



wwPDB EM Validation Summary Report ⓘ

Mar 4, 2026 – 09:20 PM UTC

PDB ID : 8QIE / pdb_00008qie
EMDB ID : EMD-18437
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
LM32Cs1C1 mutant snoRNA overexpression, class 4
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.
Deposited on : 2023-09-12
Resolution : 2.43 Å(reported)

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

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

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
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

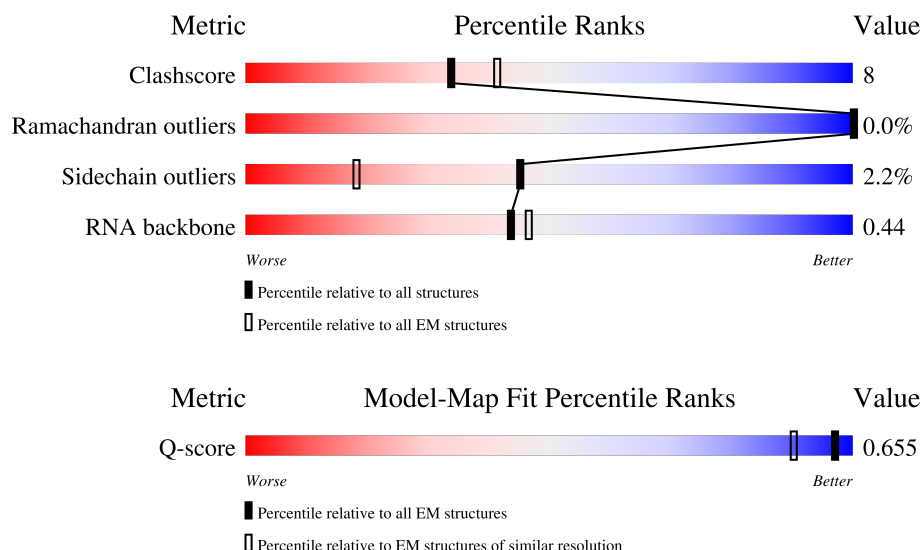
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.43 Å.

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



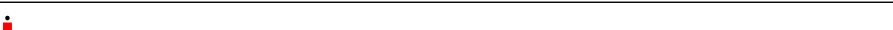
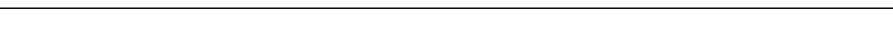
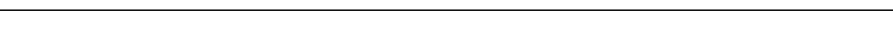
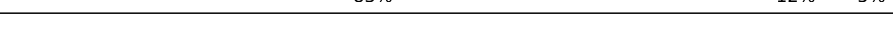
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5787 (1.94 - 2.93)

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	1	1782	
2	2	1526	
3	3	216	

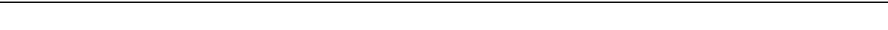
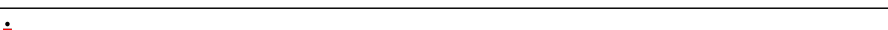
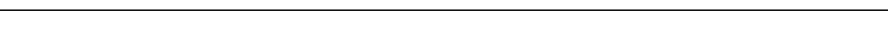
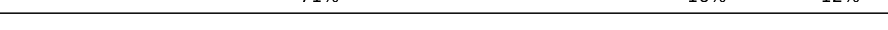
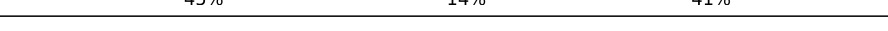
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	4	184	
5	5	135	
6	6	73	
7	7	171	
8	8	123	
9	A	260	
10	B	419	
11	C	373	
12	D	188	
13	E	190	
14	F	195	
15	G	264	
16	H	222	
17	I	220	
18	J	139	
19	K	175	
20	L	145	
21	M	204	
22	N	213	
23	O	305	
24	P	198	
25	Q	254	
26	R	179	
27	S	159	
28	S1	2204	

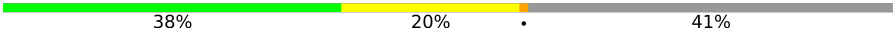
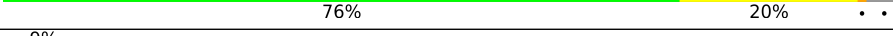
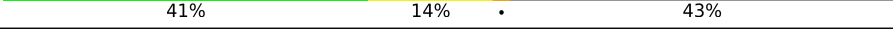
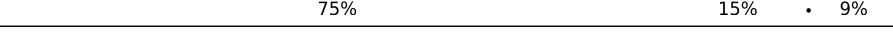
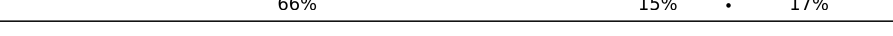
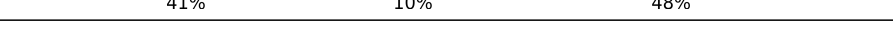
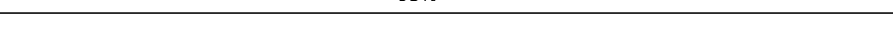
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	S4	76	
30	SA	264	
31	SB	246	
32	SC	219	
33	SD	190	
34	SE	273	
35	SF	265	
36	SG	249	
37	SH	190	
38	SI	200	
39	SJ	130	
40	SK	220	
41	SL	149	
42	SM	116	
43	SN	168	
44	SO	144	
45	SP	143	
46	SQ	141	
47	SR	153	
48	SS	57	
49	ST	151	
50	SU	173	
51	SV	143	
52	SW	152	
53	SX	161	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	SY	164	
55	SZ	137	
56	Sa	120	
57	Sb	112	
58	Sc	86	
59	Sd	87	
60	Se	66	
61	Sf	152	
62	Sg	312	
63	Sh	235	
64	T	166	
65	U	129	
66	V	145	
67	W	143	
68	X	124	
69	Y	134	
70	Z	147	
71	a	127	
72	b	70	
73	c	252	
74	d	104	
75	e	188	
76	f	133	
77	g	144	
78	h	168	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	i	105	
80	j	83	
81	k	83	
82	l	51	
83	m	128	
84	n	34	
85	o	92	
86	p	106	

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 206527 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 LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1611	Total	C	N	O	P	0	0
			34568	15451	6340	11166	1611		

- Molecule 2 is a RNA chain called LSUb_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1159	Total	C	N	O	P	0	0
			24802	11101	4482	8060	1159		

- Molecule 3 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	156	Total	C	N	O	P	0	0
			3312	1481	576	1099	156		

- Molecule 4 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	184	Total	C	N	O	P	0	0
			3937	1756	712	1285	184		

- Molecule 5 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	115	Total	C	N	O	P	0	0
			2453	1094	439	805	115		

- Molecule 6 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	71	Total	C	N	O	P	0	0
			1506	675	271	489	71		

- Molecule 7 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	164	Total	C	N	O	P	0	0
			3494	1566	621	1144	163		

- Molecule 8 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	119	Total	C	N	O	P	0	0
			2531	1132	452	828	119		

- Molecule 9 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	255	Total	C	N	O	S	1	0
			1908	1189	390	319	10		

- Molecule 10 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	399	Total	C	N	O	S	0	0
			3051	1932	599	507	13		

- Molecule 11 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	366	Total	C	N	O	S	0	0
			2777	1740	556	466	15		

- Molecule 12 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	158	Total	C	N	O	S	0	0
			1008	629	203	170	6		

- Molecule 13 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	186	Total	C	N	O	S	0	0
			1395	889	267	233	6		

- Molecule 14 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	148	Total	C	N	O	S	0	0
			1067	686	203	176	2		

- Molecule 15 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	226	Total	C	N	O	S	0	0
			1731	1097	344	283	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	220	Total	C	N	O	S	0	0
			1734	1101	349	277	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	208	Total	C	N	O	S	0	0
			1603	1001	326	269	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	203	ARG	ASN	conflict	UNP E9AEA8

- Molecule 18 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	137	Total	C	N	O	S	0	0
			999	631	190	172	6		

- Molecule 19 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	170	Total	C	N	O	S	0	0
			1266	794	252	213	7		

- Molecule 20 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	144	Total	C	N	O	S	0	0
			1124	707	226	185	6		

- Molecule 21 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	203	Total	C	N	O	S	0	0
			1696	1071	361	256	8		

- Molecule 22 is a protein called Putative 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	199	Total	C	N	O	S	0	0
			1607	1013	320	260	14		

- Molecule 23 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	276	Total	C	N	O	S	0	0
			1975	1260	379	333	3		

- Molecule 24 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	197	Total	C	N	O	S	0	0
			1528	961	305	256	6		

- Molecule 25 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	187	Total	C	N	O	S	0	0
			1433	892	316	219	6		

- Molecule 26 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	178	Total	C	N	O	S	0	0
			1413	904	273	231	5		

- Molecule 27 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	157	Total	C	N	O	S	0	0
			1234	784	240	206	4		

- Molecule 28 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S1	1787	Total	C	N	O	P	0	0
			38240	17106	6918	12429	1787		

- Molecule 29 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S4	50	Total	C	N	O	P	0	0
			1072	478	200	345	49		

- Molecule 30 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SA	225	Total	C	N	O	S	1	0
			1820	1141	346	321	12		

- Molecule 31 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SB	208	Total	C	N	O	S	0	0
			1627	1034	297	284	12		

- Molecule 32 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SC	212	Total	C	N	O	S	1	0
			1624	1029	296	286	13		

- Molecule 33 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SD	167	Total	C	N	O	S	0	0
			1366	863	270	225	8		

- Molecule 34 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SE	260	Total	C	N	O	S	0	0
			2050	1299	393	349	9		

- Molecule 35 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SF	218	Total	C	N	O	S	0	0
			1662	1063	297	293	9		

- Molecule 36 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SG	231	Total	C	N	O	S	0	0
			1831	1144	374	310	3		

- Molecule 37 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SH	182	Total	C	N	O	S	0	0
			1436	892	278	259	7		

- Molecule 38 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SI	199	Total	C	N	O	S	0	0
			1619	1032	313	267	7		

- Molecule 39 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SJ	129	Total	C	N	O	S	0	0
			1021	646	188	179	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SK	182	Total	C	N	O	S	0	0
			1443	906	305	230	2		

- Molecule 41 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SL	143	Total	C	N	O	S	0	0
			1124	724	206	191	3		

- Molecule 42 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SM	102	Total	C	N	O	S	0	0
			796	498	145	151	2		

- Molecule 43 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SN	99	Total	C	N	O	S	0	0
			808	518	141	142	7		

- Molecule 44 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SO	135	Total	C	N	O	S	0	0
			1010	624	197	181	8		

- Molecule 45 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SP	141	Total	C	N	O	S	0	0
			1100	694	217	186	3		

- Molecule 46 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SQ	100	Total	C	N	O	S	0	0
			679	419	122	133	5		

- Molecule 47 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SR	130	Total	C	N	O	S	0	0
			1034	655	201	174	4		

- Molecule 48 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SS	56	Total	C	N	O	S	0	0
			452	279	94	73	6		

- Molecule 49 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	ST	142	Total	C	N	O	S	0	0
			1155	728	229	190	8		

- Molecule 50 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SU	156	Total	C	N	O	S	0	0
			1253	796	247	205	5		

- Molecule 51 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SV	71	Total	C	N	O	S	0	0
			577	368	110	97	2		

- Molecule 52 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SW	113	Total	C	N	O	S	0	0
			907	578	172	153	4		

- Molecule 53 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SX	152	Total	C	N	O	S	0	0
			1202	764	237	197	4		

- Molecule 54 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SY	84	Total	C	N	O	S	0	0
			616	381	115	116	4		

- Molecule 55 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SZ	127	Total	C	N	O	S	0	0
			1031	662	200	166	3		

- Molecule 56 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Sa	71	Total	C	N	O	S	0	0
			558	356	99	100	3		

- Molecule 57 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Sb	103	Total	C	N	O	S	0	0
			816	505	175	129	7		

- Molecule 58 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Sc	73	Total	C	N	O	S	0	0
			570	358	107	101	4		

- Molecule 59 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Sd	66	Total	C	N	O	S	0	0
			483	295	97	87	4		

- Molecule 60 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Se	51	Total	C	N	O	S	0	0
			401	252	86	62	1		

- Molecule 61 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Sf	33	Total	C	N	O	S	0	0
			295	193	58	43	1		

- Molecule 62 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Sg	300	Total	C	N	O	S	0	0
			2284	1438	406	428	12		

- Molecule 63 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sh	134	Total	C	N	O	S	0	0
			948	603	179	164	2		

- Molecule 64 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	T	151	Total	C	N	O	S	0	0
			1211	757	240	203	11		

- Molecule 65 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	U	118	Total	C	N	O	S	0	0
			801	514	152	133	2		

- Molecule 66 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	V	118	Total	C	N	O	S	0	0
			926	587	178	159	2		

- Molecule 67 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	W	118	Total	C	N	O	S	0	0
			937	586	197	150	4		

- Molecule 68 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	X	64	Total	C	N	O	S	0	0
			548	359	105	80	4		

- Molecule 69 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Y	132	Total	C	N	O	S	0	0
			1027	661	206	157	3		

- Molecule 70 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Z	145	Total	C	N	O	S	0	0
			1095	671	234	185	5		

- Molecule 71 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	a	123	Total	C	N	O	S	0	0
			1006	630	211	161	4		

- Molecule 72 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	b	68	Total	C	N	O		0	0
			546	335	125	86			

- Molecule 73 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	c	229	Total	C	N	O	S	0	0
			1862	1185	358	308	11		

- Molecule 74 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	d	92	Total	C	N	O	S	0	0
			705	438	129	133	5		

- Molecule 75 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	e	180	Total	C	N	O	S	0	0
			1421	895	288	234	4		

- Molecule 76 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	f	125	Total	C	N	O	S	0	0
			1011	636	201	170	4		

- Molecule 77 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	g	142	Total	C	N	O	S	0	0
			1142	710	239	188	5		

- Molecule 78 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	h	127	Total	C	N	O	S	0	0
			1018	626	221	165	6		

- Molecule 79 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	i	88	Total	C	N	O	S	0	0
			689	438	143	106	2		

- Molecule 80 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	j	81	Total	C	N	O	S	0	0
			668	407	154	101	6		

- Molecule 81 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	k	72	Total	C	N	O	S	0	0
			534	338	105	88	3		

- Molecule 82 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	l	50	Total	C	N	O	S	0	0
			450	291	95	63	1		

- Molecule 83 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	m	51	Total	C	N	O	S	0	0
			378	238	74	59	7		

- Molecule 84 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	n	33	Total	C	N	O	S	0	0
			292	178	75	37	2		

- Molecule 85 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	o	88	Total	C	N	O	S	0	0
			688	428	142	112	6		

- Molecule 86 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	p	97	Total	C	N	O	S	0	0
			775	491	157	123	4		

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

Mol	Chain	Residues	Atoms		AltConf
87	1	58	Total	Mg	0
			58	58	
87	2	66	Total	Mg	0
			66	66	
87	4	3	Total	Mg	0
			3	3	
87	5	3	Total	Mg	0
			3	3	
87	6	1	Total	Mg	0
			1	1	
87	7	2	Total	Mg	0
			2	2	
87	8	1	Total	Mg	0
			1	1	
87	A	2	Total	Mg	0
			2	2	
87	J	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	S	1	Total 1	Mg 1	0
87	S1	79	Total 79	Mg 79	0
87	SX	1	Total 1	Mg 1	0
87	Sb	1	Total 1	Mg 1	0

- Molecule 88 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
88	1	11	Total 11	Na 11	0
88	2	10	Total 10	Na 10	0
88	4	3	Total 3	Na 3	0
88	S1	9	Total 9	Na 9	0
88	S4	1	Total 1	Na 1	0

- Molecule 89 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
89	1	9	Total 9	K 9	0
89	2	3	Total 3	K 3	0
89	S1	4	Total 4	K 4	0

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
90	p	1	Total 1	Zn 1	0

- Molecule 91 is water.

Mol	Chain	Residues	Atoms		AltConf
91	1	617	Total 617	O 617	0
91	2	478	Total 478	O 478	0
91	3	21	Total 21	O 21	0
91	4	62	Total 62	O 62	0
91	5	24	Total 24	O 24	0
91	6	5	Total 5	O 5	0
91	7	43	Total 43	O 43	0
91	8	5	Total 5	O 5	0
91	A	20	Total 20	O 20	0
91	B	38	Total 38	O 38	0
91	C	18	Total 18	O 18	0
91	D	1	Total 1	O 1	0
91	F	1	Total 1	O 1	0
91	G	1	Total 1	O 1	0
91	H	9	Total 9	O 9	0
91	I	10	Total 10	O 10	0
91	J	4	Total 4	O 4	0
91	L	12	Total 12	O 12	0
91	M	22	Total 22	O 22	0
91	N	1	Total 1	O 1	0
91	P	8	Total 8	O 8	0
91	Q	2	Total 2	O 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
91	R	1	Total 1	O 1	0
91	S	2	Total 2	O 2	0
91	S1	802	Total 802	O 802	0
91	S4	3	Total 3	O 3	0
91	SA	7	Total 7	O 7	0
91	SB	1	Total 1	O 1	0
91	SC	1	Total 1	O 1	0
91	SD	4	Total 4	O 4	0
91	SE	13	Total 13	O 13	0
91	SF	6	Total 6	O 6	0
91	SG	1	Total 1	O 1	0
91	SH	6	Total 6	O 6	0
91	SJ	12	Total 12	O 12	0
91	SK	13	Total 13	O 13	0
91	SL	3	Total 3	O 3	0
91	SM	6	Total 6	O 6	0
91	SN	2	Total 2	O 2	0
91	SO	7	Total 7	O 7	0
91	SP	12	Total 12	O 12	0
91	SR	4	Total 4	O 4	0
91	SS	1	Total 1	O 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
91	ST	19	Total 19	O 19	0
91	SU	5	Total 5	O 5	0
91	SX	5	Total 5	O 5	0
91	Sa	2	Total 2	O 2	0
91	Sb	23	Total 23	O 23	0
91	Sc	5	Total 5	O 5	0
91	T	9	Total 9	O 9	0
91	V	4	Total 4	O 4	0
91	W	2	Total 2	O 2	0
91	X	2	Total 2	O 2	0
91	Z	1	Total 1	O 1	0
91	b	3	Total 3	O 3	0
91	c	5	Total 5	O 5	0
91	e	3	Total 3	O 3	0
91	f	14	Total 14	O 14	0
91	g	11	Total 11	O 11	0
91	h	7	Total 7	O 7	0
91	i	1	Total 1	O 1	0
91	j	12	Total 12	O 12	0
91	l	5	Total 5	O 5	0
91	n	5	Total 5	O 5	0

Continued on next page...

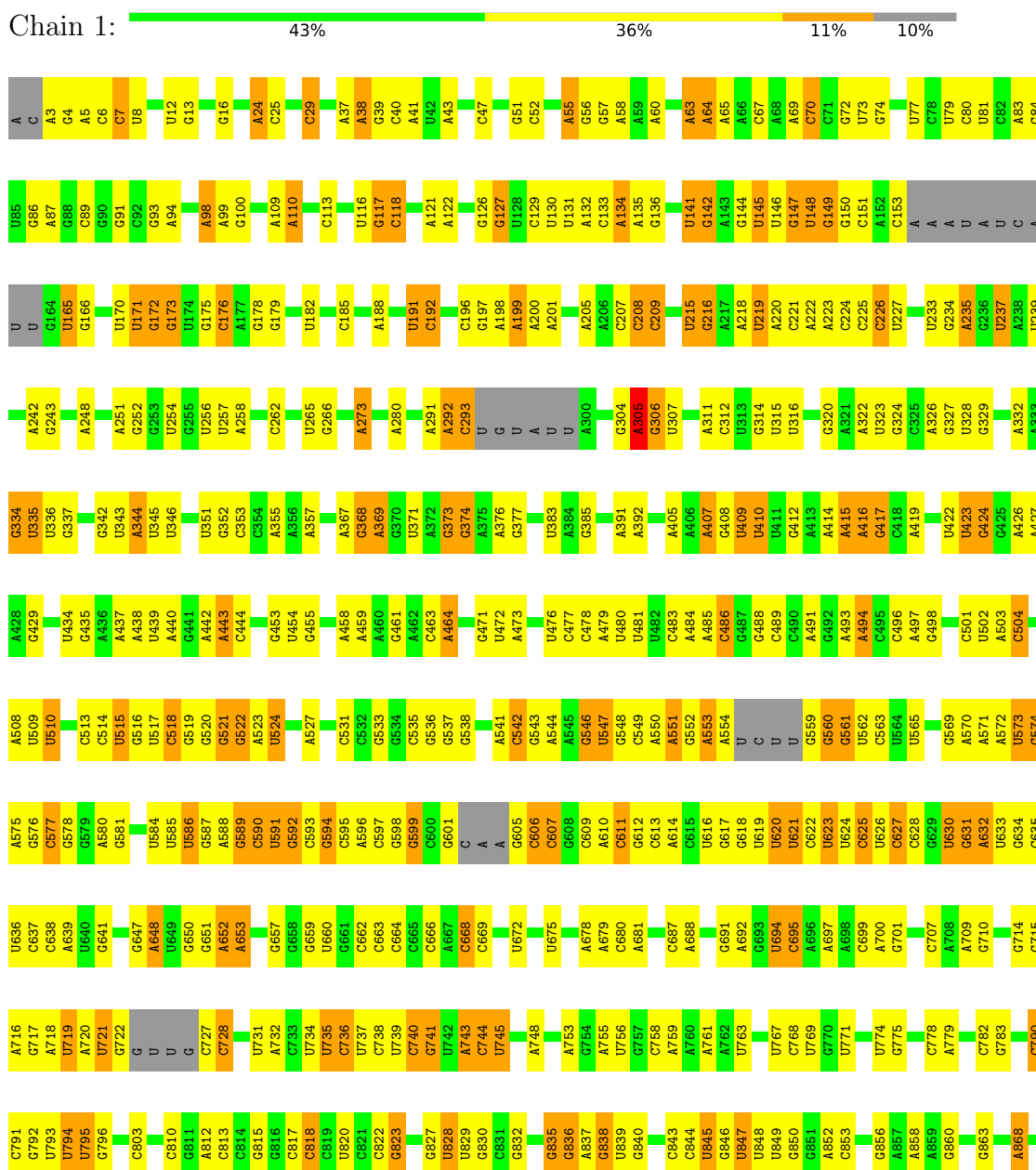
Continued from previous page...

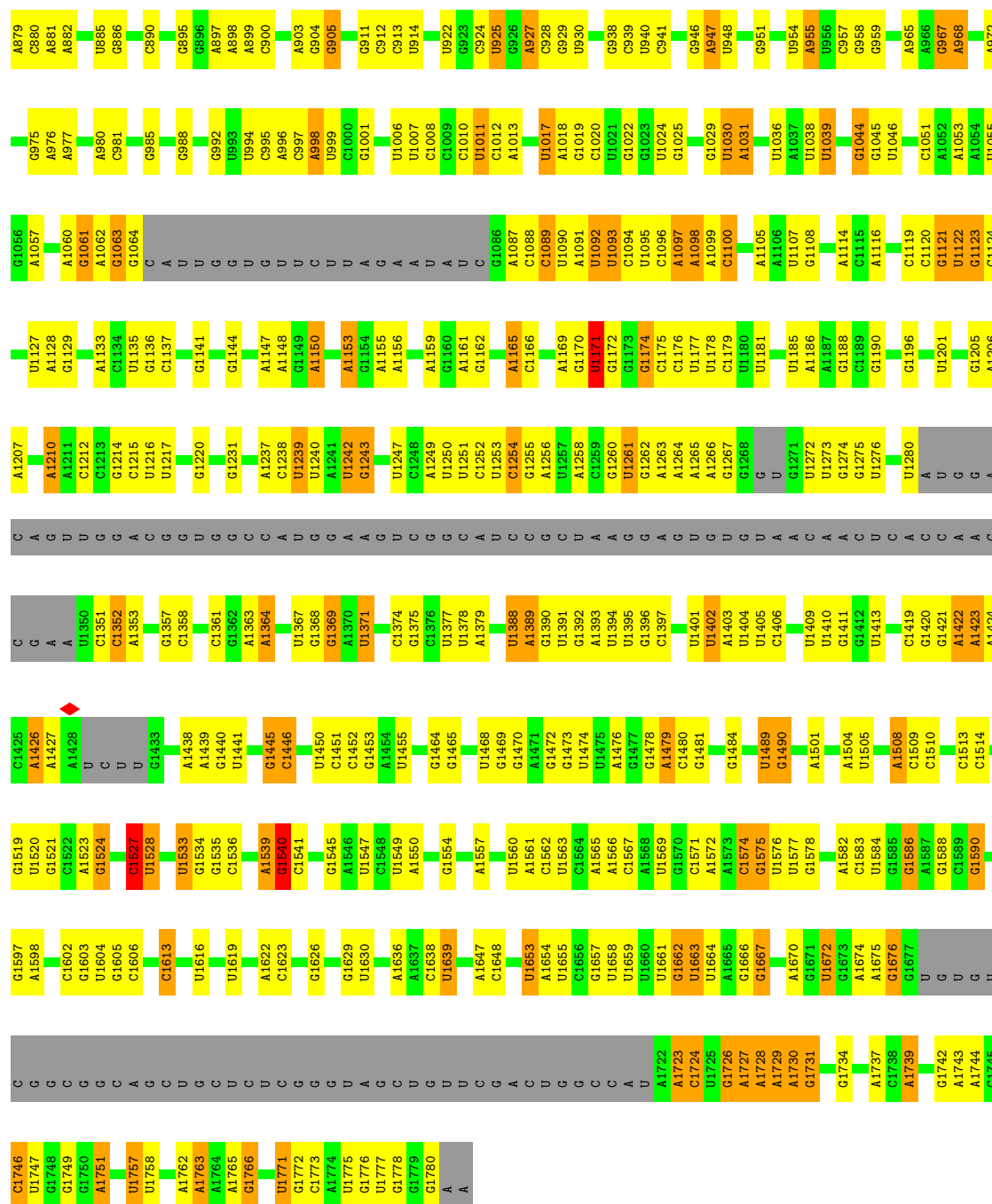
Mol	Chain	Residues	Atoms		AltConf
91	o	8	Total	O	0
			8	8	
91	p	5	Total	O	0
			5	5	

3 Residue-property plots

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

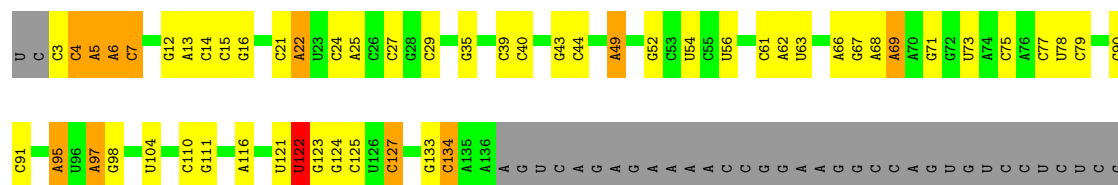
• Molecule 1: LSUa_rRNA_chain_1





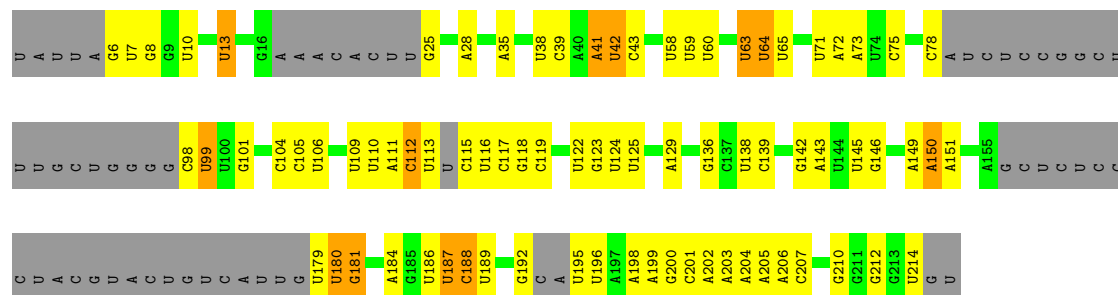
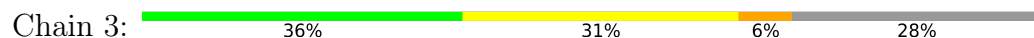
• Molecule 2: LSub_rRNA_chain_2

Chain 2: 37% 26% 12% 24%

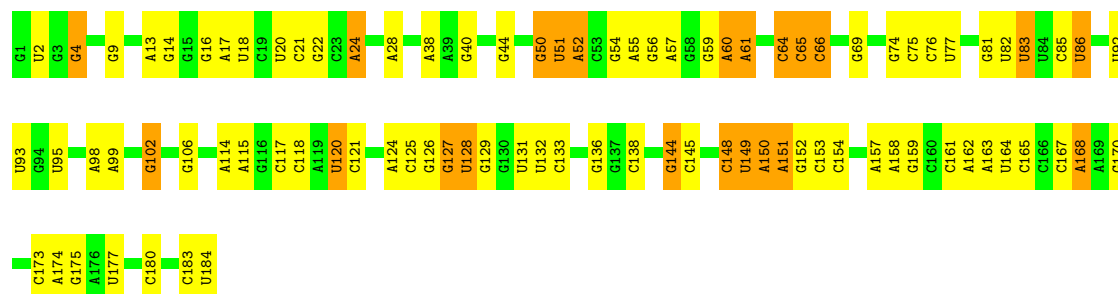




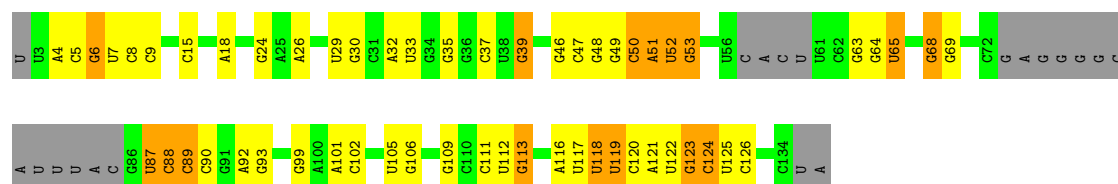
- Molecule 3: SR1 chain 3



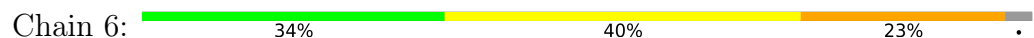
- Molecule 4: SR2 chain 4



- Molecule 5: SR4_chain_5

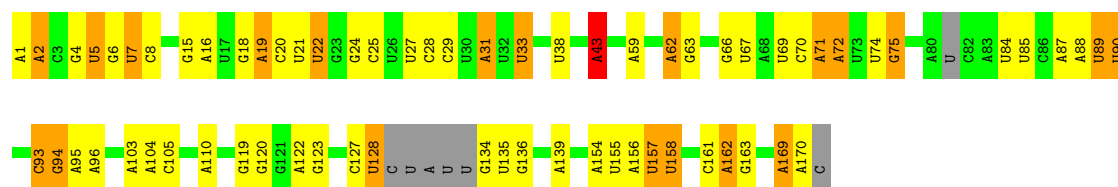


- Molecule 6: SR6 chain 6



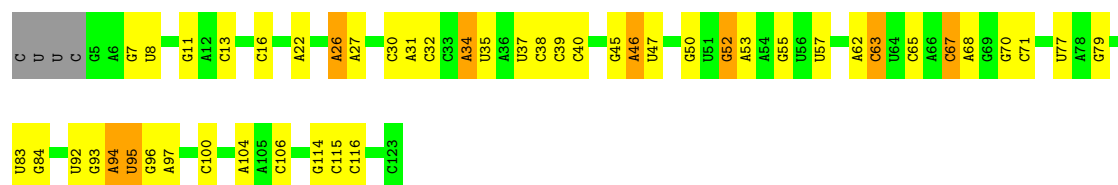
- Molecule 7: 5.8S_rRNA_chain_7

Chain 7:  56% 27% 12% ..



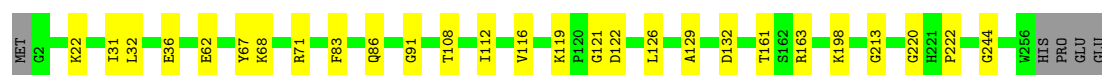
• Molecule 8: 5S_rRNA_chain_8

Chain 8:  58% 33% 7% .



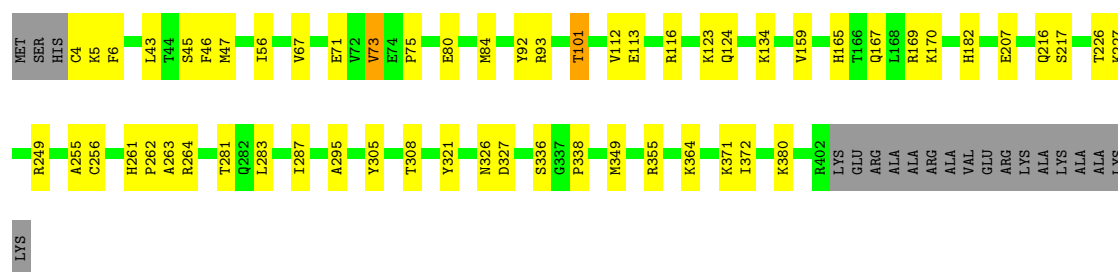
• Molecule 9: Putative 60S ribosomal protein L2

Chain A:  88% 10% .



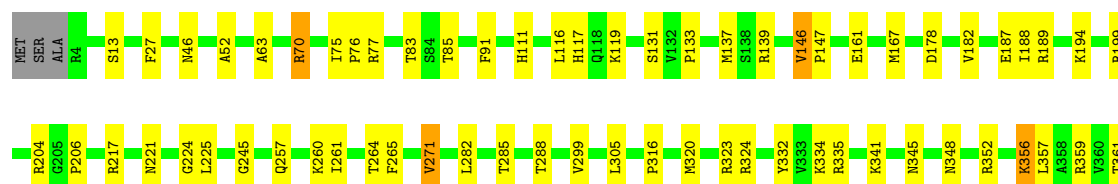
• Molecule 10: Putative ribosomal protein L3

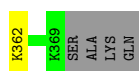
Chain B:  81% 13% 5%



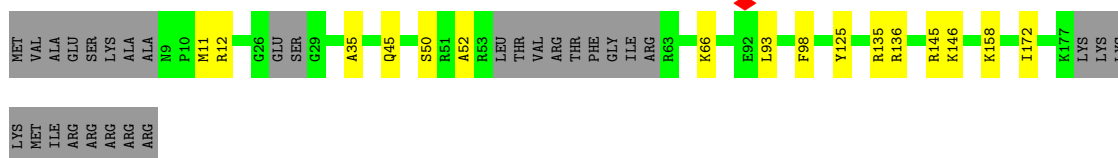
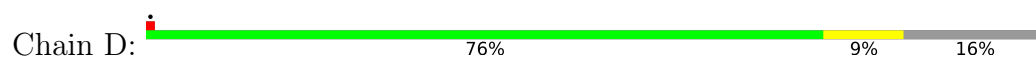
• Molecule 11: Putative ribosomal protein L1a

Chain C:  81% 16% ..

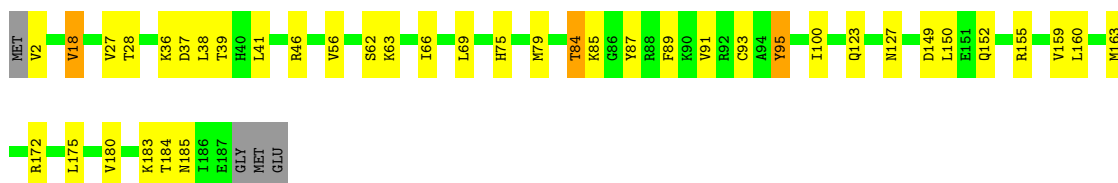
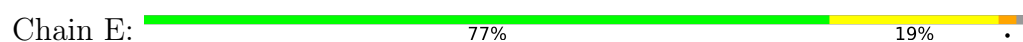




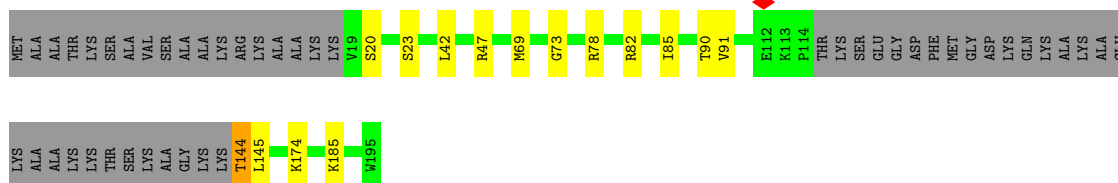
- Molecule 12: 60S ribosomal protein L11



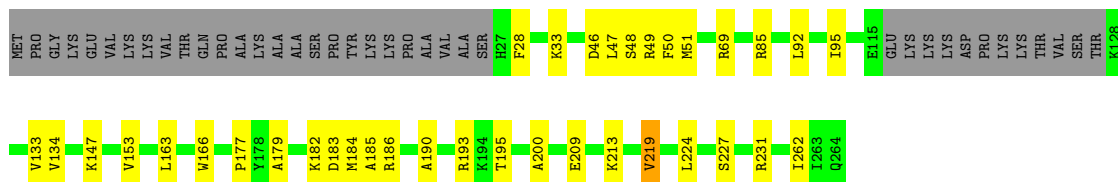
- Molecule 13: Putative 60S ribosomal protein L9



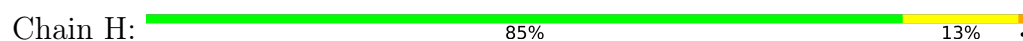
- Molecule 14: Putative 60S ribosomal protein L6



- Molecule 15: 60S ribosomal protein L7a



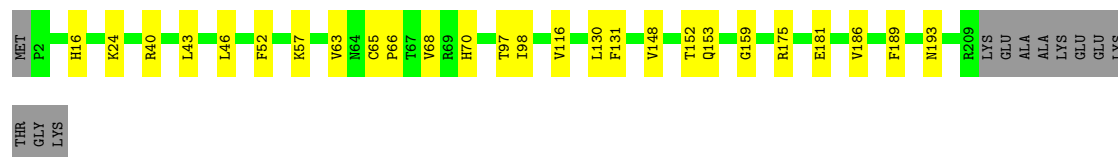
- Molecule 16: Putative 60S ribosomal protein L13a





- Molecule 17: Putative 60S ribosomal protein L13

Chain I: 83% 12% 5%



- Molecule 18: Putative 60S ribosomal protein L23

Chain J: 82% 17% .



- Molecule 19: Putative 40S ribosomal protein L14

Chain K: 82% 15% .



- Molecule 20: Putative 60S ribosomal protein L27A/L29

Chain L: 85% 14% .



- Molecule 21: Ribosomal protein L15

Chain M: 85% 15%



- Molecule 22: Putative 60S ribosomal protein L10

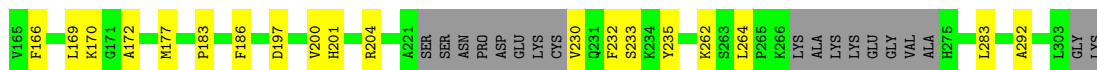
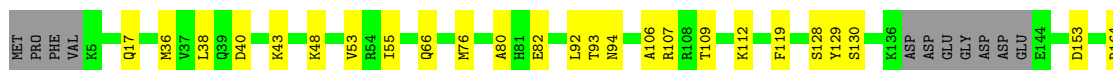
Chain N: 66% 26% 7%





• Molecule 23: Putative 60S ribosomal protein L5

Chain O: 76% 14% 10%



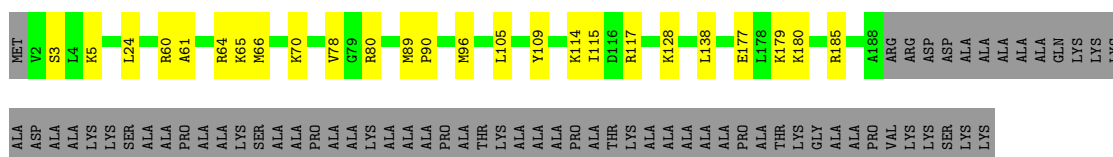
• Molecule 24: 60S ribosomal protein L18

Chain P: 85% 15%



• Molecule 25: Putative 60S ribosomal protein L19

Chain Q: 64% 10% 26%



• Molecule 26: 60S ribosomal protein L18a

Chain R: 85% 14% ..



• Molecule 27: Putative 60S ribosomal protein L21

Chain S: 77% 19% ..

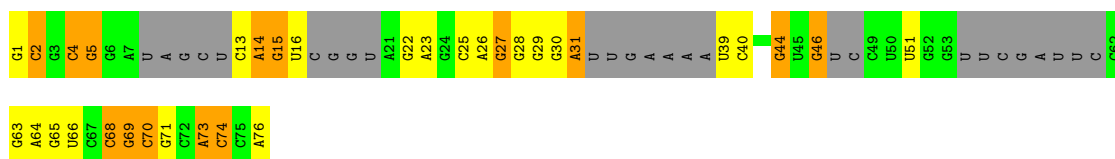


• Molecule 28: SSU_rRNA_chain_S1

Chain S1: 40% 32% 9% 19%

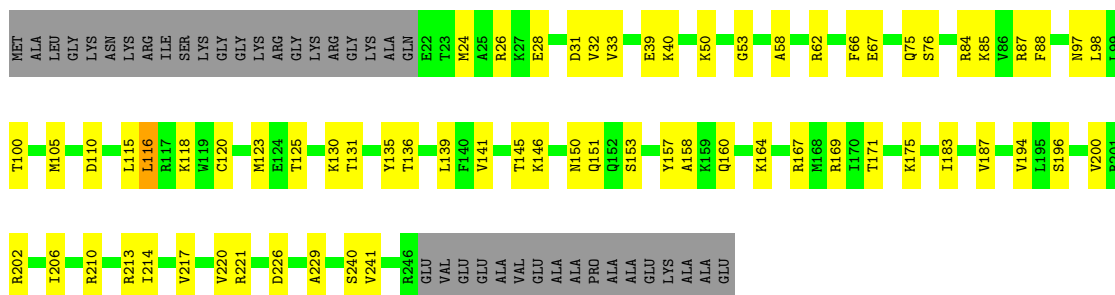






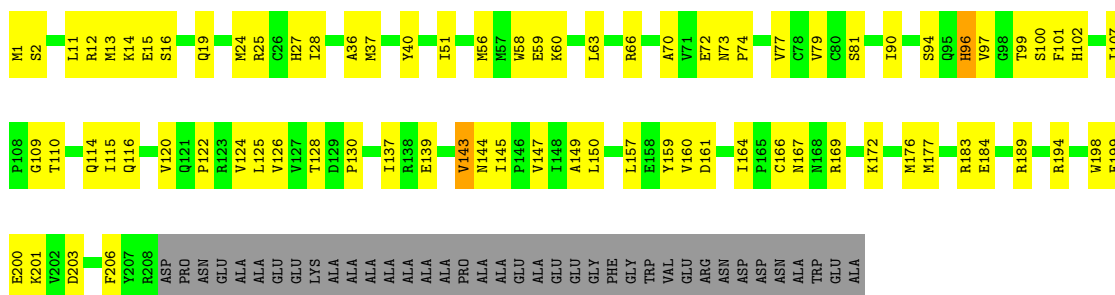
• Molecule 30: 40S ribosomal protein S3a

Chain SA:



• Molecule 31: 40S ribosomal protein SA

Chain SB:



• Molecule 32: Putative 40S ribosomal protein S3

Chain SC:



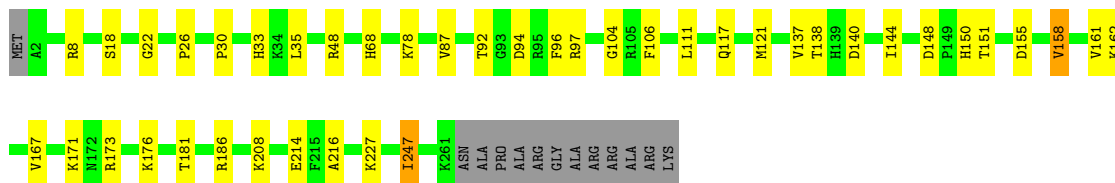
• Molecule 33: Putative 40S ribosomal protein S9

Chain SD:



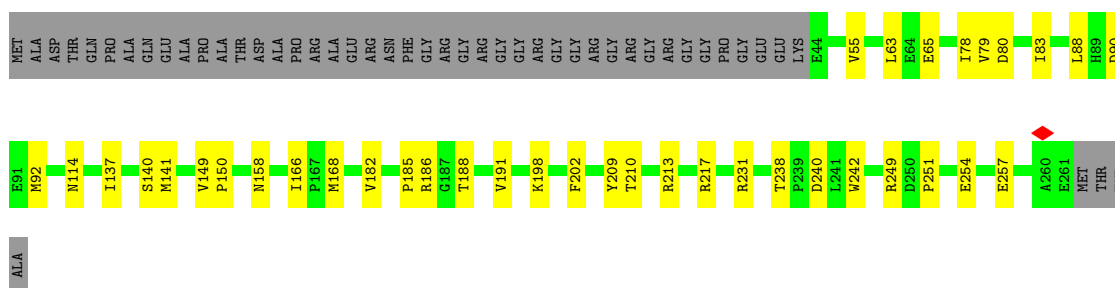
- Molecule 34: 40S ribosomal protein S4

Chain SE: 80% 15% • 5%



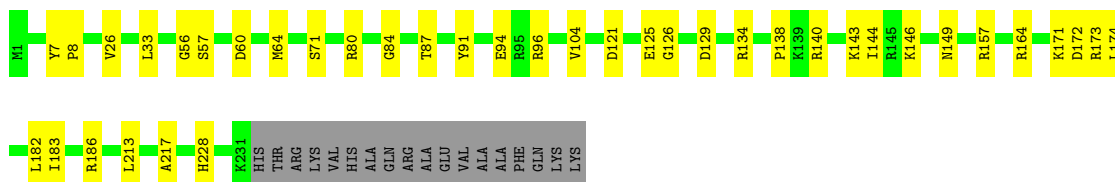
- Molecule 35: 40S ribosomal protein S2

Chain SF: 68% 14% 18%



- Molecule 36: 40S ribosomal protein S6

Chain SG: 



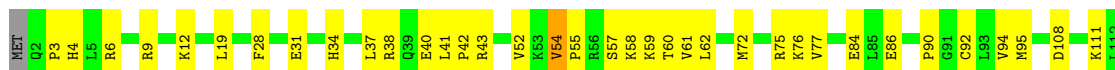
- Molecule 37: 40S ribosomal protein S5

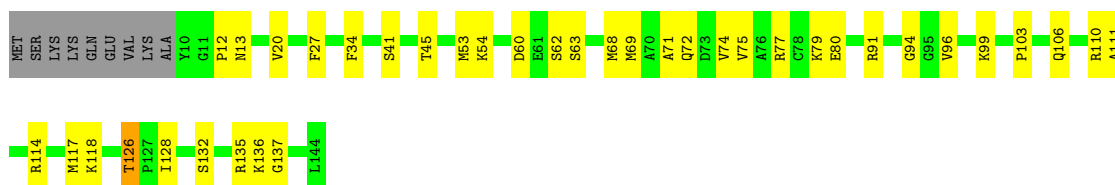
Chain SH: 85% 11% .



- Molecule 38: 40S ribosomal protein S7

Chain SI: 72% 27%





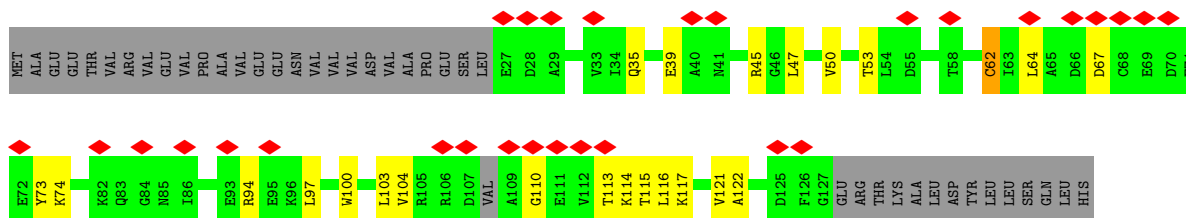
- Molecule 45: Putative 40S ribosomal protein S23

Chain SP: 82% 17% .



- Molecule 46: 40S ribosomal protein S12

Chain SQ: 21% 54% 16% 29% .



- Molecule 47: Putative 40S ribosomal protein S18

Chain SR: 70% 14% 15% .



- Molecule 48: Putative ribosomal protein S29

Chain SS: 81% 18% .



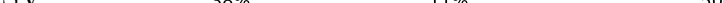
- Molecule 49: Putative 40S ribosomal protein S13

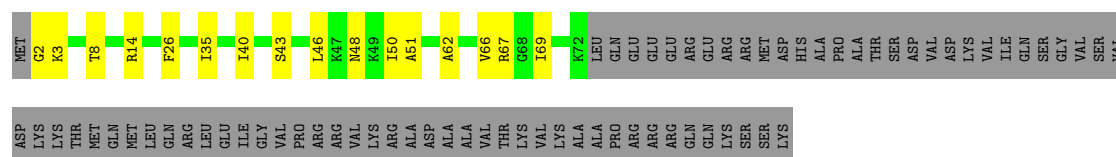
Chain ST: 75% 19% 6% .

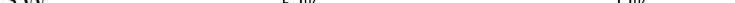


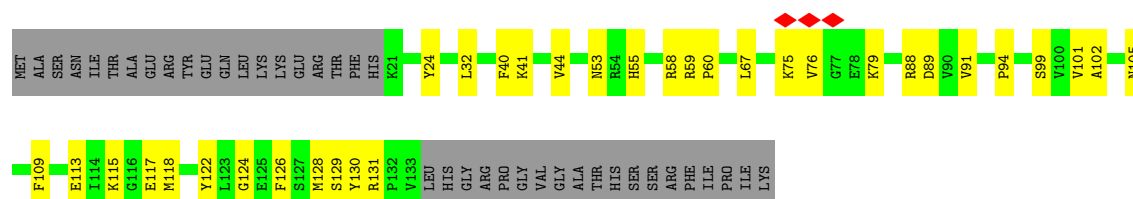
- Molecule 50: Putative 40S ribosomal protein S11

MT1	PRO	V3	Y7	V13	D14	Q18	H19	E20	K21	A28	M33	P36	K39	H40	V41	N42	H46	N65	V89	M95	T98	K110	Q113	Q116	K148	V158	SER	LYS	SER	SER	ALA	ALA	ASP	LYS	LYS	MET	GLY	LYS	LYS	PHE	ALA	LYS	ASN
-----	-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain SV: 

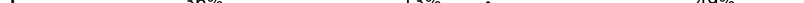


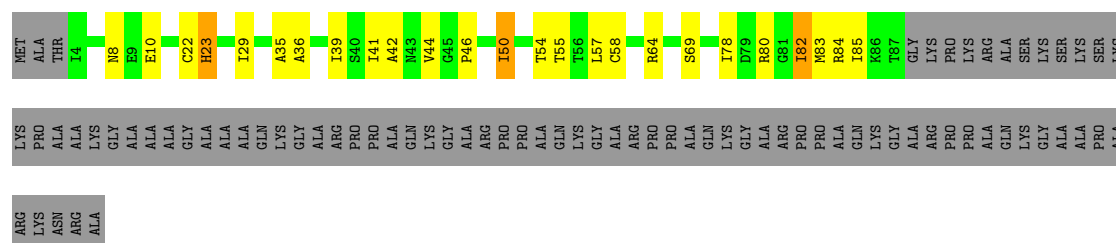
- Chain SW: 

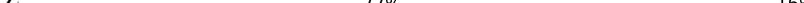


- Chain SX:



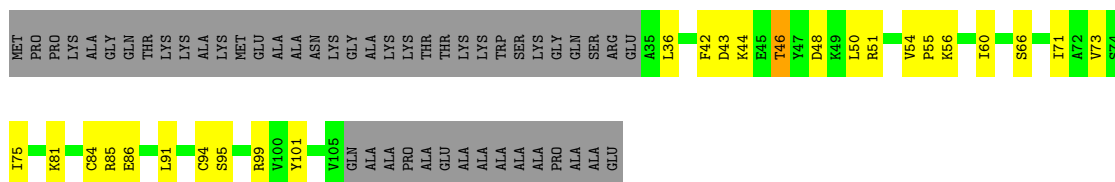
- Chain SY: 



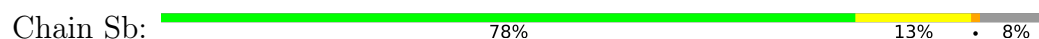
- Chain SZ: 



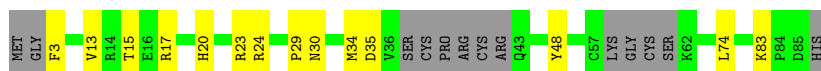
- Molecule 56: 40S ribosomal protein S25



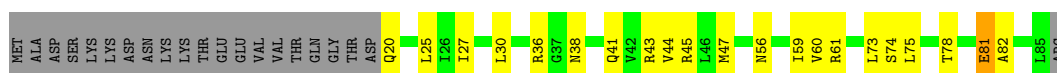
- Molecule 57: 40S ribosomal protein S26



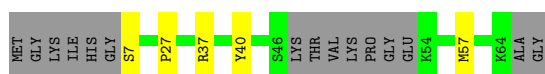
- Molecule 58: Putative 40S ribosomal protein S27-1



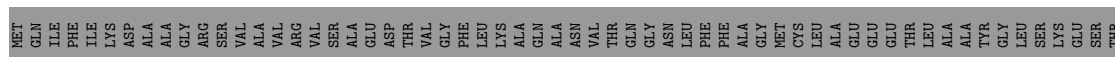
- Molecule 59: Putative 40S ribosomal protein S33

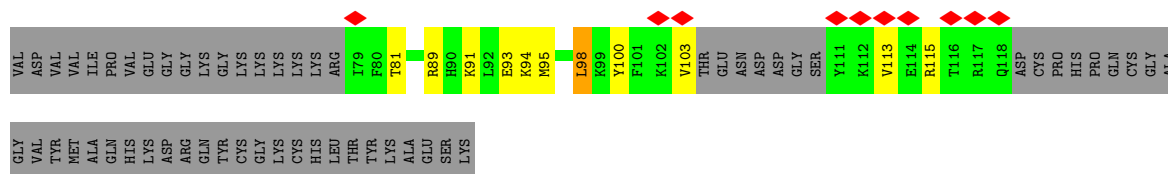


- Molecule 60: 40S ribosomal protein S30

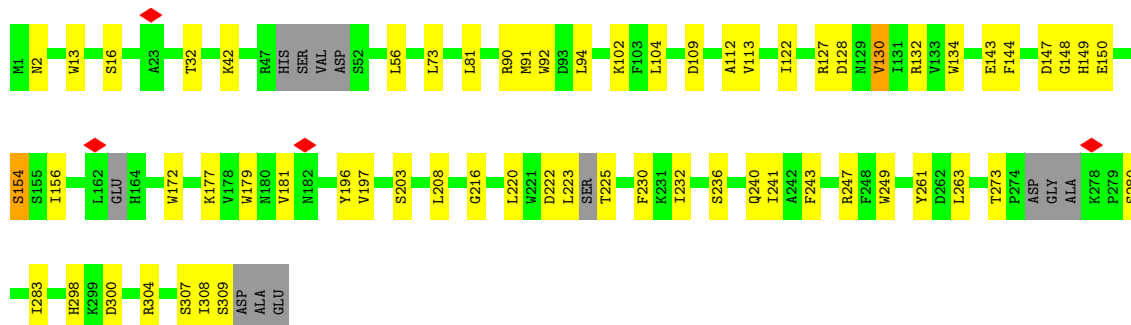
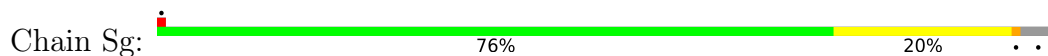


- Molecule 61: Ubiquitin-60S ribosomal protein L40

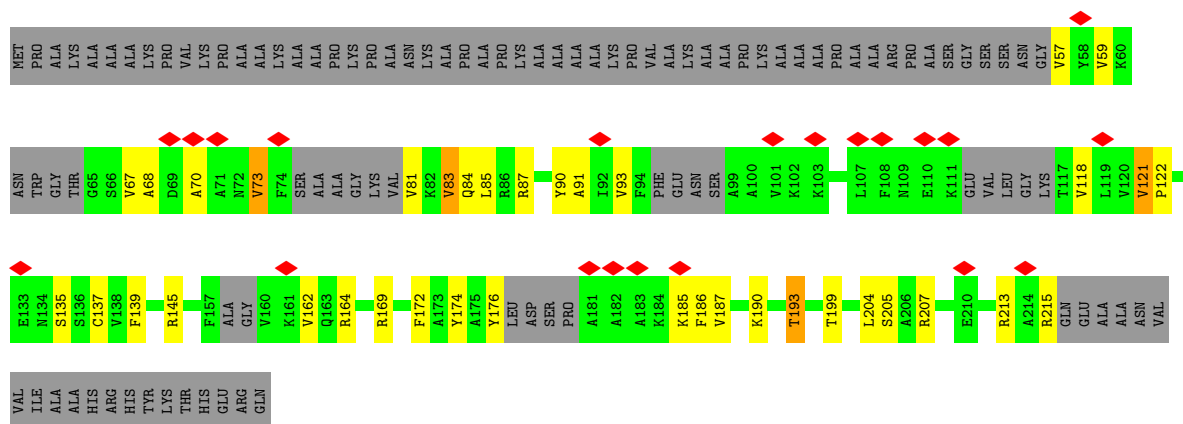
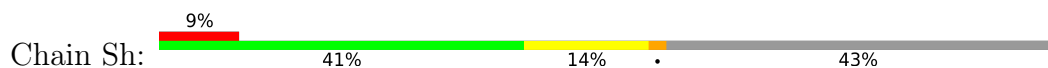




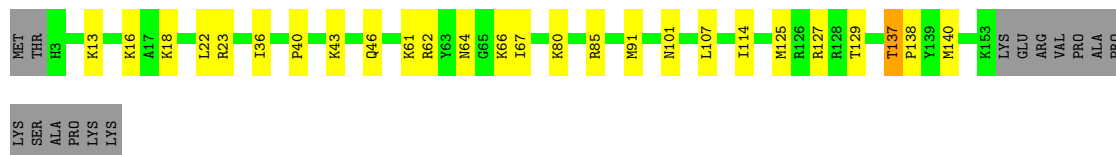
• Molecule 62: Guanine nucleotide-binding protein subunit beta-like protein



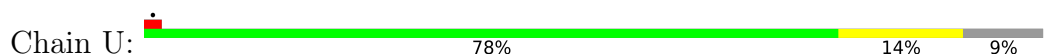
• Molecule 63: Putative RNA binding protein



• Molecule 64: Putative 60S ribosomal protein L17

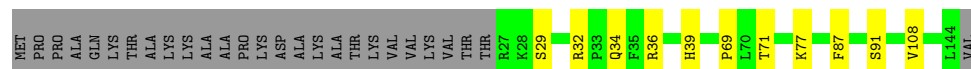


• Molecule 65: Putative 60S ribosomal protein L22

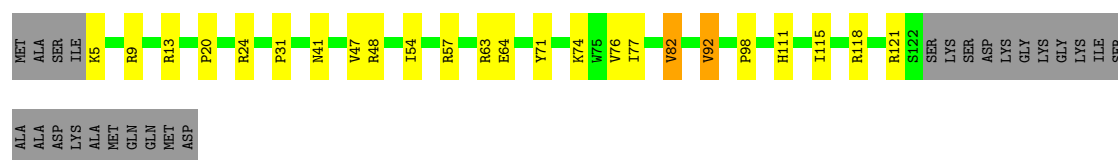




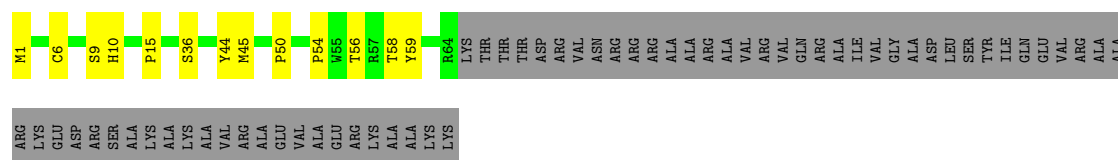
- Molecule 66: Putative 60S ribosomal protein L23a



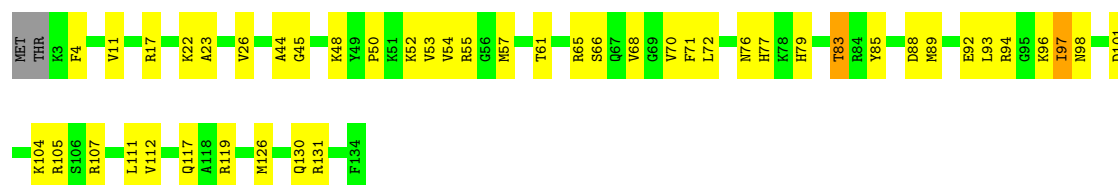
- Molecule 67: Putative 60S ribosomal protein L26



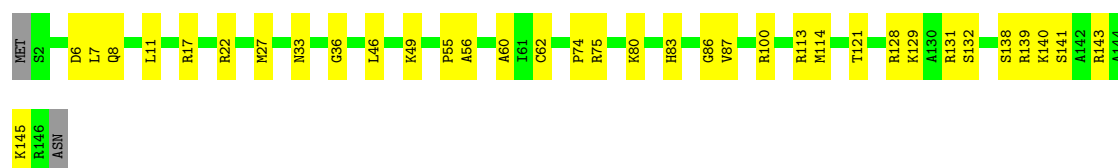
- Molecule 68: Putative ribosomal protein L24



- Molecule 69: 60S ribosomal protein L27

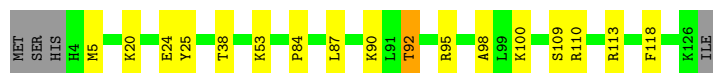


- Molecule 70: Putative 60S ribosomal protein L28



- Molecule 71: Putative 60S ribosomal protein L35

Chain a:  83% 13% ..



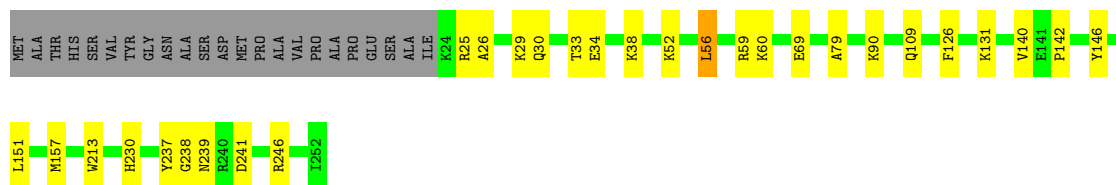
- Molecule 72: 60S ribosomal protein L29

Chain b:  93% ..



- Molecule 73: Putative 60S ribosomal protein L7

Chain c:  79% 11% 9%



- Molecule 74: 60S ribosomal protein L30

Chain d:  63% 22% 12%



- Molecule 75: Putative 60S ribosomal subunit protein L31

Chain e:  79% 16% ..



- Molecule 76: 60S ribosomal protein L32

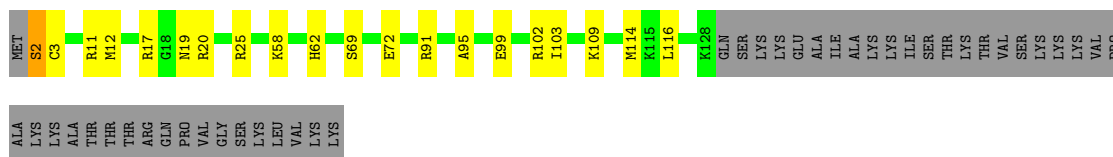
Chain f:  82% 11% 6%



- Molecule 77: Putative ribosomal protein l35a

Chain g:  86% 12% ..

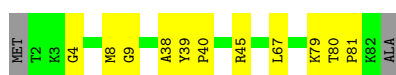
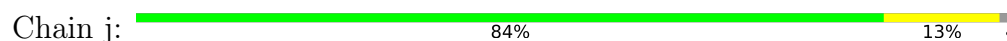
- Molecule 78: Putative 60S ribosomal protein L34



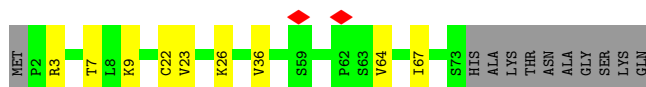
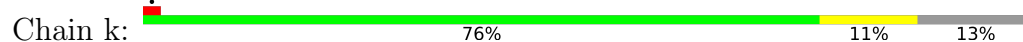
- Molecule 79: Putative 60S Ribosomal protein L36



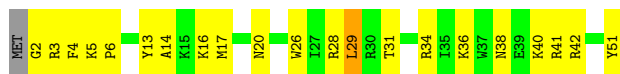
- Molecule 80: Ribosomal protein L37



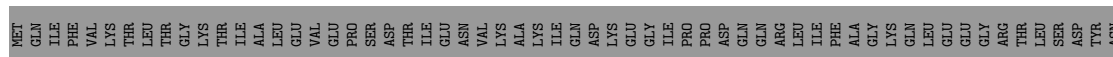
- Molecule 81: Putative ribosomal protein L38

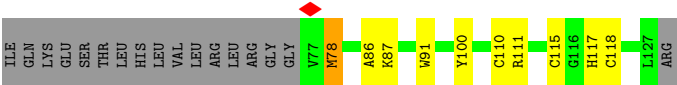


- Molecule 82: Putative 60S ribosomal protein L39



- Molecule 83: Ubiquitin-60S ribosomal protein L40

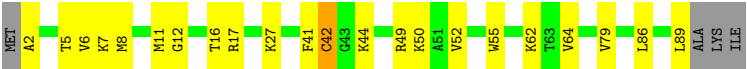




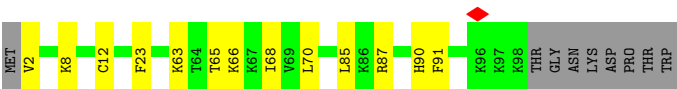
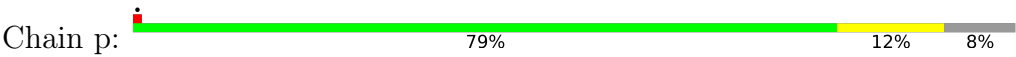
• Molecule 84: 60S ribosomal protein L41



• Molecule 85: 60S ribosomal protein L37a



• Molecule 86: Putative 60S ribosomal protein L44



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	178107	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.94	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, A2M, MA6, PSU, OMC, 7MG, OMG, NA, 5MC, 1MA, ZN, K, MG, OMU

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	1	0.24	0/37788	0.44	0/58914
2	2	0.25	5/26311 (0.0%)	0.44	0/40996
3	3	0.20	0/3671	0.41	0/5704
4	4	0.20	0/4376	0.41	0/6822
5	5	0.21	0/2739	0.46	0/4263
6	6	0.19	0/1683	0.48	0/2618
7	7	0.24	0/3758	0.42	0/5847
8	8	0.17	0/2829	0.35	0/4405
9	A	0.19	0/1950	0.44	0/2622
10	B	0.18	0/3117	0.40	0/4212
11	C	0.18	0/2827	0.43	0/3808
12	D	0.16	0/1026	0.40	0/1395
13	E	0.20	0/1415	0.49	2/1914 (0.1%)
14	F	0.18	0/1089	0.40	0/1486
15	G	0.17	0/1755	0.38	0/2370
16	H	0.18	0/1769	0.40	0/2381
17	I	0.28	0/1636	0.50	0/2202
18	J	0.19	0/1016	0.45	0/1375
19	K	0.17	0/1285	0.36	0/1736
20	L	0.20	0/1151	0.46	0/1538
21	M	0.22	0/1736	0.42	0/2320
22	N	0.19	0/1639	0.46	0/2194
23	O	0.18	0/2012	0.41	0/2724
24	P	0.18	0/1553	0.40	0/2080
25	Q	0.18	0/1452	0.37	0/1939
26	R	0.18	0/1447	0.35	0/1957
27	S	0.19	0/1263	0.42	0/1705
28	S1	0.20	3/41642 (0.0%)	0.39	0/64864
29	S4	0.17	0/1194	0.39	0/1850
30	SA	0.17	0/1848	0.43	0/2487
31	SB	0.18	0/1660	0.42	0/2246
32	SC	0.13	0/1652	0.34	0/2212

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SD	0.15	0/1393	0.32	0/1874
34	SE	0.16	0/2088	0.40	0/2814
35	SF	0.18	0/1698	0.37	0/2301
36	SG	0.16	0/1853	0.40	1/2475 (0.0%)
37	SH	0.13	0/1458	0.32	0/1955
38	SI	0.16	0/1649	0.38	0/2220
39	SJ	0.16	0/1038	0.37	0/1391
40	SK	0.17	0/1465	0.37	0/1964
41	SL	0.14	0/1145	0.34	0/1540
42	SM	0.15	0/806	0.36	0/1093
43	SN	0.14	0/831	0.34	0/1127
44	SO	0.19	0/1025	0.43	0/1377
45	SP	0.14	0/1120	0.39	0/1500
46	SQ	0.14	0/682	0.34	0/927
47	SR	0.13	0/1052	0.34	0/1414
48	SS	0.13	0/458	0.34	0/607
49	ST	0.24	0/1178	0.43	0/1580
50	SU	0.16	0/1283	0.39	0/1729
51	SV	0.14	0/584	0.31	0/777
52	SW	0.14	0/926	0.35	0/1245
53	SX	0.13	0/1233	0.34	0/1656
54	SY	0.50	1/625 (0.2%)	0.84	3/851 (0.4%)
55	SZ	0.13	0/1051	0.35	0/1399
56	Sa	0.16	0/563	0.45	0/757
57	Sb	0.32	0/833	0.47	0/1116
58	Sc	0.14	0/580	0.35	0/780
59	Sd	0.16	0/485	0.37	0/652
60	Se	1.53	1/407 (0.2%)	0.69	1/540 (0.2%)
61	Sf	0.13	0/301	0.38	0/396
62	Sg	0.14	0/2339	0.36	0/3183
63	Sh	0.17	0/957	0.42	0/1291
64	T	0.21	0/1235	0.44	0/1656
65	U	0.18	0/810	0.47	0/1086
66	V	0.17	0/941	0.38	0/1269
67	W	0.17	0/951	0.40	0/1270
68	X	0.17	0/569	0.38	0/767
69	Y	0.17	0/1048	0.41	0/1409
70	Z	0.20	0/1111	0.39	0/1492
71	a	0.18	0/1016	0.36	0/1351
72	b	0.18	0/557	0.42	0/743
73	c	0.22	0/1896	0.43	0/2540
74	d	0.20	0/715	0.40	0/968
75	e	0.17	0/1439	0.39	0/1912

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	f	0.25	0/1031	0.46	0/1380
77	g	0.18	0/1165	0.37	0/1563
78	h	0.19	0/1034	0.44	0/1378
79	i	0.17	0/699	0.36	0/929
80	j	0.19	0/682	0.45	0/910
81	k	0.15	0/542	0.39	0/733
82	l	0.20	0/463	0.42	0/617
83	m	0.25	0/384	0.55	1/518 (0.2%)
84	n	0.28	0/296	0.51	0/386
85	o	0.22	0/700	0.51	0/933
86	p	0.18	0/788	0.39	0/1043
All	All	0.22	10/215467 (0.0%)	0.42	8/316570 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
42	SM	0	1
49	ST	0	1
57	Sb	0	1
All	All	0	3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	Se	27	PRO	N-CD	-30.53	1.05	1.47
54	SY	46	PRO	CG-CD	-10.67	1.14	1.50
2	2	1419	OMU	O3'-P	5.40	1.61	1.56
2	2	527	A2M	O3'-P	5.25	1.61	1.56
28	S1	479	A2M	O3'-P	5.19	1.61	1.56

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	SY	46	PRO	N-CD-CG	-14.37	81.64	103.20
60	Se	27	PRO	N-CD-CG	12.94	122.61	103.20
54	SY	46	PRO	CA-CB-CG	-12.91	79.96	104.50
83	m	78	MET	CG-SD-CE	7.05	116.41	100.90
13	E	95	TYR	CA-C-N	-6.40	112.50	122.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	SM	65	THR	Peptide
49	ST	124	ARG	Sidechain
57	Sb	10	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	1	34568	0	17433	571	0
2	2	24802	0	12569	392	0
3	3	3312	0	1680	54	0
4	4	3937	0	1989	70	0
5	5	2453	0	1244	51	0
6	6	1506	0	768	36	0
7	7	3494	0	1774	48	0
8	8	2531	0	1283	34	0
9	A	1908	0	1940	21	0
10	B	3051	0	3080	54	0
11	C	2777	0	2856	61	0
12	D	1008	0	775	9	0
13	E	1395	0	1410	27	0
14	F	1067	0	1077	12	0
15	G	1731	0	1818	27	0
16	H	1734	0	1819	21	0
17	I	1603	0	1623	15	0
18	J	999	0	1023	15	0
19	K	1266	0	1270	27	0
20	L	1124	0	1151	16	0
21	M	1696	0	1770	26	0
22	N	1607	0	1663	43	0
23	O	1975	0	1873	30	0
24	P	1528	0	1618	20	0
25	Q	1433	0	1440	17	0
26	R	1413	0	1433	18	0
27	S	1234	0	1254	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	S1	38240	0	19316	566	0
29	S4	1072	0	551	15	0
30	SA	1820	0	1904	46	0
31	SB	1627	0	1649	62	0
32	SC	1624	0	1677	19	0
33	SD	1366	0	1406	26	0
34	SE	2050	0	2144	29	0
35	SF	1662	0	1708	28	0
36	SG	1831	0	1955	27	0
37	SH	1436	0	1467	15	0
38	SI	1619	0	1697	46	0
39	SJ	1021	0	1050	14	0
40	SK	1443	0	1524	23	0
41	SL	1124	0	1179	13	0
42	SM	796	0	838	14	0
43	SN	808	0	786	17	0
44	SO	1010	0	1034	27	0
45	SP	1100	0	1146	15	0
46	SQ	679	0	609	17	0
47	SR	1034	0	1073	13	0
48	SS	452	0	463	8	0
49	ST	1155	0	1220	27	0
50	SU	1253	0	1281	16	0
51	SV	577	0	626	13	0
52	SW	907	0	935	22	0
53	SX	1202	0	1227	16	0
54	SY	616	0	601	20	0
55	SZ	1031	0	1105	17	0
56	Sa	558	0	606	16	0
57	Sb	816	0	847	13	0
58	Sc	570	0	557	10	0
59	Sd	483	0	494	12	0
60	Se	401	0	436	6	0
61	Sf	295	0	324	9	0
62	Sg	2284	0	2172	40	0
63	Sh	948	0	881	23	0
64	T	1211	0	1247	20	0
65	U	801	0	724	14	0
66	V	926	0	973	9	0
67	W	937	0	1009	18	0
68	X	548	0	553	13	0
69	Y	1027	0	1059	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	Z	1095	0	1117	30	0
71	a	1006	0	1098	13	0
72	b	546	0	575	4	0
73	c	1862	0	1959	27	0
74	d	705	0	719	17	0
75	e	1421	0	1552	23	0
76	f	1011	0	1054	15	0
77	g	1142	0	1196	14	0
78	h	1018	0	1058	16	0
79	i	689	0	751	10	0
80	j	668	0	684	7	0
81	k	534	0	534	6	0
82	l	450	0	483	18	0
83	m	378	0	377	10	0
84	n	292	0	331	9	0
85	o	688	0	711	21	0
86	p	775	0	824	8	0
87	1	58	0	0	0	0
87	2	66	0	0	0	0
87	4	3	0	0	0	0
87	5	3	0	0	0	0
87	6	1	0	0	0	0
87	7	2	0	0	0	0
87	8	1	0	0	0	0
87	A	2	0	0	0	0
87	J	1	0	0	0	0
87	S	1	0	0	0	0
87	S1	79	0	0	2	0
87	SX	1	0	0	0	0
87	Sb	1	0	0	0	0
88	1	11	0	0	0	0
88	2	10	0	0	0	0
88	4	3	0	0	0	0
88	S1	9	0	0	0	0
88	S4	1	0	0	0	0
89	1	9	0	0	0	0
89	2	3	0	0	0	0
89	S1	4	0	0	0	0
90	p	1	0	0	0	0
91	1	617	0	0	24	0
91	2	478	0	0	9	0
91	3	21	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	4	62	0	0	2	0
91	5	24	0	0	0	0
91	6	5	0	0	0	0
91	7	43	0	0	1	0
91	8	5	0	0	0	0
91	A	20	0	0	2	0
91	B	38	0	0	2	0
91	C	18	0	0	2	0
91	D	1	0	0	0	0
91	F	1	0	0	0	0
91	G	1	0	0	0	0
91	H	9	0	0	0	0
91	I	10	0	0	0	0
91	J	4	0	0	0	0
91	L	12	0	0	0	0
91	M	22	0	0	0	0
91	N	1	0	0	0	0
91	P	8	0	0	0	0
91	Q	2	0	0	0	0
91	R	1	0	0	0	0
91	S	2	0	0	0	0
91	S1	802	0	0	16	0
91	S4	3	0	0	0	0
91	SA	7	0	0	0	0
91	SB	1	0	0	0	0
91	SC	1	0	0	0	0
91	SD	4	0	0	0	0
91	SE	13	0	0	0	0
91	SF	6	0	0	0	0
91	SG	1	0	0	0	0
91	SH	6	0	0	0	0
91	SJ	12	0	0	0	0
91	SK	13	0	0	1	0
91	SL	3	0	0	0	0
91	SM	6	0	0	0	0
91	SN	2	0	0	2	0
91	SO	7	0	0	1	0
91	SP	12	0	0	0	0
91	SR	4	0	0	0	0
91	SS	1	0	0	0	0
91	ST	19	0	0	0	0
91	SU	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	SX	5	0	0	0	0
91	Sa	2	0	0	0	0
91	Sb	23	0	0	0	0
91	Sc	5	0	0	0	0
91	T	9	0	0	0	0
91	V	4	0	0	0	0
91	W	2	0	0	1	0
91	X	2	0	0	1	0
91	Z	1	0	0	0	0
91	b	3	0	0	0	0
91	c	5	0	0	1	0
91	e	3	0	0	0	0
91	f	14	0	0	2	0
91	g	11	0	0	0	0
91	h	7	0	0	1	0
91	i	1	0	0	0	0
91	j	12	0	0	0	0
91	l	5	0	0	0	0
91	n	5	0	0	0	0
91	o	8	0	0	0	0
91	p	5	0	0	0	0
All	All	206527	0	148709	2875	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 8.

The worst 5 of 2875 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)
87:S1:2327:MG:MG	91:S1:2537:HOH:O	0.77	1.25
87:S1:2329:MG:MG	91:S1:3183:HOH:O	0.88	1.15
28:S1:955:A:N6	28:S1:980:G:H1	1.47	1.13
29:S4:26:A:H62	29:S4:44:G:N2	1.56	1.02
3:3:101:G:H1	3:3:139:C:H5	1.09	1.00

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	A	254/260 (98%)	248 (98%)	6 (2%)	0	100	100
10	B	397/419 (95%)	389 (98%)	8 (2%)	0	100	100
11	C	364/373 (98%)	351 (96%)	13 (4%)	0	100	100
12	D	152/188 (81%)	143 (94%)	9 (6%)	0	100	100
13	E	184/190 (97%)	172 (94%)	12 (6%)	0	100	100
14	F	144/195 (74%)	136 (94%)	8 (6%)	0	100	100
15	G	222/264 (84%)	216 (97%)	6 (3%)	0	100	100
16	H	218/222 (98%)	217 (100%)	1 (0%)	0	100	100
17	I	206/220 (94%)	199 (97%)	5 (2%)	2 (1%)	12	13
18	J	135/139 (97%)	131 (97%)	4 (3%)	0	100	100
19	K	168/175 (96%)	162 (96%)	6 (4%)	0	100	100
20	L	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
21	M	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
22	N	195/213 (92%)	190 (97%)	5 (3%)	0	100	100
23	O	268/305 (88%)	261 (97%)	7 (3%)	0	100	100
24	P	195/198 (98%)	187 (96%)	8 (4%)	0	100	100
25	Q	185/254 (73%)	185 (100%)	0	0	100	100
26	R	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
27	S	155/159 (98%)	151 (97%)	4 (3%)	0	100	100
30	SA	224/264 (85%)	216 (96%)	8 (4%)	0	100	100
31	SB	206/246 (84%)	194 (94%)	12 (6%)	0	100	100
32	SC	211/219 (96%)	208 (99%)	3 (1%)	0	100	100
33	SD	165/190 (87%)	165 (100%)	0	0	100	100
34	SE	258/273 (94%)	253 (98%)	5 (2%)	0	100	100
35	SF	216/265 (82%)	214 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	SG	229/249 (92%)	224 (98%)	4 (2%)	1 (0%)	30	36
37	SH	178/190 (94%)	174 (98%)	4 (2%)	0	100	100
38	SI	197/200 (98%)	194 (98%)	3 (2%)	0	100	100
39	SJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
40	SK	178/220 (81%)	174 (98%)	4 (2%)	0	100	100
41	SL	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
42	SM	100/116 (86%)	99 (99%)	1 (1%)	0	100	100
43	SN	97/168 (58%)	92 (95%)	5 (5%)	0	100	100
44	SO	133/144 (92%)	129 (97%)	4 (3%)	0	100	100
45	SP	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
46	SQ	96/141 (68%)	94 (98%)	2 (2%)	0	100	100
47	SR	128/153 (84%)	127 (99%)	1 (1%)	0	100	100
48	SS	54/57 (95%)	54 (100%)	0	0	100	100
49	ST	140/151 (93%)	135 (96%)	5 (4%)	0	100	100
50	SU	154/173 (89%)	149 (97%)	5 (3%)	0	100	100
51	SV	69/143 (48%)	66 (96%)	3 (4%)	0	100	100
52	SW	111/152 (73%)	109 (98%)	2 (2%)	0	100	100
53	SX	150/161 (93%)	144 (96%)	6 (4%)	0	100	100
54	SY	82/164 (50%)	78 (95%)	4 (5%)	0	100	100
55	SZ	125/137 (91%)	123 (98%)	2 (2%)	0	100	100
56	Sa	69/120 (58%)	69 (100%)	0	0	100	100
57	Sb	101/112 (90%)	99 (98%)	2 (2%)	0	100	100
58	Sc	67/86 (78%)	64 (96%)	3 (4%)	0	100	100
59	Sd	64/87 (74%)	63 (98%)	1 (2%)	0	100	100
60	Se	47/66 (71%)	47 (100%)	0	0	100	100
61	Sf	29/152 (19%)	26 (90%)	3 (10%)	0	100	100
62	Sg	290/312 (93%)	284 (98%)	6 (2%)	0	100	100
63	Sh	120/235 (51%)	113 (94%)	7 (6%)	0	100	100
64	T	149/166 (90%)	143 (96%)	6 (4%)	0	100	100
65	U	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
66	V	116/145 (80%)	116 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	W	116/143 (81%)	114 (98%)	2 (2%)	0	100	100
68	X	62/124 (50%)	61 (98%)	1 (2%)	0	100	100
69	Y	130/134 (97%)	127 (98%)	3 (2%)	0	100	100
70	Z	143/147 (97%)	140 (98%)	3 (2%)	0	100	100
71	a	121/127 (95%)	119 (98%)	2 (2%)	0	100	100
72	b	66/70 (94%)	64 (97%)	2 (3%)	0	100	100
73	c	227/252 (90%)	219 (96%)	8 (4%)	0	100	100
74	d	90/104 (86%)	88 (98%)	2 (2%)	0	100	100
75	e	176/188 (94%)	173 (98%)	3 (2%)	0	100	100
76	f	123/133 (92%)	119 (97%)	4 (3%)	0	100	100
77	g	140/144 (97%)	140 (100%)	0	0	100	100
78	h	125/168 (74%)	122 (98%)	2 (2%)	1 (1%)	16	18
79	i	84/105 (80%)	83 (99%)	1 (1%)	0	100	100
80	j	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
81	k	70/83 (84%)	68 (97%)	2 (3%)	0	100	100
82	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
83	m	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
84	n	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
85	o	86/92 (94%)	79 (92%)	7 (8%)	0	100	100
86	p	95/106 (90%)	92 (97%)	3 (3%)	0	100	100
All	All	11096/12926 (86%)	10802 (97%)	290 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	SG	172	ASP
78	h	62	HIS
17	I	16	HIS
17	I	152	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	A	190/204 (93%)	189 (100%)	1 (0%)	81	87
10	B	303/351 (86%)	298 (98%)	5 (2%)	53	66
11	C	277/301 (92%)	269 (97%)	8 (3%)	37	49
12	D	61/162 (38%)	60 (98%)	1 (2%)	55	68
13	E	139/172 (81%)	134 (96%)	5 (4%)	31	42
14	F	99/153 (65%)	97 (98%)	2 (2%)	48	62
15	G	170/221 (77%)	167 (98%)	3 (2%)	51	64
16	H	175/188 (93%)	170 (97%)	5 (3%)	37	49
17	I	161/183 (88%)	158 (98%)	3 (2%)	50	63
18	J	100/111 (90%)	99 (99%)	1 (1%)	68	77
19	K	118/145 (81%)	117 (99%)	1 (1%)	73	81
20	L	113/114 (99%)	111 (98%)	2 (2%)	51	64
21	M	174/180 (97%)	173 (99%)	1 (1%)	78	85
22	N	166/179 (93%)	159 (96%)	7 (4%)	26	37
23	O	162/242 (67%)	158 (98%)	4 (2%)	42	54
24	P	159/164 (97%)	158 (99%)	1 (1%)	78	85
25	Q	125/198 (63%)	123 (98%)	2 (2%)	55	68
26	R	146/159 (92%)	143 (98%)	3 (2%)	47	60
27	S	126/134 (94%)	120 (95%)	6 (5%)	23	32
30	SA	197/222 (89%)	194 (98%)	3 (2%)	57	69
31	SB	173/202 (86%)	168 (97%)	5 (3%)	37	49
32	SC	170/184 (92%)	166 (98%)	4 (2%)	43	56
33	SD	144/164 (88%)	142 (99%)	2 (1%)	59	70
34	SE	215/225 (96%)	210 (98%)	5 (2%)	44	57
35	SF	174/208 (84%)	174 (100%)	0	100	100
36	SG	189/208 (91%)	185 (98%)	4 (2%)	47	60
37	SH	151/159 (95%)	150 (99%)	1 (1%)	76	83
38	SI	175/186 (94%)	171 (98%)	4 (2%)	44	57
39	SJ	110/111 (99%)	108 (98%)	2 (2%)	51	64
40	SK	141/176 (80%)	137 (97%)	4 (3%)	38	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	SL	113/120 (94%)	111 (98%)	2 (2%)	51	64
42	SM	92/104 (88%)	92 (100%)	0	100	100
43	SN	86/128 (67%)	82 (95%)	4 (5%)	23	33
44	SO	103/113 (91%)	100 (97%)	3 (3%)	37	49
45	SP	114/117 (97%)	110 (96%)	4 (4%)	32	44
46	SQ	58/120 (48%)	57 (98%)	1 (2%)	53	66
47	SR	107/130 (82%)	104 (97%)	3 (3%)	38	51
48	SS	47/49 (96%)	46 (98%)	1 (2%)	47	60
49	ST	124/132 (94%)	124 (100%)	0	100	100
50	SU	132/152 (87%)	130 (98%)	2 (2%)	57	69
51	SV	62/126 (49%)	61 (98%)	1 (2%)	55	68
52	SW	95/130 (73%)	93 (98%)	2 (2%)	47	60
53	SX	121/131 (92%)	120 (99%)	1 (1%)	73	81
54	SY	64/116 (55%)	61 (95%)	3 (5%)	23	33
55	SZ	109/118 (92%)	105 (96%)	4 (4%)	30	41
56	Sa	63/95 (66%)	62 (98%)	1 (2%)	55	68
57	Sb	84/93 (90%)	81 (96%)	3 (4%)	31	42
58	Sc	60/76 (79%)	59 (98%)	1 (2%)	53	66
59	Sd	49/75 (65%)	47 (96%)	2 (4%)	27	38
60	Se	41/54 (76%)	40 (98%)	1 (2%)	43	56
61	Sf	32/126 (25%)	30 (94%)	2 (6%)	16	21
62	Sg	243/265 (92%)	236 (97%)	7 (3%)	37	49
63	Sh	80/177 (45%)	71 (89%)	9 (11%)	5	5
64	T	127/143 (89%)	125 (98%)	2 (2%)	55	68
65	U	57/114 (50%)	57 (100%)	0	100	100
66	V	96/124 (77%)	92 (96%)	4 (4%)	26	37
67	W	99/122 (81%)	97 (98%)	2 (2%)	48	62
68	X	58/104 (56%)	58 (100%)	0	100	100
69	Y	100/116 (86%)	96 (96%)	4 (4%)	28	39
70	Z	108/118 (92%)	104 (96%)	4 (4%)	30	41
71	a	106/118 (90%)	105 (99%)	1 (1%)	70	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	b	56/58 (97%)	56 (100%)	0	100	100
73	c	191/209 (91%)	187 (98%)	4 (2%)	47	60
74	d	80/89 (90%)	75 (94%)	5 (6%)	16	21
75	e	148/158 (94%)	145 (98%)	3 (2%)	48	62
76	f	106/115 (92%)	105 (99%)	1 (1%)	70	80
77	g	119/121 (98%)	118 (99%)	1 (1%)	73	81
78	h	104/146 (71%)	101 (97%)	3 (3%)	37	49
79	i	68/88 (77%)	67 (98%)	1 (2%)	57	69
80	j	67/70 (96%)	67 (100%)	0	100	100
81	k	52/74 (70%)	52 (100%)	0	100	100
82	l	46/47 (98%)	45 (98%)	1 (2%)	45	59
83	m	37/113 (33%)	36 (97%)	1 (3%)	39	52
84	n	30/32 (94%)	30 (100%)	0	100	100
85	o	69/74 (93%)	67 (97%)	2 (3%)	37	49
86	p	80/92 (87%)	80 (100%)	0	100	100
All	All	8886/10798 (82%)	8695 (98%)	191 (2%)	45	60

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	SV	66	VAL
63	Sh	73	VAL
54	SY	23	HIS
58	Sc	15	THR
63	Sh	193	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
62	Sg	2	ASN
73	c	177	GLN
63	Sh	191	ASN
67	W	16	HIS
76	f	28	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1600/1782 (89%)	410 (25%)	33 (2%)
2	2	1147/1526 (75%)	308 (26%)	25 (2%)
28	S1	1762/2204 (79%)	413 (23%)	25 (1%)
29	S4	45/76 (59%)	24 (53%)	1 (2%)
3	3	151/216 (69%)	31 (20%)	5 (3%)
4	4	183/184 (99%)	37 (20%)	1 (0%)
5	5	112/135 (82%)	26 (23%)	2 (1%)
6	6	70/73 (95%)	31 (44%)	3 (4%)
7	7	160/171 (93%)	34 (21%)	3 (1%)
8	8	118/123 (95%)	17 (14%)	0
All	All	5348/6490 (82%)	1331 (24%)	98 (1%)

5 of 1331 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	7	C
1	1	8	U
1	1	16	G
1	1	24	A
1	1	29	C

5 of 98 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1512	G
7	7	95	A
3	3	149	A
5	5	106	G
28	S1	276	G

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

153 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
28	PSU	S1	607	28	18,21,22	4.73	8 (44%)	21,30,33	1.83	4 (19%)
1	OMC	1	1010	1	19,22,23	2.99	8 (42%)	25,31,34	0.74	0
28	PSU	S1	2202	28	18,21,22	4.67	8 (44%)	21,30,33	1.81	5 (23%)
28	OMG	S1	1829	28,87	23,26,27	2.47	8 (34%)	32,38,41	2.05	10 (31%)
2	OMC	2	1397	2	19,22,23	2.93	8 (42%)	25,31,34	0.75	0
1	PSU	1	1664	1	18,21,22	4.74	7 (38%)	21,30,33	1.85	5 (23%)
2	PSU	2	122	2	18,21,22	4.71	8 (44%)	21,30,33	2.10	6 (28%)
2	PSU	2	437	2	18,21,22	4.65	7 (38%)	21,30,33	1.90	5 (23%)
1	OMG	1	1540	1,2	23,26,27	2.42	9 (39%)	32,38,41	2.05	10 (31%)
1	PSU	1	940	1	18,21,22	4.66	7 (38%)	21,30,33	2.06	5 (23%)
2	PSU	2	1264	2	18,21,22	4.67	8 (44%)	21,30,33	1.89	5 (23%)
1	OMG	1	856	1	23,26,27	2.47	8 (34%)	32,38,41	2.10	10 (31%)
1	A2M	1	927	1	22,25,26	3.48	9 (40%)	30,36,39	2.33	11 (36%)
2	PSU	2	1194	2	18,21,22	4.65	7 (38%)	21,30,33	1.99	5 (23%)
2	OMG	2	534	2	23,26,27	2.49	8 (34%)	32,38,41	2.07	9 (28%)
28	A2M	S1	668	28,87	22,25,26	3.45	9 (40%)	30,36,39	2.45	12 (40%)
2	PSU	2	662	2,87	18,21,22	4.68	7 (38%)	21,30,33	2.05	6 (28%)
1	PSU	1	1011	1,2	18,21,22	4.63	9 (50%)	21,30,33	1.85	6 (28%)
28	PSU	S1	2046	28	18,21,22	4.61	7 (38%)	21,30,33	1.95	5 (23%)
2	PSU	2	1265	2	18,21,22	4.69	7 (38%)	21,30,33	1.99	5 (23%)
2	OMG	2	655	2	23,26,27	2.48	8 (34%)	32,38,41	2.12	10 (31%)
2	PSU	2	1318	2	18,21,22	4.67	7 (38%)	21,30,33	1.95	6 (28%)
4	OMG	4	74	4	23,26,27	2.46	8 (34%)	32,38,41	1.99	10 (31%)
2	PSU	2	78	2	18,21,22	4.69	7 (38%)	21,30,33	1.94	5 (23%)
1	PSU	1	672	1,87	18,21,22	0.92	1 (5%)	21,30,33	0.68	0
28	A2M	S1	2021	28	22,25,26	3.47	9 (40%)	30,36,39	2.39	11 (36%)
2	OMU	2	1359	2	19,22,23	3.10	8 (42%)	25,31,34	1.79	5 (20%)
28	OMU	S1	1833	28	19,22,23	3.07	8 (42%)	25,31,34	1.97	5 (20%)
1	OMG	1	1626	1	23,26,27	2.45	8 (34%)	32,38,41	2.07	10 (31%)
2	PSU	2	597	2	18,21,22	4.66	7 (38%)	21,30,33	1.98	5 (23%)
2	OMG	2	1253	2	23,26,27	2.48	8 (34%)	32,38,41	2.08	10 (31%)
2	A2M	2	382	2	22,25,26	3.47	9 (40%)	30,36,39	2.29	11 (36%)
28	PSU	S1	609	28	18,21,22	4.70	7 (38%)	21,30,33	1.96	5 (23%)
28	OMG	S1	1623	28,87	23,26,27	2.48	8 (34%)	32,38,41	2.04	10 (31%)
28	PSU	S1	1533	28	18,21,22	4.71	7 (38%)	21,30,33	1.95	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	1MA	1	677	1,87	21,25,26	0.46	0	30,37,40	0.59	0
2	PSU	2	510	2	18,21,22	4.71	7 (38%)	21,30,33	1.96	5 (23%)
28	A2M	S1	512	28	22,25,26	3.47	9 (40%)	30,36,39	2.35	11 (36%)
28	B8N	S1	1543	28	25,29,30	3.39	6 (24%)	28,42,45	1.94	6 (21%)
2	PSU	2	1354	2	18,21,22	4.65	8 (44%)	21,30,33	1.81	5 (23%)
28	OMG	S1	2151	28,89	23,26,27	2.44	9 (39%)	32,38,41	2.09	10 (31%)
28	MA6	S1	2184	28	23,26,27	1.48	5 (21%)	33,38,41	2.85	11 (33%)
2	PSU	2	1144	2	18,21,22	4.66	7 (38%)	21,30,33	2.07	5 (23%)
2	OMU	2	73	2	19,22,23	3.01	8 (42%)	25,31,34	1.60	4 (16%)
2	OMG	2	1360	2	23,26,27	2.48	8 (34%)	32,38,41	2.08	10 (31%)
28	OMC	S1	38	28	19,22,23	3.00	8 (42%)	25,31,34	0.77	0
2	OMG	2	71	2	23,26,27	2.48	8 (34%)	32,38,41	2.14	11 (34%)
2	OMG	2	641	2,87	23,26,27	2.45	8 (34%)	32,38,41	2.07	10 (31%)
1	OMC	1	1527	1	19,22,23	2.99	8 (42%)	25,31,34	0.73	0
2	A2M	2	1185	2	22,25,26	3.46	9 (40%)	30,36,39	2.46	12 (40%)
2	5MC	2	1308	2	19,22,23	4.83	13 (68%)	26,32,35	1.34	2 (7%)
28	PSU	S1	12	28	18,21,22	4.66	7 (38%)	21,30,33	1.95	5 (23%)
2	PSU	2	1361	2	18,21,22	4.69	7 (38%)	21,30,33	2.01	6 (28%)
1	PSU	1	1017	1	18,21,22	4.67	7 (38%)	21,30,33	1.98	5 (23%)
2	OMG	2	1229	2	23,26,27	2.46	8 (34%)	32,38,41	2.03	10 (31%)
1	A2M	1	678	1,2	22,25,26	0.20	0	30,36,39	0.32	0
28	PSU	S1	1246	28	18,21,22	4.64	7 (38%)	21,30,33	2.04	5 (23%)
1	OMG	1	1190	1	23,26,27	2.45	8 (34%)	32,38,41	2.17	10 (31%)
2	A2M	2	628	2	22,25,26	3.45	9 (40%)	30,36,39	2.42	11 (36%)
2	OMC	2	359	2	19,22,23	3.01	8 (42%)	25,31,34	0.67	0
2	A2M	2	527	2,87	22,25,26	3.41	9 (40%)	30,36,39	2.70	12 (40%)
2	OMU	2	560	2,87	19,22,23	3.03	8 (42%)	25,31,34	2.25	7 (28%)
2	A2M	2	591	2	22,25,26	3.49	9 (40%)	30,36,39	2.28	9 (30%)
28	PSU	S1	1841	28	18,21,22	4.69	8 (44%)	21,30,33	1.80	5 (23%)
2	PSU	2	1060	2	18,21,22	4.67	7 (38%)	21,30,33	2.08	5 (23%)
1	OMU	1	1371	1	19,22,23	3.17	8 (42%)	25,31,34	1.99	6 (24%)
1	OMU	1	1107	1	19,22,23	3.07	8 (42%)	25,31,34	1.90	6 (24%)
2	PSU	2	472	2	18,21,22	4.60	7 (38%)	21,30,33	2.00	5 (23%)
1	A2M	1	858	1	22,25,26	3.48	9 (40%)	30,36,39	2.44	12 (40%)
1	PSU	1	1528	1	18,21,22	4.74	7 (38%)	21,30,33	1.91	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	OMG	S1	1478	28	23,26,27	2.45	8 (34%)	32,38,41	2.04	10 (31%)
2	OMG	2	1046	2	23,26,27	2.46	8 (34%)	32,38,41	2.08	10 (31%)
2	OMC	2	583	2	19,22,23	2.99	8 (42%)	25,31,34	0.70	0
28	PSU	S1	104	28	18,21,22	4.70	7 (38%)	21,30,33	2.02	5 (23%)
1	OMG	1	959	1	23,26,27	2.47	8 (34%)	32,38,41	2.09	10 (31%)
2	OMC	2	443	2	19,22,23	3.02	8 (42%)	25,31,34	0.77	0
28	A2M	S1	479	28	22,25,26	3.44	9 (40%)	30,36,39	2.36	10 (33%)
2	A2M	2	1372	2	22,25,26	3.56	10 (45%)	30,36,39	2.29	10 (33%)
2	OMU	2	1077	2	19,22,23	3.11	8 (42%)	25,31,34	1.87	5 (20%)
7	PSU	7	69	7	18,21,22	4.69	7 (38%)	21,30,33	2.06	6 (28%)
7	A2M	7	162	1,7	22,25,26	3.49	9 (40%)	30,36,39	2.39	11 (36%)
28	PSU	S1	1566	28	18,21,22	4.71	8 (44%)	21,30,33	1.82	5 (23%)
7	OMU	7	7	1,7	19,22,23	3.04	8 (42%)	25,31,34	1.87	5 (20%)
28	OMC	S1	18	28	19,22,23	2.99	8 (42%)	25,31,34	0.75	0
2	A2M	2	604	1,2	22,25,26	3.49	9 (40%)	30,36,39	2.40	12 (40%)
28	PSU	S1	1192	28	18,21,22	4.68	7 (38%)	21,30,33	1.90	5 (23%)
1	OMU	1	1659	1	19,22,23	3.07	8 (42%)	25,31,34	1.83	5 (20%)
28	OMU	S1	8	28,87	19,22,23	3.04	8 (42%)	25,31,34	1.92	5 (20%)
1	PSU	1	1181	1	18,21,22	4.75	7 (38%)	21,30,33	1.76	3 (14%)
2	OMU	2	56	1,2	19,22,23	3.05	8 (42%)	25,31,34	1.84	5 (20%)
28	OMC	S1	1866	28	19,22,23	3.03	8 (42%)	25,31,34	0.81	0
2	PSU	2	1303	2	18,21,22	4.67	7 (38%)	21,30,33	2.04	6 (28%)
28	A2M	S1	98	28,87	22,25,26	3.48	9 (40%)	30,36,39	2.33	11 (36%)
1	OMC	1	695	1	19,22,23	2.99	8 (42%)	25,31,34	0.74	0
2	OMU	2	667	2	19,22,23	3.08	8 (42%)	25,31,34	1.89	5 (20%)
7	A2M	7	43	7	22,25,26	3.47	9 (40%)	30,36,39	2.51	11 (36%)
1	A2M	1	955	1	22,25,26	3.45	9 (40%)	30,36,39	2.38	11 (36%)
2	A2M	2	1384	2,87	22,25,26	0.20	0	30,36,39	0.67	0
28	7MG	S1	1995	28	23,26,27	3.98	11 (47%)	27,39,42	2.13	9 (33%)
2	PSU	2	1382	2	18,21,22	0.92	1 (5%)	21,30,33	0.73	0
1	PSU	1	1402	1	18,21,22	4.62	9 (50%)	21,30,33	1.81	4 (19%)
28	OMG	S1	1865	28	23,26,27	2.45	8 (34%)	32,38,41	2.08	9 (28%)
28	OMC	S1	2140	28	19,22,23	3.03	8 (42%)	25,31,34	0.79	0
28	PSU	S1	1156	28	18,21,22	4.71	7 (38%)	21,30,33	1.91	5 (23%)
1	A2M	1	1539	1,2,87	22,25,26	3.46	9 (40%)	30,36,39	2.36	12 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1	1039	1	18,21,22	4.69	7 (38%)	21,30,33	1.84	5 (23%)
2	OMC	2	1159	2	19,22,23	3.02	8 (42%)	25,31,34	0.85	0
28	MA6	S1	2185	28	23,26,27	1.50	5 (21%)	33,38,41	2.79	12 (36%)
2	PSU	2	626	2	18,21,22	4.62	7 (38%)	21,30,33	1.87	5 (23%)
1	OMU	1	847	1	19,22,23	3.04	8 (42%)	25,31,34	1.76	5 (20%)
2	OMU	2	1419	2	19,22,23	0.26	0	25,31,34	0.43	0
2	PSU	2	512	2	18,21,22	4.70	7 (38%)	21,30,33	1.86	5 (23%)
28	PSU	S1	1539	28	18,21,22	4.69	8 (44%)	21,30,33	1.84	5 (23%)
28	OMU	S1	661	28	19,22,23	3.07	8 (42%)	25,31,34	1.82	5 (20%)
28	PSU	S1	2048	28	18,21,22	0.92	1 (5%)	21,30,33	0.67	0
2	OMC	2	1248	2	19,22,23	3.00	8 (42%)	25,31,34	0.86	0
1	OMG	1	1524	1	23,26,27	2.48	8 (34%)	32,38,41	2.19	10 (31%)
1	A2M	1	697	1	22,25,26	3.45	9 (40%)	30,36,39	2.36	11 (36%)
2	A2M	2	572	2	22,25,26	3.46	9 (40%)	30,36,39	2.55	12 (40%)
2	A2M	2	95	2	22,25,26	3.51	9 (40%)	30,36,39	2.44	10 (33%)
1	A2M	1	305	1	22,25,26	3.47	9 (40%)	30,36,39	2.38	11 (36%)
28	PSU	S1	33	28	18,21,22	4.71	7 (38%)	21,30,33	2.02	5 (23%)
1	PSU	1	239	1	18,21,22	4.69	7 (38%)	21,30,33	2.02	5 (23%)
1	OMU	1	845	1	19,22,23	3.04	8 (42%)	25,31,34	2.44	9 (36%)
1	PSU	1	1171	1	18,21,22	4.61	8 (44%)	21,30,33	1.89	4 (19%)
28	OMG	S1	1647	28	23,26,27	2.46	8 (34%)	32,38,41	2.14	10 (31%)
3	OMU	3	13	3	19,22,23	3.09	8 (42%)	25,31,34	1.79	5 (20%)
2	OMC	2	1317	2	19,22,23	2.97	8 (42%)	25,31,34	0.78	0
7	PSU	7	74	7	18,21,22	4.68	7 (38%)	21,30,33	1.90	5 (23%)
28	5MC	S1	2061	28	19,22,23	3.86	8 (42%)	26,32,35	0.98	3 (11%)
28	5MC	S1	1544	28	19,22,23	3.89	8 (42%)	26,32,35	0.99	1 (3%)
28	OMU	S1	29	28	19,22,23	3.11	8 (42%)	25,31,34	1.78	5 (20%)
1	PSU	1	422	1	18,21,22	4.69	7 (38%)	21,30,33	1.92	5 (23%)
2	PSU	2	1403	2	18,21,22	4.69	7 (38%)	21,30,33	2.02	6 (28%)
1	A2M	1	681	1	22,25,26	0.23	0	30,36,39	0.34	0
28	OMU	S1	1979	28	19,22,23	3.13	8 (42%)	25,31,34	1.76	5 (20%)
2	5MC	2	524	2,87	19,22,23	3.84	8 (42%)	26,32,35	0.99	2 (7%)
2	OMG	2	1078	2	23,26,27	2.80	7 (30%)	32,38,41	2.34	10 (31%)
2	PSU	2	1413	2	18,21,22	4.66	7 (38%)	21,30,33	1.89	5 (23%)
2	A2M	2	570	1,2	22,25,26	0.24	0	30,36,39	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	2	1058	2	18,21,22	4.61	7 (38%)	21,30,33	1.80	4 (19%)
28	PSU	S1	1657	28	18,21,22	4.65	7 (38%)	21,30,33	1.89	5 (23%)
28	OMG	S1	1879	28	23,26,27	2.47	8 (34%)	32,38,41	2.06	10 (31%)
28	PSU	S1	455	28	18,21,22	4.67	8 (44%)	21,30,33	1.81	5 (23%)
28	OMU	S1	1621	28	19,22,23	3.07	8 (42%)	25,31,34	1.82	5 (20%)
1	PSU	1	1533	1,2	18,21,22	4.69	7 (38%)	21,30,33	2.00	6 (28%)
1	A2M	1	235	1	22,25,26	3.49	9 (40%)	30,36,39	2.36	10 (33%)
2	PSU	2	593	2	18,21,22	4.67	8 (44%)	21,30,33	1.85	5 (23%)
7	OMG	7	75	7	23,26,27	2.43	8 (34%)	32,38,41	2.11	10 (31%)
28	OMG	S1	600	28	23,26,27	2.49	8 (34%)	32,38,41	2.05	10 (31%)
1	A2M	1	407	1	22,25,26	3.49	9 (40%)	30,36,39	2.39	12 (40%)
28	OMG	S1	1550	28	23,26,27	2.47	8 (34%)	32,38,41	2.12	10 (31%)
2	OMG	2	1231	2	23,26,27	2.46	8 (34%)	32,38,41	2.08	10 (31%)

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
28	PSU	S1	607	28	-	3/7/25/26	0/2/2/2
1	OMC	1	1010	1	-	1/9/27/28	0/2/2/2
28	PSU	S1	2202	28	-	1/7/25/26	0/2/2/2
28	OMG	S1	1829	28,87	-	1/9/27/28	0/3/3/3
2	OMC	2	1397	2	-	0/9/27/28	0/2/2/2
1	PSU	1	1664	1	-	0/7/25/26	0/2/2/2
2	PSU	2	122	2	-	2/7/25/26	0/2/2/2
2	PSU	2	437	2	-	0/7/25/26	0/2/2/2
1	OMG	1	1540	1,2	-	2/9/27/28	0/3/3/3
1	PSU	1	940	1	-	0/7/25/26	0/2/2/2
2	PSU	2	1264	2	-	2/7/25/26	0/2/2/2
1	OMG	1	856	1	-	0/9/27/28	0/3/3/3
1	A2M	1	927	1	-	0/9/27/28	0/3/3/3
2	PSU	2	1194	2	-	0/7/25/26	0/2/2/2
2	OMG	2	534	2	-	2/9/27/28	0/3/3/3
28	A2M	S1	668	28,87	-	5/9/27/28	0/3/3/3
2	PSU	2	662	2,87	-	0/7/25/26	0/2/2/2
1	PSU	1	1011	1,2	-	2/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PSU	S1	2046	28	-	0/7/25/26	0/2/2/2
2	PSU	2	1265	2	-	0/7/25/26	0/2/2/2
2	OMG	2	655	2	-	1/9/27/28	0/3/3/3
2	PSU	2	1318	2	-	0/7/25/26	0/2/2/2
4	OMG	4	74	4	-	0/9/27/28	0/3/3/3
2	PSU	2	78	2	-	0/7/25/26	0/2/2/2
1	PSU	1	672	1,87	-	0/7/25/26	0/2/2/2
28	A2M	S1	2021	28	-	3/9/27/28	0/3/3/3
2	OMU	2	1359	2	-	0/9/27/28	0/2/2/2
28	OMU	S1	1833	28	-	1/9/27/28	0/2/2/2
1	OMG	1	1626	1	-	0/9/27/28	0/3/3/3
2	PSU	2	597	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1253	2	-	0/9/27/28	0/3/3/3
2	A2M	2	382	2	-	1/9/27/28	0/3/3/3
28	PSU	S1	609	28	-	0/7/25/26	0/2/2/2
28	OMG	S1	1623	28,87	-	1/9/27/28	0/3/3/3
28	PSU	S1	1533	28	-	0/7/25/26	0/2/2/2
1	1MA	1	677	1,87	-	2/7/25/26	0/3/3/3
2	PSU	2	510	2	-	0/7/25/26	0/2/2/2
28	A2M	S1	512	28	-	1/9/27/28	0/3/3/3
28	B8N	S1	1543	28	-	8/16/34/35	0/2/2/2
2	PSU	2	1354	2	-	1/7/25/26	0/2/2/2
28	OMG	S1	2151	28,89	-	2/9/27/28	0/3/3/3
28	MA6	S1	2184	28	-	0/11/29/30	0/3/3/3
2	PSU	2	1144	2	-	0/7/25/26	0/2/2/2
2	OMU	2	73	2	-	0/9/27/28	0/2/2/2
2	OMG	2	1360	2	-	1/9/27/28	0/3/3/3
28	OMC	S1	38	28	-	0/9/27/28	0/2/2/2
2	OMG	2	71	2	-	0/9/27/28	0/3/3/3
2	OMG	2	641	2,87	-	0/9/27/28	0/3/3/3
1	OMC	1	1527	1	-	1/9/27/28	0/2/2/2
2	A2M	2	1185	2	-	3/9/27/28	0/3/3/3
2	5MC	2	1308	2	-	4/7/25/26	0/2/2/2
28	PSU	S1	12	28	-	0/7/25/26	0/2/2/2
2	PSU	2	1361	2	-	1/7/25/26	0/2/2/2
1	PSU	1	1017	1	-	0/7/25/26	0/2/2/2
2	OMG	2	1229	2	-	2/9/27/28	0/3/3/3
1	A2M	1	678	1,2	-	2/9/27/28	0/3/3/3
28	PSU	S1	1246	28	-	0/7/25/26	0/2/2/2
1	OMG	1	1190	1	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	2	628	2	-	0/9/27/28	0/3/3/3
2	OMC	2	359	2	-	0/9/27/28	0/2/2/2
2	A2M	2	527	2,87	-	2/9/27/28	0/3/3/3
2	OMU	2	560	2,87	-	2/9/27/28	0/2/2/2
2	A2M	2	591	2	-	1/9/27/28	0/3/3/3
28	PSU	S1	1841	28	-	2/7/25/26	0/2/2/2
2	PSU	2	1060	2	-	0/7/25/26	0/2/2/2
1	OMU	1	1371	1	-	3/9/27/28	0/2/2/2
1	OMU	1	1107	1	-	0/9/27/28	0/2/2/2
2	PSU	2	472	2	-	0/7/25/26	0/2/2/2
1	A2M	1	858	1	-	0/9/27/28	0/3/3/3
1	PSU	1	1528	1	-	0/7/25/26	0/2/2/2
28	OMG	S1	1478	28	-	1/9/27/28	0/3/3/3
2	OMG	2	1046	2	-	3/9/27/28	0/3/3/3
2	OMC	2	583	2	-	0/9/27/28	0/2/2/2
28	PSU	S1	104	28	-	0/7/25/26	0/2/2/2
1	OMG	1	959	1	-	0/9/27/28	0/3/3/3
2	OMC	2	443	2	-	4/9/27/28	0/2/2/2
28	A2M	S1	479	28	-	0/9/27/28	0/3/3/3
2	A2M	2	1372	2	-	0/9/27/28	0/3/3/3
2	OMU	2	1077	2	-	0/9/27/28	0/2/2/2
7	PSU	7	69	7	-	0/7/25/26	0/2/2/2
7	A2M	7	162	1,7	-	1/9/27/28	0/3/3/3
28	PSU	S1	1566	28	-	2/7/25/26	0/2/2/2
7	OMU	7	7	1,7	-	1/9/27/28	0/2/2/2
28	OMC	S1	18	28	-	0/9/27/28	0/2/2/2
2	A2M	2	604	1,2	-	0/9/27/28	0/3/3/3
28	PSU	S1	1192	28	-	2/7/25/26	0/2/2/2
1	OMU	1	1659	1	-	0/9/27/28	0/2/2/2
28	OMU	S1	8	28,87	-	7/9/27/28	0/2/2/2
1	PSU	1	1181	1	-	2/7/25/26	0/2/2/2
2	OMU	2	56	1,2	-	0/9/27/28	0/2/2/2
28	OMC	S1	1866	28	-	0/9/27/28	0/2/2/2
2	PSU	2	1303	2	-	0/7/25/26	0/2/2/2
28	A2M	S1	98	28,87	-	2/9/27/28	0/3/3/3
1	OMC	1	695	1	-	0/9/27/28	0/2/2/2
2	OMU	2	667	2	-	0/9/27/28	0/2/2/2
7	A2M	7	43	7	-	0/9/27/28	0/3/3/3
1	A2M	1	955	1	-	1/9/27/28	0/3/3/3
2	A2M	2	1384	2,87	-	1/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	7MG	S1	1995	28	-	2/7/37/38	0/3/3/3
2	PSU	2	1382	2	-	0/7/25/26	0/2/2/2
1	PSU	1	1402	1	-	0/7/25/26	0/2/2/2
28	OMG	S1	1865	28	-	0/9/27/28	0/3/3/3
28	OMC	S1	2140	28	-	0/9/27/28	0/2/2/2
28	PSU	S1	1156	28	-	0/7/25/26	0/2/2/2
1	A2M	1	1539	1,2,87	-	1/9/27/28	0/3/3/3
1	PSU	1	1039	1	-	0/7/25/26	0/2/2/2
2	OMC	2	1159	2	-	0/9/27/28	0/2/2/2
28	MA6	S1	2185	28	-	1/11/29/30	0/3/3/3
2	PSU	2	626	2	-	0/7/25/26	0/2/2/2
1	OMU	1	847	1	-	0/9/27/28	0/2/2/2
2	OMU	2	1419	2	-	0/9/27/28	0/2/2/2
2	PSU	2	512	2	-	0/7/25/26	0/2/2/2
28	PSU	S1	1539	28	-	0/7/25/26	0/2/2/2
28	OMU	S1	661	28	-	0/9/27/28	0/2/2/2
28	PSU	S1	2048	28	-	0/7/25/26	0/2/2/2
2	OMC	2	1248	2	-	2/9/27/28	0/2/2/2
1	OMG	1	1524	1	-	0/9/27/28	0/3/3/3
1	A2M	1	697	1	-	0/9/27/28	0/3/3/3
2	A2M	2	572	2	-	0/9/27/28	0/3/3/3
2	A2M	2	95	2	-	0/9/27/28	0/3/3/3
1	A2M	1	305	1	-	2/9/27/28	0/3/3/3
28	PSU	S1	33	28	-	0/7/25/26	0/2/2/2
1	PSU	1	239	1	-	0/7/25/26	0/2/2/2
1	OMU	1	845	1	-	3/9/27/28	0/2/2/2
1	PSU	1	1171	1	-	4/7/25/26	0/2/2/2
28	OMG	S1	1647	28	-	0/9/27/28	0/3/3/3
3	OMU	3	13	3	-	0/9/27/28	0/2/2/2
2	OMC	2	1317	2	-	0/9/27/28	0/2/2/2
7	PSU	7	74	7	-	0/7/25/26	0/2/2/2
28	5MC	S1	2061	28	-	0/7/25/26	0/2/2/2
28	5MC	S1	1544	28	-	2/7/25/26	0/2/2/2
28	OMU	S1	29	28	-	1/9/27/28	0/2/2/2
1	PSU	1	422	1	-	0/7/25/26	0/2/2/2
2	PSU	2	1403	2	-	0/7/25/26	0/2/2/2
1	A2M	1	681	1	-	3/9/27/28	0/3/3/3
28	OMU	S1	1979	28	-	3/9/27/28	0/2/2/2
2	5MC	2	524	2,87	-	0/7/25/26	0/2/2/2
2	OMG	2	1078	2	-	2/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	2	1413	2	-	0/7/25/26	0/2/2/2
2	A2M	2	570	1,2	-	4/9/27/28	0/3/3/3
2	PSU	2	1058	2	-	2/7/25/26	0/2/2/2
28	PSU	S1	1657	28	-	1/7/25/26	0/2/2/2
28	OMG	S1	1879	28	-	3/9/27/28	0/3/3/3
28	PSU	S1	455	28	-	3/7/25/26	0/2/2/2
28	OMU	S1	1621	28	-	1/9/27/28	0/2/2/2
1	PSU	1	1533	1,2	-	0/7/25/26	0/2/2/2
1	A2M	1	235	1	-	0/9/27/28	0/3/3/3
2	PSU	2	593	2	-	0/7/25/26	0/2/2/2
7	OMG	7	75	7	-	1/9/27/28	0/3/3/3
28	OMG	S1	600	28	-	0/9/27/28	0/3/3/3
1	A2M	1	407	1	-	0/9/27/28	0/3/3/3
28	OMG	S1	1550	28	-	0/9/27/28	0/3/3/3
2	OMG	2	1231	2	-	0/9/27/28	0/3/3/3

The worst 5 of 1144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1181	PSU	C6-C5	12.72	1.49	1.35
1	1	1664	PSU	C6-C5	12.60	1.49	1.35
1	1	1528	PSU	C6-C5	12.58	1.49	1.35
28	S1	1566	PSU	C6-C5	12.56	1.49	1.35
1	1	1171	PSU	C6-C5	12.55	1.49	1.35

The worst 5 of 946 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S1	2184	MA6	N1-C6-N6	-9.28	105.55	116.86
28	S1	2185	MA6	N1-C6-N6	-9.13	105.73	116.86
1	1	845	OMU	C4-N3-C2	-6.71	118.29	126.61
2	2	1078	OMG	C5-C4-N3	-6.52	118.01	128.39
2	2	572	A2M	N3-C2-N1	-6.09	119.37	128.58

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	7	7	OMU	C1'-C2'-O2'-CM2
7	7	75	OMG	C1'-C2'-O2'-CM2
7	7	162	A2M	C1'-C2'-O2'-CM'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1	681	A2M	O4'-C4'-C5'-O5'
1	1	845	OMU	O4'-C1'-N1-C2

There are no ring outliers.

77 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	S1	2202	PSU	1	0
2	2	122	PSU	2	0
1	1	1540	OMG	2	0
1	1	927	A2M	1	0
2	2	1194	PSU	1	0
2	2	534	OMG	1	0
28	S1	668	A2M	1	0
28	S1	2046	PSU	2	0
2	2	655	OMG	1	0
2	2	1318	PSU	1	0
2	2	1359	OMU	1	0
2	2	1253	OMG	1	0
2	2	382	A2M	5	0
28	S1	1623	OMG	1	0
28	S1	512	A2M	1	0
28	S1	1543	B8N	1	0
28	S1	2151	OMG	2	0
2	2	641	OMG	1	0
1	1	1527	OMC	1	0
2	2	1308	5MC	1	0
28	S1	12	PSU	1	0
1	1	1017	PSU	2	0
2	2	527	A2M	2	0
2	2	560	OMU	2	0
2	2	591	A2M	3	0
2	2	1060	PSU	1	0
2	2	472	PSU	1	0
1	1	1528	PSU	1	0
28	S1	1478	OMG	1	0
2	2	1046	OMG	1	0
2	2	583	OMC	1	0
28	S1	479	A2M	1	0
2	2	1372	A2M	1	0
7	7	162	A2M	2	0
7	7	7	OMU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	S1	18	OMC	1	0
2	2	604	A2M	2	0
28	S1	1192	PSU	1	0
28	S1	98	A2M	1	0
1	1	695	OMC	1	0
2	2	667	OMU	1	0
7	7	43	A2M	1	0
1	1	955	A2M	2	0
2	2	1384	A2M	1	0
2	2	1382	PSU	1	0
1	1	1402	PSU	1	0
28	S1	1865	OMG	1	0
28	S1	2140	OMC	3	0
1	1	1539	A2M	1	0
1	1	1039	PSU	1	0
28	S1	2185	MA6	3	0
2	2	626	PSU	1	0
1	1	847	OMU	1	0
2	2	512	PSU	3	0
2	2	1248	OMC	1	0
2	2	95	A2M	1	0
1	1	305	A2M	1	0
1	1	845	OMU	3	0
1	1	1171	PSU	3	0
28	S1	1647	OMG	1	0
3	3	13	OMU	1	0
28	S1	2061	5MC	1	0
28	S1	29	OMU	2	0
28	S1	1979	OMU	5	0
2	2	524	5MC	1	0
2	2	1078	OMG	1	0
2	2	1413	PSU	1	0
2	2	570	A2M	2	0
2	2	1058	PSU	1	0
28	S1	1879	OMG	1	0
28	S1	1621	OMU	1	0
1	1	1533	PSU	1	0
1	1	235	A2M	1	0
7	7	75	OMG	2	0
1	1	407	A2M	1	0
28	S1	1550	OMG	1	0
2	2	1231	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 270 ligands modelled in this entry, 270 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	7	1
28	S1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	169:A	O3'	170:A	P	4.55
1	S1	1543:B8N	O3'	1544:5MC	P	4.07

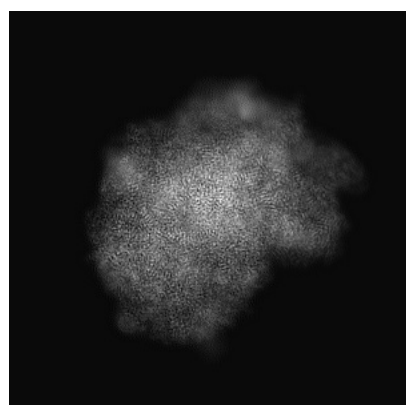
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18437. These allow visual inspection of the internal detail of the map and identification of artifacts.

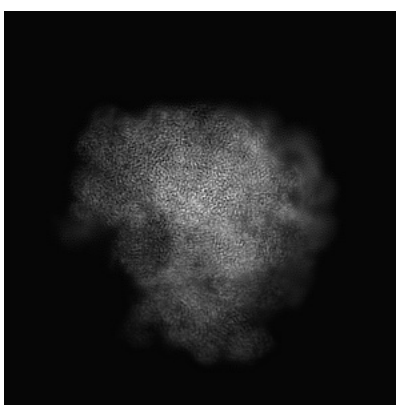
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

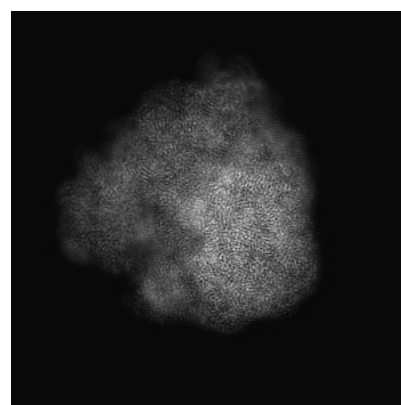
6.1.1 Primary map



X



Y

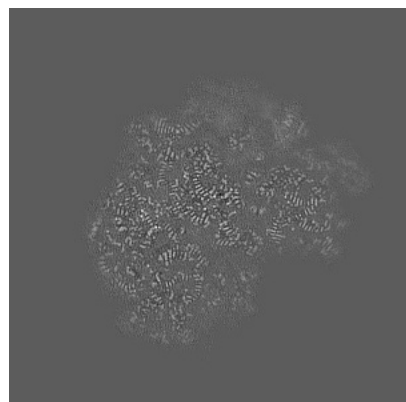


Z

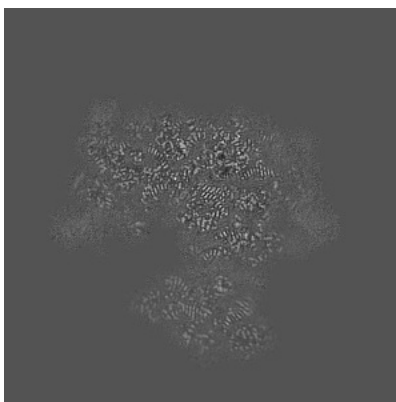
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

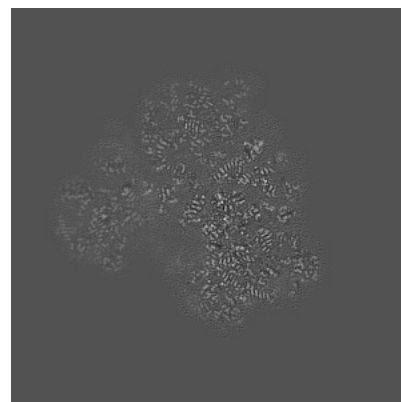
6.2.1 Primary map



X Index: 240



Y Index: 240

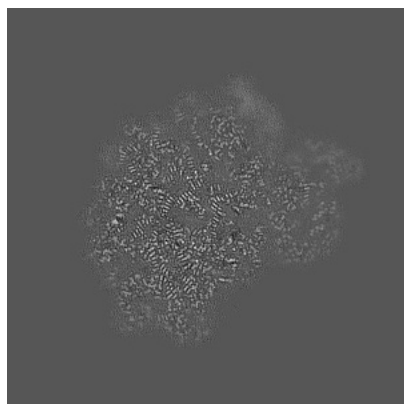


Z Index: 240

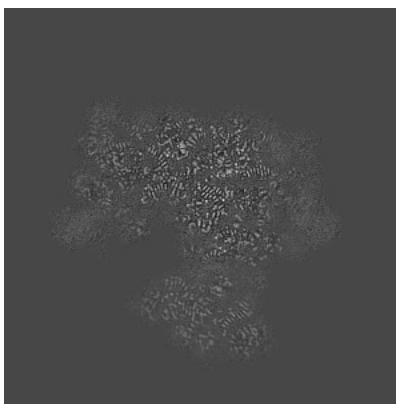
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

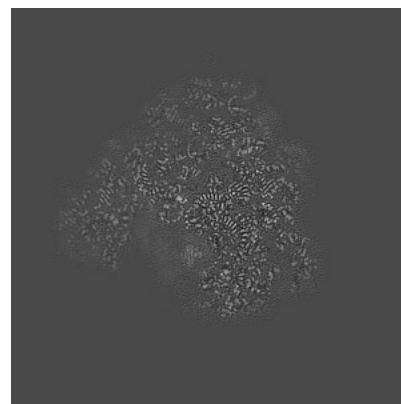
6.3.1 Primary map



X Index: 276



Y Index: 241

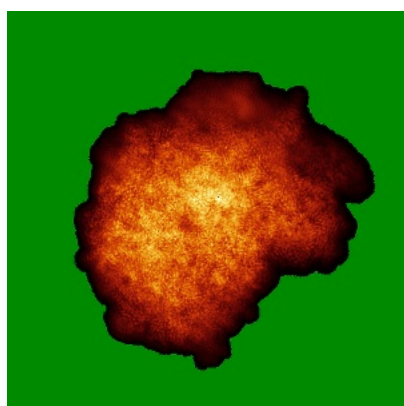


Z Index: 253

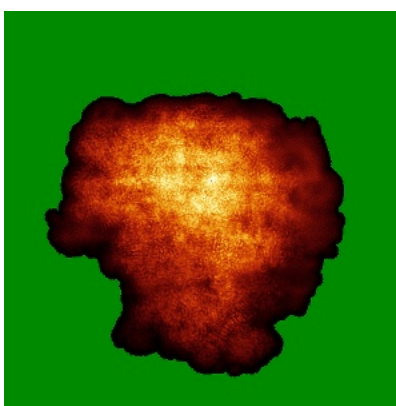
The images above show the largest variance slices of the map in three orthogonal directions.

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

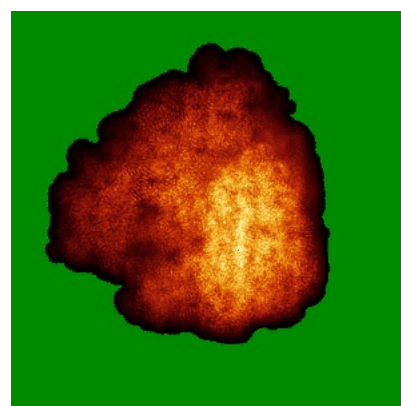
6.4.1 Primary map



X



Y

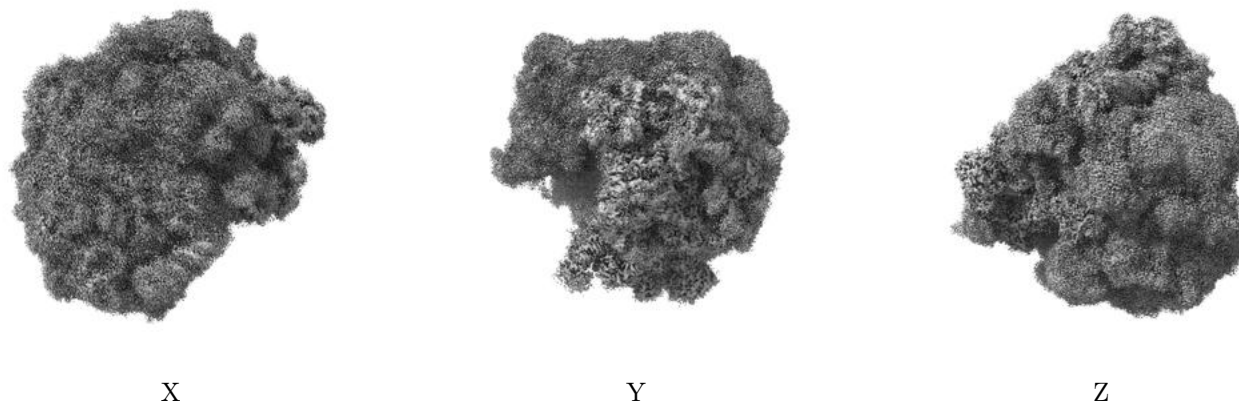


Z

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 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

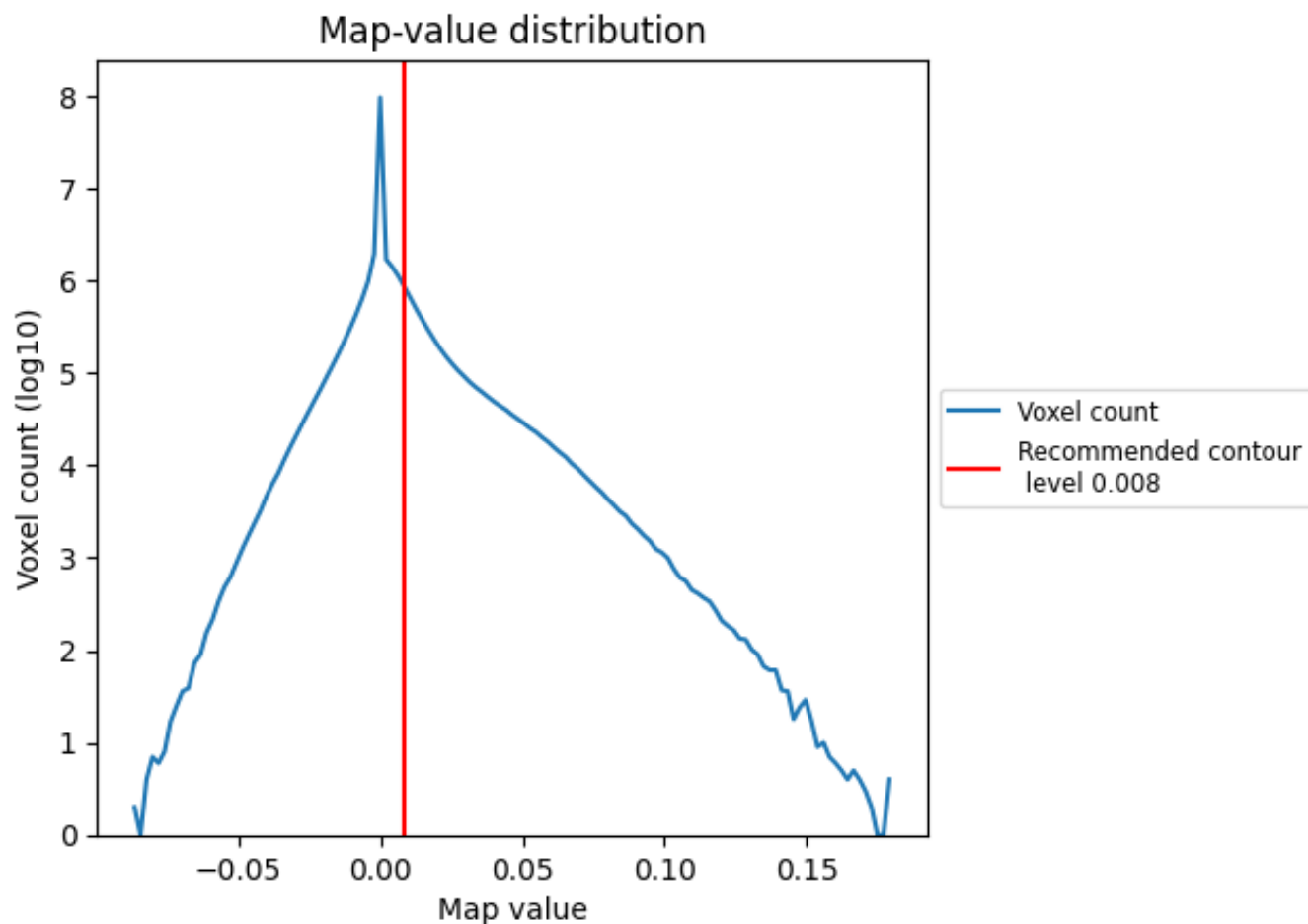
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

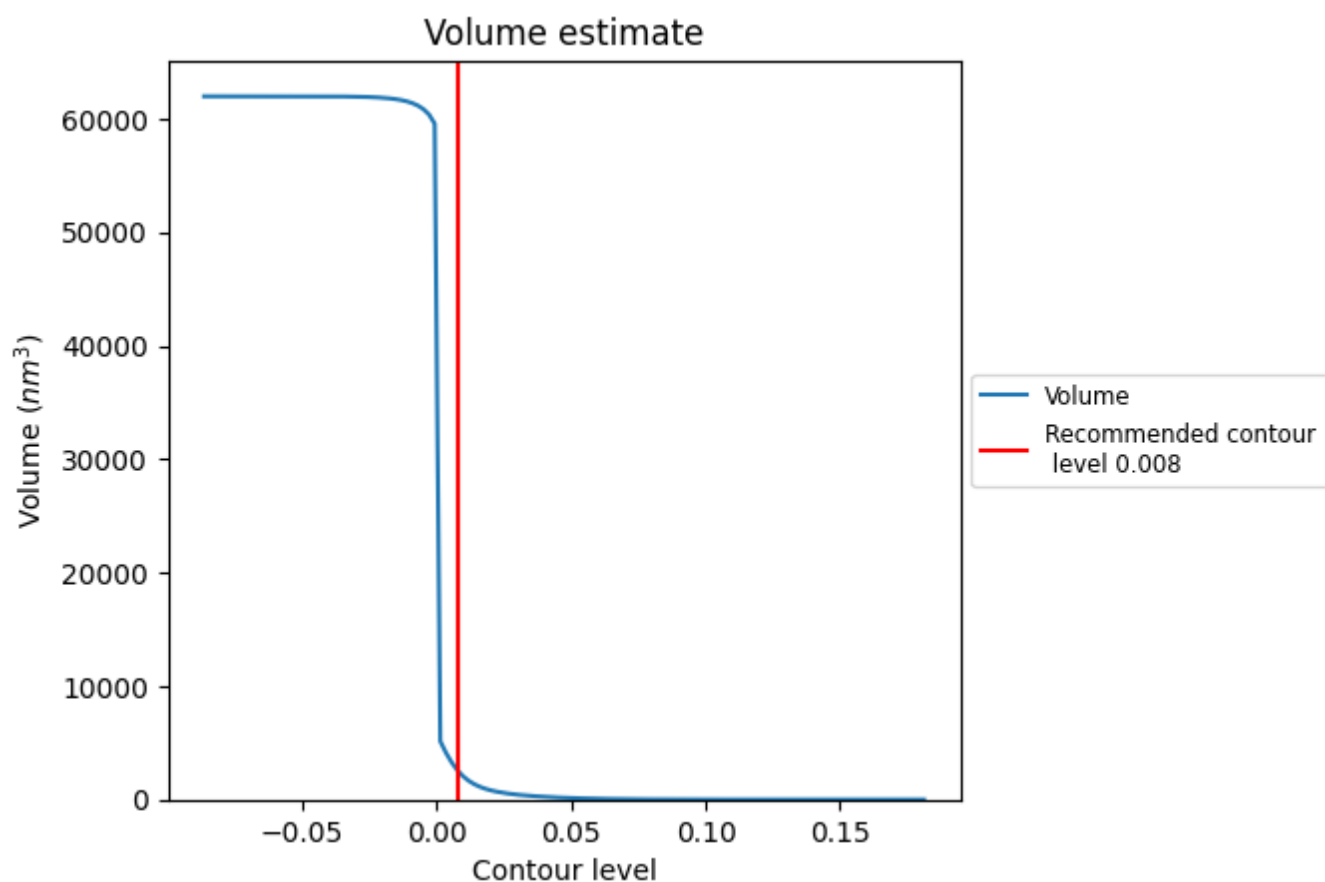
This section contains the results of statistical analysis of the map.

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.

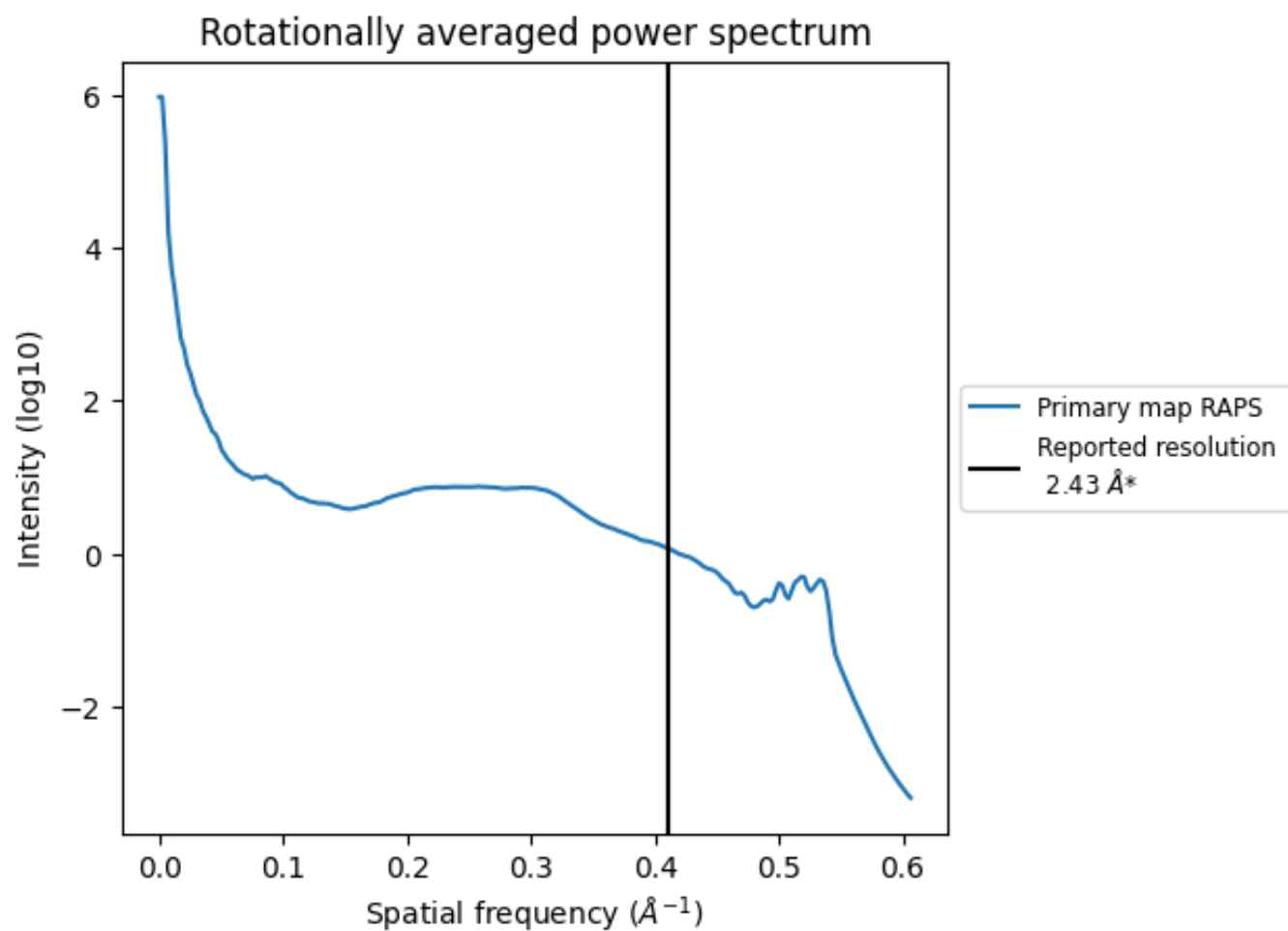
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2508 nm³; this corresponds to an approximate mass of 2266 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 ⓘ

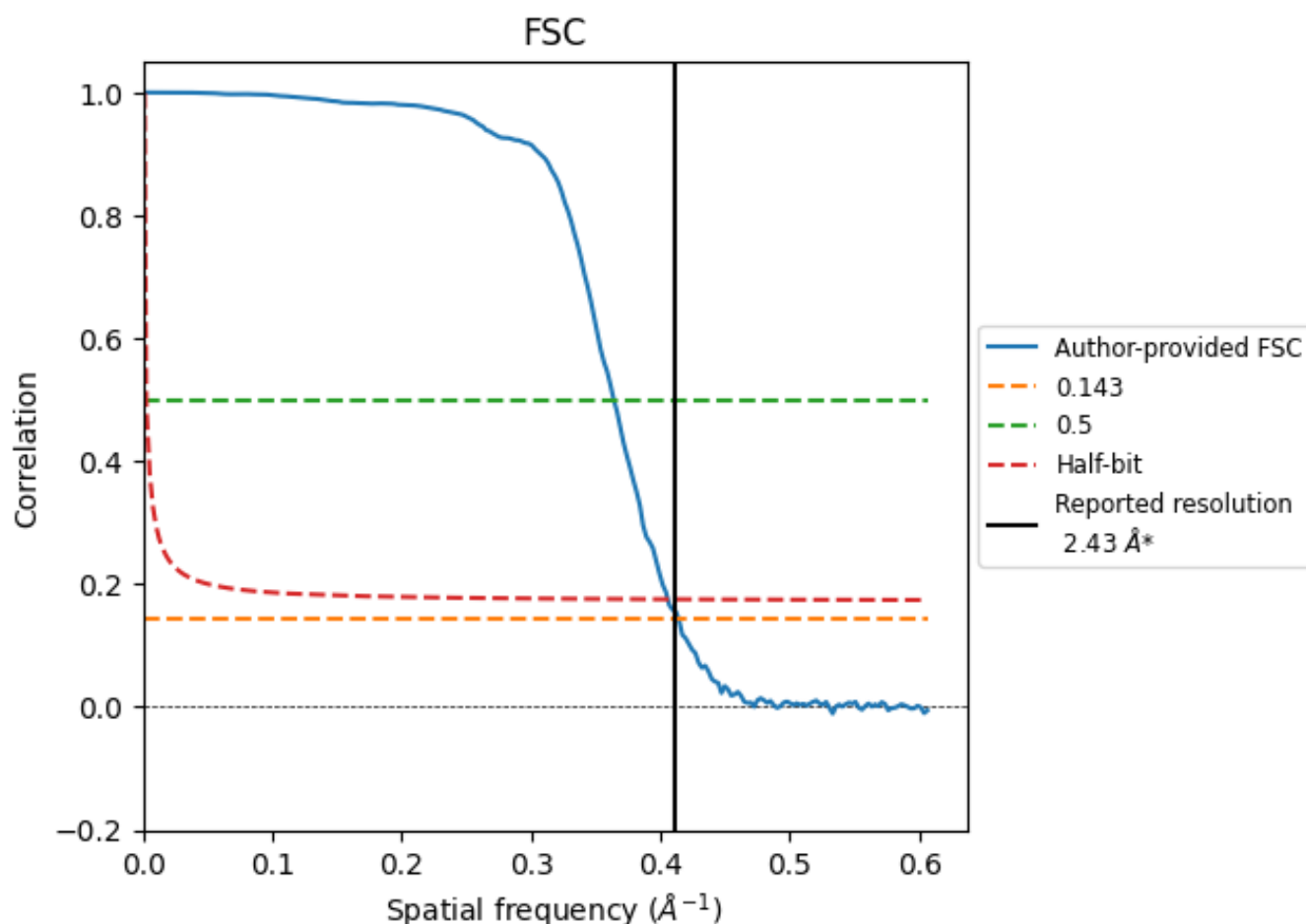


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

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 0.412 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.41	2.75	2.46
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

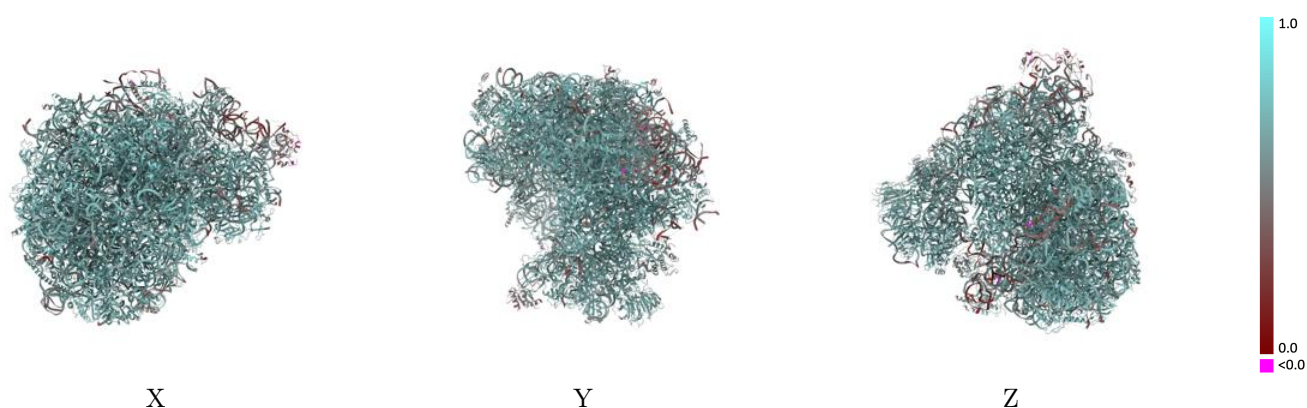
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18437 and PDB model 8QIE. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)

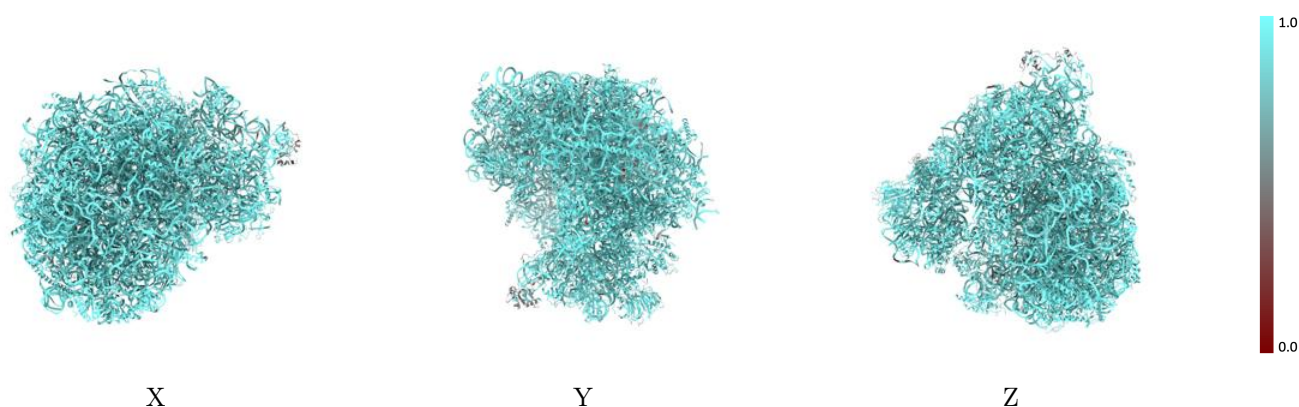
This section was not generated.

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



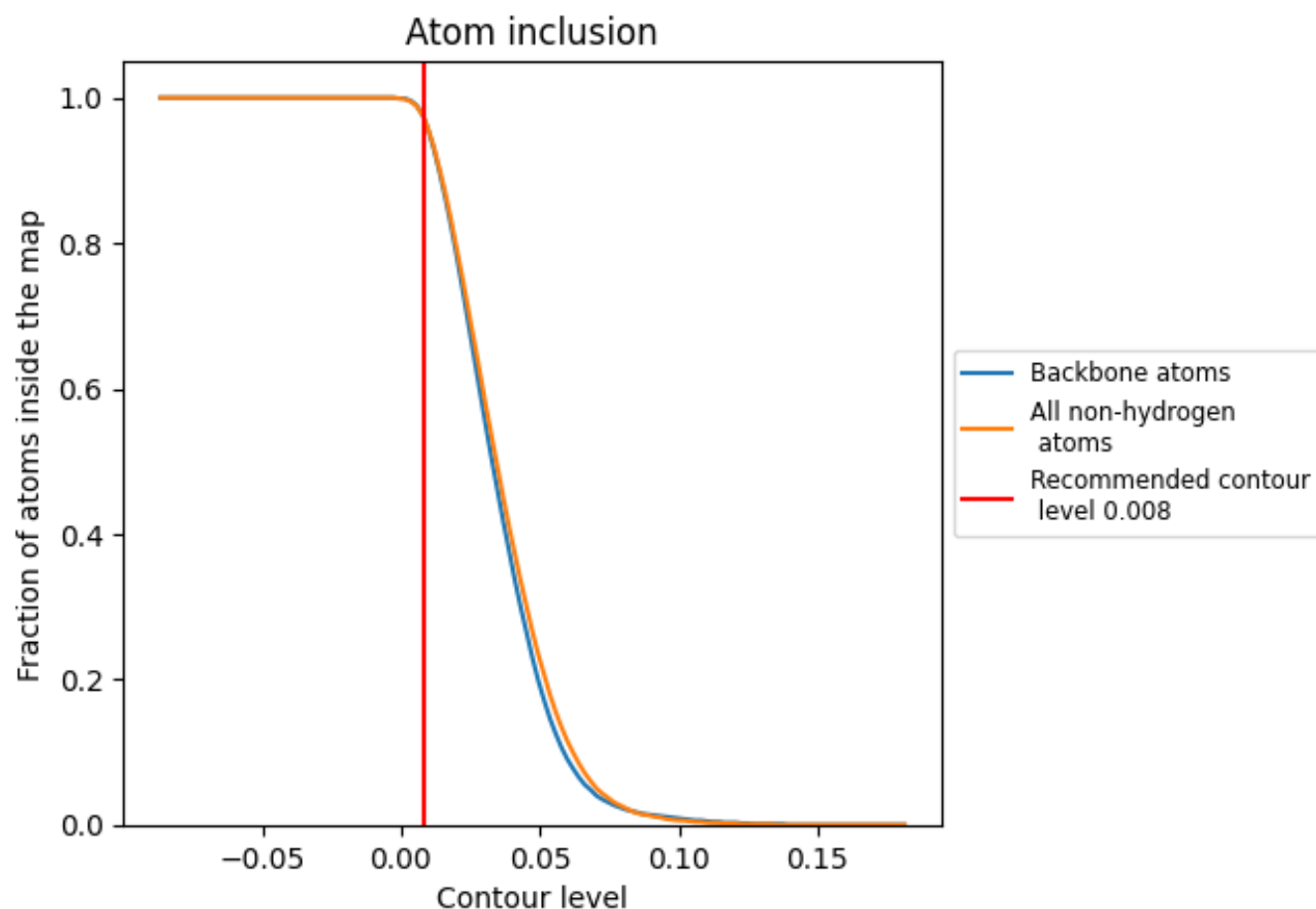
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.6550
1	 0.9840	 0.6640
2	 0.9790	 0.6420
3	 0.9870	 0.6550
4	 0.9860	 0.6700
5	 0.9770	 0.6550
6	 0.9680	 0.6310
7	 0.9890	 0.6700
8	 0.9970	 0.6660
A	 0.9980	 0.7320
B	 0.9960	 0.7300
C	 0.9930	 0.6930
D	 0.9650	 0.5600
E	 0.9830	 0.6460
F	 0.9780	 0.6620
G	 0.9930	 0.6890
H	 0.9960	 0.7200
I	 0.9880	 0.6780
J	 0.9930	 0.7180
K	 0.9750	 0.6560
L	 0.9950	 0.7090
M	 0.9990	 0.7250
N	 0.9740	 0.6390
O	 0.9830	 0.6470
P	 0.9980	 0.7030
Q	 0.9960	 0.6880
R	 0.9960	 0.7110
S	 0.9840	 0.6840
S1	 0.9720	 0.6350
S4	 0.7840	 0.2720
SA	 0.9780	 0.6600
SB	 0.9400	 0.5660
SC	 0.9420	 0.6230
SD	 0.9840	 0.6660
SE	 0.9760	 0.6720



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SF	 0.9640	 0.6660
SG	 0.9690	 0.6430
SH	 0.9830	 0.6710
SI	 0.9740	 0.6510
SJ	 0.9910	 0.7100
SK	 0.9800	 0.6710
SL	 0.9850	 0.6770
SM	 0.9270	 0.6290
SN	 0.9390	 0.6280
SO	 0.9930	 0.6870
SP	 0.9900	 0.6980
SQ	 0.5530	 0.4310
SR	 0.9460	 0.6300
SS	 0.9890	 0.6740
ST	 0.9960	 0.6970
SU	 0.9850	 0.6900
SV	 0.9840	 0.6580
SW	 0.9170	 0.6200
SX	 0.9640	 0.6570
SY	 0.9440	 0.6040
SZ	 0.9770	 0.6560
Sa	 0.9500	 0.6400
Sb	 0.9910	 0.7050
Sc	 0.9510	 0.6630
Sd	 0.9640	 0.6320
Se	 0.9950	 0.6520
Sf	 0.5610	 0.4380
Sg	 0.9430	 0.6280
Sh	 0.7140	 0.4000
T	 0.9960	 0.7300
U	 0.9350	 0.5420
V	 0.9980	 0.7070
W	 0.9950	 0.6870
X	 0.9980	 0.7150
Y	 0.9930	 0.6540
Z	 0.9820	 0.6660
a	 0.9870	 0.6650
b	 0.9850	 0.6810
c	 0.9930	 0.7020
d	 0.9930	 0.6750
e	 0.9790	 0.6840
f	 0.9970	 0.7070

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.9920	 0.7010
h	 0.9650	 0.6540
i	 0.9870	 0.6600
j	 0.9950	 0.7250
k	 0.9540	 0.6040
l	 0.9930	 0.7130
m	 0.9400	 0.5970
n	 0.9960	 0.6810
o	 0.9920	 0.7150
p	 0.9710	 0.6610