Molecule 56: Small ribosomal subunit protein eS7



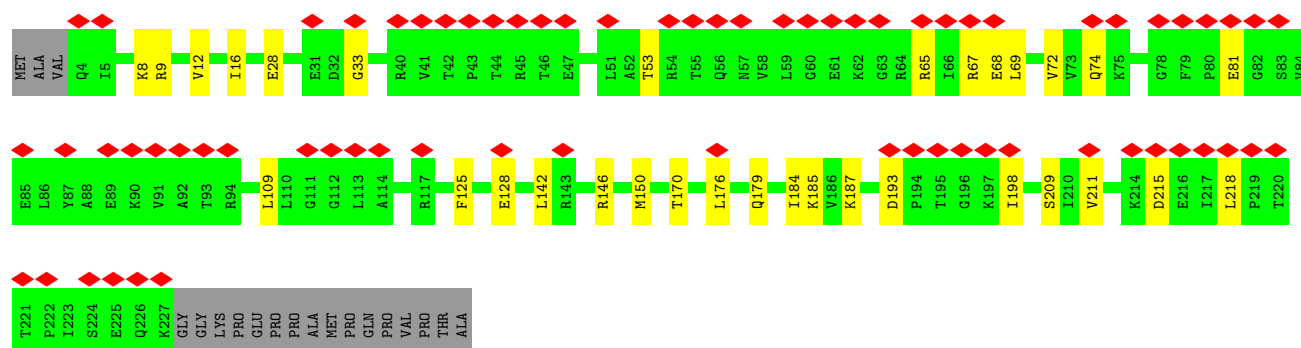
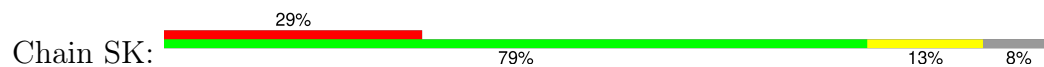
• Molecule 57: Small ribosomal subunit protein eS8



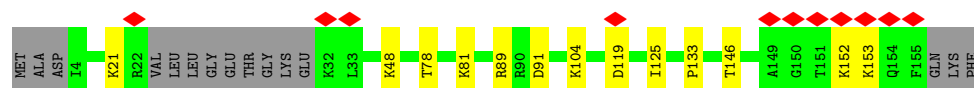
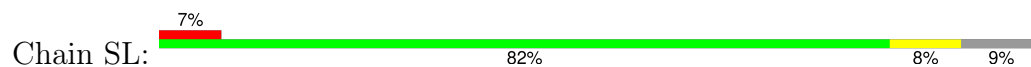
• Molecule 58: Small ribosomal subunit protein uS4



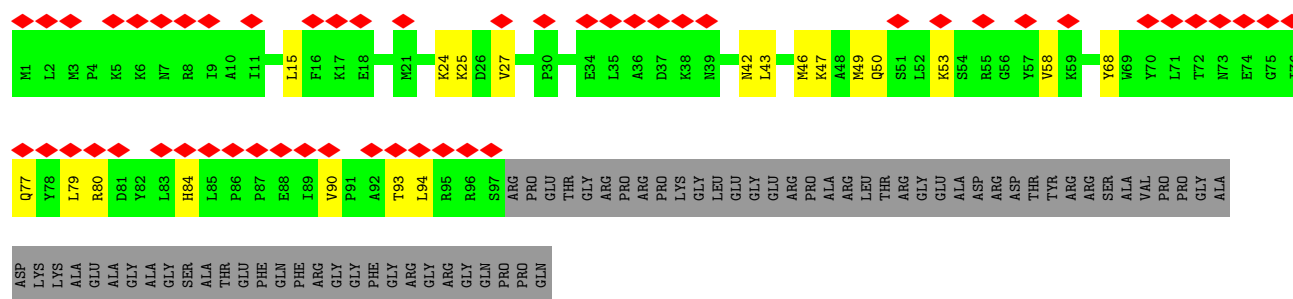
- Molecule 59: Small ribosomal subunit protein uS3



- Molecule 60: Small ribosomal subunit protein uS17



- Molecule 61: Small ribosomal subunit protein eS10



- Molecule 62: Small ribosomal subunit protein uS15



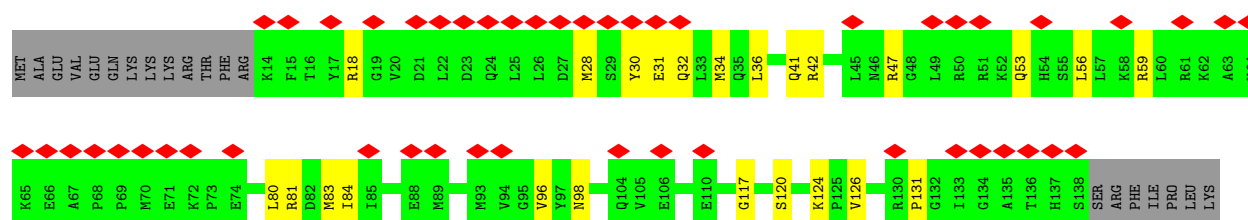
- Molecule 63: Small ribosomal subunit protein uS11

Chain SO: 



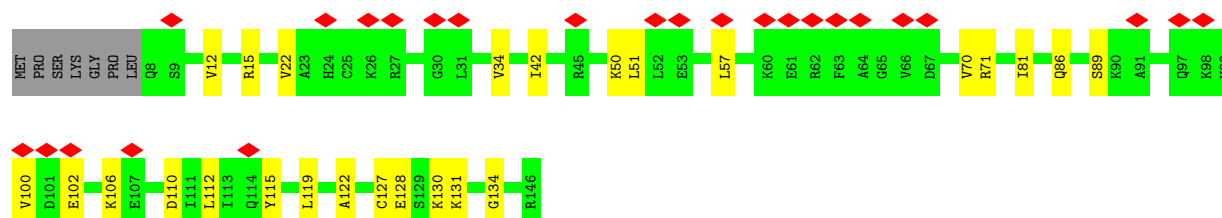
- Molecule 64: Small ribosomal subunit protein uS19

Chain SP: 



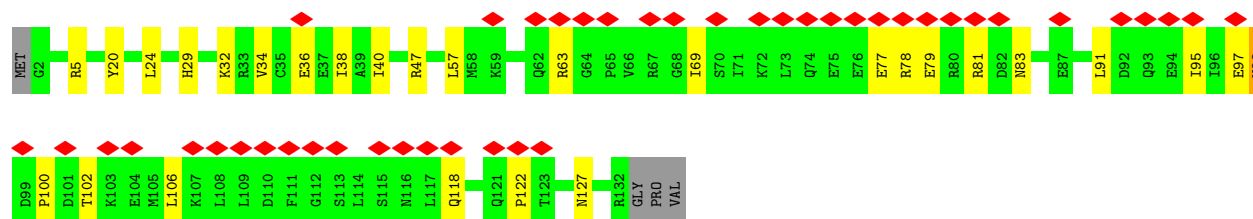
- Molecule 65: Small ribosomal subunit protein uS9

Chain SQ: 



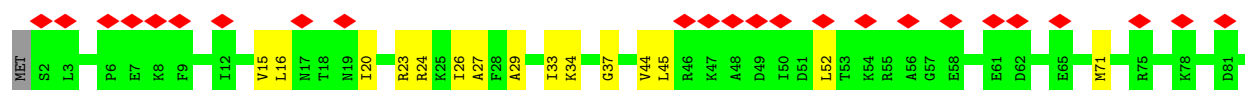
- Molecule 66: Small ribosomal subunit protein eS17

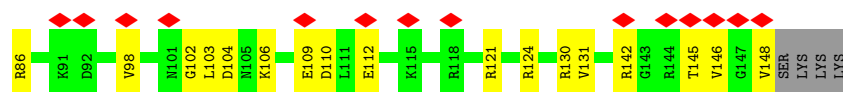
Chain SS: 



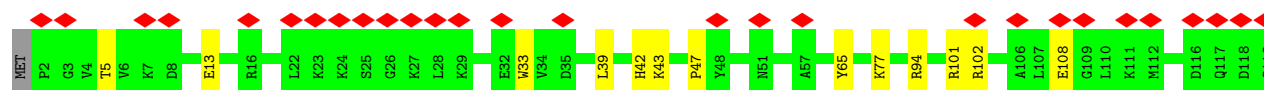
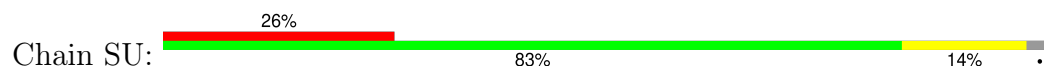
- Molecule 67: Small ribosomal subunit protein uS13

Chain ST: 

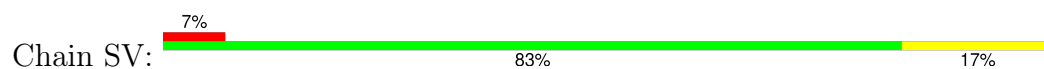




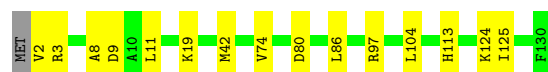
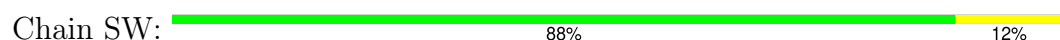
- Molecule 68: Small ribosomal subunit protein eS19



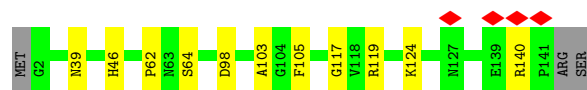
- Molecule 69: Small ribosomal subunit protein eS21



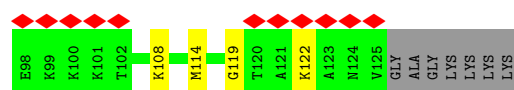
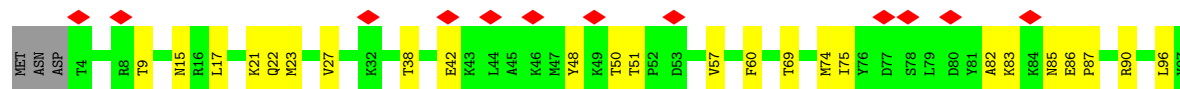
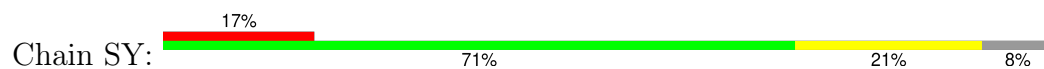
- Molecule 70: Small ribosomal subunit protein uS8



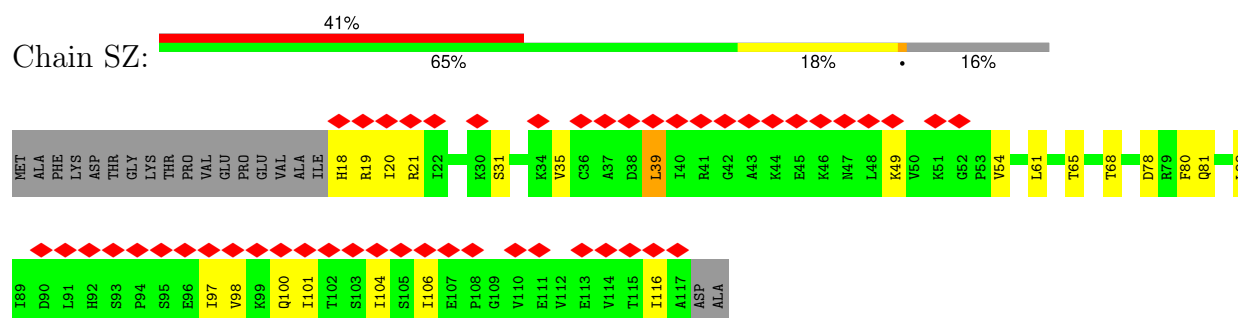
- Molecule 71: Small ribosomal subunit protein uS12



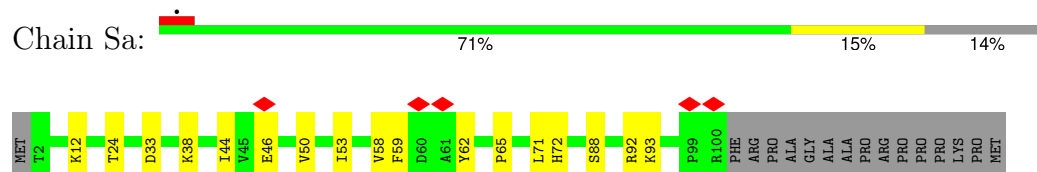
- Molecule 72: Isoform 3 of Small ribosomal subunit protein eS24



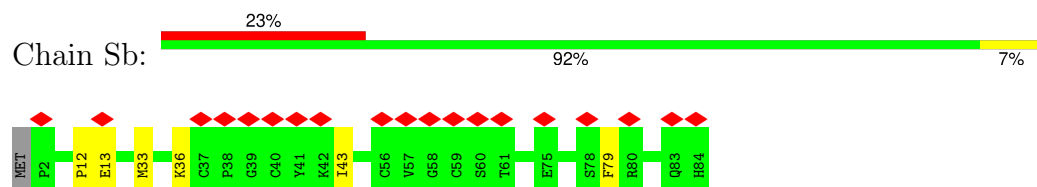
- Molecule 73: Small ribosomal subunit protein uS10



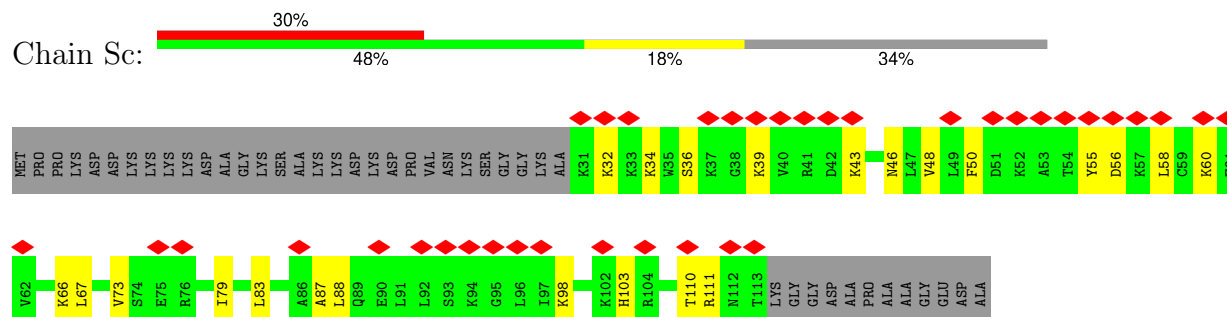
- Molecule 74: Small ribosomal subunit protein eS26



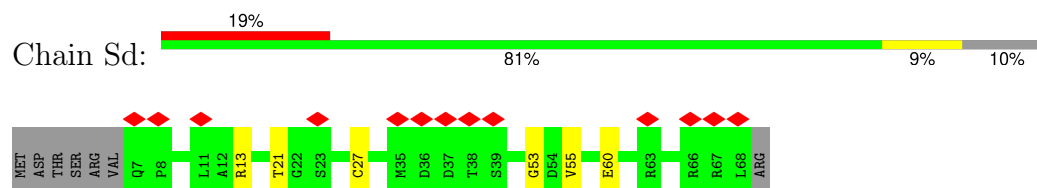
- Molecule 75: Small ribosomal subunit protein eS27



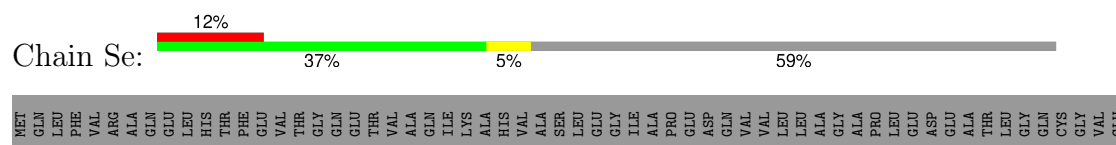
- Molecule 76: Small ribosomal subunit protein eS25



- Molecule 77: Small ribosomal subunit protein eS28

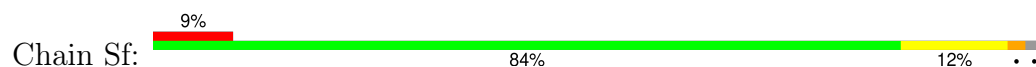


- Molecule 78: FAU ubiquitin-like and ribosomal protein S30

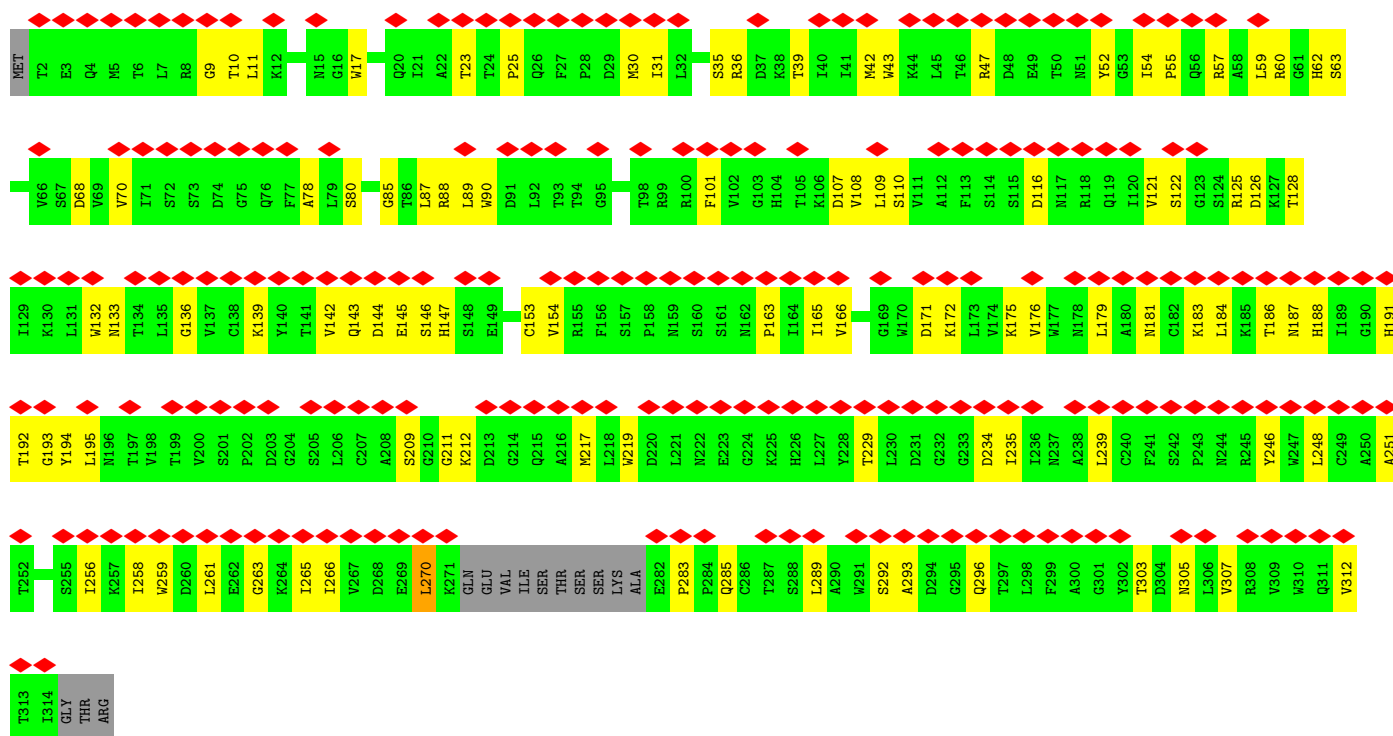




- Molecule 79: Small ribosomal subunit protein uS14



- Molecule 80: Receptor of activated protein C kinase 1



- Molecule 81: Small ribosomal subunit protein eS32

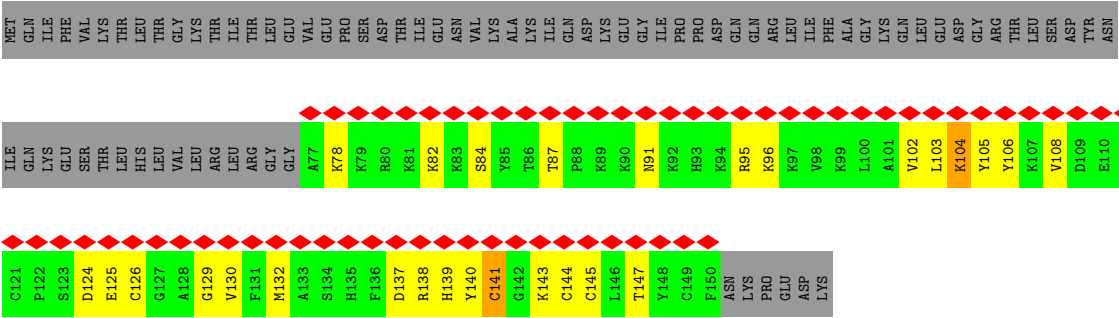
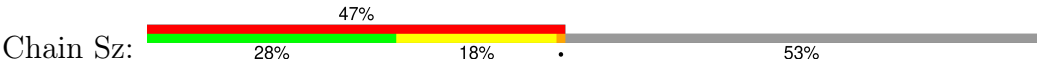


- Molecule 82: Small ribosomal subunit protein eS12





● Molecule 83: Ubiquitin-40S ribosomal protein S27a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	276000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	17	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.242	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0175	Depositor
Map size ($\text{\AA}$)	419.328, 419.328, 419.328	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.936, 0.936, 0.936	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B3P, ACE, 1MG, K, 4AC, PSU, UY1, B8N, MA6, H2U, JMH, OMG, 1MA, A2M, 5MC, OMU, 7MG, 2MG, V5N, UR3, OMC, 5MU, 6MZ, M3L, MG, M2G, MLZ, HIC, IAS, ZN, HY3

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	L1	0.25	0/3450	0.31	0/5372
2	L5	0.26	2/81683 (0.0%)	0.34	0/127409
3	L8	0.14	0/2432	0.32	0/3256
4	L9	0.24	0/2858	0.29	0/4455
5	LB	0.16	0/3289	0.35	0/4399
6	S4	0.70	0/1530	0.86	0/2384
7	LC	0.16	0/2962	0.35	0/3977
8	LD	0.16	0/1924	0.40	0/2578
9	LE	0.13	0/1132	0.31	0/1504
10	LF	0.18	0/1905	0.36	0/2540
11	LG	0.15	0/1781	0.33	0/2397
12	LH	0.15	0/1537	0.32	0/2066
13	LI	0.18	0/1071	0.38	0/1429
14	LJ	0.15	0/1363	0.37	0/1824
15	LK	0.13	0/1814	0.32	0/2435
16	LM	0.15	0/1133	0.33	0/1516
17	LN	0.17	0/1745	0.38	0/2338
18	LO	0.15	0/1022	0.30	0/1351
19	LP	0.17	0/720	0.39	0/952
20	LQ	0.14	0/1695	0.31	0/2270
21	LR	0.15	0/1574	0.30	0/2080
22	LS	0.15	0/1500	0.34	0/2013
23	LT	0.14	0/1312	0.33	0/1753
24	LU	0.16	0/453	0.32	0/599
25	LV	0.15	0/986	0.36	0/1324
26	LW	0.14	0/907	0.31	0/1202
27	LY	0.18	0/1656	0.36	0/2216
28	LZ	0.14	0/1129	0.31	0/1507
29	La	0.17	0/1178	0.37	0/1573
30	Lb	0.15	0/850	0.30	0/1121
31	Lc	0.19	0/796	0.35	0/1068

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.16	0/877	0.35	0/1181
33	Le	0.16	0/866	0.32	0/1141
34	Lf	0.17	0/894	0.34	0/1198
35	Lg	0.15	0/892	0.33	0/1189
36	Lh	0.16	0/1317	0.36	0/1769
37	Li	0.13	0/843	0.27	0/1115
38	Lj	0.17	0/1536	0.38	0/2052
39	Lk	0.13	0/565	0.26	0/750
40	Ll	0.19	0/1003	0.35	0/1346
41	Lm	0.14	0/830	0.36	0/1114
42	Ln	0.14	0/966	0.32	0/1301
43	Lo	0.14	0/433	0.31	0/575
44	Lp	0.16	0/691	0.37	0/919
45	Lz	0.15	0/1744	0.31	0/2331
46	NC	0.13	0/226	0.30	0/299
47	S1	0.13	0/1816	0.30	0/2427
48	S2	0.28	3/37683 (0.0%)	0.31	0/58736
49	S5	0.21	0/212	0.29	0/328
50	SA	0.15	0/1766	0.30	0/2399
51	SB	0.34	0/1959	0.68	0/2618
52	SC	0.14	0/1737	0.31	0/2347
53	SD	0.13	0/1483	0.30	0/1993
54	SE	0.13	0/2117	0.30	0/2849
55	SG	0.13	0/1876	0.30	0/2499
56	SH	0.14	0/1532	0.31	0/2053
57	SI	0.13	0/1724	0.30	0/2298
58	SJ	0.13	0/1520	0.30	0/2030
59	SK	0.12	0/1773	0.32	0/2387
60	SL	0.14	0/1201	0.31	0/1604
61	SM	0.12	0/840	0.30	0/1133
62	SN	0.14	0/1231	0.31	0/1656
63	SO	0.14	0/959	0.32	0/1284
64	SP	0.12	0/1041	0.29	0/1392
65	SQ	0.14	0/1125	0.31	0/1506
66	SS	0.13	0/1078	0.30	0/1447
67	ST	0.12	0/1226	0.30	0/1643
68	SU	0.12	0/1113	0.29	0/1493
69	SV	0.12	0/643	0.30	0/860
70	SW	0.15	0/1050	0.32	0/1406
71	SX	0.13	0/1096	0.32	0/1461
72	SY	0.12	0/1019	0.28	0/1354
73	SZ	0.14	0/805	0.33	0/1081
74	Sa	0.14	0/805	0.32	0/1079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sb	0.12	0/664	0.28	0/891
76	Sc	0.11	0/678	0.27	0/906
77	Sd	0.11	0/490	0.27	0/656
78	Se	0.11	0/442	0.28	0/582
79	Sf	0.12	0/469	0.30	0/623
80	Sg	0.12	0/2420	0.35	0/3294
81	So	0.18	0/240	0.33	0/305
82	Sy	0.14	0/949	0.34	0/1273
83	Sz	0.14	0/619	0.39	0/818
All	All	0.23	5/222471 (0.0%)	0.34	0/325899

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
16	LM	0	1
51	SB	0	4
57	SI	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1288	OMU	O3'-P	5.14	1.61	1.56
48	S2	1383	A2M	O3'-P	5.11	1.61	1.56
2	L5	1773	OMU	O3'-P	5.06	1.61	1.56
48	S2	576	A2M	O3'-P	5.03	1.61	1.56
2	L5	2837	OMU	O3'-P	5.00	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	LM	35	ARG	Sidechain
51	SB	13	ARG	Sidechain
51	SB	177	ARG	Sidechain
51	SB	57	ARG	Sidechain
51	SB	90	ARG	Sidechain

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	L1	3153	0	1603	40	0
2	L5	75768	0	38369	657	0
3	L8	2386	0	2421	29	0
4	L9	2558	0	1295	18	0
5	LB	3234	0	3372	31	0
6	S4	1634	0	839	15	0
7	LC	2908	0	3082	25	0
8	LD	1899	0	1985	12	0
9	LE	1115	0	1205	11	0
10	LF	1870	0	1996	23	0
11	LG	1752	0	1877	15	0
12	LH	1518	0	1601	21	0
13	LI	1053	0	1147	10	0
14	LJ	1340	0	1377	23	0
15	LK	1780	0	1938	26	0
16	LM	1111	0	1174	24	0
17	LN	1700	0	1749	14	0
18	LO	1014	0	1148	12	0
19	LP	705	0	736	7	0
20	LQ	1664	0	1773	19	0
21	LR	1558	0	1718	14	0
22	LS	1460	0	1502	18	0
23	LT	1284	0	1352	7	0
24	LU	443	0	483	6	0
25	LV	972	0	1034	7	0
26	LW	893	0	936	25	0
27	LY	1624	0	1771	22	0
28	LZ	1106	0	1182	12	0
29	La	1162	0	1206	9	0
30	Lb	848	0	918	14	0
31	Lc	785	0	825	10	0
32	Ld	862	0	912	12	0
33	Le	863	0	929	4	0
34	Lf	875	0	912	4	0
35	Lg	882	0	972	12	0
36	Lh	1289	0	1324	15	0
37	Li	832	0	917	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Lj	1512	0	1628	5	0
39	Lk	559	0	624	8	0
40	Ll	990	0	1054	10	0
41	Lm	816	0	842	15	0
42	Ln	949	0	1016	10	0
43	Lo	436	0	477	13	0
44	Lp	681	0	731	4	0
45	Lz	1705	0	1757	14	0
46	NC	227	0	236	1	0
47	S1	1790	0	1873	18	0
48	S2	35485	0	17959	399	0
49	S5	191	0	98	0	0
50	SA	1731	0	1734	34	0
51	SB	1937	0	1951	42	0
52	SC	1700	0	1784	14	0
53	SD	1463	0	1517	24	0
54	SE	2075	0	2177	32	0
55	SG	1853	0	2005	41	0
56	SH	1509	0	1604	35	0
57	SI	1695	0	1785	30	0
58	SJ	1495	0	1615	17	0
59	SK	1745	0	1839	27	0
60	SL	1180	0	1253	11	0
61	SM	816	0	841	15	0
62	SN	1207	0	1293	7	0
63	SO	956	0	981	11	0
64	SP	1021	0	1065	18	0
65	SQ	1108	0	1174	17	0
66	SS	1064	0	1118	19	0
67	ST	1208	0	1270	20	0
68	SU	1094	0	1120	15	0
69	SV	636	0	637	8	0
70	SW	1033	0	1080	15	0
71	SX	1088	0	1149	6	0
72	SY	1002	0	1075	24	0
73	SZ	795	0	862	18	0
74	Sa	792	0	841	10	0
75	Sb	650	0	672	3	0
76	Sc	670	0	745	25	0
77	Sd	488	0	514	4	0
78	Se	437	0	484	4	0
79	Sf	458	0	448	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Sg	2364	0	2318	65	0
81	So	239	0	289	2	0
82	Sy	939	0	974	36	0
83	Sz	607	0	633	31	0
84	L1	4	0	0	0	0
84	L5	204	0	0	0	0
84	L9	3	0	0	0	0
84	LD	1	0	0	0	0
84	LI	2	0	0	0	0
84	LN	1	0	0	0	0
84	LR	2	0	0	0	0
84	LV	1	0	0	0	0
84	La	1	0	0	0	0
84	Lh	1	0	0	0	0
84	S2	97	0	0	0	0
84	S4	6	0	0	0	0
84	SG	1	0	0	0	0
84	ST	1	0	0	0	0
84	SX	1	0	0	0	0
85	L1	3	0	0	0	0
85	L5	42	0	0	0	0
85	L9	1	0	0	0	0
85	LC	1	0	0	0	0
85	LD	2	0	0	0	0
85	LV	1	0	0	0	0
85	Lz	1	0	0	0	0
85	S2	39	0	0	0	0
85	SE	1	0	0	0	0
85	SO	1	0	0	0	0
85	ST	1	0	0	0	0
85	Sf	1	0	0	0	0
86	L5	19	0	26	0	0
87	LP	1	0	0	0	0
87	Le	1	0	0	0	0
87	Lg	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
87	Sa	1	0	0	0	0
87	Sf	1	0	0	0	0
87	Sz	1	0	0	0	0
88	L1	153	0	0	0	0
88	L5	4961	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	L8	25	0	0	0	0
88	L9	93	0	0	0	0
88	LB	85	0	0	0	0
88	LC	104	0	0	2	0
88	LD	91	0	0	1	0
88	LE	10	0	0	0	0
88	LF	52	0	0	0	0
88	LG	16	0	0	0	0
88	LH	18	0	0	0	0
88	LI	64	0	0	0	0
88	LJ	3	0	0	0	0
88	LK	12	0	0	0	0
88	LM	7	0	0	1	0
88	LN	89	0	0	0	0
88	LO	13	0	0	0	0
88	LP	33	0	0	1	0
88	LQ	45	0	0	1	0
88	LR	23	0	0	0	0
88	LS	39	0	0	0	0
88	LT	41	0	0	0	0
88	LU	10	0	0	0	0
88	LV	27	0	0	0	0
88	LW	7	0	0	0	0
88	LY	42	0	0	0	0
88	LZ	10	0	0	0	0
88	La	46	0	0	0	0
88	Lb	15	0	0	1	0
88	Lc	8	0	0	0	0
88	Ld	15	0	0	0	0
88	Le	19	0	0	0	0
88	Lf	33	0	0	0	0
88	Lg	30	0	0	0	0
88	Lh	42	0	0	0	0
88	Li	4	0	0	1	0
88	Lj	69	0	0	0	0
88	Lk	4	0	0	1	0
88	Ll	27	0	0	0	0
88	Lm	1	0	0	0	0
88	Ln	18	0	0	1	0
88	Lo	3	0	0	0	0
88	Lp	25	0	0	0	0
88	Lz	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	S1	25	0	0	0	0
88	S2	2334	0	0	18	0
88	S4	52	0	0	0	0
88	S5	11	0	0	0	0
88	SA	9	0	0	0	0
88	SB	9	0	0	1	0
88	SC	36	0	0	0	0
88	SD	25	0	0	0	0
88	SE	45	0	0	0	0
88	SG	16	0	0	0	0
88	SH	6	0	0	0	0
88	SI	31	0	0	1	0
88	SJ	34	0	0	2	0
88	SK	6	0	0	0	0
88	SL	43	0	0	1	0
88	SM	4	0	0	1	0
88	SN	32	0	0	2	0
88	SO	33	0	0	0	0
88	SP	14	0	0	0	0
88	SQ	32	0	0	0	0
88	SS	5	0	0	1	0
88	ST	23	0	0	0	0
88	SU	20	0	0	0	0
88	SV	8	0	0	0	0
88	SW	39	0	0	0	0
88	SX	47	0	0	1	0
88	SY	10	0	0	0	0
88	SZ	12	0	0	0	0
88	Sa	38	0	0	1	0
88	Sb	11	0	0	0	0
88	Sc	3	0	0	0	0
88	Sd	2	0	0	0	0
88	Se	10	0	0	0	0
88	Sf	8	0	0	0	0
88	Sg	1	0	0	0	0
88	So	3	0	0	0	0
All	All	222228	0	158748	2057	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 2057 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)
40:L1:30:ASN:OD1	40:L1:50:GLY:HA3	1.51	1.10
50:SA:206:ASP:OD1	50:SA:207:PRO:HD2	1.53	1.07
43:Lo:127:VAL:CG1	43:Lo:128:LYS:HE2	1.85	1.06
26:LW:97:LYS:HD3	55:SG:146:ASN:ND2	1.72	1.03
80:Sg:109:LEU:CD2	80:Sg:125:ARG:HG3	1.87	1.03

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L8	291/297 (98%)	282 (97%)	9 (3%)	0	100	100
5	LB	398/403 (99%)	394 (99%)	4 (1%)	0	100	100
7	LC	363/427 (85%)	352 (97%)	11 (3%)	0	100	100
8	LD	245/257 (95%)	237 (97%)	8 (3%)	0	100	100
9	LE	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
10	LF	223/248 (90%)	218 (98%)	5 (2%)	0	100	100
11	LG	212/266 (80%)	209 (99%)	3 (1%)	0	100	100
12	LH	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
13	LI	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
14	LJ	165/178 (93%)	163 (99%)	2 (1%)	0	100	100
15	LK	216/288 (75%)	210 (97%)	6 (3%)	0	100	100
16	LM	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
17	LN	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
18	LO	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
19	LP	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
20	LQ	204/211 (97%)	202 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	LR	184/196 (94%)	183 (100%)	1 (0%)	0	100	100
22	LS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
23	LT	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
24	LU	48/51 (94%)	48 (100%)	0	0	100	100
25	LV	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
26	LW	106/157 (68%)	103 (97%)	3 (3%)	0	100	100
27	LY	196/203 (97%)	193 (98%)	3 (2%)	0	100	100
28	LZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	La	144/148 (97%)	140 (97%)	3 (2%)	1 (1%)	18	14
30	Lb	99/159 (62%)	97 (98%)	2 (2%)	0	100	100
31	Lc	99/115 (86%)	99 (100%)	0	0	100	100
32	Ld	102/125 (82%)	102 (100%)	0	0	100	100
33	Le	102/106 (96%)	102 (100%)	0	0	100	100
34	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
35	Lg	109/117 (93%)	107 (98%)	2 (2%)	0	100	100
36	Lh	157/184 (85%)	153 (98%)	4 (2%)	0	100	100
37	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
38	Lj	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
39	Lk	66/70 (94%)	64 (97%)	2 (3%)	0	100	100
40	Ll	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
41	Lm	98/128 (77%)	91 (93%)	7 (7%)	0	100	100
42	Ln	114/156 (73%)	113 (99%)	1 (1%)	0	100	100
43	Lo	50/99 (50%)	50 (100%)	0	0	100	100
44	Lp	86/92 (94%)	82 (95%)	4 (5%)	0	100	100
45	Lz	209/214 (98%)	209 (100%)	0	0	100	100
46	NC	23/25 (92%)	23 (100%)	0	0	100	100
47	S1	217/264 (82%)	214 (99%)	3 (1%)	0	100	100
50	SA	218/295 (74%)	217 (100%)	1 (0%)	0	100	100
51	SB	230/609 (38%)	219 (95%)	10 (4%)	1 (0%)	30	27
52	SC	217/293 (74%)	211 (97%)	6 (3%)	0	100	100
53	SD	180/204 (88%)	172 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	SE	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
55	SG	227/249 (91%)	222 (98%)	5 (2%)	0	100	100
56	SH	185/194 (95%)	177 (96%)	8 (4%)	0	100	100
57	SI	205/208 (99%)	203 (99%)	2 (1%)	0	100	100
58	SJ	177/194 (91%)	173 (98%)	4 (2%)	0	100	100
59	SK	222/243 (91%)	217 (98%)	5 (2%)	0	100	100
60	SL	139/158 (88%)	137 (99%)	2 (1%)	0	100	100
61	SM	95/165 (58%)	91 (96%)	4 (4%)	0	100	100
62	SN	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
63	SO	123/151 (82%)	120 (98%)	3 (2%)	0	100	100
64	SP	123/145 (85%)	121 (98%)	2 (2%)	0	100	100
65	SQ	137/146 (94%)	135 (98%)	2 (2%)	0	100	100
66	SS	129/135 (96%)	127 (98%)	2 (2%)	0	100	100
67	ST	145/152 (95%)	142 (98%)	3 (2%)	0	100	100
68	SU	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
69	SV	81/83 (98%)	81 (100%)	0	0	100	100
70	SW	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
71	SX	137/143 (96%)	136 (99%)	1 (1%)	0	100	100
72	SY	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
73	SZ	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
74	Sa	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
75	Sb	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
76	Sc	81/125 (65%)	78 (96%)	3 (4%)	0	100	100
77	Sd	60/69 (87%)	60 (100%)	0	0	100	100
78	Se	53/133 (40%)	53 (100%)	0	0	100	100
79	Sf	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
80	Sg	299/317 (94%)	284 (95%)	15 (5%)	0	100	100
81	So	23/25 (92%)	23 (100%)	0	0	100	100
82	Sy	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
83	Sz	72/156 (46%)	63 (88%)	8 (11%)	1 (1%)	9	4
All	All	11414/13366 (85%)	11166 (98%)	245 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	SB	97	GLU
83	Sz	91	ASN
29	La	15	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L8	247/250 (99%)	245 (99%)	2 (1%)	73	80
5	LB	347/348 (100%)	345 (99%)	2 (1%)	78	85
7	LC	304/348 (87%)	302 (99%)	2 (1%)	76	82
8	LD	189/198 (96%)	189 (100%)	0	100	100
9	LE	124/135 (92%)	124 (100%)	0	100	100
10	LF	195/216 (90%)	194 (100%)	1 (0%)	81	87
11	LG	187/223 (84%)	186 (100%)	1 (0%)	81	87
12	LH	169/171 (99%)	168 (99%)	1 (1%)	78	85
13	LI	114/121 (94%)	113 (99%)	1 (1%)	70	78
14	LJ	141/149 (95%)	140 (99%)	1 (1%)	76	82
15	LK	196/252 (78%)	195 (100%)	1 (0%)	81	87
16	LM	115/161 (71%)	115 (100%)	0	100	100
17	LN	171/172 (99%)	171 (100%)	0	100	100
18	LO	109/110 (99%)	107 (98%)	2 (2%)	51	58
19	LP	73/80 (91%)	73 (100%)	0	100	100
20	LQ	172/177 (97%)	170 (99%)	2 (1%)	63	70
21	LR	165/175 (94%)	165 (100%)	0	100	100
22	LS	157/157 (100%)	156 (99%)	1 (1%)	78	85
23	LT	138/140 (99%)	136 (99%)	2 (1%)	59	66
24	LU	47/48 (98%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	LV	100/107 (94%)	100 (100%)	0	100	100
26	LW	90/126 (71%)	89 (99%)	1 (1%)	65	73
27	LY	170/174 (98%)	170 (100%)	0	100	100
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	119/120 (99%)	119 (100%)	0	100	100
30	Lb	85/125 (68%)	85 (100%)	0	100	100
31	Lc	86/97 (89%)	86 (100%)	0	100	100
32	Ld	95/110 (86%)	95 (100%)	0	100	100
33	Le	92/93 (99%)	92 (100%)	0	100	100
34	Lf	88/89 (99%)	88 (100%)	0	100	100
35	Lg	95/100 (95%)	95 (100%)	0	100	100
36	Lh	140/163 (86%)	140 (100%)	0	100	100
37	Li	86/89 (97%)	86 (100%)	0	100	100
38	Lj	164/165 (99%)	164 (100%)	0	100	100
39	Lk	63/65 (97%)	63 (100%)	0	100	100
40	Ll	107/120 (89%)	107 (100%)	0	100	100
41	Lm	90/115 (78%)	90 (100%)	0	100	100
42	Ln	104/133 (78%)	103 (99%)	1 (1%)	68	75
43	Lo	48/90 (53%)	48 (100%)	0	100	100
44	Lp	71/75 (95%)	71 (100%)	0	100	100
45	Lz	179/181 (99%)	178 (99%)	1 (1%)	78	85
46	NC	25/25 (100%)	25 (100%)	0	100	100
47	S1	200/231 (87%)	199 (100%)	1 (0%)	81	87
50	SA	182/242 (75%)	181 (100%)	1 (0%)	81	87
51	SB	215/509 (42%)	212 (99%)	3 (1%)	59	66
52	SC	185/225 (82%)	184 (100%)	1 (0%)	81	87
53	SD	157/170 (92%)	156 (99%)	1 (1%)	78	85
54	SE	224/225 (100%)	220 (98%)	4 (2%)	51	58
55	SG	199/218 (91%)	198 (100%)	1 (0%)	81	87
56	SH	168/174 (97%)	164 (98%)	4 (2%)	43	47
57	SI	179/180 (99%)	178 (99%)	1 (1%)	78	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	SJ	160/168 (95%)	159 (99%)	1 (1%)	78	85
59	SK	188/202 (93%)	188 (100%)	0	100	100
60	SL	130/142 (92%)	129 (99%)	1 (1%)	73	80
61	SM	88/136 (65%)	88 (100%)	0	100	100
62	SN	130/131 (99%)	130 (100%)	0	100	100
63	SO	99/118 (84%)	99 (100%)	0	100	100
64	SP	111/130 (85%)	111 (100%)	0	100	100
65	SQ	115/121 (95%)	112 (97%)	3 (3%)	40	44
66	SS	119/122 (98%)	118 (99%)	1 (1%)	73	80
67	ST	127/132 (96%)	126 (99%)	1 (1%)	73	80
68	SU	111/115 (96%)	111 (100%)	0	100	100
69	SV	67/67 (100%)	66 (98%)	1 (2%)	57	64
70	SW	112/113 (99%)	111 (99%)	1 (1%)	70	78
71	SX	111/114 (97%)	110 (99%)	1 (1%)	70	78
72	SY	107/114 (94%)	107 (100%)	0	100	100
73	SZ	92/107 (86%)	90 (98%)	2 (2%)	45	50
74	Sa	86/98 (88%)	86 (100%)	0	100	100
75	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	68
76	Sc	74/103 (72%)	74 (100%)	0	100	100
77	Sd	55/62 (89%)	55 (100%)	0	100	100
78	Se	45/104 (43%)	44 (98%)	1 (2%)	45	50
79	Sf	48/49 (98%)	47 (98%)	1 (2%)	47	52
80	Sg	263/275 (96%)	259 (98%)	4 (2%)	57	64
81	So	24/24 (100%)	24 (100%)	0	100	100
82	Sy	103/108 (95%)	102 (99%)	1 (1%)	68	75
83	Sz	66/140 (47%)	63 (96%)	3 (4%)	24	23
All	All	9989/11356 (88%)	9927 (99%)	62 (1%)	76	85

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	SD	41	VAL
80	Sg	132	TRP

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Mol	Chain	Res	Type
56	SH	162	GLN
80	Sg	70	VAL
83	Sz	104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
41	Lm	116	GLN
67	ST	19	ASN
47	S1	158	HIS
67	ST	11	HIS
64	SP	79	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	145/157 (92%)	12 (8%)	0
2	L5	3511/5069 (69%)	519 (14%)	10 (0%)
4	L9	119/121 (98%)	9 (7%)	0
48	S2	1655/1869 (88%)	248 (14%)	4 (0%)
49	S5	8/9 (88%)	1 (12%)	0
6	S4	75/76 (98%)	24 (32%)	2 (2%)
All	All	5513/7301 (75%)	813 (14%)	16 (0%)

5 of 813 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	34	U
1	L1	35	C
1	L1	48	A
1	L1	59	A
1	L1	62	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	S2	912	C
48	S2	874	G
2	L5	3876	A
48	S2	836	G

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Mol	Chain	Res	Type
2	L5	2587	A

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

235 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
6	1MG	S4	37	6	23,26,27	0.61	0	33,39,42	0.71	1 (3%)
48	OMC	S2	462	48	19,22,23	0.80	0	25,31,34	0.85	0
71	HY3	SX	62	71,85	7,8,9	0.98	0	7,10,12	1.08	1 (14%)
2	A2M	L5	1524	2	22,25,26	1.41	2 (9%)	30,36,39	0.94	2 (6%)
48	PSU	S2	36	48	18,21,22	1.39	3 (16%)	21,30,33	1.97	4 (19%)
48	OMU	S2	1442	48	19,22,23	1.24	4 (21%)	25,31,34	1.80	4 (16%)
2	PSU	L5	4972	2	18,21,22	1.35	2 (11%)	21,30,33	2.00	4 (19%)
48	OMU	S2	116	48	19,22,23	1.20	3 (15%)	25,31,34	1.82	5 (20%)
2	PSU	L5	4420	2	18,21,22	1.40	2 (11%)	21,30,33	2.00	4 (19%)
48	OMC	S2	174	48	19,22,23	0.79	0	25,31,34	0.83	0
48	PSU	S2	1244	48	18,21,22	1.36	2 (11%)	21,30,33	2.06	3 (14%)
48	OMU	S2	1288	48	19,22,23	1.21	2 (10%)	25,31,34	1.90	6 (24%)
48	PSU	S2	918	48	18,21,22	1.40	3 (16%)	21,30,33	2.10	5 (23%)
2	PSU	L5	3884	2	18,21,22	1.40	3 (16%)	21,30,33	2.03	4 (19%)
2	OMG	L5	4623	2	23,26,27	1.20	3 (13%)	32,38,41	2.08	5 (15%)
6	H2U	S4	16	6	18,21,22	0.63	0	19,30,33	0.54	0
2	OMC	L5	1340	2	19,22,23	0.80	0	25,31,34	0.85	1 (4%)
2	PSU	L5	4689	2	18,21,22	1.42	3 (16%)	21,30,33	2.04	4 (19%)
2	OMG	L5	1522	2	23,26,27	1.17	2 (8%)	32,38,41	2.07	7 (21%)
48	PSU	S2	1347	48	18,21,22	1.36	2 (11%)	21,30,33	2.16	4 (19%)
48	A2M	S2	1031	48	22,25,26	1.30	1 (4%)	30,36,39	1.03	1 (3%)
6	1MA	S4	58	6	21,25,26	0.41	0	30,37,40	0.55	0
6	5MU	S4	54	6	19,22,23	0.25	0	27,32,35	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	S2	801	48	18,21,22	1.39	3 (16%)	21,30,33	2.07	5 (23%)
48	6MZ	S2	1832	84,85,48	22,25,26	1.54	4 (18%)	29,36,39	2.09	9 (31%)
2	A2M	L5	3825	2	22,25,26	1.34	2 (9%)	30,36,39	0.95	1 (3%)
48	OMC	S2	1391	48	19,22,23	0.79	0	25,31,34	0.81	0
2	PSU	L5	2508	2	18,21,22	1.32	3 (16%)	21,30,33	2.00	4 (19%)
48	A2M	S2	99	84,48	22,25,26	1.31	1 (4%)	30,36,39	1.01	2 (6%)
2	A2M	L5	2787	2	22,25,26	1.44	2 (9%)	30,36,39	0.99	1 (3%)
48	PSU	S2	93	48	18,21,22	1.39	3 (16%)	21,30,33	2.02	3 (14%)
2	OMG	L5	3944	2	23,26,27	1.21	3 (13%)	32,38,41	1.96	6 (18%)
2	PSU	L5	4471	2	18,21,22	1.44	3 (16%)	21,30,33	1.95	4 (19%)
48	MA6	S2	1850	48	23,26,27	1.58	5 (21%)	33,38,41	2.26	14 (42%)
48	PSU	S2	814	48	18,21,22	1.39	2 (11%)	21,30,33	2.04	4 (19%)
48	OMC	S2	1710	48	19,22,23	0.80	0	25,31,34	0.96	1 (4%)
2	5MC	L5	3782	2,84	19,22,23	1.65	3 (15%)	26,32,35	1.04	2 (7%)
2	A2M	L5	3867	2	22,25,26	1.30	1 (4%)	30,36,39	0.95	2 (6%)
2	PSU	L5	3920	2,84	18,21,22	1.38	2 (11%)	21,30,33	2.13	6 (28%)
2	OMU	L5	3925	2	19,22,23	1.23	2 (10%)	25,31,34	1.85	5 (20%)
2	PSU	L5	3853	2,84	18,21,22	1.40	2 (11%)	21,30,33	2.01	3 (14%)
2	PSU	L5	4431	2	18,21,22	1.35	2 (11%)	21,30,33	2.07	4 (19%)
2	OMG	L5	2364	2	23,26,27	1.14	3 (13%)	32,38,41	2.02	7 (21%)
2	OMG	L5	3744	2	23,26,27	1.17	3 (13%)	32,38,41	1.96	6 (18%)
2	OMC	L5	4456	2	19,22,23	0.78	0	25,31,34	0.88	1 (4%)
48	A2M	S2	1383	48	22,25,26	1.30	2 (9%)	30,36,39	1.16	5 (16%)
48	OMG	S2	867	48	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
2	OMC	L5	3701	85,2	19,22,23	0.77	0	25,31,34	0.87	1 (4%)
2	PSU	L5	4552	2	18,21,22	1.33	2 (11%)	21,30,33	2.21	3 (14%)
2	PSU	L5	2632	2	18,21,22	1.42	3 (16%)	21,30,33	2.02	3 (14%)
2	PSU	L5	4457	2	18,21,22	1.33	2 (11%)	21,30,33	2.08	4 (19%)
48	OMG	S2	683	48	23,26,27	1.16	2 (8%)	32,38,41	2.04	6 (18%)
2	UY1	L5	3818	85,2	19,22,23	1.55	5 (26%)	21,31,34	1.88	5 (23%)
2	PSU	L5	4521	85,2,84	18,21,22	1.36	2 (11%)	21,30,33	2.11	4 (19%)
48	PSU	S2	210	48	18,21,22	1.37	2 (11%)	21,30,33	1.98	4 (19%)
2	OMG	L5	4618	2	23,26,27	1.17	3 (13%)	32,38,41	2.03	6 (18%)
2	PSU	L5	1792	85,2	18,21,22	1.32	2 (11%)	21,30,33	1.98	3 (14%)
48	A2M	S2	468	48	22,25,26	1.41	2 (9%)	30,36,39	0.98	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	M3L	Lo	98	43	10,11,12	1.04	0	9,14,16	0.67	0
2	OMC	L5	3808	2	19,22,23	0.75	0	25,31,34	0.78	0
48	OMU	S2	1326	84,48	19,22,23	1.21	3 (15%)	25,31,34	1.84	5 (20%)
2	6MZ	L5	4220	2	22,25,26	1.56	4 (18%)	29,36,39	2.14	9 (31%)
2	OMG	L5	2050	2	23,26,27	1.17	3 (13%)	32,38,41	1.95	5 (15%)
2	A2M	L5	1534	2,84	22,25,26	1.33	2 (9%)	30,36,39	1.07	1 (3%)
8	V5N	LD	216	8	8,11,12	1.62	2 (25%)	8,14,16	1.77	3 (37%)
2	PSU	L5	4299	2	18,21,22	1.39	3 (16%)	21,30,33	1.96	4 (19%)
2	A2M	L5	2815	2	22,25,26	1.34	2 (9%)	30,36,39	0.90	1 (3%)
2	OMC	L5	4536	2	19,22,23	0.76	0	25,31,34	0.87	0
2	JMH	L5	1456	2	18,22,23	2.83	6 (33%)	23,32,35	0.91	1 (4%)
48	PSU	S2	1445	48	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
2	PSU	L5	4423	2	18,21,22	1.34	2 (11%)	21,30,33	2.09	4 (19%)
48	PSU	S2	866	48	18,21,22	1.39	2 (11%)	21,30,33	2.05	3 (14%)
2	OMG	L5	1316	2	23,26,27	1.21	4 (17%)	32,38,41	1.94	6 (18%)
48	A2M	S2	484	48	22,25,26	1.34	3 (13%)	30,36,39	0.90	1 (3%)
2	OMG	L5	1625	85,2	23,26,27	1.21	3 (13%)	32,38,41	1.98	6 (18%)
2	PSU	L5	3768	2	18,21,22	1.37	2 (11%)	21,30,33	2.20	4 (19%)
2	PSU	L5	4628	2	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
48	PSU	S2	218	48	18,21,22	1.38	3 (16%)	21,30,33	1.96	4 (19%)
48	OMU	S2	428	48	19,22,23	1.18	2 (10%)	25,31,34	1.84	5 (20%)
48	PSU	S2	1643	84,48	18,21,22	1.34	2 (11%)	21,30,33	2.01	4 (19%)
2	2MG	L5	1517	2	23,26,27	1.31	2 (8%)	33,38,41	1.44	4 (12%)
2	OMC	L5	2365	2	19,22,23	0.75	0	25,31,34	0.78	0
2	OMU	L5	1773	2	19,22,23	1.22	3 (15%)	25,31,34	1.84	5 (20%)
48	PSU	S2	681	48	18,21,22	1.32	2 (11%)	21,30,33	2.08	4 (19%)
2	PSU	L5	4579	2	18,21,22	1.38	2 (11%)	21,30,33	2.05	3 (14%)
48	PSU	S2	1232	48	18,21,22	1.38	2 (11%)	21,30,33	2.02	3 (14%)
2	PSU	L5	5001	2	18,21,22	1.35	2 (11%)	21,30,33	2.09	3 (14%)
2	PSU	L5	4500	2	18,21,22	1.36	2 (11%)	21,30,33	2.11	5 (23%)
2	PSU	L5	1683	85,2	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
48	PSU	S2	1625	48	18,21,22	1.36	2 (11%)	21,30,33	2.02	3 (14%)
48	4AC	S2	1842	85,48	21,24,25	3.13	11 (52%)	28,34,37	0.98	1 (3%)
2	A2M	L5	2401	2	22,25,26	1.36	2 (9%)	30,36,39	0.94	1 (3%)
2	A2M	L5	1871	2,84	22,25,26	1.36	3 (13%)	30,36,39	1.06	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	3637	85,2	18,21,22	1.34	2 (11%)	21,30,33	2.13	4 (19%)
2	OMC	L5	3869	2	19,22,23	0.76	0	25,31,34	0.71	0
6	M2G	S4	26	6	24,27,28	0.42	0	33,40,43	0.44	0
2	OMG	L5	4499	2	23,26,27	1.16	3 (13%)	32,38,41	2.09	7 (21%)
48	PSU	S2	1692	48	18,21,22	1.40	2 (11%)	21,30,33	2.06	4 (19%)
2	OMC	L5	1881	2,84	19,22,23	0.77	0	25,31,34	0.96	1 (4%)
48	PSU	S2	966	48	18,21,22	1.39	3 (16%)	21,30,33	2.02	4 (19%)
2	OMC	L5	3887	2	19,22,23	0.78	0	25,31,34	0.83	0
2	OMC	L5	2824	2	19,22,23	0.78	0	25,31,34	0.74	0
48	7MG	S2	1639	6,48	23,26,27	1.09	1 (4%)	27,39,42	0.85	2 (7%)
2	OMU	L5	2837	2	19,22,23	1.25	3 (15%)	25,31,34	1.90	5 (20%)
2	PSU	L5	4353	2	18,21,22	1.32	3 (16%)	21,30,33	2.05	4 (19%)
2	OMU	L5	4306	2	19,22,23	1.24	3 (15%)	25,31,34	1.75	4 (16%)
48	PSU	S2	1174	85,48	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
48	PSU	S2	1238	48	18,21,22	1.39	2 (11%)	21,30,33	2.13	4 (19%)
48	PSU	S2	1367	48	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)
48	PSU	S2	406	48	18,21,22	1.38	3 (16%)	21,30,33	2.11	4 (19%)
2	OMG	L5	3899	2	23,26,27	1.18	3 (13%)	32,38,41	2.10	6 (18%)
48	OMG	S2	436	48	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
2	OMU	L5	4498	2	19,22,23	1.20	3 (15%)	25,31,34	1.91	5 (20%)
2	PSU	L5	3851	2	18,21,22	1.39	2 (11%)	21,30,33	1.98	5 (23%)
6	PSU	S4	27	6	18,21,22	0.92	1 (5%)	21,30,33	0.66	0
2	PSU	L5	3715	2	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
48	A2M	S2	1678	48	22,25,26	1.42	3 (13%)	30,36,39	1.00	2 (6%)
2	PSU	L5	5010	2	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
1	OMG	L1	75	1	23,26,27	1.17	3 (13%)	32,38,41	2.00	6 (18%)
30	MLZ	Lb	5	30	8,9,10	0.65	0	4,9,11	0.96	0
2	A2M	L5	398	2	22,25,26	1.42	2 (9%)	30,36,39	0.99	3 (10%)
48	PSU	S2	863	48	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
2	PSU	L5	3730	2	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
2	OMG	L5	4870	2	23,26,27	1.18	3 (13%)	32,38,41	1.93	6 (18%)
2	OMU	L5	4620	2	19,22,23	1.23	3 (15%)	25,31,34	1.64	5 (20%)
1	PSU	L1	69	1	18,21,22	1.44	2 (11%)	21,30,33	2.14	5 (23%)
2	2MG	L5	4872	2	23,26,27	1.28	2 (8%)	33,38,41	1.43	4 (12%)
2	PSU	L5	4673	2	18,21,22	1.38	2 (11%)	21,30,33	2.08	4 (19%)
48	MA6	S2	1851	48	23,26,27	1.56	4 (17%)	33,38,41	2.30	13 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	S2	1046	48	18,21,22	1.35	2 (11%)	21,30,33	1.91	4 (19%)
2	PSU	L5	1781	2	18,21,22	1.43	3 (16%)	21,30,33	1.99	3 (14%)
2	PSU	L5	4403	2	18,21,22	1.38	2 (11%)	21,30,33	2.04	4 (19%)
2	A2M	L5	3785	2	22,25,26	1.36	3 (13%)	30,36,39	1.30	3 (10%)
2	PSU	L5	3770	2	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
2	OMC	L5	2351	2,84	19,22,23	0.78	0	25,31,34	0.92	1 (4%)
2	OMG	L5	2876	2	23,26,27	1.17	3 (13%)	32,38,41	1.99	6 (18%)
48	OMU	S2	121	48	19,22,23	1.19	3 (15%)	25,31,34	1.80	5 (20%)
48	PSU	S2	686	48	18,21,22	1.37	2 (11%)	21,30,33	2.03	4 (19%)
48	PSU	S2	822	48	18,21,22	1.36	2 (11%)	21,30,33	1.97	4 (19%)
48	A2M	S2	166	48	22,25,26	1.40	3 (13%)	30,36,39	1.05	2 (6%)
2	OMG	L5	2424	2	23,26,27	1.20	3 (13%)	32,38,41	1.94	6 (18%)
48	OMU	S2	172	48	19,22,23	1.20	2 (10%)	25,31,34	1.89	5 (20%)
48	OMG	S2	1328	85,48	23,26,27	1.17	3 (13%)	32,38,41	1.94	6 (18%)
6	1MG	S4	9	6,84	23,26,27	0.63	0	33,39,42	0.78	1 (3%)
2	A2M	L5	3718	2	22,25,26	1.27	2 (9%)	30,36,39	1.01	2 (6%)
6	PSU	S4	55	6	18,21,22	0.92	1 (5%)	21,30,33	0.72	0
2	A2M	L5	4590	2	22,25,26	1.34	2 (9%)	30,36,39	1.03	1 (3%)
48	PSU	S2	109	48	18,21,22	1.37	3 (16%)	21,30,33	2.01	3 (14%)
48	PSU	S2	609	48	18,21,22	1.38	2 (11%)	21,30,33	1.99	3 (14%)
48	PSU	S2	1004	48	18,21,22	1.39	2 (11%)	21,30,33	2.04	4 (19%)
48	PSU	S2	1056	48	18,21,22	1.37	3 (16%)	21,30,33	1.97	4 (19%)
48	A2M	S2	159	48	22,25,26	1.38	3 (13%)	30,36,39	1.03	3 (10%)
2	OMG	L5	3792	85,2	23,26,27	1.22	3 (13%)	32,38,41	2.02	6 (18%)
2	PSU	L5	3764	2	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)
48	OMC	S2	517	48	19,22,23	0.78	0	25,31,34	0.83	0
2	OMG	L5	4392	2	23,26,27	1.17	4 (17%)	32,38,41	2.00	6 (18%)
48	PSU	S2	815	48	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
5	HIC	LB	245	5	10,11,12	1.25	0	9,14,16	2.58	3 (33%)
2	A2M	L5	4571	2	22,25,26	1.38	2 (9%)	30,36,39	0.94	2 (6%)
2	PSU	L5	4361	2	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
1	PSU	L1	55	1	18,21,22	1.39	3 (16%)	21,30,33	2.13	4 (19%)
2	PSU	L5	1582	2	18,21,22	1.41	2 (11%)	21,30,33	2.05	3 (14%)
2	PSU	L5	4532	2	18,21,22	1.42	3 (16%)	21,30,33	2.03	3 (14%)
2	PSU	L5	3734	2	18,21,22	1.41	2 (11%)	21,30,33	2.03	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	V5N	La	39	29	8,11,12	1.56	1 (12%)	8,14,16	1.94	3 (37%)
48	A2M	S2	576	85,48	22,25,26	1.31	2 (9%)	30,36,39	1.04	2 (6%)
48	PSU	S2	823	48	18,21,22	1.35	2 (11%)	21,30,33	2.11	5 (23%)
48	PSU	S2	1177	48	18,21,22	1.34	2 (11%)	21,30,33	2.19	4 (19%)
48	OMC	S2	1703	84,48	19,22,23	0.76	0	25,31,34	0.78	0
2	PSU	L5	4312	2	18,21,22	1.36	2 (11%)	21,30,33	1.99	3 (14%)
6	H2U	S4	47	6	18,21,22	0.63	0	19,30,33	0.45	0
2	OMG	L5	4228	2	23,26,27	1.20	3 (13%)	32,38,41	2.02	6 (18%)
48	OMG	S2	509	84,48	23,26,27	1.21	3 (13%)	32,38,41	1.96	5 (15%)
2	2MG	L5	729	2	23,26,27	1.30	2 (8%)	33,38,41	1.44	4 (12%)
48	OMG	S2	1490	84,48	23,26,27	1.18	3 (13%)	32,38,41	1.90	6 (18%)
2	A2M	L5	1326	2	22,25,26	1.36	2 (9%)	30,36,39	0.95	2 (6%)
48	PSU	S2	649	48	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
2	OMC	L5	2861	2	19,22,23	0.78	0	25,31,34	0.80	0
2	OMG	L5	4196	6,2	23,26,27	1.17	3 (13%)	32,38,41	2.03	7 (21%)
48	A2M	S2	512	48	22,25,26	1.38	2 (9%)	30,36,39	1.02	1 (3%)
48	A2M	S2	27	84,48	22,25,26	1.32	1 (4%)	30,36,39	0.99	1 (3%)
2	PSU	L5	4576	2	18,21,22	1.36	2 (11%)	21,30,33	2.08	3 (14%)
48	OMG	S2	601	48	23,26,27	1.18	3 (13%)	32,38,41	1.98	6 (18%)
2	OMC	L5	2804	2	19,22,23	0.79	1 (5%)	25,31,34	0.75	0
48	PSU	S2	1045	48	18,21,22	1.37	2 (11%)	21,30,33	2.09	4 (19%)
2	PSU	L5	3695	85,2,84	18,21,22	1.35	2 (11%)	21,30,33	2.15	5 (23%)
48	PSU	S2	119	48	18,21,22	1.37	2 (11%)	21,30,33	2.04	3 (14%)
48	PSU	S2	572	85,48	18,21,22	1.41	2 (11%)	21,30,33	2.08	4 (19%)
2	PSU	L5	1862	2	18,21,22	1.35	2 (11%)	21,30,33	2.07	4 (19%)
2	OMG	L5	4370	2	23,26,27	1.15	3 (13%)	32,38,41	2.09	7 (21%)
6	2MG	S4	10	6	23,26,27	0.36	0	33,38,41	0.44	0
2	PSU	L5	4442	2	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
48	OMU	S2	799	48	19,22,23	1.25	4 (21%)	25,31,34	1.78	5 (20%)
2	OMU	L5	2415	2	19,22,23	1.25	4 (21%)	25,31,34	1.72	5 (20%)
2	OMU	L5	4227	2	19,22,23	1.24	3 (15%)	25,31,34	1.83	5 (20%)
6	OMG	S4	18	6	23,26,27	0.33	0	32,38,41	0.44	0
48	OMU	S2	1804	48	19,22,23	1.24	3 (15%)	25,31,34	1.82	4 (16%)
48	A2M	S2	668	84,48	22,25,26	1.48	5 (22%)	30,36,39	1.00	1 (3%)
48	PSU	S2	105	48	18,21,22	1.35	2 (11%)	21,30,33	2.05	3 (14%)
2	PSU	L5	3758	2	18,21,22	1.37	3 (16%)	21,30,33	2.03	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	L5	400	2	22,25,26	1.36	2 (9%)	30,36,39	0.91	0
2	PSU	L5	3639	2	18,21,22	1.41	2 (11%)	21,30,33	2.08	6 (28%)
2	PSU	L5	1782	2	18,21,22	1.36	2 (11%)	21,30,33	2.09	3 (14%)
2	OMC	L5	3841	2	19,22,23	0.78	0	25,31,34	0.79	0
2	OMG	L5	4494	2	23,26,27	1.18	2 (8%)	32,38,41	1.97	6 (18%)
63	IAS	SO	138	63	6,7,8	1.10	0	3,8,10	2.15	1 (33%)
2	PSU	L5	1860	2	18,21,22	1.37	3 (16%)	21,30,33	1.92	4 (19%)
2	5MC	L5	4447	85,2	19,22,23	1.70	3 (15%)	26,32,35	1.27	2 (7%)
2	A2M	L5	4523	2,84	22,25,26	1.43	4 (18%)	30,36,39	1.15	2 (6%)
2	PSU	L5	1536	2	18,21,22	1.37	2 (11%)	21,30,33	1.99	4 (19%)
2	PSU	L5	4296	2	18,21,22	1.40	2 (11%)	21,30,33	2.08	4 (19%)
6	H2U	S4	20	6	18,21,22	0.68	1 (5%)	19,30,33	0.51	0
2	PSU	L5	3762	2	18,21,22	1.42	2 (11%)	21,30,33	2.10	4 (19%)
2	A2M	L5	2363	2,84	22,25,26	1.32	2 (9%)	30,36,39	0.95	2 (6%)
2	PSU	L5	3844	2	18,21,22	1.38	3 (16%)	21,30,33	2.03	3 (14%)
2	UR3	L5	4530	2	19,22,23	0.94	0	26,32,35	1.70	2 (7%)
2	A2M	L5	3830	2	22,25,26	1.40	2 (9%)	30,36,39	1.05	2 (6%)
2	1MA	L5	1322	2,84	21,25,26	0.78	1 (4%)	30,37,40	1.15	3 (10%)
2	OMG	L5	1760	2	23,26,27	1.19	3 (13%)	32,38,41	2.01	6 (18%)
48	A2M	S2	590	48	22,25,26	1.48	3 (13%)	30,36,39	1.02	3 (10%)
2	PSU	L5	4636	2	18,21,22	1.41	3 (16%)	21,30,33	2.04	4 (19%)
48	PSU	S2	34	48	18,21,22	1.39	3 (16%)	21,30,33	2.02	4 (19%)
2	A2M	L5	3760	2,48	22,25,26	1.44	3 (13%)	30,36,39	0.99	1 (3%)
48	OMG	S2	644	48	23,26,27	1.20	3 (13%)	32,38,41	2.02	6 (18%)
2	PSU	L5	4293	2	18,21,22	1.38	2 (11%)	21,30,33	2.01	3 (14%)
48	PSU	S2	651	48	18,21,22	1.36	2 (11%)	21,30,33	2.12	4 (19%)
2	PSU	L5	1744	85,2	18,21,22	1.33	2 (11%)	21,30,33	2.08	4 (19%)
48	B8N	S2	1248	48	25,29,30	3.33	8 (32%)	28,42,45	2.04	8 (28%)
2	PSU	L5	1677	2	18,21,22	1.44	3 (16%)	21,30,33	2.08	4 (19%)
48	PSU	S2	1081	48	18,21,22	1.42	2 (11%)	21,30,33	2.09	5 (23%)
48	4AC	S2	1337	48	21,24,25	3.20	11 (52%)	28,34,37	1.08	3 (10%)
48	OMU	S2	627	48	19,22,23	1.20	2 (10%)	25,31,34	1.77	5 (20%)
2	OMC	L5	2422	2,84	19,22,23	0.79	0	25,31,34	0.74	0
33	MLZ	Le	53	33	8,9,10	0.68	0	4,9,11	0.80	0
2	OMG	L5	4637	85,2	23,26,27	1.16	3 (13%)	32,38,41	2.05	7 (21%)

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
6	1MG	S4	37	6	-	0/7/25/26	0/3/3/3
48	OMC	S2	462	48	-	0/9/27/28	0/2/2/2
71	HY3	SX	62	71,85	-	0/1/12/14	0/1/1/1
2	A2M	L5	1524	2	-	1/9/27/28	0/3/3/3
48	PSU	S2	36	48	-	0/7/25/26	0/2/2/2
48	OMU	S2	1442	48	-	0/9/27/28	0/2/2/2
2	PSU	L5	4972	2	-	0/7/25/26	0/2/2/2
48	OMU	S2	116	48	-	0/9/27/28	0/2/2/2
2	PSU	L5	4420	2	-	0/7/25/26	0/2/2/2
48	OMC	S2	174	48	-	1/9/27/28	0/2/2/2
48	PSU	S2	1244	48	-	0/7/25/26	0/2/2/2
48	OMU	S2	1288	48	-	0/9/27/28	0/2/2/2
48	PSU	S2	918	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	3884	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4623	2	-	0/9/27/28	0/3/3/3
6	H2U	S4	16	6	-	3/7/38/39	0/2/2/2
2	OMC	L5	1340	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4689	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	1522	2	-	0/9/27/28	0/3/3/3
48	PSU	S2	1347	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	1031	48	-	0/9/27/28	0/3/3/3
6	1MA	S4	58	6	-	2/7/25/26	0/3/3/3
6	5MU	S4	54	6	-	0/7/25/26	0/2/2/2
48	PSU	S2	801	48	-	0/7/25/26	0/2/2/2
48	6MZ	S2	1832	84,85,48	-	2/9/27/28	0/3/3/3
2	A2M	L5	3825	2	-	0/9/27/28	0/3/3/3
48	OMC	S2	1391	48	-	0/9/27/28	0/2/2/2
2	PSU	L5	2508	2	-	0/7/25/26	0/2/2/2
48	A2M	S2	99	84,48	-	1/9/27/28	0/3/3/3
2	A2M	L5	2787	2	-	4/9/27/28	0/3/3/3
48	PSU	S2	93	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	3944	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	4471	2	-	0/7/25/26	0/2/2/2
48	MA6	S2	1850	48	-	1/11/29/30	0/3/3/3
48	PSU	S2	814	48	-	0/7/25/26	0/2/2/2
48	OMC	S2	1710	48	-	0/9/27/28	0/2/2/2
2	5MC	L5	3782	2,84	-	0/7/25/26	0/2/2/2
2	A2M	L5	3867	2	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	3920	2,84	-	0/7/25/26	0/2/2/2
2	OMU	L5	3925	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3853	2,84	-	0/7/25/26	0/2/2/2
2	PSU	L5	4431	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	2364	2	-	1/9/27/28	0/3/3/3
2	OMG	L5	3744	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	4456	2	-	0/9/27/28	0/2/2/2
48	A2M	S2	1383	48	-	1/9/27/28	0/3/3/3
48	OMG	S2	867	48	-	0/9/27/28	0/3/3/3
2	OMC	L5	3701	85,2	-	4/9/27/28	0/2/2/2
2	PSU	L5	4552	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	2632	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4457	2	-	0/7/25/26	0/2/2/2
48	OMG	S2	683	48	-	1/9/27/28	0/3/3/3
2	UY1	L5	3818	85,2	-	1/9/27/28	0/2/2/2
2	PSU	L5	4521	85,2,84	-	0/7/25/26	0/2/2/2
48	PSU	S2	210	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	4618	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	1792	85,2	-	0/7/25/26	0/2/2/2
48	A2M	S2	468	48	-	0/9/27/28	0/3/3/3
43	M3L	Lo	98	43	-	0/9/10/12	-
2	OMC	L5	3808	2	-	0/9/27/28	0/2/2/2
48	OMU	S2	1326	84,48	-	0/9/27/28	0/2/2/2
2	6MZ	L5	4220	2	-	0/9/27/28	0/3/3/3
2	OMG	L5	2050	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	1534	2,84	-	1/9/27/28	0/3/3/3
8	V5N	LD	216	8	-	1/9/10/12	0/1/1/1
2	PSU	L5	4299	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2815	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	4536	2	-	0/9/27/28	0/2/2/2
2	JMH	L5	1456	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	1445	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	4423	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	866	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	1316	2	-	0/9/27/28	0/3/3/3
48	A2M	S2	484	48	-	0/9/27/28	0/3/3/3
2	OMG	L5	1625	85,2	-	1/9/27/28	0/3/3/3
2	PSU	L5	3768	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4628	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	218	48	-	0/7/25/26	0/2/2/2
48	OMU	S2	428	48	-	4/9/27/28	0/2/2/2
48	PSU	S2	1643	84,48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2MG	L5	1517	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	2365	2	-	0/9/27/28	0/2/2/2
2	OMU	L5	1773	2	-	0/9/27/28	0/2/2/2
48	PSU	S2	681	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	4579	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	1232	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	5001	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4500	2	-	3/7/25/26	0/2/2/2
2	PSU	L5	1683	85,2	-	0/7/25/26	0/2/2/2
48	PSU	S2	1625	48	-	0/7/25/26	0/2/2/2
48	4AC	S2	1842	85,48	-	0/11/29/30	0/2/2/2
2	A2M	L5	2401	2	-	2/9/27/28	0/3/3/3
2	A2M	L5	1871	2,84	-	0/9/27/28	0/3/3/3
2	PSU	L5	3637	85,2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3869	2	-	1/9/27/28	0/2/2/2
6	M2G	S4	26	6	-	0/11/29/30	0/3/3/3
2	OMG	L5	4499	2	-	1/9/27/28	0/3/3/3
48	PSU	S2	1692	48	-	0/7/25/26	0/2/2/2
2	OMC	L5	1881	2,84	-	0/9/27/28	0/2/2/2
48	PSU	S2	966	48	-	0/7/25/26	0/2/2/2
2	OMC	L5	3887	2	-	0/9/27/28	0/2/2/2
2	OMC	L5	2824	2	-	0/9/27/28	0/2/2/2
48	7MG	S2	1639	6,48	-	2/7/37/38	0/3/3/3
2	OMU	L5	2837	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4353	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4306	2	-	0/9/27/28	0/2/2/2
48	PSU	S2	1174	85,48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1238	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1367	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	406	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	3899	2	-	0/9/27/28	0/3/3/3
48	OMG	S2	436	48	-	0/9/27/28	0/3/3/3
2	OMU	L5	4498	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3851	2	-	2/7/25/26	0/2/2/2
6	PSU	S4	27	6	-	0/7/25/26	0/2/2/2
2	PSU	L5	3715	2	-	0/7/25/26	0/2/2/2
48	A2M	S2	1678	48	-	1/9/27/28	0/3/3/3
2	PSU	L5	5010	2	-	0/7/25/26	0/2/2/2
1	OMG	L1	75	1	-	0/9/27/28	0/3/3/3
30	MLZ	Lb	5	30	-	2/7/8/10	-
2	A2M	L5	398	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	S2	863	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	3730	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4870	2	-	3/9/27/28	0/3/3/3
2	OMU	L5	4620	2	-	0/9/27/28	0/2/2/2
1	PSU	L1	69	1	-	0/7/25/26	0/2/2/2
2	2MG	L5	4872	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4673	2	-	0/7/25/26	0/2/2/2
48	MA6	S2	1851	48	-	4/11/29/30	0/3/3/3
48	PSU	S2	1046	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	1781	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4403	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3785	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	3770	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	2351	2,84	-	2/9/27/28	0/2/2/2
2	OMG	L5	2876	2	-	0/9/27/28	0/3/3/3
48	OMU	S2	121	48	-	0/9/27/28	0/2/2/2
48	PSU	S2	686	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	822	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	166	48	-	0/9/27/28	0/3/3/3
2	OMG	L5	2424	2	-	0/9/27/28	0/3/3/3
48	OMU	S2	172	48	-	0/9/27/28	0/2/2/2
48	OMG	S2	1328	85,48	-	0/9/27/28	0/3/3/3
6	1MG	S4	9	6,84	-	1/7/25/26	0/3/3/3
2	A2M	L5	3718	2	-	0/9/27/28	0/3/3/3
6	PSU	S4	55	6	-	0/7/25/26	0/2/2/2
2	A2M	L5	4590	2	-	1/9/27/28	0/3/3/3
48	PSU	S2	109	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	609	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1004	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1056	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	159	48	-	0/9/27/28	0/3/3/3
2	OMG	L5	3792	85,2	-	0/9/27/28	0/3/3/3
2	PSU	L5	3764	2	-	0/7/25/26	0/2/2/2
48	OMC	S2	517	48	-	0/9/27/28	0/2/2/2
2	OMG	L5	4392	2	-	0/9/27/28	0/3/3/3
48	PSU	S2	815	48	-	0/7/25/26	0/2/2/2
5	HIC	LB	245	5	-	0/5/6/8	0/1/1/1
2	A2M	L5	4571	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4361	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	55	1	-	0/7/25/26	0/2/2/2
2	PSU	L5	1582	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	4532	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3734	2	-	0/7/25/26	0/2/2/2
29	V5N	La	39	29	-	0/9/10/12	0/1/1/1
48	A2M	S2	576	85,48	-	2/9/27/28	0/3/3/3
48	PSU	S2	823	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1177	48	-	0/7/25/26	0/2/2/2
48	OMC	S2	1703	84,48	-	0/9/27/28	0/2/2/2
2	PSU	L5	4312	2	-	0/7/25/26	0/2/2/2
6	H2U	S4	47	6	-	2/7/38/39	0/2/2/2
2	OMG	L5	4228	2	-	0/9/27/28	0/3/3/3
48	OMG	S2	509	84,48	-	0/9/27/28	0/3/3/3
2	2MG	L5	729	2	-	0/9/27/28	0/3/3/3
48	OMG	S2	1490	84,48	-	1/9/27/28	0/3/3/3
2	A2M	L5	1326	2	-	2/9/27/28	0/3/3/3
48	PSU	S2	649	48	-	0/7/25/26	0/2/2/2
2	OMC	L5	2861	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4196	6,2	-	0/9/27/28	0/3/3/3
48	A2M	S2	512	48	-	2/9/27/28	0/3/3/3
48	A2M	S2	27	84,48	-	0/9/27/28	0/3/3/3
2	PSU	L5	4576	2	-	0/7/25/26	0/2/2/2
48	OMG	S2	601	48	-	0/9/27/28	0/3/3/3
2	OMC	L5	2804	2	-	0/9/27/28	0/2/2/2
48	PSU	S2	1045	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	3695	85,2,84	-	0/7/25/26	0/2/2/2
48	PSU	S2	119	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	572	85,48	-	0/7/25/26	0/2/2/2
2	PSU	L5	1862	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4370	2	-	0/9/27/28	0/3/3/3
6	2MG	S4	10	6	-	0/9/27/28	0/3/3/3
2	PSU	L5	4442	2	-	0/7/25/26	0/2/2/2
48	OMU	S2	799	48	-	1/9/27/28	0/2/2/2
2	OMU	L5	2415	2	-	0/9/27/28	0/2/2/2
2	OMU	L5	4227	2	-	0/9/27/28	0/2/2/2
6	OMG	S4	18	6	-	2/9/27/28	0/3/3/3
48	OMU	S2	1804	48	-	0/9/27/28	0/2/2/2
48	A2M	S2	668	84,48	-	2/9/27/28	0/3/3/3
48	PSU	S2	105	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	3758	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	400	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	3639	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1782	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	L5	3841	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4494	2	-	0/9/27/28	0/3/3/3
63	IAS	SO	138	63	-	1/7/7/8	-
2	PSU	L5	1860	2	-	0/7/25/26	0/2/2/2
2	5MC	L5	4447	85,2	-	4/7/25/26	0/2/2/2
2	A2M	L5	4523	2,84	-	0/9/27/28	0/3/3/3
2	PSU	L5	1536	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4296	2	-	0/7/25/26	0/2/2/2
6	H2U	S4	20	6	-	2/7/38/39	0/2/2/2
2	PSU	L5	3762	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2363	2,84	-	1/9/27/28	0/3/3/3
2	PSU	L5	3844	2	-	1/7/25/26	0/2/2/2
2	UR3	L5	4530	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3830	2	-	0/9/27/28	0/3/3/3
2	1MA	L5	1322	2,84	-	2/7/25/26	0/3/3/3
2	OMG	L5	1760	2	-	0/9/27/28	0/3/3/3
48	A2M	S2	590	48	-	3/9/27/28	0/3/3/3
2	PSU	L5	4636	2	-	2/7/25/26	0/2/2/2
48	PSU	S2	34	48	-	0/7/25/26	0/2/2/2
2	A2M	L5	3760	2,48	-	5/9/27/28	0/3/3/3
48	OMG	S2	644	48	-	1/9/27/28	0/3/3/3
2	PSU	L5	4293	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	651	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	1744	85,2	-	0/7/25/26	0/2/2/2
48	B8N	S2	1248	48	-	4/16/34/35	0/2/2/2
2	PSU	L5	1677	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	1081	48	-	1/7/25/26	0/2/2/2
48	4AC	S2	1337	48	-	0/11/29/30	0/2/2/2
48	OMU	S2	627	48	-	2/9/27/28	0/2/2/2
2	OMC	L5	2422	2,84	-	0/9/27/28	0/2/2/2
33	MLZ	Le	53	33	-	2/7/8/10	-
2	OMG	L5	4637	85,2	-	0/9/27/28	0/3/3/3

The worst 5 of 513 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1248	B8N	C4-N3	-8.14	1.26	1.40
48	S2	1248	B8N	C6-N1	7.66	1.55	1.36
2	L5	1456	JMH	C2-N1	7.61	1.49	1.38
48	S2	1337	4AC	C4-N3	7.02	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1248	B8N	C4-C5	6.97	1.63	1.47

The worst 5 of 805 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3920	PSU	N1-C2-N3	6.85	122.39	115.17
1	L1	55	PSU	N1-C2-N3	6.77	122.31	115.17
2	L5	4530	UR3	C4-N3-C2	-6.77	119.13	124.58
2	L5	3768	PSU	N1-C2-N3	6.77	122.31	115.17
48	S2	1177	PSU	N1-C2-N3	6.73	122.27	115.17

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L5	3701	OMC	C2'-C1'-N1-C6
2	L5	3760	A2M	C1'-C2'-O2'-CM'
2	L5	4590	A2M	C4'-C5'-O5'-P
6	S4	18	OMG	C1'-C2'-O2'-CM2
6	S4	47	H2U	O4'-C4'-C5'-O5'

There are no ring outliers.

64 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	S2	1442	OMU	1	0
48	S2	116	OMU	2	0
2	L5	4420	PSU	1	0
6	S4	16	H2U	1	0
2	L5	1340	OMC	2	0
2	L5	4689	PSU	1	0
6	S4	54	5MU	1	0
48	S2	801	PSU	2	0
48	S2	1391	OMC	2	0
48	S2	99	A2M	1	0
2	L5	3944	OMG	1	0
48	S2	1850	MA6	1	0
48	S2	814	PSU	1	0
48	S2	1710	OMC	1	0
2	L5	3867	A2M	1	0
2	L5	4431	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L5	4456	OMC	1	0
2	L5	2632	PSU	1	0
2	L5	4457	PSU	1	0
2	L5	3818	UY1	1	0
2	L5	4521	PSU	1	0
2	L5	4618	OMG	1	0
48	S2	468	A2M	1	0
2	L5	3808	OMC	1	0
2	L5	4220	6MZ	1	0
2	L5	2050	OMG	1	0
2	L5	4536	OMC	1	0
48	S2	1643	PSU	1	0
2	L5	4579	PSU	2	0
48	S2	1232	PSU	2	0
2	L5	1871	A2M	1	0
2	L5	3637	PSU	1	0
6	S4	26	M2G	1	0
48	S2	1692	PSU	1	0
48	S2	1639	7MG	1	0
48	S2	436	OMG	1	0
48	S2	1678	A2M	2	0
1	L1	75	OMG	1	0
2	L5	398	A2M	1	0
2	L5	4870	OMG	1	0
2	L5	4620	OMU	2	0
2	L5	4872	2MG	1	0
48	S2	1851	MA6	1	0
2	L5	3785	A2M	1	0
2	L5	2351	OMC	1	0
2	L5	2876	OMG	2	0
2	L5	2424	OMG	2	0
48	S2	1328	OMG	1	0
2	L5	3718	A2M	3	0
6	S4	55	PSU	1	0
48	S2	159	A2M	1	0
2	L5	3792	OMG	1	0
2	L5	3734	PSU	1	0
48	S2	576	A2M	2	0
6	S4	47	H2U	3	0
48	S2	509	OMG	1	0
2	L5	2415	OMU	1	0
6	S4	18	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	S2	1804	OMU	1	0
2	L5	2363	A2M	1	0
2	L5	4530	UR3	1	0
2	L5	4636	PSU	1	0
48	S2	1337	4AC	1	0
2	L5	2422	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 429 ligands modelled in this entry, 428 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	B3P	L5	5129	-	18,18,18	0.72	0	23,23,23	0.97	1 (4%)

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
86	B3P	L5	5129	-	-	9/28/28/28	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	L5	5129	B3P	C11-C8-C10	-2.51	104.51	110.02

There are no chirality outliers.

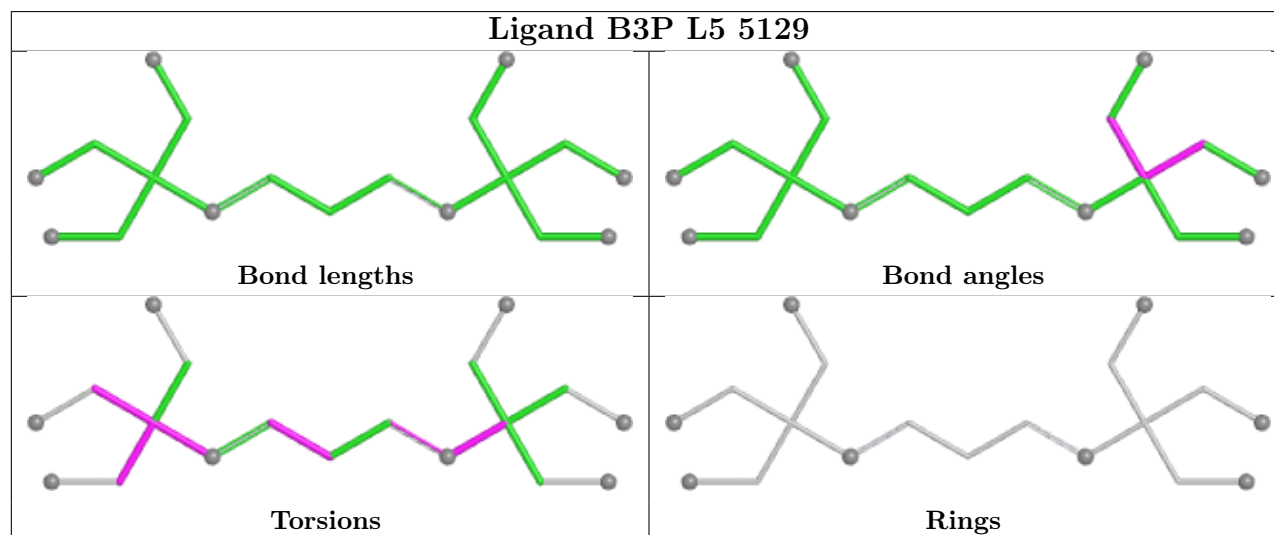
5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	L5	5129	B3P	N1-C4-C7-O6
86	L5	5129	B3P	C1-C2-N2-C8
86	L5	5129	B3P	C5-C4-N1-C3
86	L5	5129	B3P	C7-C4-N1-C3
86	L5	5129	B3P	C10-C8-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

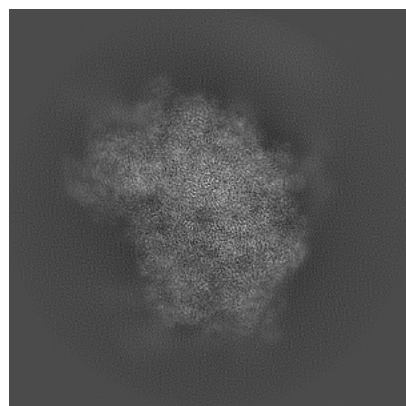
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45170. These allow visual inspection of the internal detail of the map and identification of artifacts.

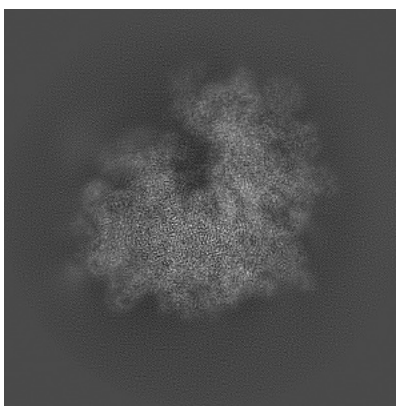
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

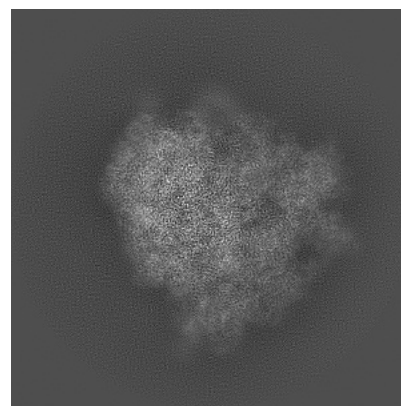
6.1.1 Primary map



X

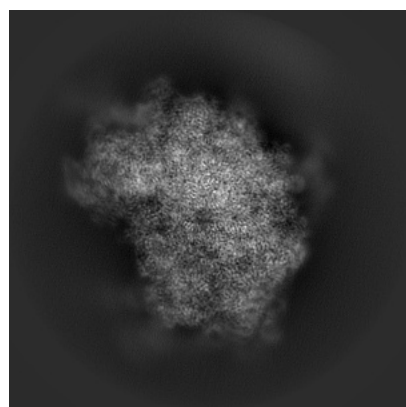


Y

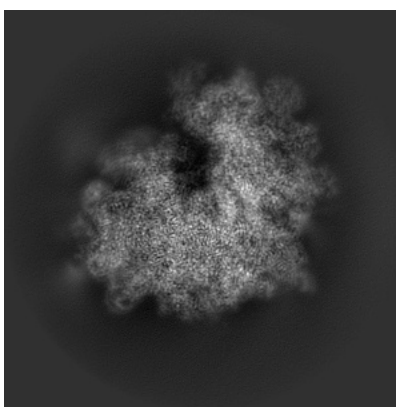


Z

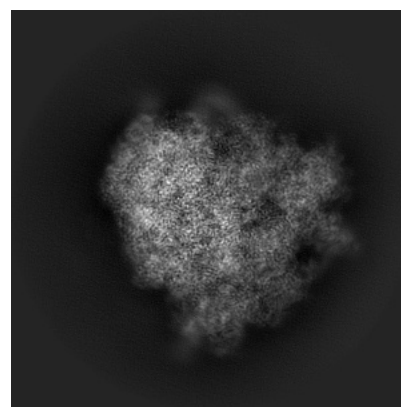
6.1.2 Raw map



X



Y

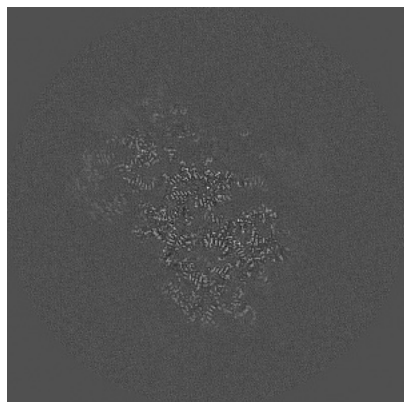


Z

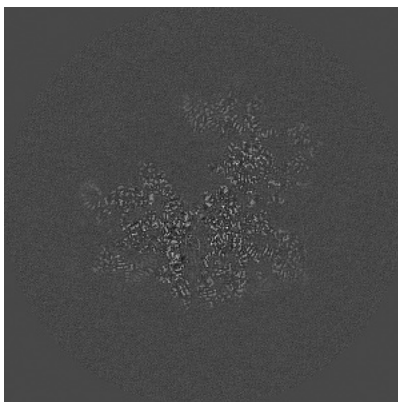
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

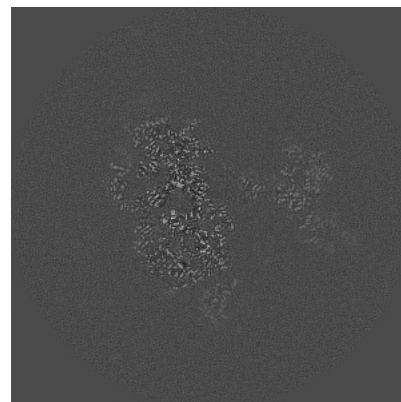
6.2.1 Primary map



X Index: 224

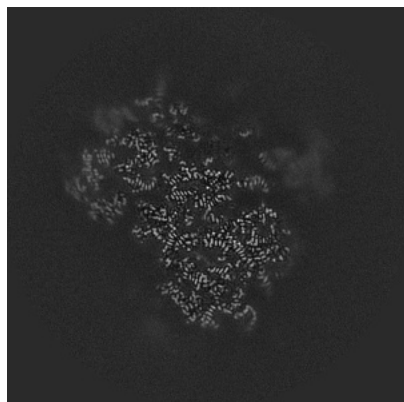


Y Index: 224

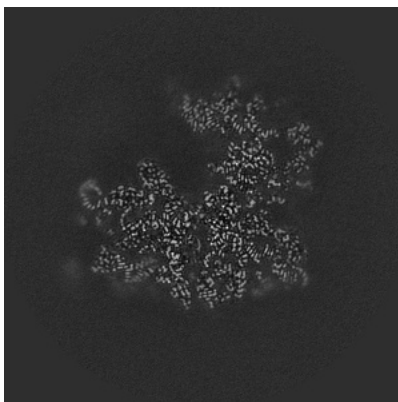


Z Index: 224

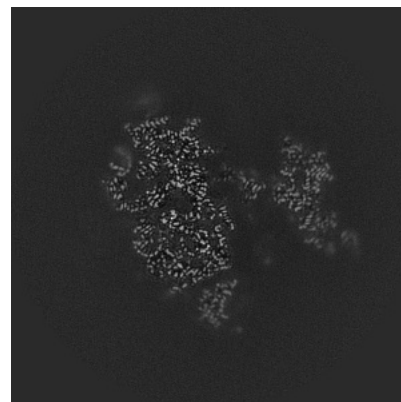
6.2.2 Raw map



X Index: 224



Y Index: 224

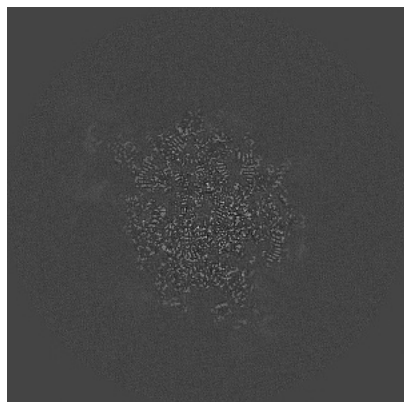


Z Index: 224

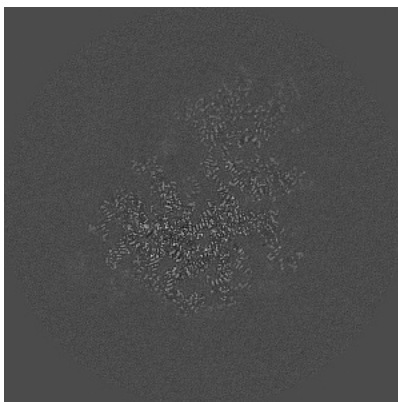
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

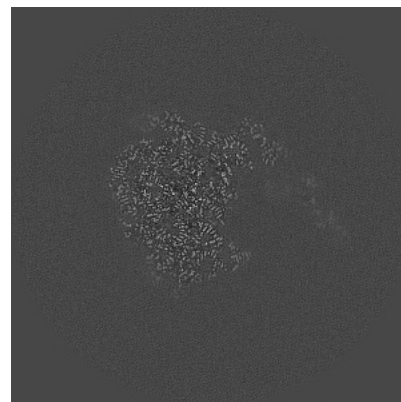
6.3.1 Primary map



X Index: 200

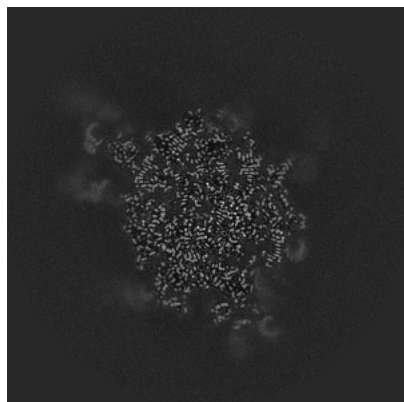


Y Index: 238

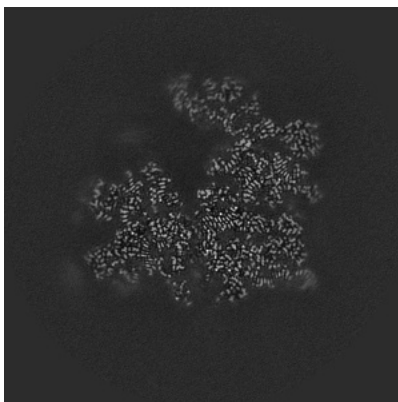


Z Index: 190

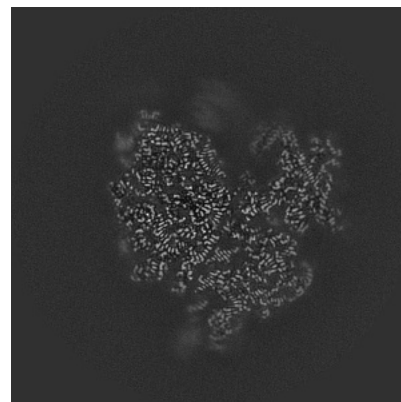
6.3.2 Raw map



X Index: 200



Y Index: 215

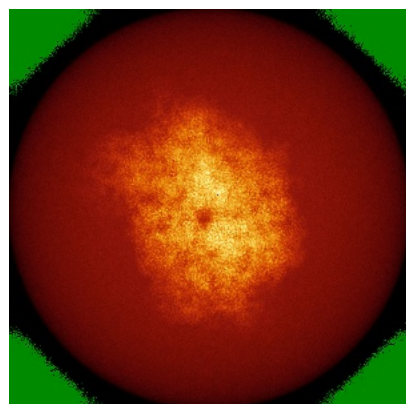


Z Index: 252

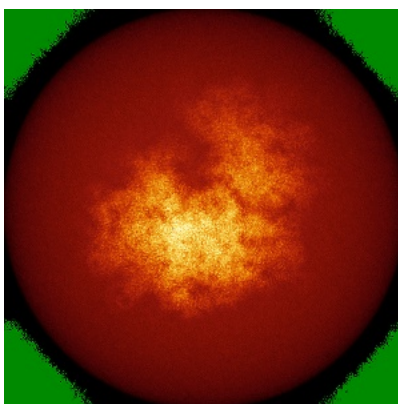
The images above show the largest variance slices of the map in three orthogonal directions.

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

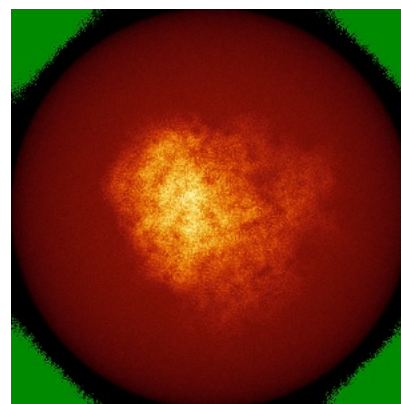
6.4.1 Primary map



X

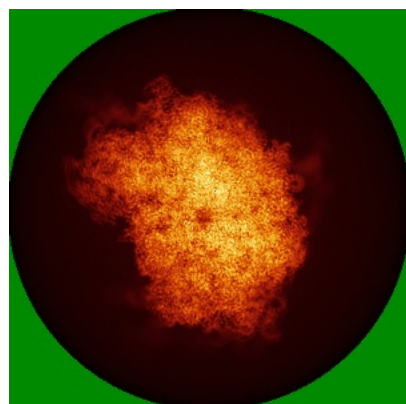


Y

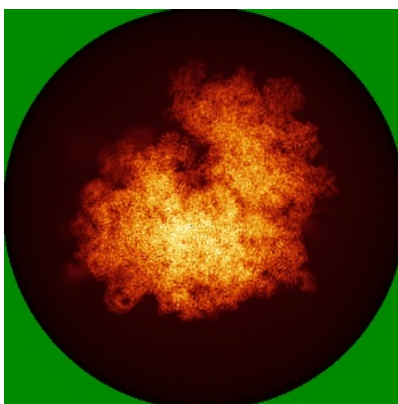


Z

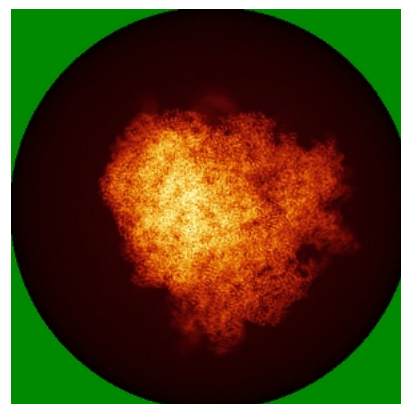
6.4.2 Raw map



X



Y

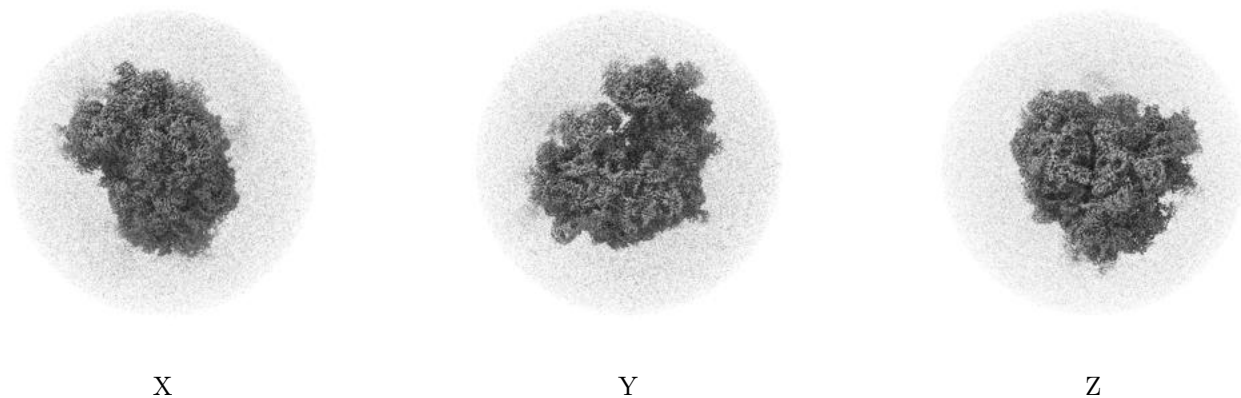


Z

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.

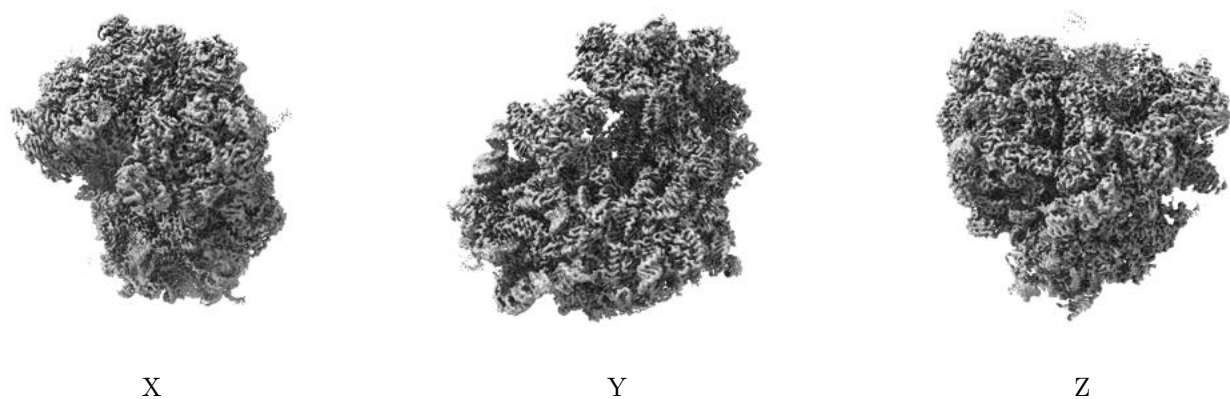
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0175. 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.

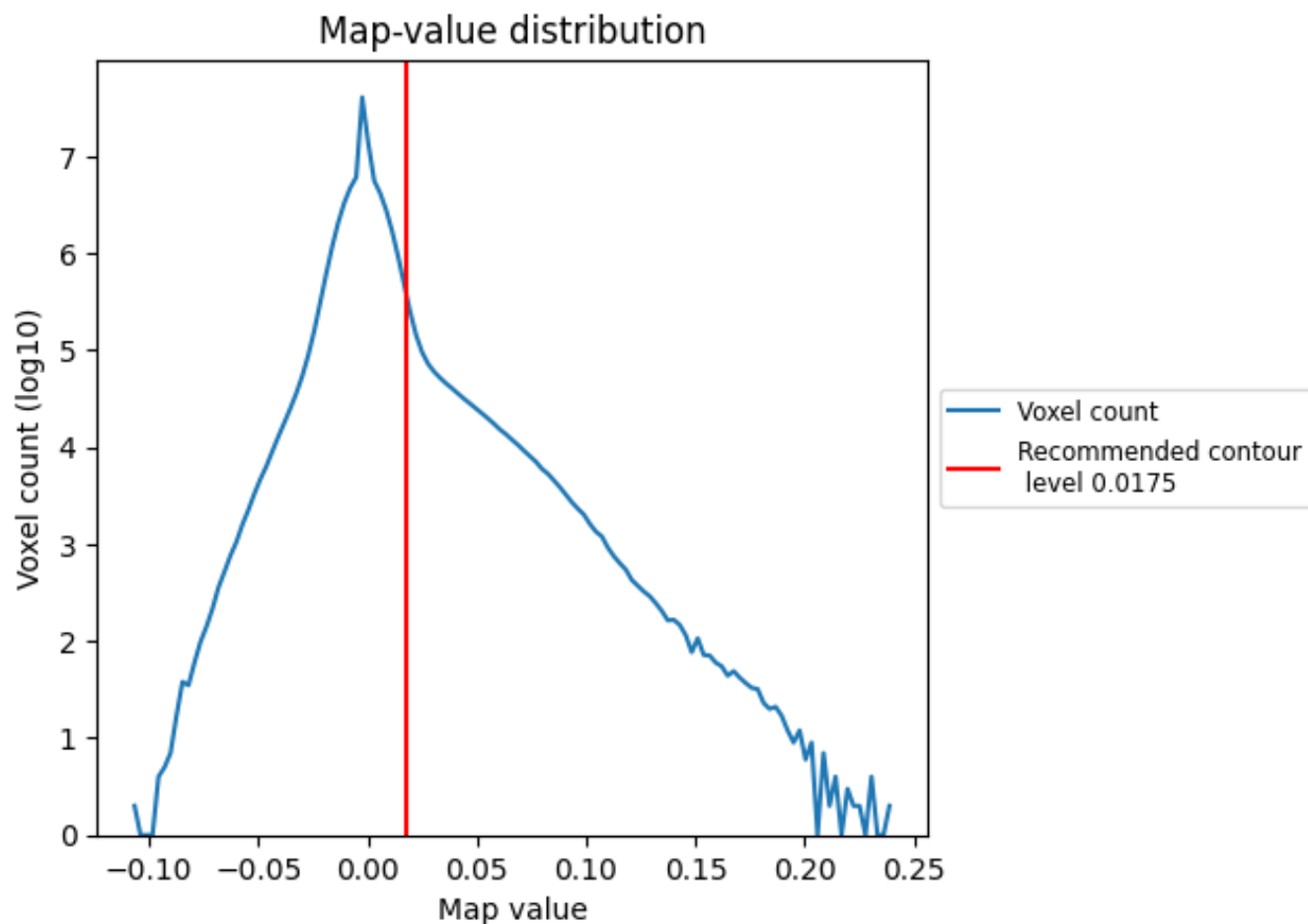
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

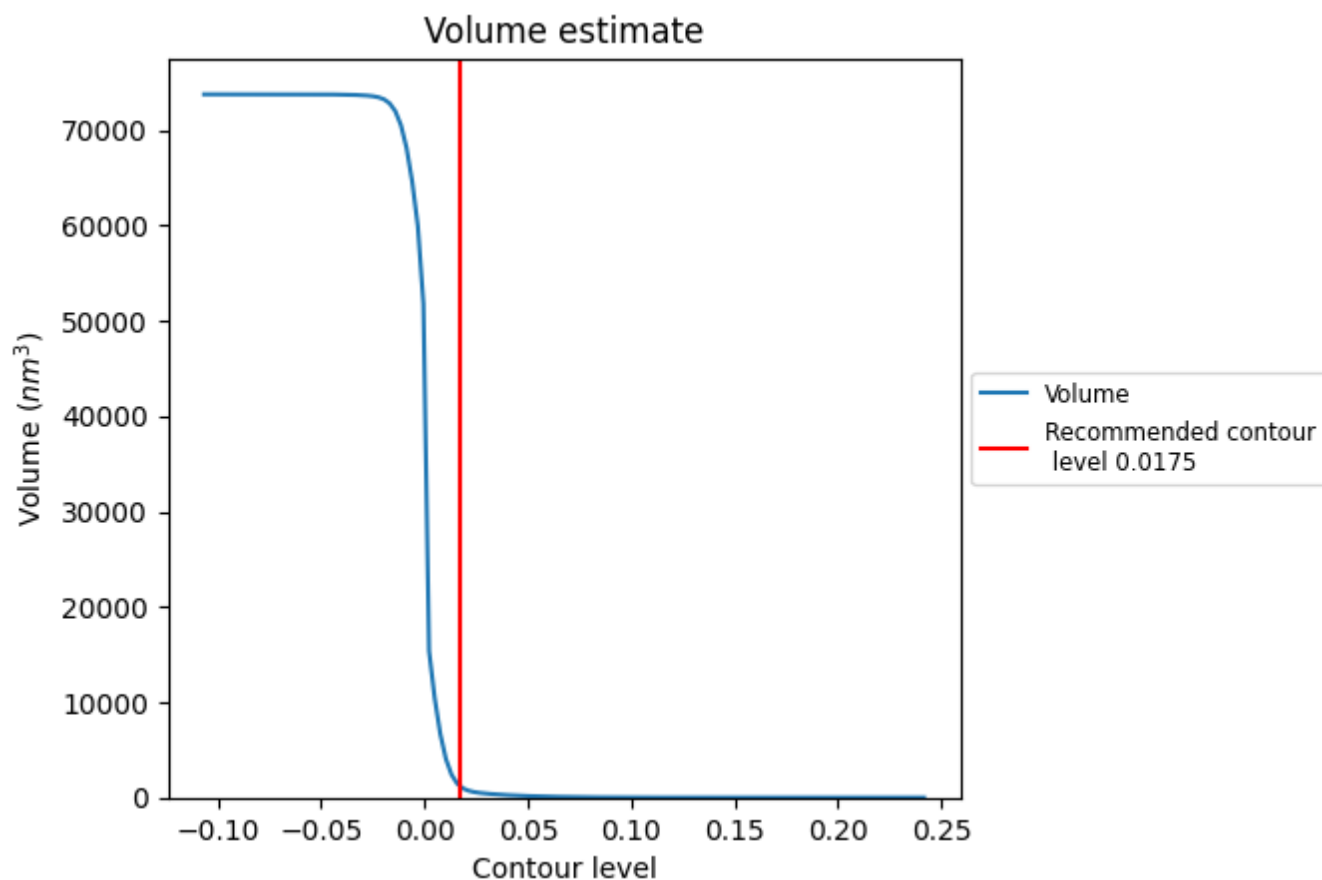
This section contains the results of statistical analysis of the map.

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.

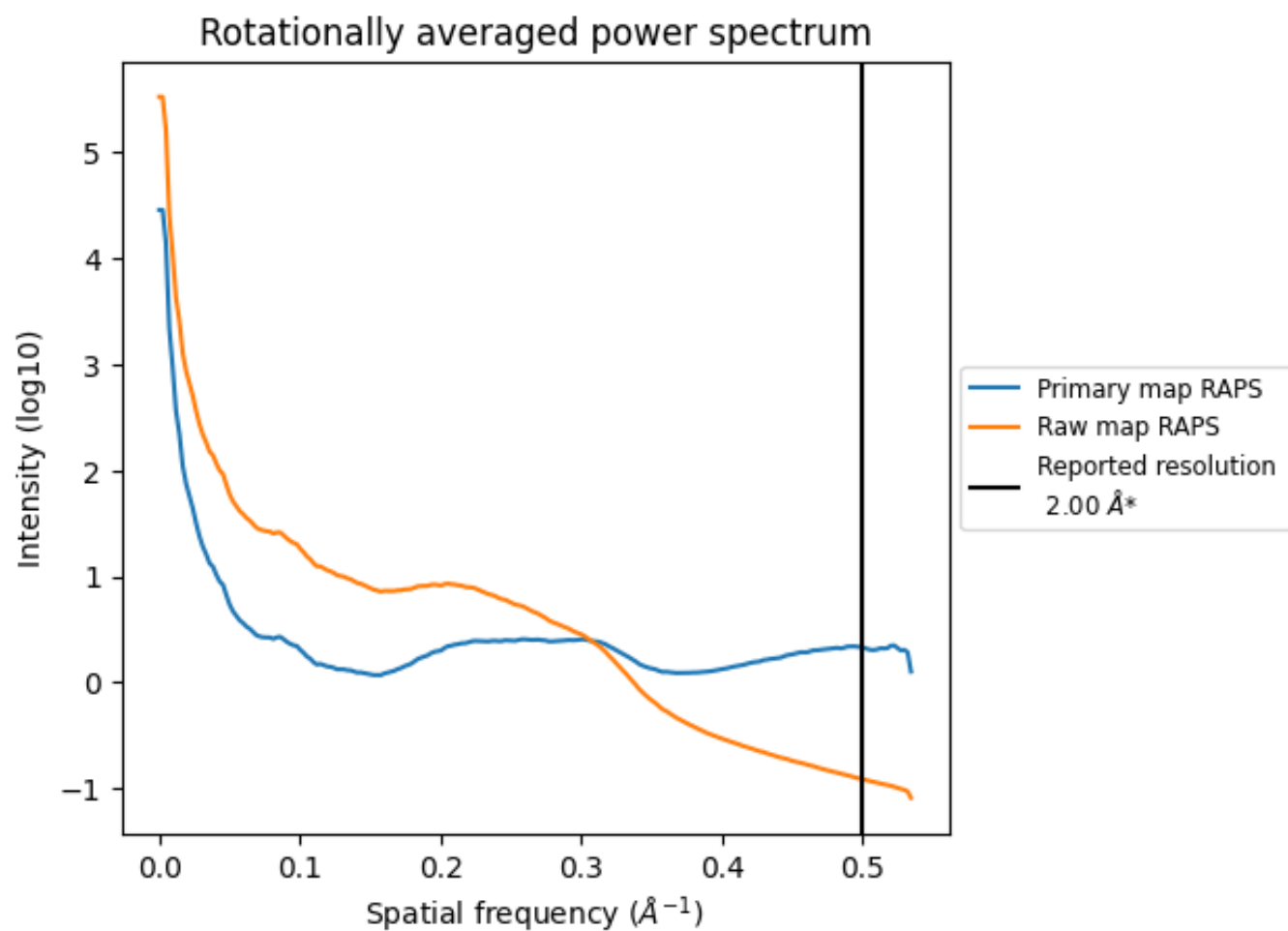
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1154 nm^3 ; this corresponds to an approximate mass of 1042 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 ⓘ

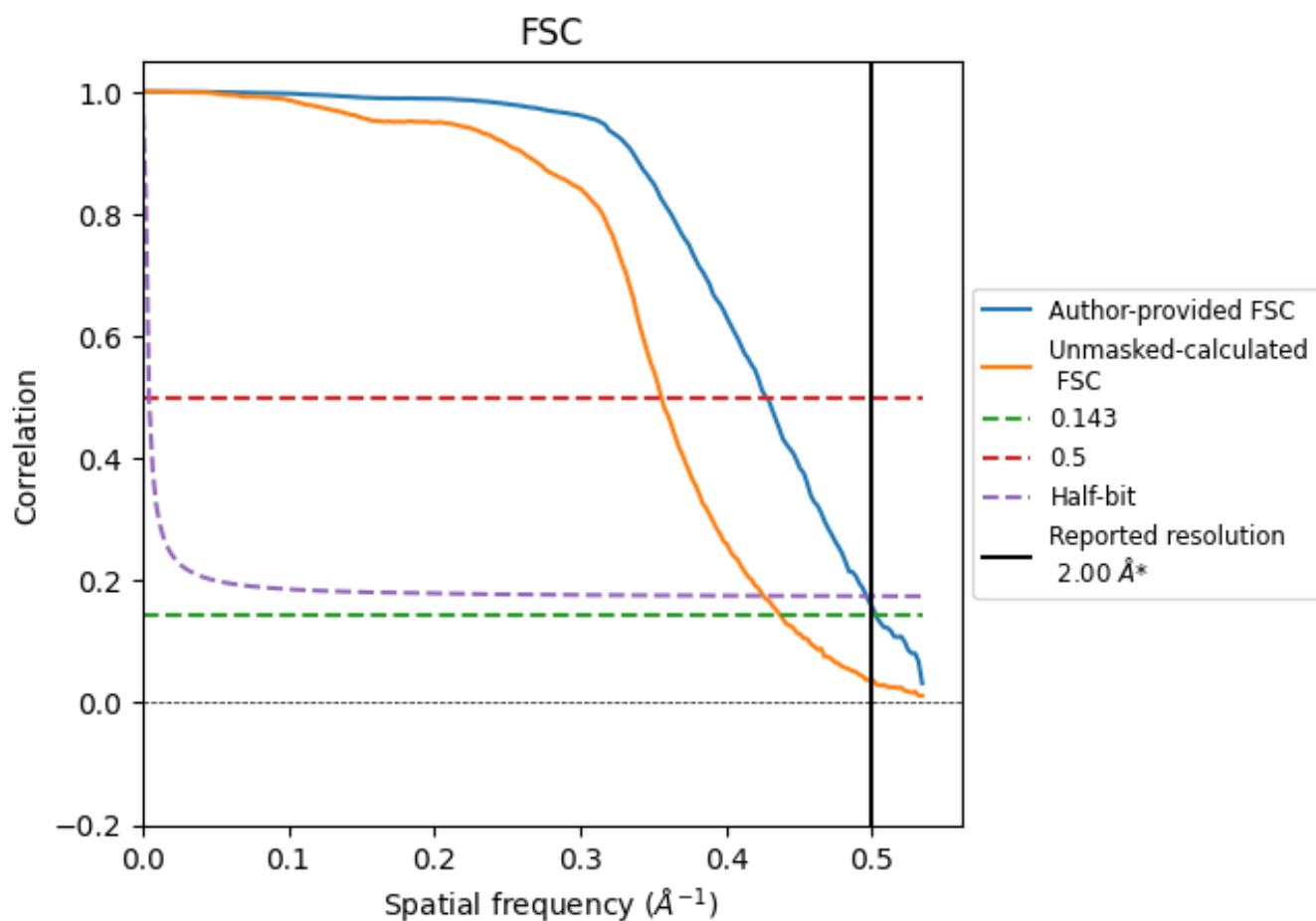


*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

8.2 Resolution estimates [i](#)

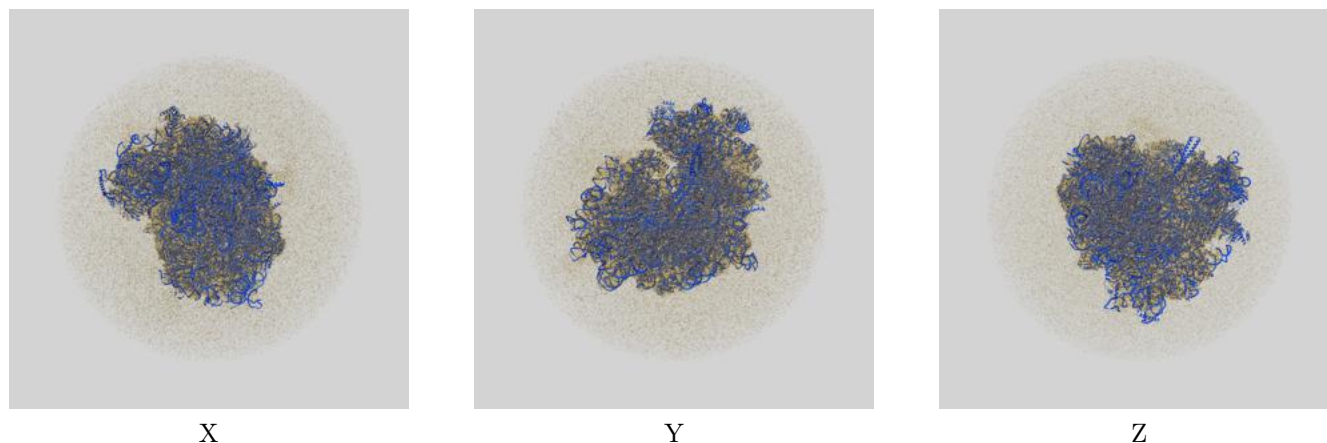
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	1.99	2.34	2.02
Unmasked-calculated*	2.29	2.81	2.35

*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 2.29 differs from the reported value 2.0 by more than 10 %

9 Map-model fit [i](#)

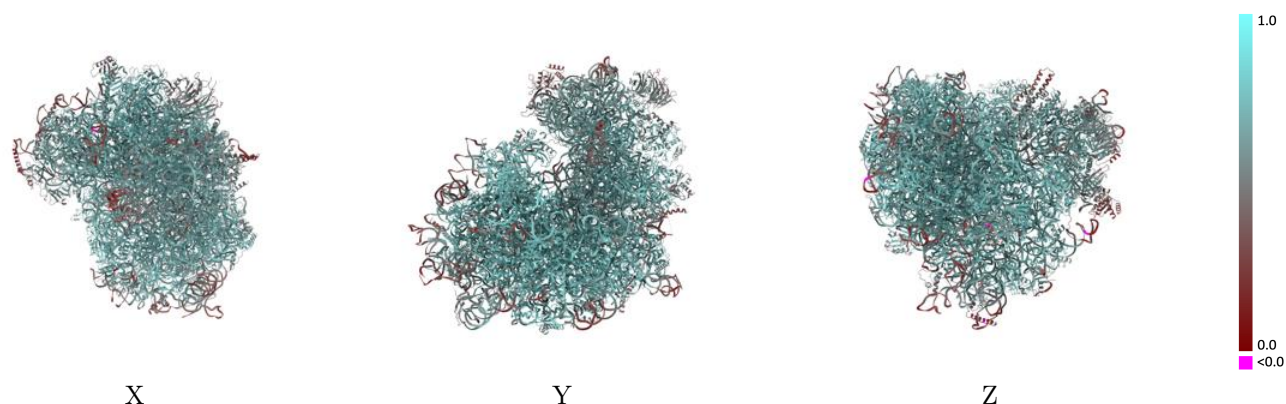
This section contains information regarding the fit between EMDB map EMD-45170 and PDB model 9C3H. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



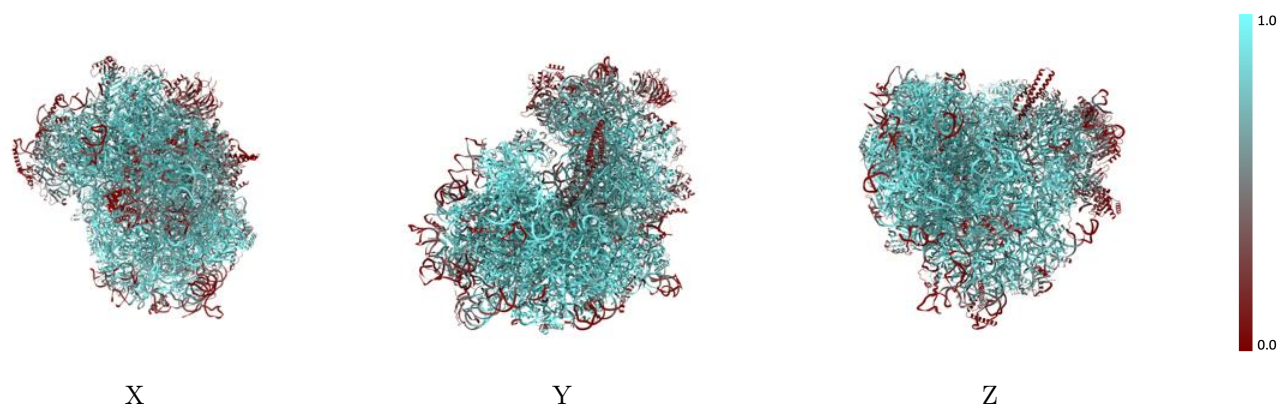
The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



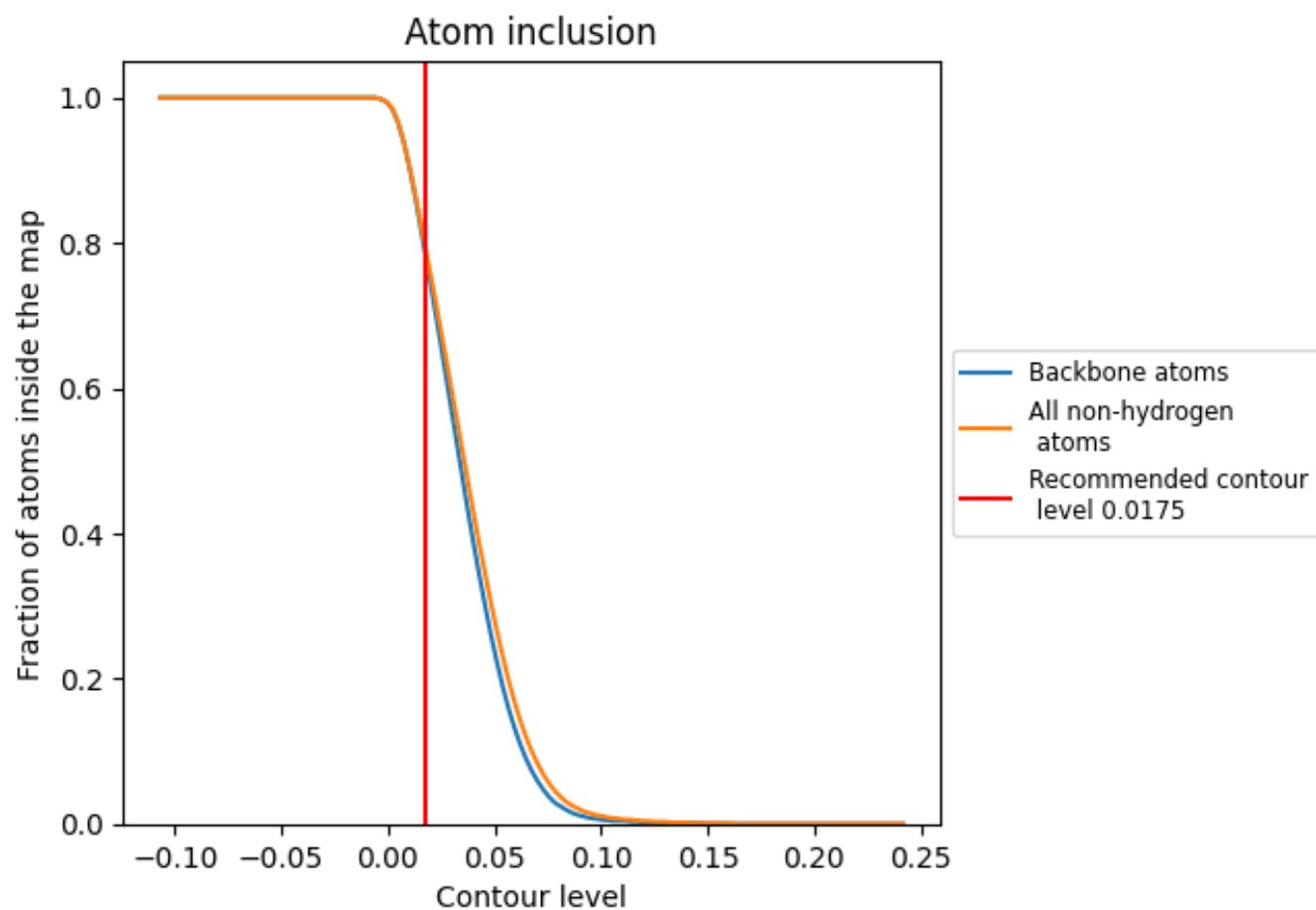
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0175).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7960	 0.6840
L1	 0.9300	 0.7300
L5	 0.8260	 0.6900
L8	 0.8170	 0.6940
L9	 0.9590	 0.7290
LB	 0.9070	 0.7620
LC	 0.9150	 0.7580
LD	 0.9670	 0.7980
LE	 0.8660	 0.7310
LF	 0.9190	 0.7660
LG	 0.8140	 0.6910
LH	 0.8680	 0.7170
LI	 0.9440	 0.7780
LJ	 0.7340	 0.6530
LK	 0.7900	 0.6870
LM	 0.8760	 0.7220
LN	 0.9900	 0.7950
LO	 0.8420	 0.7120
LP	 0.9570	 0.7860
LQ	 0.8410	 0.7190
LR	 0.7860	 0.6910
LS	 0.9430	 0.7700
LT	 0.8500	 0.7320
LU	 0.9290	 0.7620
LV	 0.9450	 0.7820
LW	 0.5460	 0.5580
LY	 0.9220	 0.7670
LZ	 0.8460	 0.7070
La	 0.9480	 0.7810
Lb	 0.7250	 0.6580
Lc	 0.8530	 0.7260
Ld	 0.8530	 0.7320
Le	 0.8710	 0.7520
Lf	 0.9610	 0.7890
Lg	 0.8900	 0.7490



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Chain	Atom inclusion	Q-score
Lh	 0.8950	 0.7620
Li	 0.8220	 0.7050
Lj	 0.9580	 0.7850
Lk	 0.6380	 0.6390
Ll	 0.9330	 0.7610
Lm	 0.5580	 0.5820
Ln	 0.8940	 0.7330
Lo	 0.8970	 0.7570
Lp	 0.9380	 0.7800
Lz	 0.8890	 0.7440
NC	 0.7850	 0.7310
S1	 0.7900	 0.7010
S2	 0.8130	 0.6640
S4	 0.6970	 0.6070
S5	 0.6810	 0.6390
SA	 0.8100	 0.6880
SB	 0.1950	 0.4830
SC	 0.8710	 0.7160
SD	 0.7280	 0.6620
SE	 0.7310	 0.6680
SG	 0.4090	 0.5340
SH	 0.4950	 0.5730
SI	 0.7380	 0.6670
SJ	 0.7400	 0.6660
SK	 0.5540	 0.5990
SL	 0.8510	 0.7180
SM	 0.4130	 0.5430
SN	 0.8860	 0.7330
SO	 0.9000	 0.7400
SP	 0.4790	 0.5850
SQ	 0.6670	 0.6440
SS	 0.5800	 0.6090
ST	 0.5820	 0.6090
SU	 0.5910	 0.6100
SV	 0.8040	 0.6990
SW	 0.9320	 0.7530
SX	 0.9010	 0.7420
SY	 0.5650	 0.6070
SZ	 0.4730	 0.5500
Sa	 0.8770	 0.7360
Sb	 0.6980	 0.6580
Sc	 0.4800	 0.5800

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Chain	Atom inclusion	Q-score
Sd	 0.6380	 0.6400
Se	 0.6070	 0.6140
Sf	 0.7870	 0.6790
Sg	 0.2680	 0.5080
So	 0.8580	 0.7470
Sy	 0.0440	 0.2790
Sz	 0.0850	 0.3440