



## wwPDB EM Validation Summary Report ⓘ

Jun 19, 2026 – 07:40 am BST

PDB ID : 9RU8 / pdb\_00009ru8  
EMDB ID : EMD-54266  
Title : WT-HEK 80S ribosome bound to TISU mRNA (WT-TISU)  
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.  
Deposited on : 2025-07-03  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

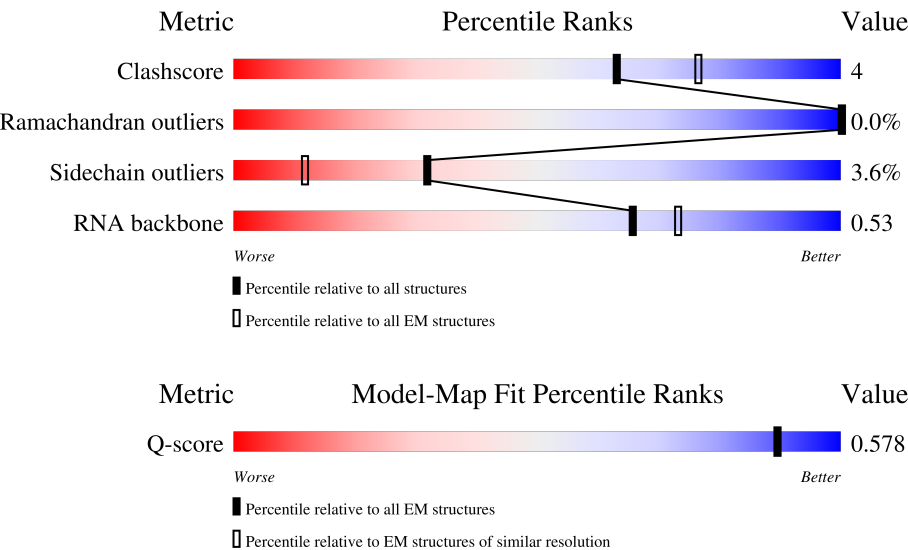
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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 3.00 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.








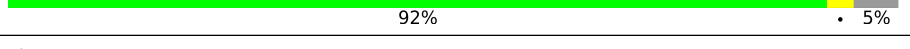
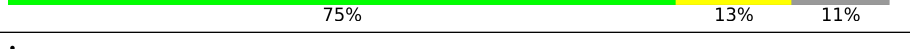
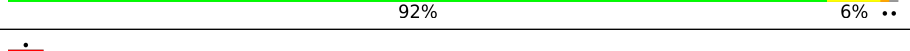
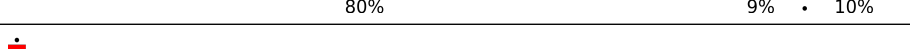
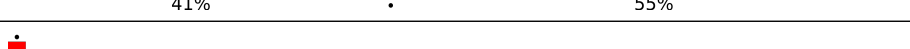
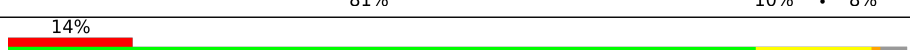

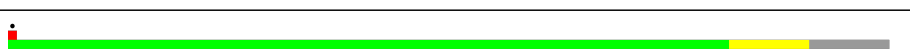







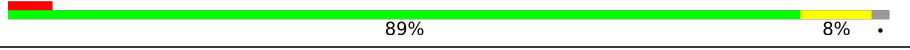
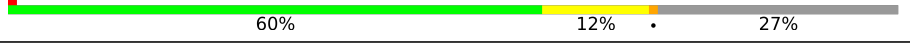



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Lm	128	<div><div>35%5%60%</div></div>
2	Ll	51	<div><div>75%20%.</div></div>
3	Lo	106	<div><div>83%15%..</div></div>







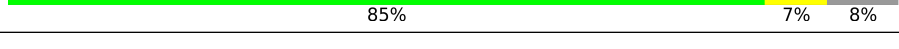
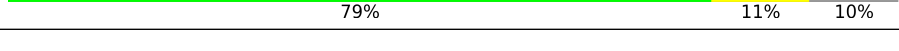
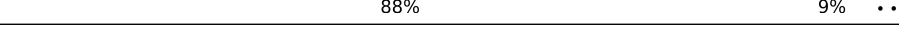
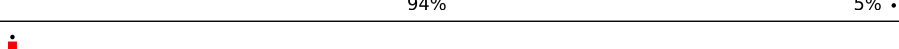
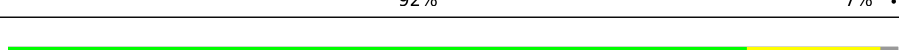

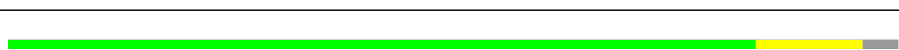

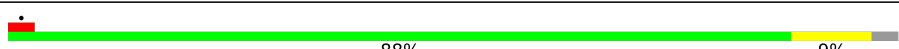





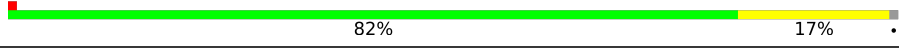
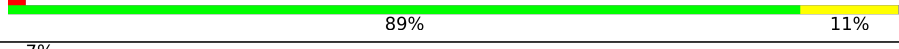



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Mol	Chain	Length	Quality of chain
4	SY	133	
5	SX	143	
6	SW	130	
7	SV	83	
8	SR	135	
9	SQ	146	
10	SO	151	
11	SN	151	
12	SL	158	
13	SK	165	
14	SJ	194	
15	SH	194	
16	Sg	317	
17	SF	204	
18	SE	263	
19	Se	133	
20	SD	243	
21	Sd	56	
22	SC	293	
23	Sc	69	
24	SB	264	
25	Sb	84	
26	SA	295	
27	LZ	136	
28	LY	145	













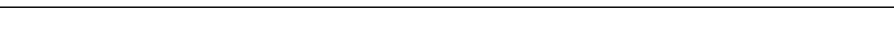

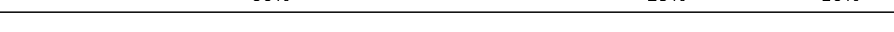

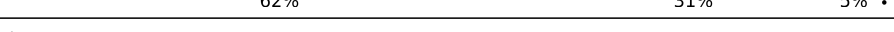







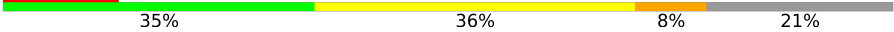
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Mol	Chain	Length	Quality of chain
29	LX	156	
30	LW	157	
31	LV	140	
32	LU	128	
33	LT	160	
34	LS	176	
35	LR	196	
36	Lr	137	
37	LQ	188	
38	LP	154	
39	Lp	91	
40	LO	203	
41	LN	204	
42	Ln	25	
43	LM	215	
44	LL	211	
45	Lk	70	
46	LJ	178	
47	Lj	97	
48	LI	214	
49	Li	105	
50	LH	192	
51	Lh	123	
52	LG	266	
53	Lg	112	



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Mol	Chain	Length	Quality of chain
54	LF	248	
55	Lf	111	
56	LE	288	
57	Le	135	
58	LD	297	
59	Ld	125	
60	LC	427	
61	Lc	115	
62	LB	397	
63	Lb	159	
64	LA	257	
65	La	148	
66	L7	119	
67	Pt	77	
68	Sa	115	
69	L8	156	
70	L5	5069	
71	SZ	125	
72	ST	145	
73	SP	145	
74	S2	1869	
75	SG	249	
76	SI	208	
77	S6	75	
78	SS	152	

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Mol	Chain	Length	Quality of chain
79	mR	27	
80	SU	119	

## 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 201487 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 protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Lm	51	Total	C	N	O	S	0	0
			407	251	87	63	6		

- Molecule 2 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ll	50	Total	C	N	O	S	0	0
			434	275	94	64	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ll	34	ILE	LYS	conflict	UNP P62891

- Molecule 3 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Lo	105	Total	C	N	O	S	0	0
			822	516	166	134	6		

- Molecule 4 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SY	123	Total	C	N	O	S	0	0
			900	565	181	151	3		

- Molecule 5 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SX	141	Total	C	N	O	S	0	0
			1060	669	214	174	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SX	62	HIS	PRO	conflict	UNP P62266

- Molecule 6 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SW	129	Total	C	N	O	S	0	0
			1023	653	192	172	6		

- Molecule 7 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SV	83	Total	C	N	O	S	0	0
			623	388	117	113	5		

- Molecule 8 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SR	132	Total	C	N	O	S	0	0
			936	591	173	169	3		

- Molecule 9 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SQ	139	Total	C	N	O	S	0	0
			918	570	181	166	1		

- Molecule 10 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SO	134	Total	C	N	O	S	0	0
			977	600	196	175	6		

- Molecule 11 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SN	150	Total	C	N	O	S	0	0
			1186	761	221	203	1		

- Molecule 12 is a protein called Small ribosomal subunit protein uS17.



Mol	Chain	Residues	Atoms					AltConf	Trace
12	SL	142	Total	C	N	O	S	0	0
			1158	737	218	197	6		

- Molecule 13 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SK	74	Total	C	N	O	S	0	0
			468	302	86	79	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SK	68	PHE	TYR	conflict	UNP P46783

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SJ	178	Total	C	N	O	S	0	0
			1430	915	285	228	2		

- Molecule 15 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SH	189	Total	C	N	O	S	0	0
			1408	905	263	239	1		

- Molecule 16 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Sg	241	Total	C	N	O		0	0
			1259	757	255	247			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Sg	155	PHE	ARG	conflict	UNP P63244

- Molecule 17 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SF	185	Total	C	N	O	S	0	0
			1327	835	251	238	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SF	15	LYS	PRO	conflict	UNP P46782

- Molecule 18 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SE	260	Total	C	N	O	S	0	0
			2037	1304	383	342	8		

- Molecule 19 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Se	51	Total	C	N	O	S	0	0
			399	243	90	65	1		

- Molecule 20 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SD	175	Total	C	N	O	S	0	0
			1094	689	201	201	3		

- Molecule 21 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Sd	55	Total	C	N	O	S	0	0
			430	270	87	68	5		

- Molecule 22 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SC	220	Total	C	N	O	S	0	0
			1694	1097	292	295	10		

- Molecule 23 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sc	61	Total	C	N	O	S	0	0
			434	264	87	81	2		

- Molecule 24 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SB	212	Total	C	N	O	S	1	0
			1694	1078	306	295	15		

- Molecule 25 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Sb	82	Total	C	N	O	S	0	0
			613	383	113	110	7		

- Molecule 26 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SA	215	Total	C	N	O	S	0	0
			1658	1056	292	303	7		

- Molecule 27 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LZ	135	Total	C	N	O	S	0	0
			1095	709	207	176	3		

- Molecule 28 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LY	133	Total	C	N	O	S	0	0
			1060	666	215	176	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LY	52	LYS	ASP	conflict	UNP P61254

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 30 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LW	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 31 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LV	131	Total	C	N	O	S	1	0
			987	623	187	172	5		

- Molecule 32 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LU	99	Total	C	N	O	S	0	0
			800	513	140	145	2		

- Molecule 33 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LT	159	Total	C	N	O	S	0	0
			1297	823	252	216	6		

- Molecule 34 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LS	176	Total	C	N	O	S	0	0
			1456	927	283	235	11		

- Molecule 35 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LR	181	Total	C	N	O	S	0	0
			1458	903	312	234	9		

- Molecule 36 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lr	123	Total	C	N	O	S	0	0
			987	612	205	166	4		

- Molecule 37 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LQ	187	Total	C	N	O	S	0	0
			1505	940	312	248	5		

- Molecule 38 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LP	153	Total	C	N	O	S	0	0
			1230	769	240	212	9		

- Molecule 39 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lp	90	Total	C	N	O	S	0	0
			695	439	134	115	7		

- Molecule 40 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LO	199	Total	C	N	O	S	0	0
			1620	1044	318	253	5		

- Molecule 41 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LN	203	Total	C	N	O	S	0	0
			1694	1069	356	265	4		

- Molecule 42 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	24	Total	C	N	O	S	0	0
			235	142	65	25	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ln	24	ARG	SER	conflict	UNP P62945

- Molecule 43 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LM	136	Total	C	N	O	S	0	0
			1116	716	214	179	7		

- Molecule 44 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LL	205	Total	C	N	O	S	0	0
			1638	1026	342	266	4		

- Molecule 45 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lk	69	Total	C	N	O	S	0	0
			557	358	101	97	1		

- Molecule 46 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LJ	169	Total	C	N	O	S	0	0
			1329	843	246	234	6		

- Molecule 47 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lj	86	Total	C	N	O	S	0	0
			701	432	154	110	5		

- Molecule 48 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LI	203	Total	C	N	O	S	0	0
			1632	1038	314	267	13		

- Molecule 49 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Li	102	Total	C	N	O	S	0	0
			812	509	171	127	5		

- Molecule 50 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LH	190	Total	C	N	O	S	0	0
			1499	946	281	266	6		

- Molecule 51 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lh	122	Total	C	N	O	S	0	0
			1010	638	204	167	1		

- Molecule 52 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LG	228	Total	C	N	O	S	0	0
			1791	1142	346	299	4		

- Molecule 53 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lg	110	Total	C	N	O	S	1	0
			871	545	181	139	6		

- Molecule 54 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LF	225	Total	C	N	O	S	0	0
			1835	1178	350	298	9		

- Molecule 55 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lf	109	Total	C	N	O	S	0	0
			868	549	173	143	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lf	111	LYS	-	expression tag	UNP P18077

- Molecule 56 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LE	217	Total	C	N	O	S	1	0
			1721	1108	327	282	4		

- Molecule 57 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Le	127	Total	C	N	O	S	0	0
			1044	660	215	164	5		

- Molecule 58 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LD	292	Total	C	N	O	S	0	0
			2354	1487	429	424	14		

- Molecule 59 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ld	106	Total	C	N	O	S	0	0
			840	534	165	139	2		

- Molecule 60 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LC	359	Total	C	N	O	S	0	0
			2862	1802	572	475	13		

- Molecule 61 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Lc	98	Total	C	N	O	S	0	0
			760	482	134	138	6		

- Molecule 62 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LB	396	Total	C	N	O	S	0	0
			3174	2022	597	542	13		

- Molecule 63 is a protein called Large ribosomal subunit protein eL29.



Mol	Chain	Residues	Atoms					AltConf	Trace
63	Lb	101	Total	C	N	O	S	0	0
			815	506	178	127	4		

- Molecule 64 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LA	248	Total	C	N	O	S	1	0
			1899	1190	389	314	6		

- Molecule 65 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	La	147	Total	C	N	O	S	0	0
			1157	732	236	186	3		

- Molecule 66 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	L7	119	Total	C	N	O	P	0	0
			2542	1132	454	837	119		

- Molecule 67 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	Pt	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

- Molecule 68 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Sa	99	Total	C	N	O	S	0	0
			775	484	159	128	4		

- Molecule 69 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	L8	153	Total	C	N	O	P	0	0
			3256	1453	574	1076	153		

- Molecule 70 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	L5	3446	Total	C	N	O	P	1	0
			73960	32974	13527	24012	3447		

- Molecule 71 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	SZ	63	Total	C	N	O	0	0
			383	245	69	69		

- Molecule 72 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	ST	129	Total	C	N	O	S	0	0
			837	529	163	143	2		

- Molecule 73 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SP	126	Total	C	N	O	S	0	0
			806	504	155	144	3		

- Molecule 74 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	S2	1569	Total	C	N	O	P	0	0
			33557	15003	6040	10945	1569		

- Molecule 75 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SG	220	Total	C	N	O	S	0	0
			1663	1043	329	284	7		

- Molecule 76 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SI	206	Total	C	N	O	S	0	0
			1648	1035	326	282	5		

- Molecule 77 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	S6	59	Total	C	N	O	P	0	0
			1263	565	238	402	58		

- Molecule 78 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SS	138	Total	C	N	O		0	0
			903	565	178	160			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SS	115	ILE	LYS	conflict	UNP P62269
SS	117	ALA	ILE	conflict	UNP P62269
SS	119	PHE	ALA	conflict	UNP P62269

- Molecule 79 is a RNA chain called TISU mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	mR	7	Total	C	N	O	P	0	0
			152	68	30	47	7		

- Molecule 80 is a protein called 40S ribosomal protein S20.

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

- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	Lm	1	Total	Zn	0
			1	1	
81	Lo	1	Total	Zn	0
			1	1	
81	Sd	1	Total	Zn	0
			1	1	
81	Lp	1	Total	Zn	0
			1	1	
81	Lg	1	Total	Zn	0
			1	1	

- Molecule 82 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
82	SQ	1	Total K 1 1	0
82	Lf	1	Total K 1 1	0
82	LC	1	Total K 1 1	0
82	LB	1	Total K 1 1	0
82	L8	1	Total K 1 1	0
82	L5	60	Total K 60 60	0
82	S2	11	Total K 11 11	0

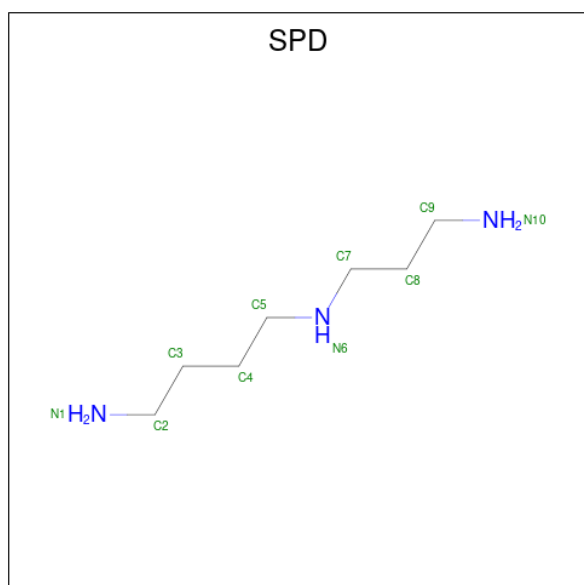
- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
83	Sd	1	Total Mg 1 1	0
83	LV	1	Total Mg 1 1	0
83	LS	1	Total Mg 1 1	0
83	LP	1	Total Mg 1 1	0
83	LM	1	Total Mg 1 1	0
83	LI	2	Total Mg 2 2	0
83	Le	1	Total Mg 1 1	0
83	LB	1	Total Mg 1 1	0
83	L7	5	Total Mg 5 5	0
83	Pt	1	Total Mg 1 1	0
83	L8	3	Total Mg 3 3	0
83	L5	81	Total Mg 81 81	0
83	S2	21	Total Mg 21 21	0

- Molecule 84 is SODIUM ION (CCD ID: NA) (formula: Na).

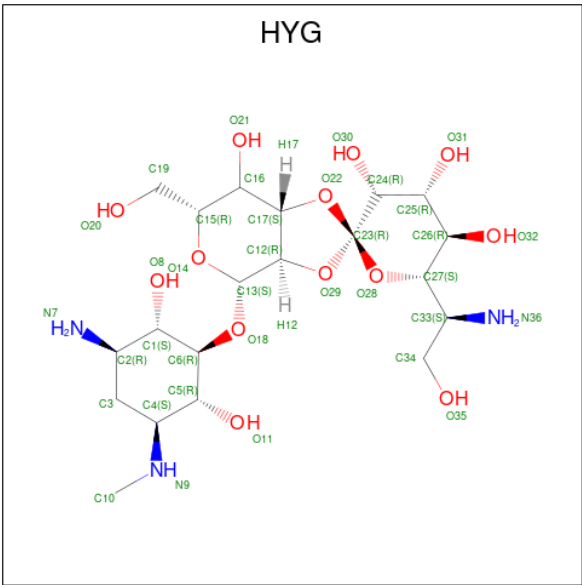
Mol	Chain	Residues	Atoms		AltConf
84	LN	1	Total	Na	0
			1	1	
84	Le	1	Total	Na	0
			1	1	
84	LB	1	Total	Na	0
			1	1	
84	L5	46	Total	Na	0
			46	46	
84	S2	12	Total	Na	0
			12	12	

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	

- Molecule 86 is HYGROMYCIN B (CCD ID: HYG) (formula: C<sub>20</sub>H<sub>37</sub>N<sub>3</sub>O<sub>13</sub>).



Mol	Chain	Residues	Atoms				AltConf
86	S2	1	Total	C	N	O	0
			36	20	3	13	

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	Ll	2	Total	O	0
			2	2	
87	Lo	1	Total	O	0
			1	1	
87	SN	3	Total	O	0
			3	3	
87	SL	1	Total	O	0
			1	1	
87	SF	1	Total	O	0
			1	1	
87	LW	1	Total	O	0
			1	1	
87	LV	2	Total	O	0
			2	2	
87	LT	4	Total	O	0
			4	4	
87	LS	5	Total	O	0
			5	5	
87	LR	3	Total	O	0
			3	3	
87	LQ	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
87	LP	3	Total 3	O 3	0
87	Lp	1	Total 1	O 1	0
87	LN	5	Total 5	O 5	0
87	Ln	2	Total 2	O 2	0
87	LM	1	Total 1	O 1	0
87	LL	2	Total 2	O 2	0
87	Lj	2	Total 2	O 2	0
87	LI	1	Total 1	O 1	0
87	LH	1	Total 1	O 1	0
87	Lh	2	Total 2	O 2	0
87	LG	1	Total 1	O 1	0
87	Lg	3	Total 3	O 3	0
87	LF	3	Total 3	O 3	0
87	Le	3	Total 3	O 3	0
87	LD	1	Total 1	O 1	0
87	LC	1	Total 1	O 1	0
87	Lc	2	Total 2	O 2	0
87	LB	7	Total 7	O 7	0
87	Lb	4	Total 4	O 4	0
87	LA	4	Total 4	O 4	0
87	La	3	Total 3	O 3	0

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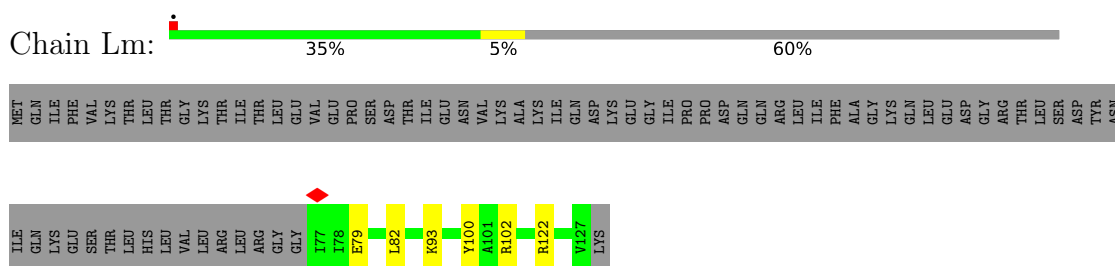
Mol	Chain	Residues	Atoms		AltConf
87	L7	9	Total 9	O 9	0
87	Pt	1	Total 1	O 1	0
87	Sa	1	Total 1	O 1	0
87	L8	16	Total 16	O 16	0
87	L5	473	Total 473	O 473	0
87	S2	101	Total 101	O 101	0
87	SI	5	Total 5	O 5	0
87	SS	2	Total 2	O 2	0



### 3 Residue-property plots [i](#)

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.

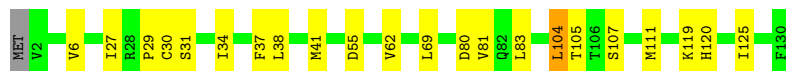
- Molecule 1: Ubiquitin-60S ribosomal protein L40





- Molecule 6: 40S ribosomal protein S15a

Chain SW: 82% 16% ..



- Molecule 7: 40S ribosomal protein S21

Chain SV: 87% 13%



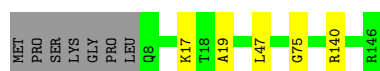
- Molecule 8: 40S ribosomal protein S17

Chain SR: 85% 11% ..



- Molecule 9: 40S ribosomal protein S16

Chain SQ: 92% 5%



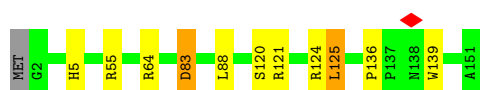
- Molecule 10: 40S ribosomal protein S14

Chain SO: 75% 13% 11%




- Molecule 11: 40S ribosomal protein S13

Chain SN: 92% 6% ..



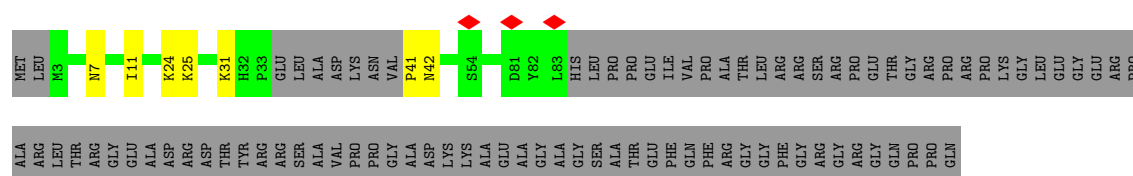
- Molecule 12: Small ribosomal subunit protein uS17

Chain SL:  80% 9% 10%




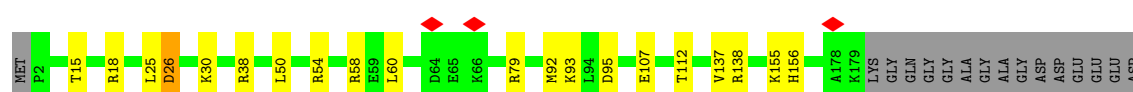
- Molecule 13: Small ribosomal subunit protein eS10

Chain SK:  41% 55%




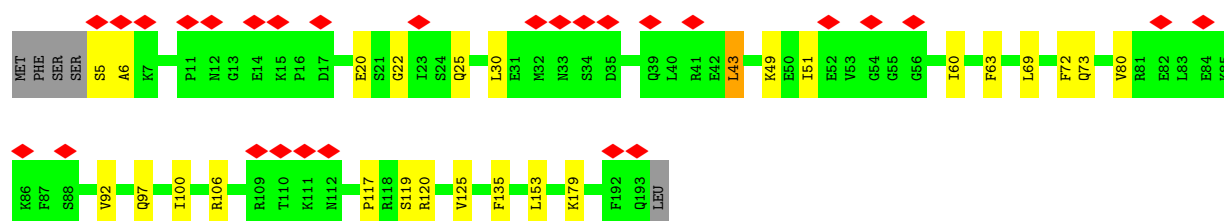
- Molecule 14: 40S ribosomal protein S9

Chain SJ:  81% 10% 8%




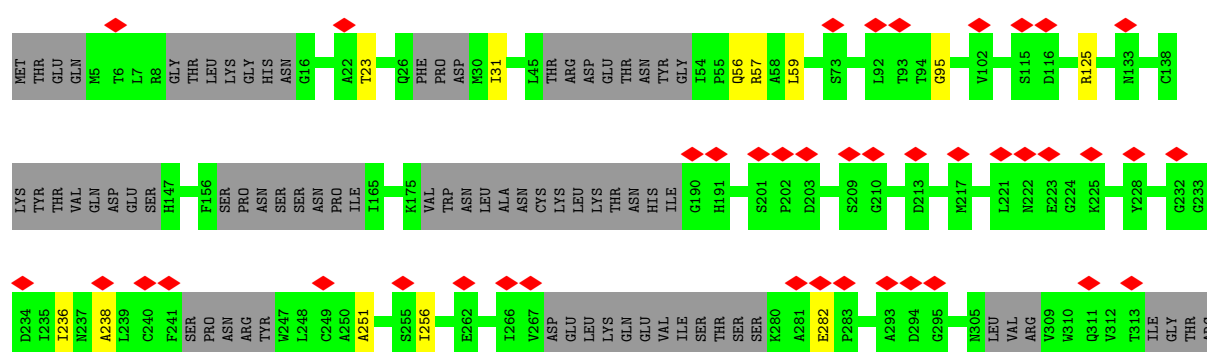
- Molecule 15: 40S ribosomal protein S7

Chain SH:  14% 84% 13%



- Molecule 16: Small ribosomal subunit protein RACK1

Chain Sg:  13% 72% 24%



- Molecule 17: Small ribosomal subunit protein uS7

[illegible]

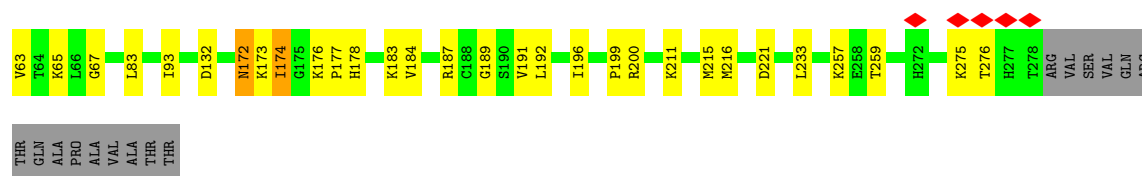
- [illegible]

- [illegible]

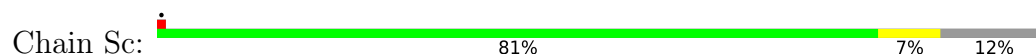
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- |     |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | G2 | H10 | K13 | C21 | R22 | V23 | C24 | S25 | N26 | L30 | K33 | Y34 | G35 | L36 | N37 | M38 | C39 | C42 | F52 | I53 | D56 |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

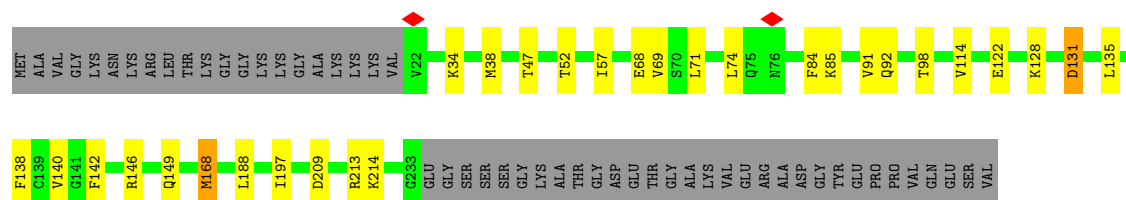
- [illegible]



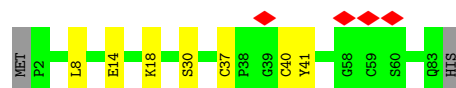
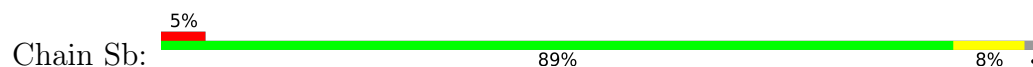
- Molecule 23: 40S ribosomal protein S28



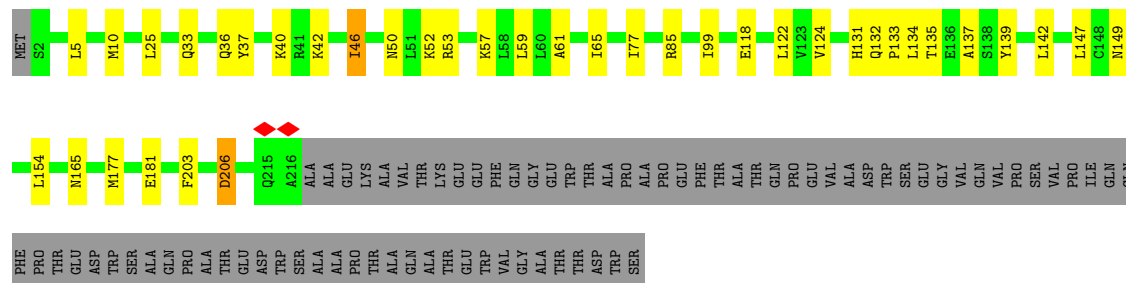
- Molecule 24: 40S ribosomal protein S3a



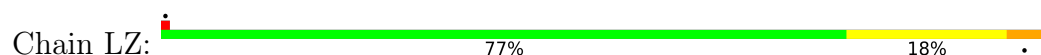
- Molecule 25: 40S ribosomal protein S27

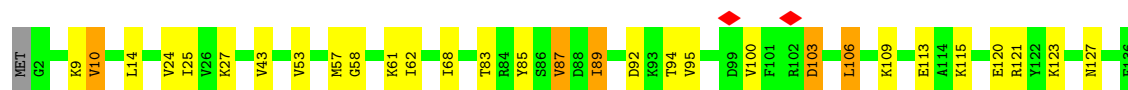


- Molecule 26: 40S ribosomal protein SA



- Molecule 27: 60S ribosomal protein L27





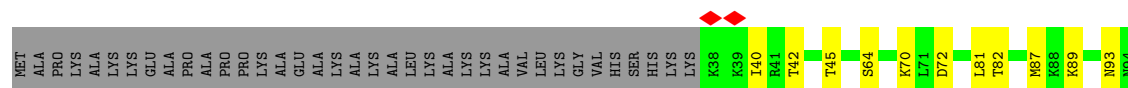
- Molecule 28: Large ribosomal subunit protein uL24

Chain LY: 87% 5% 8%



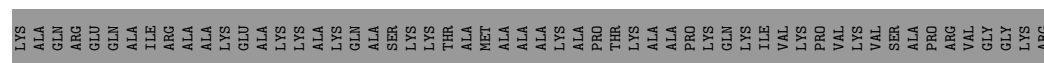
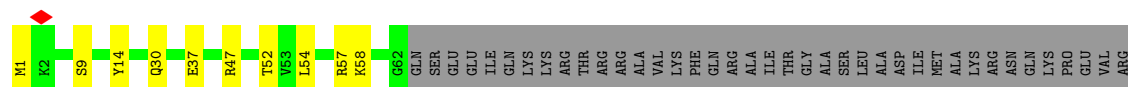
- Molecule 29: 60S ribosomal protein L23a

Chain LX: 64% 12% 24%



- Molecule 30: 60S ribosomal protein L24

Chain LW: 33% 6% 61%



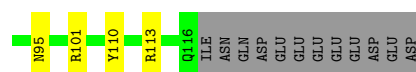
- Molecule 31: 60S ribosomal protein L23

Chain LV: 85% 8% 6%

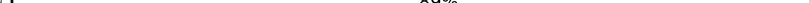


- Molecule 32: 60S ribosomal protein L22

Chain LU: 8% 59% 17% 23%

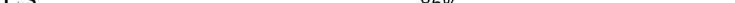


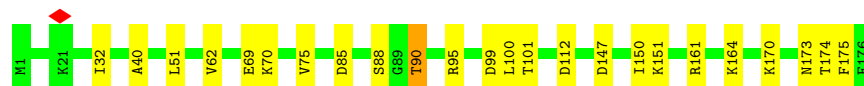
- Molecule 33: 60S ribosomal protein L21

Chain LT:  89% 9% ..




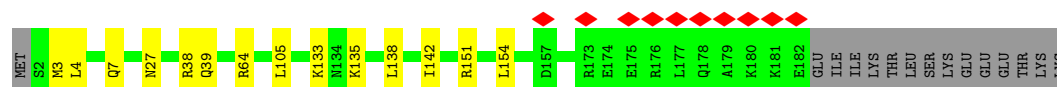
- Molecule 34: 60S ribosomal protein L18a

Chain LS:  86% 13%



- Molecule 35: 60S ribosomal protein L19

Chain LR: 

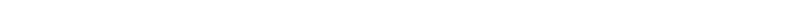


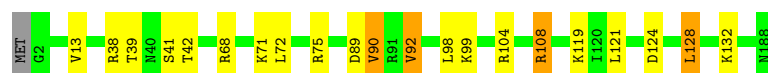
- Molecule 36: Large ribosomal subunit protein eL28

Chain Lr:  79% 11% 10%



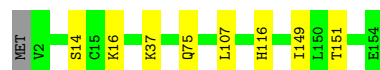
- Molecule 37: 60S ribosomal protein L18

Chain LQ:  88% 9% 3%



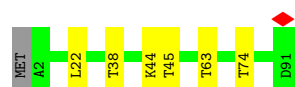
- Molecule 38: Large ribosomal subunit protein uL22

Chain LP:  94% 5% 1%

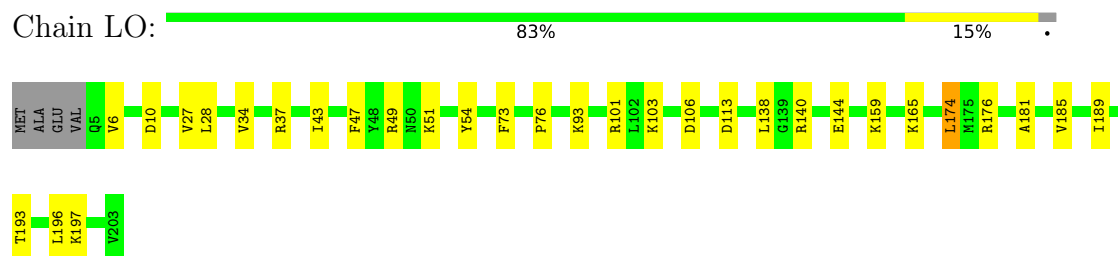


- Molecule 39: Large ribosomal subunit protein eL43

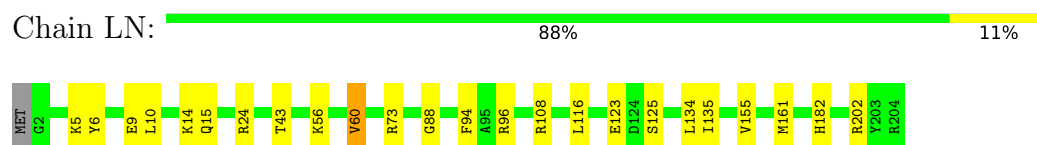
Chain Lp:  92% 7%



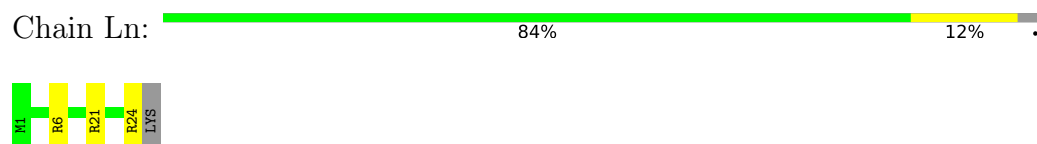
- Molecule 40: 60S ribosomal protein L13a



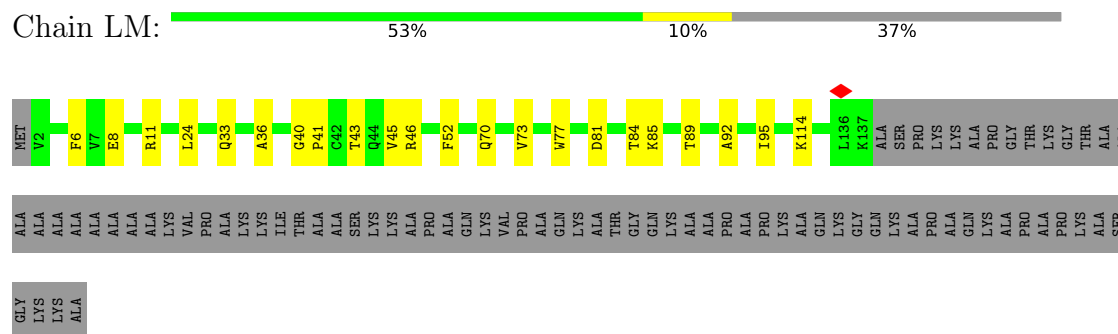
- Molecule 41: 60S ribosomal protein L15



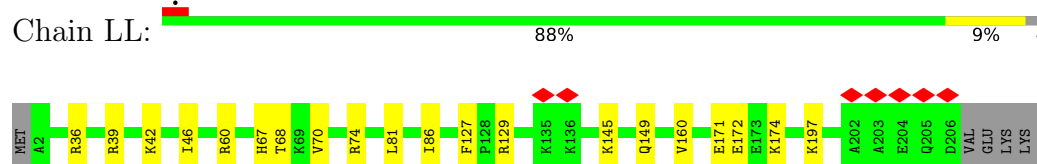
- Molecule 42: Small ribosomal subunit protein eS32



- Molecule 43: 60S ribosomal protein L14



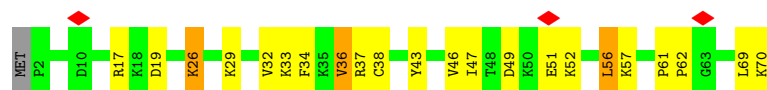
- Molecule 44: 60S ribosomal protein L13



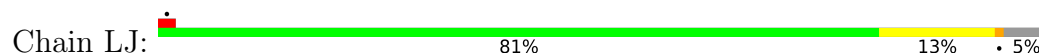
- Molecule 45: 60S ribosomal protein L38



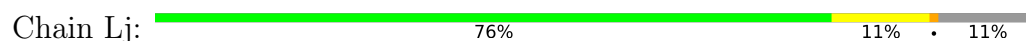




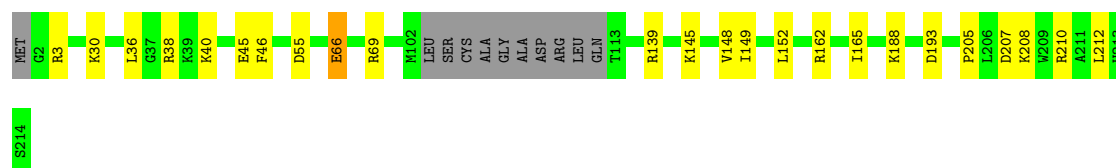
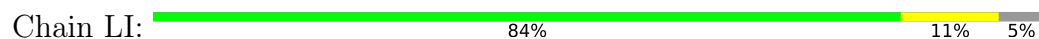
- Molecule 46: 60S ribosomal protein L11



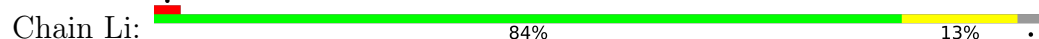
- Molecule 47: Large ribosomal subunit protein eL37



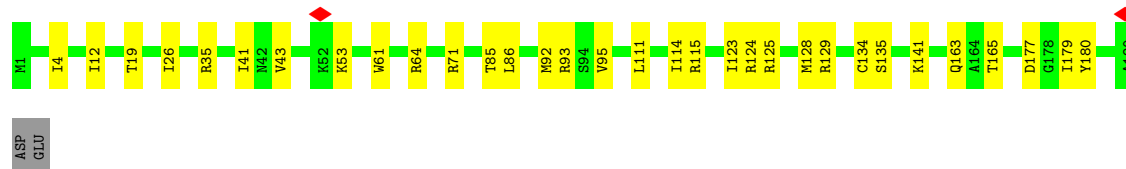
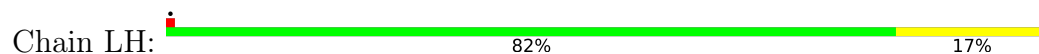
- Molecule 48: 60S ribosomal protein L10



- Molecule 49: 60S ribosomal protein L36

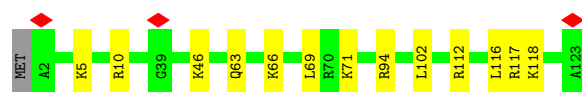


- Molecule 50: 60S ribosomal protein L9

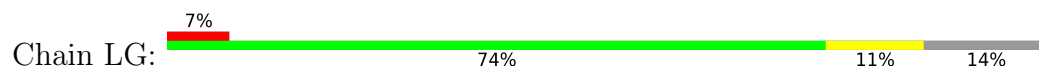


- Molecule 51: 60S ribosomal protein L35

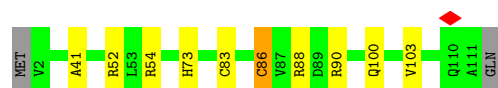




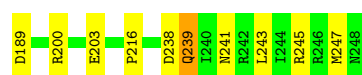
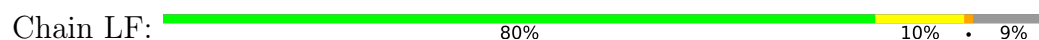
- Molecule 52: 60S ribosomal protein L7a



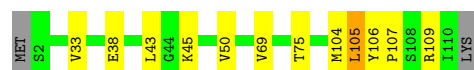
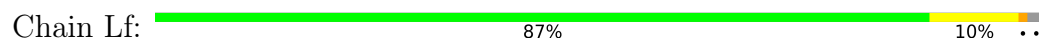
- Molecule 53: Large ribosomal subunit protein eL34



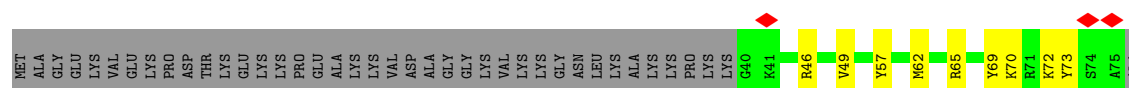
- Molecule 54: Large ribosomal subunit protein uL30

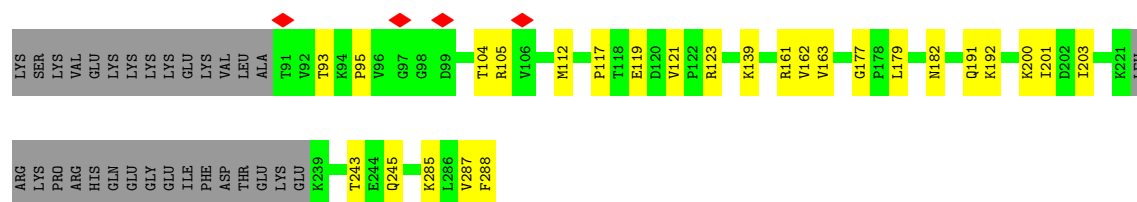


- Molecule 55: Large ribosomal subunit protein eL33



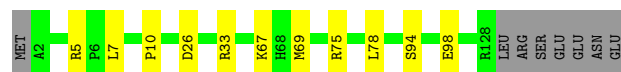
- Molecule 56: Large ribosomal subunit protein eL6





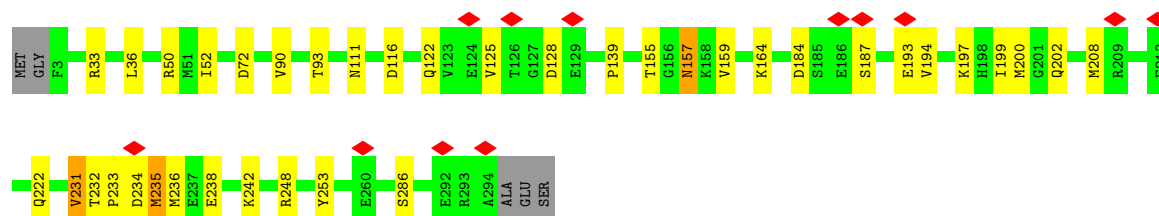
• Molecule 57: 60S ribosomal protein L32

Chain Le: 86% 8% 6%



• Molecule 58: 60S ribosomal protein L5

Chain LD: 86% 12% ..



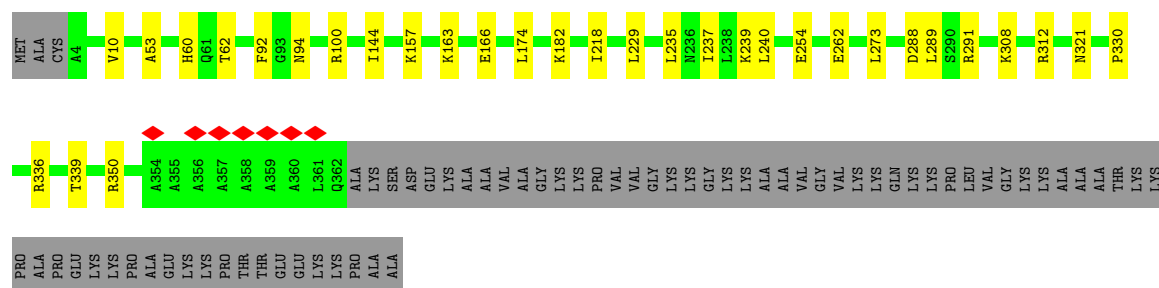
• Molecule 59: 60S ribosomal protein L31

Chain Ld: 74% 10% 15%



• Molecule 60: 60S ribosomal protein L4

Chain LC: 77% 7% 16%

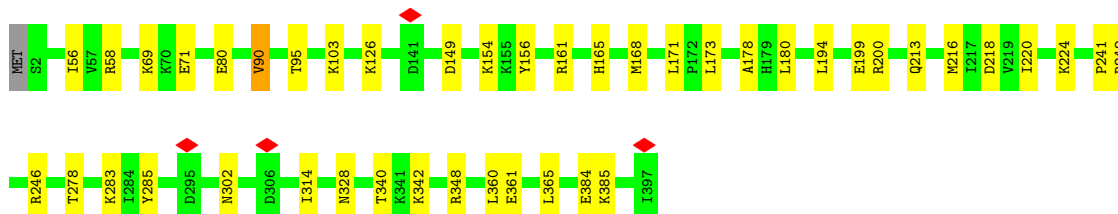


• Molecule 61: 60S ribosomal protein L30

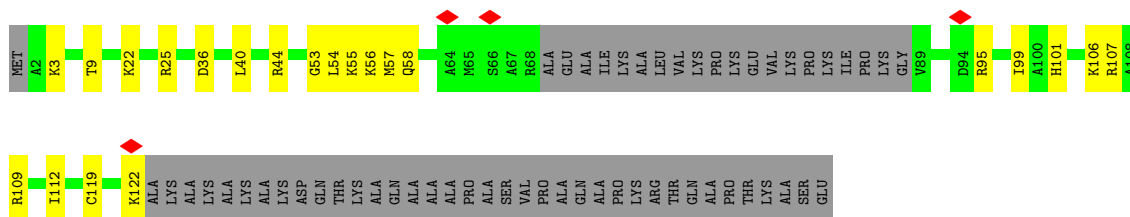
Chain Lc: 73% 11% 15%



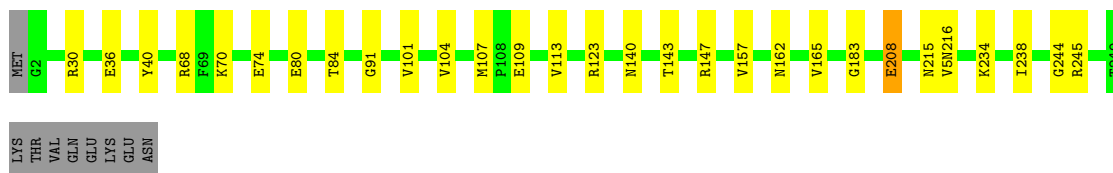
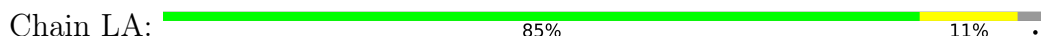
- Molecule 62: Large ribosomal subunit protein uL3



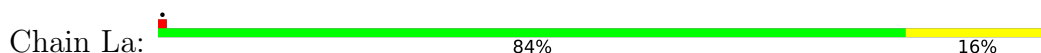
- Molecule 63: Large ribosomal subunit protein eL29



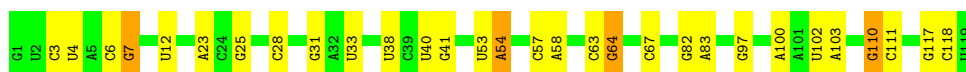
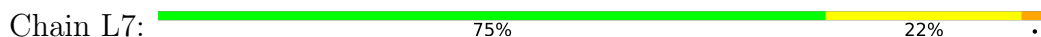
- Molecule 64: Large ribosomal subunit protein uL2



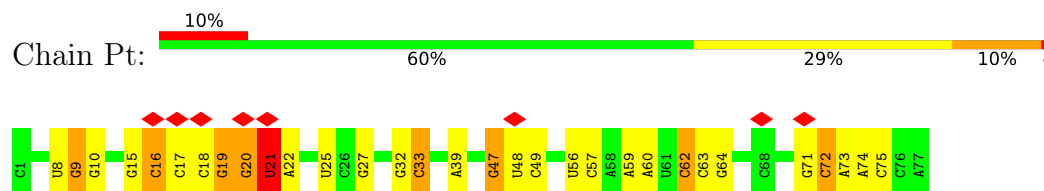
- Molecule 65: Large ribosomal subunit protein uL15



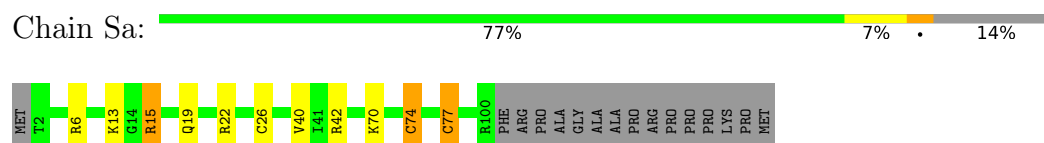
- Molecule 66: 5S rRNA



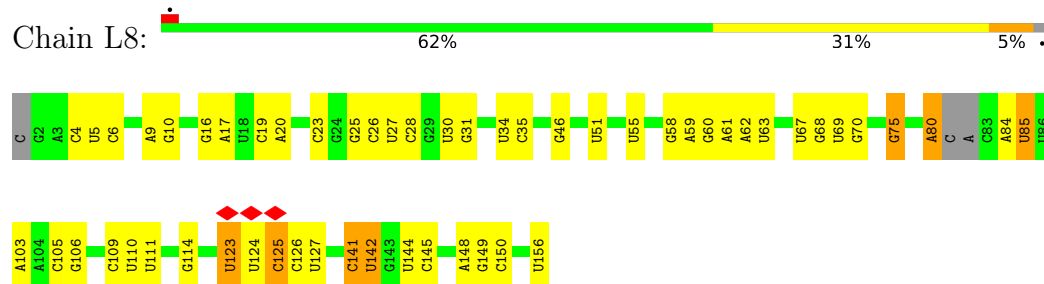
- Molecule 67: P site tRNA



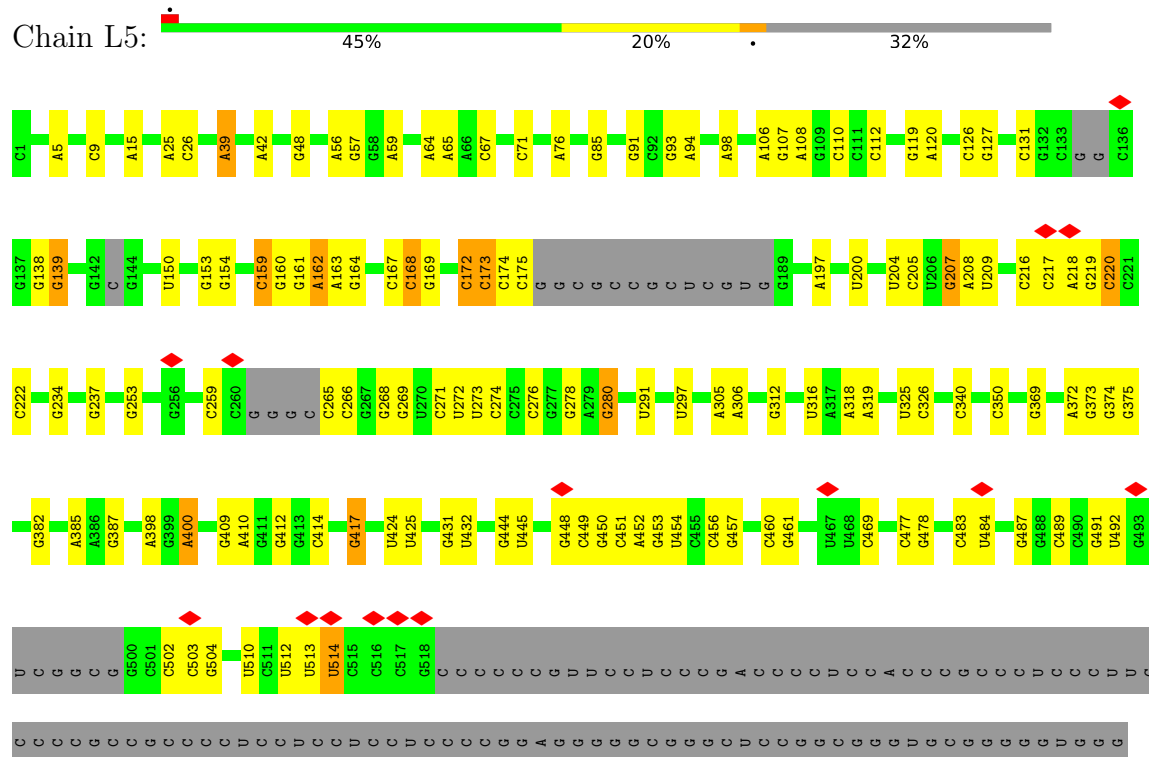
- Molecule 68: 40S ribosomal protein S26

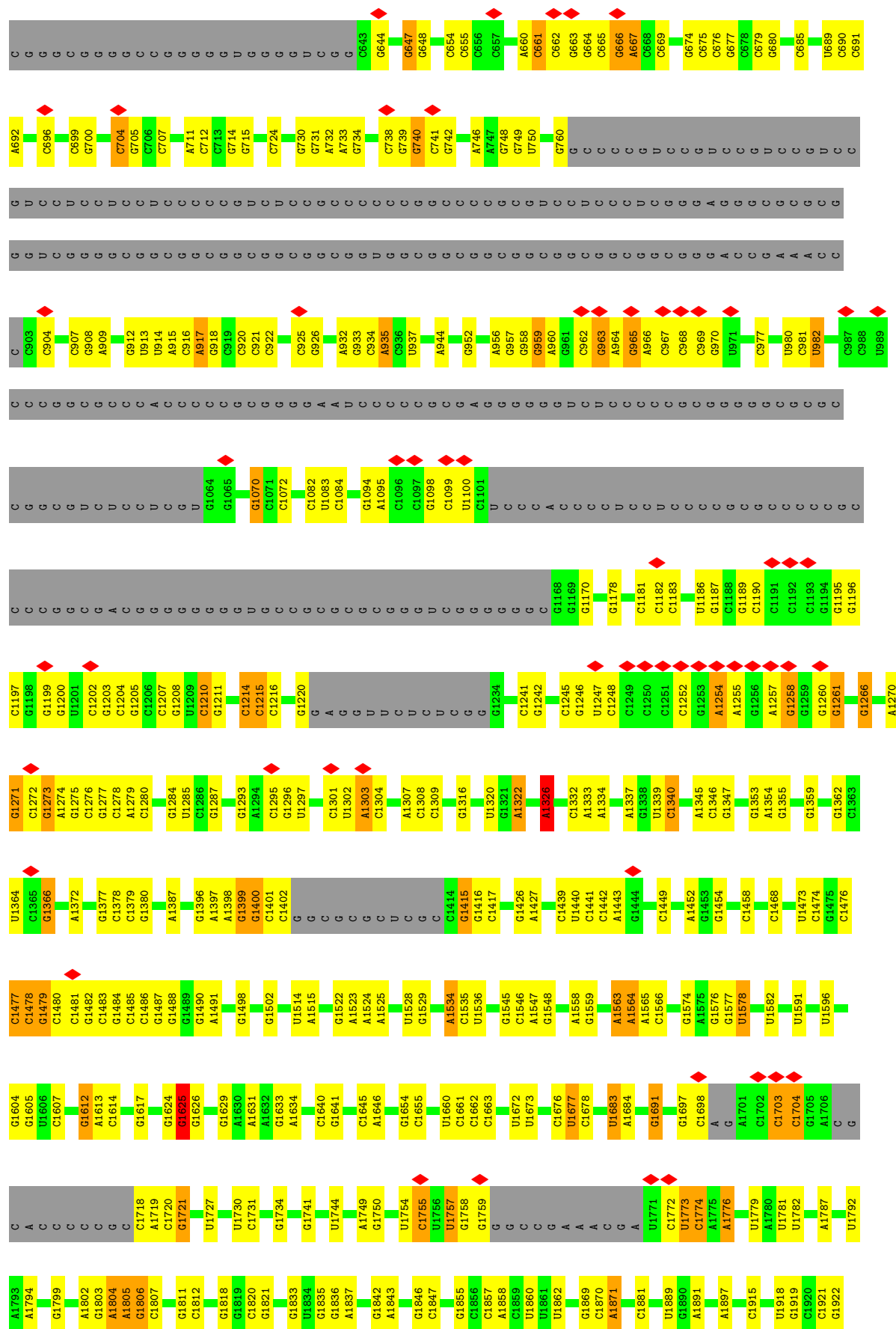


- Molecule 69: 5.8S rRNA



- Molecule 70: 28S rRNA

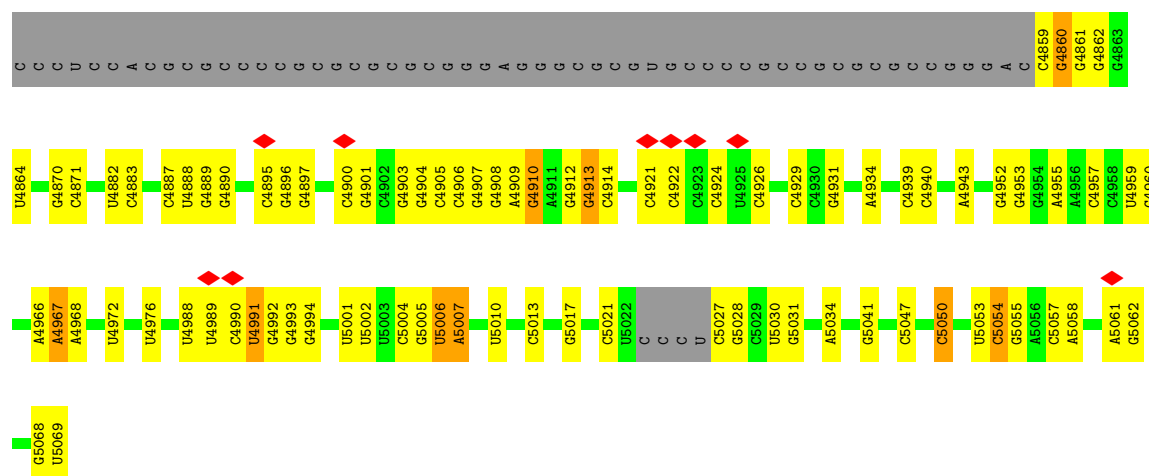




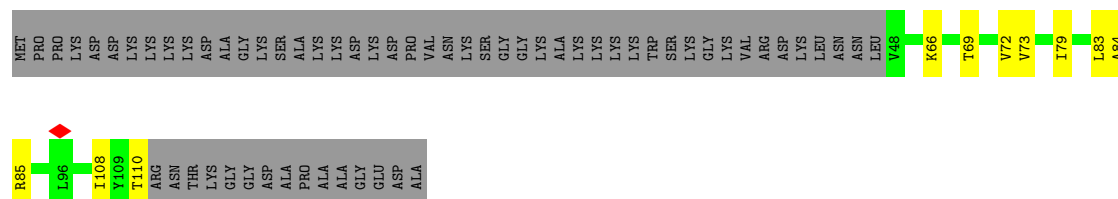




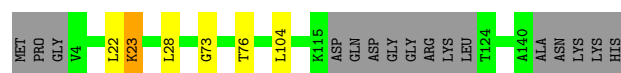
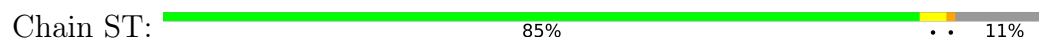




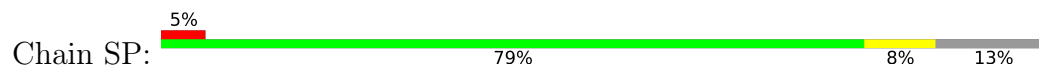
- Molecule 71: Small ribosomal subunit protein eS25



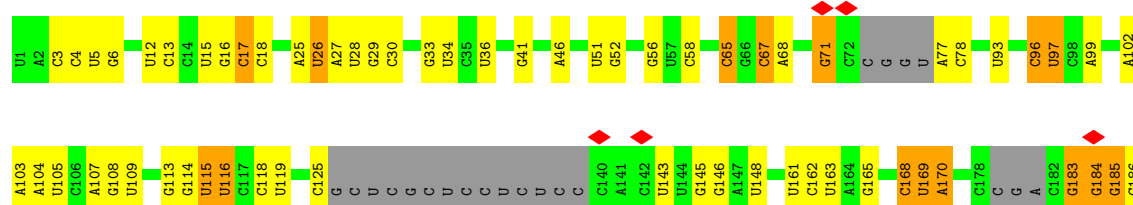
- Molecule 72: 40S ribosomal protein S19



- Molecule 73: 40S ribosomal protein S15

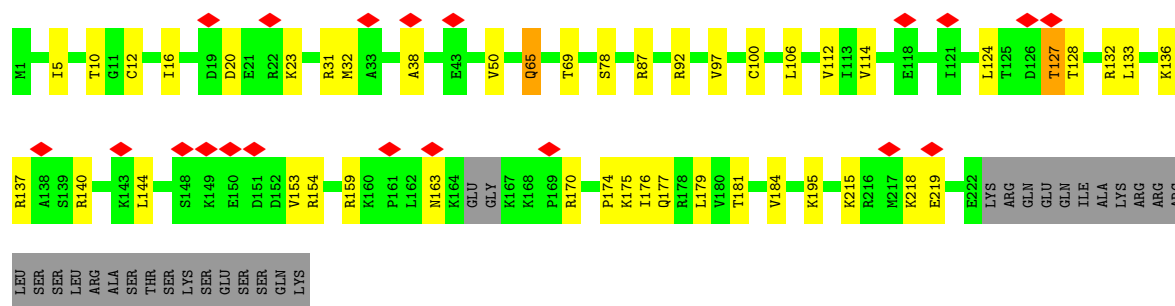
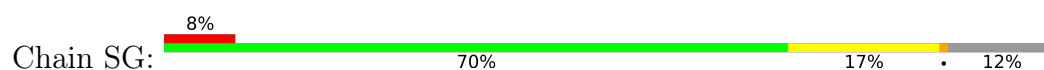


- Molecule 74: 18S rRNA

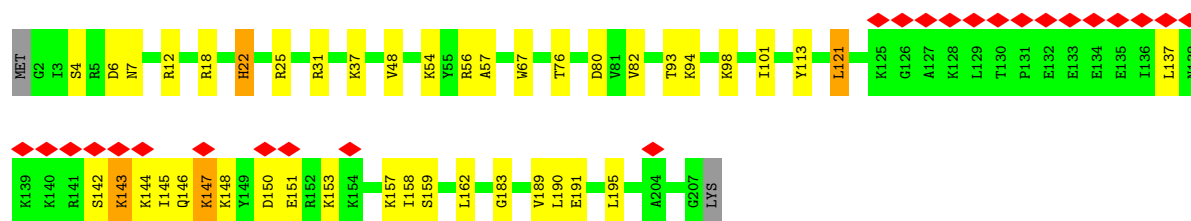
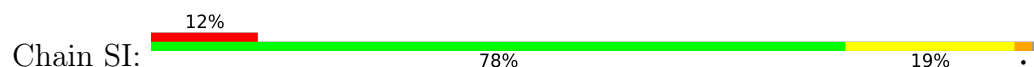




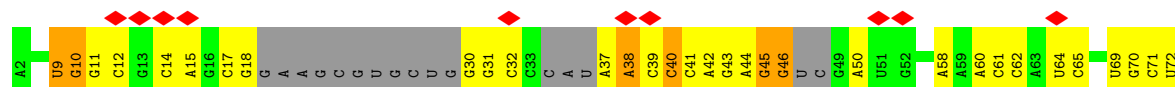
- Molecule 75: 40S ribosomal protein S6



- Molecule 76: 40S ribosomal protein S8



- Molecule 77: E site tRNA





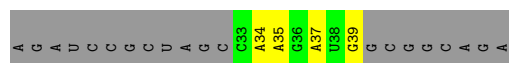
- Molecule 78: Small ribosomal subunit protein uS13

Chain SS: 83% 7% 9%



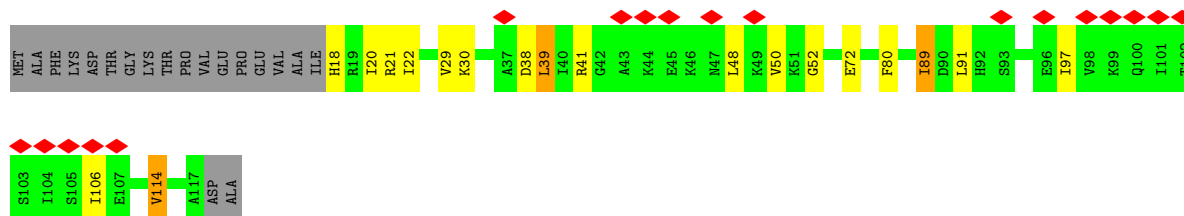
- Molecule 79: TISU mRNA

Chain mR: 11% 15% 74%



- Molecule 80: 40S ribosomal protein S20

Chain SU: 15% 68% 13% 16%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	404.16, 404.16, 404.16	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.842, 0.842, 0.842	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, H2U, HYG, V5N, MA6, B8N, G7M, K, OMU, MG, MLZ, 4SU, 1MA, OMC, UR3, 5MC, SPD, OMG, A2M, 4AC, NA, 6MZ, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Lm	0.15	0/413	0.33	0/549
2	Ll	0.17	0/444	0.33	0/588
3	Lo	0.15	0/823	0.31	0/1088
4	SY	0.15	0/917	0.33	0/1234
5	SX	0.15	0/1077	0.33	0/1441
6	SW	0.17	0/1040	0.30	0/1393
7	SV	0.14	0/630	0.32	0/843
8	SR	0.15	0/950	0.35	0/1291
9	SQ	0.15	0/927	0.32	0/1258
10	SO	0.18	0/990	0.37	0/1330
11	SN	0.17	0/1210	0.32	0/1633
12	SL	0.15	0/1178	0.28	0/1578
13	SK	0.14	0/481	0.29	0/662
14	SJ	0.15	0/1455	0.30	0/1954
15	SH	0.15	0/1429	0.33	0/1929
16	Sg	0.14	0/1259	0.38	0/1730
17	SF	0.15	0/1345	0.33	0/1827
18	SE	0.14	0/2079	0.32	0/2801
19	Se	0.13	0/401	0.33	0/524
20	SD	0.14	0/1103	0.29	0/1505
21	Sd	0.15	0/441	0.28	0/589
22	SC	0.16	0/1731	0.34	0/2341
23	Sc	0.14	0/435	0.26	0/587
24	SB	0.16	0/1721	0.34	0/2304
25	Sb	0.14	0/625	0.31	0/842
26	SA	0.16	0/1695	0.31	0/2310
27	LZ	0.15	0/1118	0.30	0/1494
28	LY	0.15	0/1077	0.32	0/1440
29	LX	0.17	0/993	0.34	0/1334
30	LW	0.15	0/532	0.30	0/708
31	LV	0.15	0/1004	0.31	0/1346

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	LU	0.15	0/814	0.38	0/1094
33	LT	0.15	0/1325	0.27	0/1770
34	LS	0.16	0/1496	0.30	0/2009
35	LR	0.18	0/1474	0.32	0/1957
36	Lr	0.19	0/1002	0.35	0/1344
37	LQ	0.17	0/1529	0.33	0/2044
38	LP	0.16	0/1256	0.33	0/1687
39	Lp	0.17	0/705	0.34	0/937
40	LO	0.18	0/1652	0.30	0/2211
41	LN	0.17	0/1739	0.34	0/2331
42	Ln	0.21	0/236	0.32	0/300
43	LM	0.17	0/1138	0.34	0/1523
44	LL	0.15	0/1669	0.29	0/2237
45	Lk	0.17	0/563	0.37	0/748
46	LJ	0.15	0/1352	0.32	0/1812
47	Lj	0.15	0/716	0.32	0/947
48	LI	0.16	0/1670	0.29	0/2230
49	Li	0.14	0/823	0.31	0/1092
50	LH	0.16	0/1518	0.31	0/2043
51	Lh	0.17	0/1018	0.34	0/1347
52	LG	0.16	0/1824	0.33	0/2465
53	Lg	0.19	0/884	0.35	0/1179
54	LF	0.18	0/1869	0.33	0/2498
55	Lf	0.17	0/887	0.33	0/1190
56	LE	0.14	0/1758	0.29	0/2360
57	Le	0.17	0/1062	0.31	0/1416
58	LD	0.14	0/2400	0.33	0/3220
59	Ld	0.16	0/854	0.34	0/1153
60	LC	0.16	0/2916	0.31	0/3917
61	Lc	0.18	0/770	0.36	0/1034
62	LB	0.15	0/3242	0.32	0/4343
63	Lb	0.17	0/817	0.37	0/1080
64	LA	0.16	0/1927	0.33	0/2582
65	La	0.16	0/1173	0.32	0/1566
66	L7	0.16	0/2840	0.26	0/4425
67	Pt	0.23	0/1721	0.31	0/2679
68	Sa	0.21	0/788	0.44	1/1059 (0.1%)
69	L8	0.17	0/3564	0.30	0/5550
70	L5	0.19	3/79828 (0.0%)	0.30	0/124490
71	SZ	0.18	0/385	0.33	0/530
72	ST	0.15	0/851	0.28	0/1157
73	SP	0.14	0/814	0.34	0/1109
74	S2	0.21	2/35763 (0.0%)	0.31	0/55704

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	SG	0.13	0/1683	0.29	0/2261
76	SI	0.17	0/1677	0.33	0/2243
77	S6	0.14	0/1411	0.32	0/2192
78	SS	0.14	0/916	0.32	0/1256
79	mR	0.30	0/170	0.66	0/263
80	SU	0.21	0/805	0.43	0/1081
All	All	0.18	5/210817 (0.0%)	0.31	1/310118 (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
26	SA	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	3830	A2M	O3'-P	5.09	1.61	1.56
70	L5	4523	A2M	O3'-P	5.06	1.61	1.56
74	S2	668	A2M	O3'-P	5.05	1.61	1.56
70	L5	3785	A2M	O3'-P	5.02	1.61	1.56
74	S2	512	A2M	O3'-P	5.00	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	Sa	77	CYS	CA-CB-SG	5.08	126.08	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	SA	147	LEU	Peptide

## 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	Lm	407	0	423	4	0
2	Ll	434	0	461	6	0
3	Lo	822	0	856	8	0
4	SY	900	0	831	15	0
5	SX	1060	0	1087	5	0
6	SW	1023	0	1063	11	0
7	SV	623	0	627	8	0
8	SR	936	0	866	8	0
9	SQ	918	0	804	4	0
10	SO	977	0	994	10	0
11	SN	1186	0	1247	8	0
12	SL	1158	0	1214	8	0
13	SK	468	0	317	4	0
14	SJ	1430	0	1498	13	0
15	SH	1408	0	1432	12	0
16	Sg	1259	0	646	6	0
17	SF	1327	0	1251	12	0
18	SE	2037	0	2131	11	0
19	Se	399	0	433	2	0
20	SD	1094	0	910	6	0
21	Sd	430	0	397	9	0
22	SC	1694	0	1769	17	0
23	Sc	434	0	419	3	0
24	SB	1694	0	1744	17	0
25	Sb	613	0	614	4	0
26	SA	1658	0	1630	23	0
27	LZ	1095	0	1164	16	0
28	LY	1060	0	1101	5	0
29	LX	976	0	1053	11	0
30	LW	519	0	533	6	0
31	LV	987	0	1052	5	0
32	LU	800	0	816	13	0
33	LT	1297	0	1366	9	0
34	LS	1456	0	1491	16	0
35	LR	1458	0	1555	8	0
36	Lr	987	0	1050	8	0
37	LQ	1505	0	1613	14	0
38	LP	1230	0	1250	4	0
39	Lp	695	0	746	3	0
40	LO	1620	0	1753	19	0
41	LN	1694	0	1738	16	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	Ln	235	0	284	2	0
43	LM	1116	0	1176	15	0
44	LL	1638	0	1737	14	0
45	Lk	557	0	611	14	0
46	LJ	1329	0	1346	13	0
47	Lj	701	0	735	9	0
48	LI	1632	0	1675	15	0
49	Li	812	0	870	12	0
50	LH	1499	0	1572	20	0
51	Lh	1010	0	1137	10	0
52	LG	1791	0	1883	19	0
53	Lg	871	0	953	5	0
54	LF	1835	0	1926	19	0
55	Lf	868	0	892	9	0
56	LE	1721	0	1839	22	0
57	Le	1044	0	1132	6	0
58	LD	2354	0	2345	21	0
59	Ld	840	0	859	8	0
60	LC	2862	0	3036	19	0
61	Lc	760	0	793	6	0
62	LB	3174	0	3294	27	0
63	Lb	815	0	869	13	0
64	LA	1899	0	1983	20	0
65	La	1157	0	1190	14	0
66	L7	2542	0	1284	14	0
67	Pt	1645	0	844	15	0
68	Sa	775	0	813	10	0
69	L8	3256	0	1652	30	0
70	L5	73960	0	37478	514	0
71	SZ	383	0	313	7	0
72	ST	837	0	694	3	0
73	SP	806	0	652	3	0
74	S2	33557	0	16987	250	0
75	SG	1663	0	1701	25	0
76	SI	1648	0	1700	28	0
77	S6	1263	0	647	15	0
78	SS	903	0	728	7	0
79	mR	152	0	77	2	0
80	SU	795	0	862	13	0
81	Lg	1	0	0	0	0
81	Lm	1	0	0	0	0
81	Lo	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	Lp	1	0	0	0	0
81	Sd	1	0	0	0	0
82	L5	60	0	0	0	0
82	L8	1	0	0	0	0
82	LB	1	0	0	0	0
82	LC	1	0	0	0	0
82	Lf	1	0	0	0	0
82	S2	11	0	0	0	0
82	SQ	1	0	0	0	0
83	L5	81	0	0	0	0
83	L7	5	0	0	0	0
83	L8	3	0	0	0	0
83	LB	1	0	0	0	0
83	LI	2	0	0	0	0
83	LM	1	0	0	0	0
83	LP	1	0	0	0	0
83	LS	1	0	0	0	0
83	LV	1	0	0	0	0
83	Le	1	0	0	0	0
83	Pt	1	0	0	0	0
83	S2	21	0	0	0	0
83	Sd	1	0	0	0	0
84	L5	46	0	0	0	0
84	LB	1	0	0	0	0
84	LN	1	0	0	0	0
84	Le	1	0	0	0	0
84	S2	12	0	0	0	0
85	L5	30	0	55	4	0
86	S2	36	0	37	0	0
87	L5	473	0	0	9	0
87	L7	9	0	0	0	0
87	L8	16	0	0	0	0
87	LA	4	0	0	0	0
87	LB	7	0	0	0	0
87	LC	1	0	0	0	0
87	LD	1	0	0	0	0
87	LF	3	0	0	0	0
87	LG	1	0	0	0	0
87	LH	1	0	0	0	0
87	LI	1	0	0	0	0
87	LL	2	0	0	0	0
87	LM	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	LN	5	0	0	0	0
87	LP	3	0	0	0	0
87	LQ	3	0	0	0	0
87	LR	3	0	0	1	0
87	LS	5	0	0	0	0
87	LT	4	0	0	0	0
87	LV	2	0	0	0	0
87	LW	1	0	0	0	0
87	La	3	0	0	0	0
87	Lb	4	0	0	0	0
87	Lc	2	0	0	1	0
87	Le	3	0	0	0	0
87	Lg	3	0	0	0	0
87	Lh	2	0	0	0	0
87	Lj	2	0	0	0	0
87	Ll	2	0	0	0	0
87	Ln	2	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
87	Pt	1	0	0	0	0
87	S2	101	0	0	1	0
87	SF	1	0	0	0	0
87	SI	5	0	0	0	0
87	SL	1	0	0	0	0
87	SN	3	0	0	0	0
87	SS	2	0	0	0	0
87	Sa	1	0	0	1	0
All	All	201487	0	144606	1404	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 4.

The worst 5 of 1404 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)
70:L5:1100:U:H3	70:L5:1195:G:H1	1.22	0.87
74:S2:885:U:H3	74:S2:901:G:H1	1.21	0.85
70:L5:3634:G:H1	70:L5:3826:C:H5	1.31	0.77
52:LG:180:PRO:HG3	52:LG:223:ARG:HE	1.51	0.76
52:LG:249:ARG:NH2	70:L5:4075:U:OP1	2.19	0.76

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	
1	Lm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
2	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
3	Lo	102/106 (96%)	99 (97%)	3 (3%)	0	100	100
4	SY	121/133 (91%)	118 (98%)	3 (2%)	0	100	100
5	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
6	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
7	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
8	SR	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
9	SQ	137/146 (94%)	127 (93%)	10 (7%)	0	100	100
10	SO	132/151 (87%)	125 (95%)	7 (5%)	0	100	100
11	SN	148/151 (98%)	148 (100%)	0	0	100	100
12	SL	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
13	SK	70/165 (42%)	69 (99%)	1 (1%)	0	100	100
14	SJ	176/194 (91%)	168 (96%)	8 (4%)	0	100	100
15	SH	187/194 (96%)	181 (97%)	6 (3%)	0	100	100
16	Sg	221/317 (70%)	180 (81%)	39 (18%)	2 (1%)	14	48
17	SF	181/204 (89%)	173 (96%)	8 (4%)	0	100	100
18	SE	258/263 (98%)	251 (97%)	7 (3%)	0	100	100
19	Se	47/133 (35%)	47 (100%)	0	0	100	100
20	SD	165/243 (68%)	161 (98%)	4 (2%)	0	100	100
21	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
22	SC	218/293 (74%)	211 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Sc	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
24	SB	211/264 (80%)	205 (97%)	6 (3%)	0	100	100
25	Sb	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
26	SA	213/295 (72%)	206 (97%)	7 (3%)	0	100	100
27	LZ	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
28	LY	131/145 (90%)	128 (98%)	3 (2%)	0	100	100
29	LX	117/156 (75%)	114 (97%)	3 (3%)	0	100	100
30	LW	60/157 (38%)	60 (100%)	0	0	100	100
31	LV	130/140 (93%)	128 (98%)	2 (2%)	0	100	100
32	LU	97/128 (76%)	91 (94%)	6 (6%)	0	100	100
33	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
34	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
35	LR	179/196 (91%)	173 (97%)	6 (3%)	0	100	100
36	Lr	121/137 (88%)	118 (98%)	3 (2%)	0	100	100
37	LQ	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
38	LP	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
39	Lp	88/91 (97%)	85 (97%)	3 (3%)	0	100	100
40	LO	197/203 (97%)	193 (98%)	4 (2%)	0	100	100
41	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	LM	134/215 (62%)	133 (99%)	1 (1%)	0	100	100
44	LL	203/211 (96%)	196 (97%)	7 (3%)	0	100	100
45	Lk	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
46	LJ	167/178 (94%)	162 (97%)	5 (3%)	0	100	100
47	Lj	84/97 (87%)	84 (100%)	0	0	100	100
48	LI	199/214 (93%)	197 (99%)	2 (1%)	0	100	100
49	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
50	LH	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
51	Lh	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
52	LG	226/266 (85%)	217 (96%)	9 (4%)	0	100	100
53	Lg	109/112 (97%)	107 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	LF	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
55	Lf	107/111 (96%)	106 (99%)	1 (1%)	0	100	100
56	LE	212/288 (74%)	205 (97%)	7 (3%)	0	100	100
57	Le	125/135 (93%)	122 (98%)	3 (2%)	0	100	100
58	LD	290/297 (98%)	285 (98%)	5 (2%)	0	100	100
59	Ld	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
60	LC	357/427 (84%)	346 (97%)	11 (3%)	0	100	100
61	Lc	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
62	LB	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
63	Lb	96/159 (60%)	92 (96%)	4 (4%)	0	100	100
64	LA	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
65	La	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
68	Sa	97/115 (84%)	94 (97%)	3 (3%)	0	100	100
71	SZ	61/125 (49%)	56 (92%)	5 (8%)	0	100	100
72	ST	125/145 (86%)	122 (98%)	3 (2%)	0	100	100
73	SP	124/145 (86%)	117 (94%)	7 (6%)	0	100	100
75	SG	216/249 (87%)	210 (97%)	6 (3%)	0	100	100
76	SI	204/208 (98%)	199 (98%)	5 (2%)	0	100	100
78	SS	136/152 (90%)	124 (91%)	11 (8%)	1 (1%)	18	53
80	SU	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
All	All	10686/12433 (86%)	10331 (97%)	352 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
78	SS	119	PHE
16	Sg	236	ILE
16	Sg	282	GLU

### 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	
1	Lm	43/116 (37%)	42 (98%)	1 (2%)	44	74
2	Ll	45/48 (94%)	40 (89%)	5 (11%)	6	25
3	Lo	82/93 (88%)	75 (92%)	7 (8%)	10	36
4	SY	75/115 (65%)	72 (96%)	3 (4%)	28	62
5	SX	101/115 (88%)	96 (95%)	5 (5%)	22	56
6	SW	109/113 (96%)	101 (93%)	8 (7%)	13	42
7	SV	63/67 (94%)	62 (98%)	1 (2%)	55	79
8	SR	83/122 (68%)	74 (89%)	9 (11%)	6	26
9	SQ	66/121 (54%)	66 (100%)	0	100	100
10	SO	97/119 (82%)	92 (95%)	5 (5%)	21	55
11	SN	125/131 (95%)	123 (98%)	2 (2%)	55	79
12	SL	127/142 (89%)	125 (98%)	2 (2%)	55	79
13	SK	24/136 (18%)	24 (100%)	0	100	100
14	SJ	145/168 (86%)	140 (97%)	5 (3%)	32	66
15	SH	139/174 (80%)	131 (94%)	8 (6%)	18	51
16	Sg	17/275 (6%)	17 (100%)	0	100	100
17	SF	117/170 (69%)	114 (97%)	3 (3%)	40	72
18	SE	215/225 (96%)	210 (98%)	5 (2%)	44	74
19	Se	39/104 (38%)	37 (95%)	2 (5%)	21	55
20	SD	74/202 (37%)	68 (92%)	6 (8%)	11	38
21	Sd	41/49 (84%)	38 (93%)	3 (7%)	13	42
22	SC	182/225 (81%)	174 (96%)	8 (4%)	25	60
23	Sc	42/62 (68%)	41 (98%)	1 (2%)	43	73
24	SB	183/231 (79%)	173 (94%)	10 (6%)	19	53
25	Sb	68/76 (90%)	67 (98%)	1 (2%)	57	80
26	SA	169/243 (70%)	165 (98%)	4 (2%)	43	73
27	LZ	113/118 (96%)	105 (93%)	8 (7%)	13	43
28	LY	111/135 (82%)	110 (99%)	1 (1%)	70	85
29	LX	107/133 (80%)	102 (95%)	5 (5%)	23	58
30	LW	54/126 (43%)	51 (94%)	3 (6%)	19	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	LV	102/107 (95%)	97 (95%)	5 (5%)	22	56
32	LU	87/115 (76%)	83 (95%)	4 (5%)	24	58
33	LT	139/140 (99%)	136 (98%)	3 (2%)	45	74
34	LS	156/157 (99%)	150 (96%)	6 (4%)	29	63
35	LR	147/175 (84%)	145 (99%)	2 (1%)	59	80
36	Lr	107/121 (88%)	104 (97%)	3 (3%)	38	70
37	LQ	162/165 (98%)	156 (96%)	6 (4%)	30	64
38	LP	131/135 (97%)	129 (98%)	2 (2%)	57	80
39	Lp	72/74 (97%)	70 (97%)	2 (3%)	38	70
40	LO	167/174 (96%)	162 (97%)	5 (3%)	36	69
41	LN	170/172 (99%)	167 (98%)	3 (2%)	51	77
42	Ln	23/24 (96%)	22 (96%)	1 (4%)	26	60
43	LM	115/161 (71%)	113 (98%)	2 (2%)	53	78
44	LL	166/177 (94%)	160 (96%)	6 (4%)	31	65
45	Lk	61/65 (94%)	57 (93%)	4 (7%)	15	46
46	LJ	136/149 (91%)	129 (95%)	7 (5%)	21	55
47	Lj	72/80 (90%)	69 (96%)	3 (4%)	26	61
48	LI	170/181 (94%)	168 (99%)	2 (1%)	63	82
49	Li	80/89 (90%)	77 (96%)	3 (4%)	29	63
50	LH	164/171 (96%)	162 (99%)	2 (1%)	63	82
51	Lh	108/110 (98%)	104 (96%)	4 (4%)	30	64
52	LG	184/223 (82%)	179 (97%)	5 (3%)	39	71
53	Lg	92/96 (96%)	88 (96%)	4 (4%)	26	60
54	LF	186/215 (86%)	183 (98%)	3 (2%)	55	79
55	Lf	86/90 (96%)	85 (99%)	1 (1%)	63	82
56	LE	184/252 (73%)	177 (96%)	7 (4%)	29	63
57	Le	113/121 (93%)	110 (97%)	3 (3%)	39	71
58	LD	239/250 (96%)	230 (96%)	9 (4%)	29	63
59	Ld	85/110 (77%)	83 (98%)	2 (2%)	43	73
60	LC	299/348 (86%)	293 (98%)	6 (2%)	48	76
61	Lc	82/97 (84%)	77 (94%)	5 (6%)	17	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	LB	339/346 (98%)	332 (98%)	7 (2%)	47	75
63	Lb	81/125 (65%)	77 (95%)	4 (5%)	22	56
64	LA	188/198 (95%)	186 (99%)	2 (1%)	65	83
65	La	117/120 (98%)	114 (97%)	3 (3%)	40	72
68	Sa	82/98 (84%)	79 (96%)	3 (4%)	30	64
71	SZ	22/103 (21%)	22 (100%)	0	100	100
72	ST	52/115 (45%)	50 (96%)	2 (4%)	29	63
73	SP	51/130 (39%)	45 (88%)	6 (12%)	5	22
75	SG	163/218 (75%)	152 (93%)	11 (7%)	15	46
76	SI	168/180 (93%)	159 (95%)	9 (5%)	20	53
78	SS	59/132 (45%)	54 (92%)	5 (8%)	10	36
80	SU	92/107 (86%)	86 (94%)	6 (6%)	15	47
All	All	8355/10570 (79%)	8056 (96%)	299 (4%)	32	65

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
60	LC	144	ILE
76	SI	143	LYS
61	Lc	68	LYS
72	ST	23	LYS
24	SB	168	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
50	LH	140	GLN
58	LD	131	ASN
50	LH	188	GLN
54	LF	119	ASN
60	LC	116	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
66	L7	118/119 (99%)	11 (9%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
67	Pt	76/77 (98%)	16 (21%)	0
69	L8	151/156 (96%)	26 (17%)	0
70	L5	3414/5069 (67%)	552 (16%)	10 (0%)
74	S2	1550/1869 (82%)	269 (17%)	6 (0%)
77	S6	55/75 (73%)	18 (32%)	1 (1%)
79	mR	6/27 (22%)	2 (33%)	0
All	All	5370/7392 (72%)	894 (16%)	17 (0%)

5 of 894 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
66	L7	7	G
66	L7	25	G
66	L7	31	G
66	L7	33	U
66	L7	53	U

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
74	S2	1508	A
77	S6	60	A
70	L5	2541	G
70	L5	4281	A
70	L5	4699	U

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

208 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	$\# Z  > 2$
3	MLZ	Lo	53	3	8,9,10	0.73	0	4,9,11	0.61	0
70	PSU	L5	3920	70,83	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
74	OMG	S2	1490	74	23,26,27	2.41	8 (34%)	33,38,41	2.02	10 (30%)
74	PSU	S2	1004	74	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
70	PSU	L5	4552	70	18,21,22	1.02	1 (5%)	22,30,33	1.71	4 (18%)
70	OMC	L5	4536	70	19,22,23	2.98	8 (42%)	26,31,34	0.78	0
70	A2M	L5	400	70	22,25,26	3.42	9 (40%)	31,36,39	2.38	9 (29%)
70	PSU	L5	1744	70	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
70	PSU	L5	2839	70	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
70	UR3	L5	4530	70	19,22,23	2.77	7 (36%)	26,32,35	1.34	2 (7%)
74	PSU	S2	119	74	18,21,22	1.03	1 (5%)	22,30,33	1.58	4 (18%)
74	PSU	S2	1232	74	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)
74	PSU	S2	1243	74	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
70	OMU	L5	2837	70	19,22,23	2.98	8 (42%)	26,31,34	1.77	5 (19%)
74	G7M	S2	1639	67,74	23,26,27	2.59	9 (39%)	35,39,42	2.49	11 (31%)
74	PSU	S2	572	74	18,21,22	1.02	1 (5%)	22,30,33	1.70	5 (22%)
70	OMC	L5	3841	70	19,22,23	2.97	8 (42%)	26,31,34	0.80	0
70	OMC	L5	2422	70,84	19,22,23	2.99	8 (42%)	26,31,34	0.78	0
67	OMC	Pt	33	67	19,22,23	3.01	8 (42%)	26,31,34	1.02	2 (7%)
70	6MZ	L5	4220	70	22,25,26	2.62	4 (18%)	30,36,39	2.30	11 (36%)
70	A2M	L5	1871	70	22,25,26	3.48	9 (40%)	31,36,39	2.39	10 (32%)
70	PSU	L5	4532	70	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)
70	PSU	L5	2632	70	18,21,22	1.02	1 (5%)	22,30,33	1.63	4 (18%)
70	1MA	L5	1322	70,84	21,25,26	2.91	6 (28%)	31,37,40	2.87	8 (25%)
70	PSU	L5	3762	70	18,21,22	1.09	1 (5%)	22,30,33	1.63	4 (18%)
70	PSU	L5	4636	70	18,21,22	1.06	1 (5%)	22,30,33	1.80	3 (13%)
74	PSU	S2	1445	74	18,21,22	1.08	1 (5%)	22,30,33	1.85	5 (22%)
74	PSU	S2	36	74	18,21,22	1.03	1 (5%)	22,30,33	1.76	4 (18%)
70	PSU	L5	4423	70	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
70	PSU	L5	2508	70	18,21,22	1.03	1 (5%)	22,30,33	1.68	4 (18%)
74	PSU	S2	573	74	18,21,22	1.05	1 (5%)	22,30,33	1.72	3 (13%)
70	A2M	L5	4523	70,83	22,25,26	3.42	9 (40%)	31,36,39	2.35	9 (29%)
70	PSU	L5	4296	70	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
74	A2M	S2	27	74,83	22,25,26	3.42	10 (45%)	31,36,39	2.38	10 (32%)
74	PSU	S2	866	74	18,21,22	1.11	1 (5%)	22,30,33	1.76	4 (18%)
70	OMG	L5	1522	70	23,26,27	2.42	8 (34%)	33,38,41	2.09	10 (30%)
74	PSU	S2	1643	74,83	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
70	PSU	L5	5001	70	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
70	PSU	L5	1782	70	18,21,22	1.02	1 (5%)	22,30,33	1.69	3 (13%)
70	OMU	L5	3925	70	19,22,23	2.96	8 (42%)	26,31,34	1.72	5 (19%)
70	PSU	L5	4493	70	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
74	MA6	S2	1851	74	23,26,27	1.37	4 (17%)	34,38,41	3.78	11 (32%)
70	OMC	L5	1881	70,82	19,22,23	2.97	8 (42%)	26,31,34	0.81	0
70	OMC	L5	2365	70,83	19,22,23	2.94	8 (42%)	26,31,34	0.68	0
74	PSU	S2	1367	74	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
70	A2M	L5	3830	70	22,25,26	3.40	9 (40%)	31,36,39	2.43	11 (35%)
70	OMU	L5	4227	70	19,22,23	2.95	8 (42%)	26,31,34	1.72	4 (15%)
70	PSU	L5	3734	70	18,21,22	1.00	1 (5%)	22,30,33	1.69	4 (18%)
74	PSU	S2	822	74	18,21,22	1.12	2 (11%)	22,30,33	1.83	5 (22%)
70	A2M	L5	3760	70	22,25,26	3.41	9 (40%)	31,36,39	2.52	11 (35%)
70	OMG	L5	4370	70	23,26,27	2.41	8 (34%)	33,38,41	2.06	9 (27%)
70	OMU	L5	4498	70	19,22,23	2.99	8 (42%)	26,31,34	1.70	4 (15%)
70	OMG	L5	4623	70	23,26,27	2.43	8 (34%)	33,38,41	2.05	10 (30%)
74	OMG	S2	1328	74	23,26,27	2.43	8 (34%)	33,38,41	2.05	10 (30%)
70	PSU	L5	3639	70	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
74	B8N	S2	1248	74	24,29,30	3.16	8 (33%)	29,42,45	1.79	7 (24%)
74	PSU	S2	863	74	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
70	OMG	L5	1625	70	23,26,27	2.44	8 (34%)	33,38,41	2.03	10 (30%)
69	OMG	L8	75	69	23,26,27	2.44	8 (34%)	33,38,41	2.04	10 (30%)
70	5MC	L5	4447	70	18,22,23	3.66	7 (38%)	26,32,35	1.08	1 (3%)
74	PSU	S2	609	74	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
70	PSU	L5	4521	70,83	18,21,22	1.11	1 (5%)	22,30,33	1.79	4 (18%)
70	PSU	L5	3764	70	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
74	OMC	S2	1703	74	19,22,23	3.00	8 (42%)	26,31,34	0.71	0
63	MLZ	Lb	5	63	8,9,10	0.77	0	4,9,11	0.65	0
70	OMG	L5	4228	70	23,26,27	2.42	9 (39%)	33,38,41	2.09	10 (30%)
70	OMC	L5	1340	70	19,22,23	2.94	8 (42%)	26,31,34	0.76	0
74	PSU	S2	218	74	18,21,22	1.06	1 (5%)	22,30,33	1.74	5 (22%)
70	PSU	L5	1536	70	18,21,22	1.06	1 (5%)	22,30,33	1.68	4 (18%)
70	OMG	L5	2424	70	23,26,27	2.43	8 (34%)	33,38,41	2.03	9 (27%)
70	PSU	L5	3637	70	18,21,22	1.05	1 (5%)	22,30,33	1.79	4 (18%)
70	A2M	L5	3785	70	22,25,26	3.35	9 (40%)	31,36,39	2.60	13 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
74	OMU	S2	428	74	19,22,23	2.98	8 (42%)	26,31,34	1.73	4 (15%)
70	PSU	L5	1862	70	18,21,22	1.01	1 (5%)	22,30,33	1.80	4 (18%)
74	PSU	S2	1244	74	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
69	PSU	L8	55	69	18,21,22	1.07	1 (5%)	22,30,33	1.72	4 (18%)
70	A2M	L5	2815	70	22,25,26	3.42	9 (40%)	31,36,39	2.41	10 (32%)
70	OMG	L5	3627	70	23,26,27	2.43	8 (34%)	33,38,41	2.10	10 (30%)
67	4SU	Pt	8	67	18,21,22	3.51	7 (38%)	26,30,33	2.20	5 (19%)
70	PSU	L5	4673	70	18,21,22	1.09	1 (5%)	22,30,33	1.75	4 (18%)
74	OMG	S2	867	74	23,26,27	2.41	8 (34%)	33,38,41	2.07	10 (30%)
74	A2M	S2	468	74	22,25,26	3.43	9 (40%)	31,36,39	2.32	10 (32%)
70	PSU	L5	3695	70	18,21,22	1.07	1 (5%)	22,30,33	1.78	5 (22%)
70	OMC	L5	3701	70,82,84	19,22,23	2.93	8 (42%)	26,31,34	0.73	0
70	PSU	L5	4500	70	18,21,22	1.11	1 (5%)	22,30,33	1.84	5 (22%)
70	A2M	L5	1524	70	22,25,26	3.41	10 (45%)	31,36,39	2.47	11 (35%)
74	A2M	S2	512	74	22,25,26	3.39	10 (45%)	31,36,39	2.47	10 (32%)
67	PSU	Pt	56	67	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
74	A2M	S2	484	74	22,25,26	3.42	9 (40%)	31,36,39	2.37	9 (29%)
70	PSU	L5	4689	70	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
74	PSU	S2	814	74	18,21,22	1.02	1 (5%)	22,30,33	1.61	4 (18%)
74	PSU	S2	918	74	18,21,22	1.12	2 (11%)	22,30,33	1.83	5 (22%)
74	A2M	S2	1031	74	22,25,26	3.46	9 (40%)	31,36,39	2.41	11 (35%)
70	OMG	L5	2876	70	23,26,27	2.44	8 (34%)	33,38,41	2.10	10 (30%)
74	OMU	S2	1804	74	19,22,23	3.04	8 (42%)	26,31,34	1.70	4 (15%)
74	PSU	S2	1347	74	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
70	OMG	L5	4494	70	23,26,27	2.43	8 (34%)	33,38,41	2.05	9 (27%)
74	PSU	S2	801	74	18,21,22	1.11	1 (5%)	22,30,33	1.72	4 (18%)
74	4AC	S2	1337	74	21,24,25	3.47	9 (42%)	29,34,37	1.03	2 (6%)
74	PSU	S2	109	74	18,21,22	1.11	1 (5%)	22,30,33	1.78	4 (18%)
74	PSU	S2	1177	74	18,21,22	1.04	1 (5%)	22,30,33	1.68	4 (18%)
70	OMC	L5	3869	70	19,22,23	2.99	8 (42%)	26,31,34	0.73	0
70	OMG	L5	3744	70	23,26,27	2.42	8 (34%)	33,38,41	2.03	10 (30%)
70	A2M	L5	2363	70,83,84	22,25,26	3.47	9 (40%)	31,36,39	2.39	10 (32%)
74	PSU	S2	1174	74	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
74	A2M	S2	590	74	22,25,26	3.41	9 (40%)	31,36,39	2.54	11 (35%)
67	H2U	Pt	21	67	18,21,22	3.04	5 (27%)	21,30,33	1.93	4 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
70	OMC	L5	2351	70	19,22,23	2.95	8 (42%)	26,31,34	1.08	3 (11%)
70	PSU	L5	1781	70	18,21,22	1.08	1 (5%)	22,30,33	1.64	4 (18%)
70	OMG	L5	4392	70	23,26,27	2.40	8 (34%)	33,38,41	2.06	10 (30%)
70	OMC	L5	4456	70	19,22,23	2.94	8 (42%)	26,31,34	0.84	1 (3%)
70	PSU	L5	4531	70	18,21,22	1.04	1 (5%)	22,30,33	1.77	5 (22%)
70	A2M	L5	4571	70	22,25,26	3.45	9 (40%)	31,36,39	2.32	10 (32%)
70	A2M	L5	398	70	22,25,26	3.42	9 (40%)	31,36,39	2.37	11 (35%)
70	PSU	L5	1683	70	18,21,22	1.09	1 (5%)	22,30,33	1.78	4 (18%)
74	PSU	S2	1238	74	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
70	PSU	L5	4299	70	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
70	A2M	L5	3867	70	22,25,26	3.43	9 (40%)	31,36,39	2.43	10 (32%)
74	PSU	S2	1625	74	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
70	OMG	L5	4637	70	23,26,27	2.40	8 (34%)	33,38,41	2.07	10 (30%)
70	PSU	L5	4576	70	18,21,22	1.05	1 (5%)	22,30,33	1.70	4 (18%)
74	PSU	S2	1081	74	18,21,22	0.96	1 (5%)	22,30,33	1.70	2 (9%)
70	PSU	L5	3851	70	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
70	PSU	L5	2843	70	18,21,22	1.04	1 (5%)	22,30,33	1.86	4 (18%)
74	PSU	S2	686	74	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
74	OMG	S2	644	74	23,26,27	2.42	8 (34%)	33,38,41	2.04	10 (30%)
70	PSU	L5	4569	70	18,21,22	1.06	1 (5%)	22,30,33	1.71	4 (18%)
70	OMG	L5	3792	70	23,26,27	2.41	8 (34%)	33,38,41	2.05	9 (27%)
74	OMG	S2	509	74	23,26,27	2.39	8 (34%)	33,38,41	2.00	9 (27%)
74	PSU	S2	1136	74	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
70	OMG	L5	1316	70	23,26,27	2.43	8 (34%)	33,38,41	2.03	10 (30%)
74	4AC	S2	1842	74	21,24,25	3.34	9 (42%)	29,34,37	1.06	3 (10%)
70	OMC	L5	2861	70	19,22,23	2.98	8 (42%)	26,31,34	0.78	0
70	OMG	L5	4499	70	23,26,27	2.43	8 (34%)	33,38,41	2.04	10 (30%)
74	PSU	S2	296	74	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
70	PSU	L5	4431	70	18,21,22	1.11	1 (5%)	22,30,33	1.71	4 (18%)
70	PSU	L5	5010	70	18,21,22	1.09	1 (5%)	22,30,33	1.75	4 (18%)
70	PSU	L5	4457	70	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
74	A2M	S2	576	74	22,25,26	3.40	9 (40%)	31,36,39	2.31	9 (29%)
70	OMG	L5	3899	70,83	23,26,27	2.40	8 (34%)	33,38,41	2.06	10 (30%)
70	PSU	L5	3768	70	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
69	PSU	L8	69	69	18,21,22	1.03	1 (5%)	22,30,33	1.71	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
74	PSU	S2	1692	74	18,21,22	1.05	1 (5%)	22,30,33	1.67	4 (18%)
74	6MZ	S2	1832	74,83	22,25,26	2.63	4 (18%)	30,36,39	2.33	10 (33%)
74	OMG	S2	436	74	23,26,27	2.39	8 (34%)	33,38,41	2.06	10 (30%)
70	OMG	L5	4196	70	23,26,27	2.43	8 (34%)	33,38,41	2.02	10 (30%)
70	PSU	L5	1677	70	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
74	PSU	S2	651	74	18,21,22	1.03	1 (5%)	22,30,33	1.71	4 (18%)
70	OMC	L5	2824	70	19,22,23	3.02	8 (42%)	26,31,34	0.75	0
70	PSU	L5	4353	70	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
67	G7M	Pt	47	67	23,26,27	2.63	9 (39%)	35,39,42	2.46	11 (31%)
70	5MC	L5	3782	70,83	18,22,23	3.65	7 (38%)	26,32,35	1.09	2 (7%)
70	A2M	L5	3718	70	22,25,26	3.42	9 (40%)	31,36,39	2.36	9 (29%)
70	PSU	L5	4293	70	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
74	OMC	S2	462	74	19,22,23	3.00	8 (42%)	26,31,34	0.78	0
74	MA6	S2	1850	74	23,26,27	1.38	4 (17%)	34,38,41	3.66	11 (32%)
70	OMG	L5	4618	70	23,26,27	2.41	8 (34%)	33,38,41	2.06	10 (30%)
74	PSU	S2	406	74	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
70	PSU	L5	4471	70	18,21,22	1.07	1 (5%)	22,30,33	1.66	4 (18%)
70	PSU	L5	4361	70	18,21,22	1.02	1 (5%)	22,30,33	1.73	4 (18%)
74	PSU	S2	1056	74	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
74	PSU	S2	815	74	18,21,22	0.98	1 (5%)	22,30,33	1.65	4 (18%)
74	PSU	S2	34	74	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
70	PSU	L5	3853	70,84	18,21,22	1.09	1 (5%)	22,30,33	1.69	4 (18%)
74	PSU	S2	105	74	18,21,22	1.07	1 (5%)	22,30,33	1.71	4 (18%)
70	A2M	L5	3825	70	22,25,26	3.43	10 (45%)	31,36,39	2.40	11 (35%)
70	PSU	L5	3729	70	18,21,22	1.10	1 (5%)	22,30,33	1.76	4 (18%)
74	PSU	S2	681	74	18,21,22	1.05	1 (5%)	22,30,33	1.71	4 (18%)
74	OMC	S2	517	74	19,22,23	3.00	8 (42%)	26,31,34	0.77	0
74	OMG	S2	683	74	23,26,27	2.44	8 (34%)	33,38,41	2.03	10 (30%)
74	PSU	S2	966	74	18,21,22	0.99	1 (5%)	22,30,33	1.60	3 (13%)
70	OMG	L5	2364	70	23,26,27	2.39	8 (34%)	33,38,41	2.05	10 (30%)
70	A2M	L5	1534	70,83	22,25,26	3.46	9 (40%)	31,36,39	2.36	9 (29%)
70	A2M	L5	2401	70	22,25,26	3.41	10 (45%)	31,36,39	2.38	10 (32%)
70	PSU	L5	3770	70	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
74	PSU	S2	1239	74	18,21,22	1.05	1 (5%)	22,30,33	1.74	3 (13%)
70	PSU	L5	3844	70	18,21,22	1.00	1 (5%)	22,30,33	1.75	4 (18%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
70	PSU	L5	4403	70	18,21,22	1.04	1 (5%)	22,30,33	1.80	5 (22%)
74	A2M	S2	1678	74	22,25,26	3.49	9 (40%)	31,36,39	2.53	11 (35%)
70	PSU	L5	4312	70	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
70	PSU	L5	4420	70	18,21,22	1.05	1 (5%)	22,30,33	1.65	5 (22%)
70	PSU	L5	4442	70	18,21,22	1.03	1 (5%)	22,30,33	1.73	5 (22%)
74	A2M	S2	668	74,83	22,25,26	3.40	10 (45%)	31,36,39	2.45	11 (35%)
70	OMU	L5	4620	70	19,22,23	2.93	8 (42%)	26,31,34	1.67	4 (15%)
70	OMC	L5	3887	70	19,22,23	2.97	8 (42%)	26,31,34	0.77	0
70	PSU	L5	4579	70	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
70	PSU	L5	4628	70	18,21,22	1.06	1 (5%)	22,30,33	1.87	4 (18%)
64	V5N	LA	216	64	9,11,12	2.65	2 (22%)	9,14,16	1.18	1 (11%)
74	OMU	S2	627	74	19,22,23	3.03	8 (42%)	26,31,34	1.73	5 (19%)
65	V5N	La	39	65	9,11,12	2.68	2 (22%)	9,14,16	1.27	1 (11%)
70	PSU	L5	1779	70	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
70	PSU	L5	3884	70	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
70	PSU	L5	4972	70	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
74	PSU	S2	93	74	18,21,22	1.00	1 (5%)	22,30,33	1.65	4 (18%)
70	PSU	L5	1860	70	18,21,22	1.05	1 (5%)	22,30,33	1.69	4 (18%)
70	A2M	L5	4590	70	22,25,26	3.43	9 (40%)	31,36,39	2.43	9 (29%)
74	A2M	S2	99	74,83	22,25,26	3.44	9 (40%)	31,36,39	2.35	10 (32%)
70	PSU	L5	1582	70	18,21,22	1.03	1 (5%)	22,30,33	1.58	4 (18%)
74	PSU	S2	649	74	18,21,22	1.04	1 (5%)	22,30,33	1.77	4 (18%)
74	OMU	S2	116	74	19,22,23	2.99	8 (42%)	26,31,34	1.66	5 (19%)
74	OMC	S2	1391	74	19,22,23	2.98	8 (42%)	26,31,34	0.79	0
70	PSU	L5	1792	70,82	18,21,22	1.03	1 (5%)	22,30,33	1.61	4 (18%)
70	OMC	L5	2804	70	19,22,23	2.96	8 (42%)	26,31,34	0.66	0
70	PSU	L5	3715	70	18,21,22	1.06	1 (5%)	22,30,33	1.67	4 (18%)
70	A2M	L5	1326	70	22,25,26	3.41	10 (45%)	31,36,39	2.35	8 (25%)
70	OMC	L5	3808	70	19,22,23	2.94	8 (42%)	26,31,34	0.85	0
70	PSU	L5	3758	70,84	18,21,22	1.04	1 (5%)	22,30,33	1.76	4 (18%)
74	A2M	S2	1383	74	22,25,26	3.42	9 (40%)	31,36,39	2.38	9 (29%)

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
3	MLZ	Lo	53	3	-	4/7/8/10	-
70	PSU	L5	3920	70,83	-	0/7/25/26	0/2/2/2
74	OMG	S2	1490	74	-	1/9/27/28	0/3/3/3
74	PSU	S2	1004	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4552	70	-	0/7/25/26	0/2/2/2
70	OMC	L5	4536	70	-	0/9/27/28	0/2/2/2
70	A2M	L5	400	70	-	1/9/27/28	0/3/3/3
70	PSU	L5	1744	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	2839	70	-	0/7/25/26	0/2/2/2
70	UR3	L5	4530	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	119	74	-	1/7/25/26	0/2/2/2
74	PSU	S2	1232	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	1243	74	-	2/7/25/26	0/2/2/2
70	OMU	L5	2837	70	-	0/9/27/28	0/2/2/2
74	G7M	S2	1639	67,74	-	0/7/25/26	0/3/3/3
74	PSU	S2	572	74	-	0/7/25/26	0/2/2/2
70	OMC	L5	3841	70	-	0/9/27/28	0/2/2/2
70	OMC	L5	2422	70,84	-	2/9/27/28	0/2/2/2
67	OMC	Pt	33	67	-	2/9/27/28	0/2/2/2
70	6MZ	L5	4220	70	-	0/9/27/28	0/3/3/3
70	A2M	L5	1871	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	4532	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	2632	70	-	0/7/25/26	0/2/2/2
70	1MA	L5	1322	70,84	-	0/7/25/26	0/3/3/3
70	PSU	L5	3762	70	-	2/7/25/26	0/2/2/2
70	PSU	L5	4636	70	-	4/7/25/26	0/2/2/2
74	PSU	S2	1445	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	36	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4423	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	2508	70	-	2/7/25/26	0/2/2/2
74	PSU	S2	573	74	-	0/7/25/26	0/2/2/2
70	A2M	L5	4523	70,83	-	0/9/27/28	0/3/3/3
70	PSU	L5	4296	70	-	0/7/25/26	0/2/2/2
74	A2M	S2	27	74,83	-	0/9/27/28	0/3/3/3
74	PSU	S2	866	74	-	0/7/25/26	0/2/2/2
70	OMG	L5	1522	70	-	0/9/27/28	0/3/3/3
74	PSU	S2	1643	74,83	-	1/7/25/26	0/2/2/2
70	PSU	L5	5001	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	1782	70	-	0/7/25/26	0/2/2/2
70	OMU	L5	3925	70	-	1/9/27/28	0/2/2/2
70	PSU	L5	4493	70	-	0/7/25/26	0/2/2/2
74	MA6	S2	1851	74	-	1/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	OMC	L5	1881	70,82	-	0/9/27/28	0/2/2/2
70	OMC	L5	2365	70,83	-	0/9/27/28	0/2/2/2
74	PSU	S2	1367	74	-	0/7/25/26	0/2/2/2
70	A2M	L5	3830	70	-	0/9/27/28	0/3/3/3
70	OMU	L5	4227	70	-	0/9/27/28	0/2/2/2
70	PSU	L5	3734	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	822	74	-	2/7/25/26	0/2/2/2
70	A2M	L5	3760	70	-	3/9/27/28	0/3/3/3
70	OMG	L5	4370	70	-	0/9/27/28	0/3/3/3
70	OMU	L5	4498	70	-	0/9/27/28	0/2/2/2
70	OMG	L5	4623	70	-	1/9/27/28	0/3/3/3
74	OMG	S2	1328	74	-	1/9/27/28	0/3/3/3
70	PSU	L5	3639	70	-	0/7/25/26	0/2/2/2
74	B8N	S2	1248	74	-	4/16/34/35	0/2/2/2
74	PSU	S2	863	74	-	0/7/25/26	0/2/2/2
70	OMG	L5	1625	70	-	2/9/27/28	0/3/3/3
69	OMG	L8	75	69	-	1/9/27/28	0/3/3/3
70	5MC	L5	4447	70	-	4/7/25/26	0/2/2/2
74	PSU	S2	609	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4521	70,83	-	1/7/25/26	0/2/2/2
70	PSU	L5	3764	70	-	2/7/25/26	0/2/2/2
74	OMC	S2	1703	74	-	1/9/27/28	0/2/2/2
63	MLZ	Lb	5	63	-	5/7/8/10	-
70	OMG	L5	4228	70	-	0/9/27/28	0/3/3/3
70	OMC	L5	1340	70	-	0/9/27/28	0/2/2/2
74	PSU	S2	218	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	1536	70	-	0/7/25/26	0/2/2/2
70	OMG	L5	2424	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	3637	70	-	0/7/25/26	0/2/2/2
70	A2M	L5	3785	70	-	1/9/27/28	0/3/3/3
74	OMU	S2	428	74	-	6/9/27/28	0/2/2/2
70	PSU	L5	1862	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	1244	74	-	0/7/25/26	0/2/2/2
69	PSU	L8	55	69	-	0/7/25/26	0/2/2/2
70	A2M	L5	2815	70	-	0/9/27/28	0/3/3/3
70	OMG	L5	3627	70	-	0/9/27/28	0/3/3/3
67	4SU	Pt	8	67	-	0/7/25/26	0/2/2/2
70	PSU	L5	4673	70	-	0/7/25/26	0/2/2/2
74	OMG	S2	867	74	-	1/9/27/28	0/3/3/3
74	A2M	S2	468	74	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PSU	L5	3695	70	-	0/7/25/26	0/2/2/2
70	OMC	L5	3701	70,82,84	-	4/9/27/28	0/2/2/2
70	PSU	L5	4500	70	-	1/7/25/26	0/2/2/2
70	A2M	L5	1524	70	-	1/9/27/28	0/3/3/3
74	A2M	S2	512	74	-	2/9/27/28	0/3/3/3
67	PSU	Pt	56	67	-	0/7/25/26	0/2/2/2
74	A2M	S2	484	74	-	0/9/27/28	0/3/3/3
70	PSU	L5	4689	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	814	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	918	74	-	2/7/25/26	0/2/2/2
74	A2M	S2	1031	74	-	0/9/27/28	0/3/3/3
70	OMG	L5	2876	70	-	1/9/27/28	0/3/3/3
74	OMU	S2	1804	74	-	1/9/27/28	0/2/2/2
74	PSU	S2	1347	74	-	0/7/25/26	0/2/2/2
70	OMG	L5	4494	70	-	0/9/27/28	0/3/3/3
74	PSU	S2	801	74	-	0/7/25/26	0/2/2/2
74	4AC	S2	1337	74	-	0/11/29/30	0/2/2/2
74	PSU	S2	109	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	1177	74	-	0/7/25/26	0/2/2/2
70	OMC	L5	3869	70	-	1/9/27/28	0/2/2/2
70	OMG	L5	3744	70	-	0/9/27/28	0/3/3/3
70	A2M	L5	2363	70,83,84	-	0/9/27/28	0/3/3/3
74	PSU	S2	1174	74	-	0/7/25/26	0/2/2/2
74	A2M	S2	590	74	-	3/9/27/28	0/3/3/3
67	H2U	Pt	21	67	-	4/7/38/39	0/2/2/2
70	OMC	L5	2351	70	-	3/9/27/28	0/2/2/2
70	PSU	L5	1781	70	-	0/7/25/26	0/2/2/2
70	OMG	L5	4392	70	-	0/9/27/28	0/3/3/3
70	OMC	L5	4456	70	-	0/9/27/28	0/2/2/2
70	PSU	L5	4531	70	-	0/7/25/26	0/2/2/2
70	A2M	L5	4571	70	-	0/9/27/28	0/3/3/3
70	A2M	L5	398	70	-	1/9/27/28	0/3/3/3
70	PSU	L5	1683	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	1238	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4299	70	-	0/7/25/26	0/2/2/2
70	A2M	L5	3867	70	-	1/9/27/28	0/3/3/3
74	PSU	S2	1625	74	-	0/7/25/26	0/2/2/2
70	OMG	L5	4637	70	-	2/9/27/28	0/3/3/3
70	PSU	L5	4576	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	1081	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	3851	70	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PSU	L5	2843	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	686	74	-	0/7/25/26	0/2/2/2
74	OMG	S2	644	74	-	3/9/27/28	0/3/3/3
70	PSU	L5	4569	70	-	0/7/25/26	0/2/2/2
70	OMG	L5	3792	70	-	0/9/27/28	0/3/3/3
74	OMG	S2	509	74	-	1/9/27/28	0/3/3/3
74	PSU	S2	1136	74	-	0/7/25/26	0/2/2/2
70	OMG	L5	1316	70	-	0/9/27/28	0/3/3/3
74	4AC	S2	1842	74	-	0/11/29/30	0/2/2/2
70	OMC	L5	2861	70	-	0/9/27/28	0/2/2/2
70	OMG	L5	4499	70	-	2/9/27/28	0/3/3/3
74	PSU	S2	296	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4431	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	5010	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4457	70	-	0/7/25/26	0/2/2/2
74	A2M	S2	576	74	-	2/9/27/28	0/3/3/3
70	OMG	L5	3899	70,83	-	0/9/27/28	0/3/3/3
70	PSU	L5	3768	70	-	0/7/25/26	0/2/2/2
69	PSU	L8	69	69	-	1/7/25/26	0/2/2/2
74	PSU	S2	1692	74	-	0/7/25/26	0/2/2/2
74	6MZ	S2	1832	74,83	-	2/9/27/28	0/3/3/3
74	OMG	S2	436	74	-	0/9/27/28	0/3/3/3
70	OMG	L5	4196	70	-	3/9/27/28	0/3/3/3
70	PSU	L5	1677	70	-	4/7/25/26	0/2/2/2
74	PSU	S2	651	74	-	0/7/25/26	0/2/2/2
70	OMC	L5	2824	70	-	0/9/27/28	0/2/2/2
70	PSU	L5	4353	70	-	0/7/25/26	0/2/2/2
67	G7M	Pt	47	67	-	1/7/25/26	0/3/3/3
70	5MC	L5	3782	70,83	-	0/7/25/26	0/2/2/2
70	A2M	L5	3718	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	4293	70	-	2/7/25/26	0/2/2/2
74	OMC	S2	462	74	-	1/9/27/28	0/2/2/2
74	MA6	S2	1850	74	-	0/11/29/30	0/3/3/3
70	OMG	L5	4618	70	-	0/9/27/28	0/3/3/3
74	PSU	S2	406	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4471	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4361	70	-	1/7/25/26	0/2/2/2
74	PSU	S2	1056	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	815	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	34	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	3853	70,84	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	PSU	S2	105	74	-	0/7/25/26	0/2/2/2
70	A2M	L5	3825	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	3729	70	-	2/7/25/26	0/2/2/2
74	PSU	S2	681	74	-	0/7/25/26	0/2/2/2
74	OMC	S2	517	74	-	0/9/27/28	0/2/2/2
74	OMG	S2	683	74	-	0/9/27/28	0/3/3/3
74	PSU	S2	966	74	-	0/7/25/26	0/2/2/2
70	OMG	L5	2364	70	-	0/9/27/28	0/3/3/3
70	A2M	L5	1534	70,83	-	2/9/27/28	0/3/3/3
70	A2M	L5	2401	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	3770	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	1239	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	3844	70	-	3/7/25/26	0/2/2/2
70	PSU	L5	4403	70	-	0/7/25/26	0/2/2/2
74	A2M	S2	1678	74	-	0/9/27/28	0/3/3/3
70	PSU	L5	4312	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4420	70	-	4/7/25/26	0/2/2/2
70	PSU	L5	4442	70	-	1/7/25/26	0/2/2/2
74	A2M	S2	668	74,83	-	3/9/27/28	0/3/3/3
70	OMU	L5	4620	70	-	1/9/27/28	0/2/2/2
70	OMC	L5	3887	70	-	0/9/27/28	0/2/2/2
70	PSU	L5	4579	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4628	70	-	0/7/25/26	0/2/2/2
64	V5N	LA	216	64	-	1/9/10/12	0/1/1/1
74	OMU	S2	627	74	-	1/9/27/28	0/2/2/2
65	V5N	La	39	65	-	0/9/10/12	0/1/1/1
70	PSU	L5	1779	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	3884	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4972	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	93	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	1860	70	-	0/7/25/26	0/2/2/2
70	A2M	L5	4590	70	-	2/9/27/28	0/3/3/3
74	A2M	S2	99	74,83	-	1/9/27/28	0/3/3/3
70	PSU	L5	1582	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	649	74	-	0/7/25/26	0/2/2/2
74	OMU	S2	116	74	-	1/9/27/28	0/2/2/2
74	OMC	S2	1391	74	-	0/9/27/28	0/2/2/2
70	PSU	L5	1792	70,82	-	0/7/25/26	0/2/2/2
70	OMC	L5	2804	70	-	0/9/27/28	0/2/2/2
70	PSU	L5	3715	70	-	0/7/25/26	0/2/2/2
70	A2M	L5	1326	70	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	OMC	L5	3808	70	-	0/9/27/28	0/2/2/2
70	PSU	L5	3758	70,84	-	1/7/25/26	0/2/2/2
74	A2M	S2	1383	74	-	0/9/27/28	0/3/3/3

The worst 5 of 926 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	S2	1832	6MZ	C6-N6	10.79	1.45	1.34
70	L5	4220	6MZ	C6-N6	10.58	1.45	1.34
67	Pt	21	H2U	C2-N1	9.64	1.49	1.35
70	L5	4447	5MC	C6-C5	9.55	1.50	1.34
70	L5	3782	5MC	C6-C5	9.33	1.49	1.34

The worst 5 of 1125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	S2	1851	MA6	N1-C6-N6	-15.79	99.82	117.08
74	S2	1850	MA6	N1-C6-N6	-15.05	100.62	117.08
70	L5	1322	1MA	C1'-N9-C8	-9.09	100.81	126.70
74	S2	1851	MA6	C5-C6-N6	8.87	140.75	125.30
70	L5	1322	1MA	C1'-N9-C4	8.83	152.73	126.50

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Lo	53	MLZ	N-CA-CB-CG
3	Lo	53	MLZ	C-CA-CB-CG
63	Lb	5	MLZ	N-CA-CB-CG
63	Lb	5	MLZ	C-CA-CB-CG
64	LA	216	V5N	O-C-CA-CB

There are no ring outliers.

48 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	S2	1490	OMG	1	0
70	L5	4552	PSU	1	0
70	L5	400	A2M	1	0
74	S2	1232	PSU	1	0
70	L5	2837	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	S2	1639	G7M	1	0
67	Pt	33	OMC	1	0
70	L5	4220	6MZ	1	0
70	L5	1871	A2M	1	0
70	L5	1322	1MA	1	0
74	S2	573	PSU	1	0
70	L5	4523	A2M	1	0
70	L5	3925	OMU	1	0
70	L5	3830	A2M	1	0
70	L5	4623	OMG	1	0
70	L5	1625	OMG	1	0
69	L8	75	OMG	2	0
70	L5	4521	PSU	1	0
74	S2	1703	OMC	1	0
70	L5	1340	OMC	1	0
70	L5	2424	OMG	1	0
74	S2	1244	PSU	2	0
70	L5	2815	A2M	1	0
74	S2	867	OMG	1	0
74	S2	512	A2M	1	0
74	S2	484	A2M	1	0
74	S2	1031	A2M	1	0
74	S2	1804	OMU	1	0
70	L5	2363	A2M	1	0
67	Pt	21	H2U	1	0
70	L5	2351	OMC	1	0
70	L5	4456	OMC	1	0
70	L5	1683	PSU	1	0
70	L5	3867	A2M	1	0
70	L5	4637	OMG	1	0
74	S2	509	OMG	2	0
74	S2	576	A2M	1	0
74	S2	436	OMG	1	0
70	L5	4196	OMG	1	0
70	L5	3718	A2M	2	0
70	L5	4618	OMG	1	0
70	L5	3770	PSU	2	0
70	L5	4620	OMU	2	0
70	L5	4579	PSU	1	0
74	S2	627	OMU	1	0
74	S2	116	OMU	2	0
74	S2	1391	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	L5	1326	A2M	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 266 ligands modelled in this entry, 262 are monoatomic - leaving 4 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
85	SPD	L5	5101	-	9,9,9	0.28	0	8,8,8	0.19	0
86	HYG	S2	1901	-	35,39,39	3.13	12 (34%)	43,60,60	1.88	8 (18%)
85	SPD	L5	5102	-	9,9,9	0.28	0	8,8,8	0.22	0
85	SPD	L5	5103	70	9,9,9	0.28	0	8,8,8	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	L5	5101	-	-	2/7/7/7	-
86	HYG	S2	1901	-	-	2/12/87/87	0/4/4/4
85	SPD	L5	5102	-	-	4/7/7/7	-
85	SPD	L5	5103	70	-	4/7/7/7	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	S2	1901	HYG	O29-C12	11.00	1.61	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	S2	1901	HYG	O22-C17	6.65	1.54	1.43
86	S2	1901	HYG	O14-C13	6.47	1.58	1.41
86	S2	1901	HYG	O28-C23	6.07	1.47	1.40
86	S2	1901	HYG	C16-C15	4.31	1.62	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	1901	HYG	O28-C27-C26	6.61	117.91	108.52
86	S2	1901	HYG	O29-C12-C13	4.84	123.57	110.86
86	S2	1901	HYG	O22-C17-C16	4.08	121.16	111.22
86	S2	1901	HYG	C23-O28-C27	3.91	119.44	112.00
86	S2	1901	HYG	O22-C17-C12	2.75	107.97	103.58

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	L5	5103	SPD	C3-C4-C5-N6
85	L5	5102	SPD	C3-C4-C5-N6
86	S2	1901	HYG	O14-C13-O18-C6
85	L5	5103	SPD	C7-C8-C9-N10
85	L5	5103	SPD	N6-C7-C8-C9

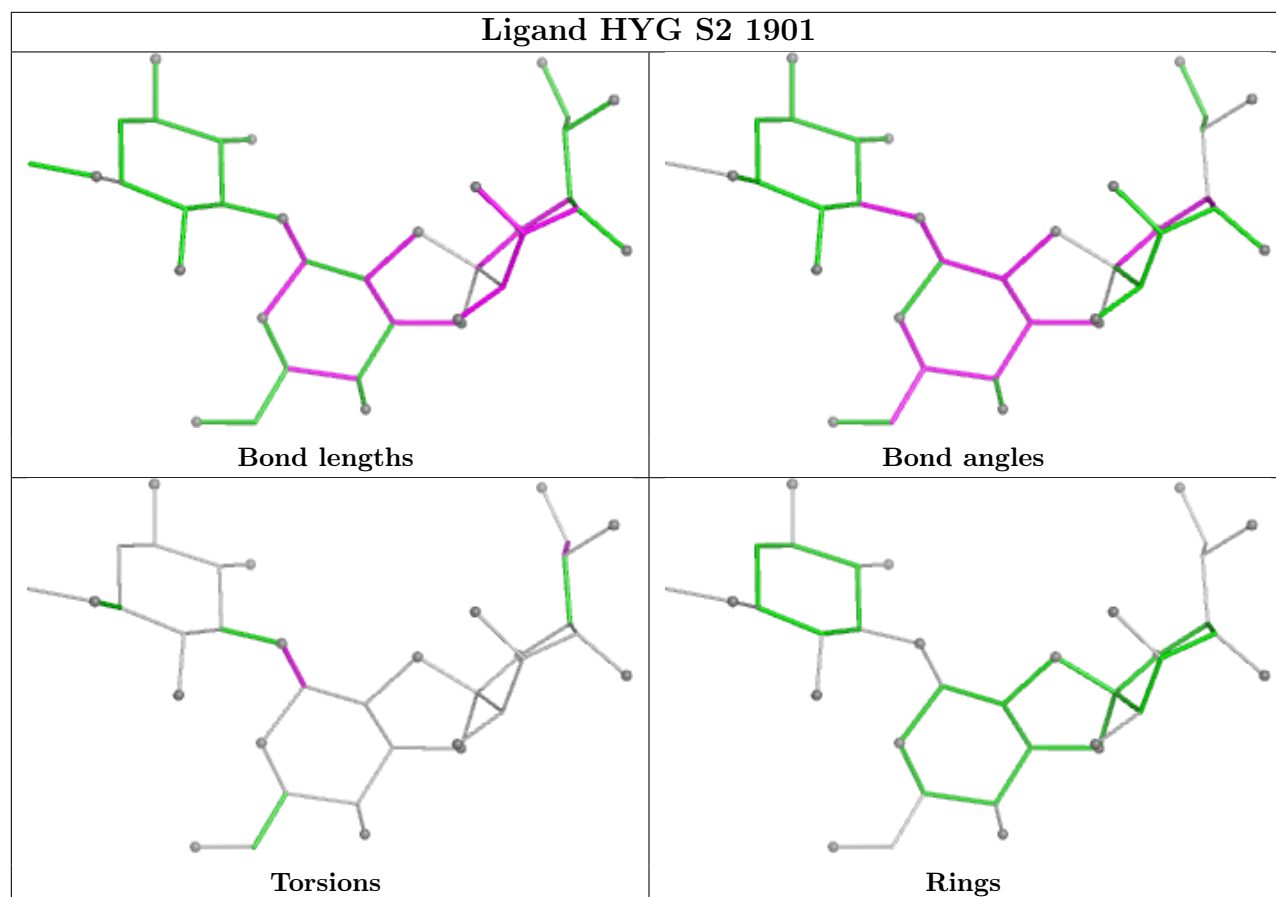
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	L5	5101	SPD	1	0
85	L5	5102	SPD	3	0

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

equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

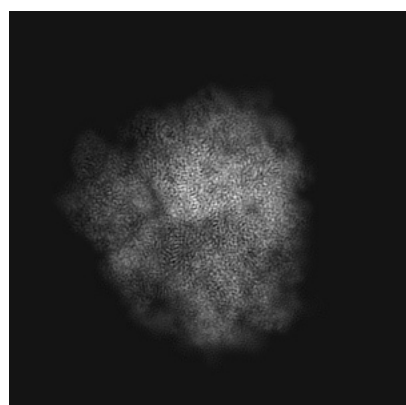
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54266. These allow visual inspection of the internal detail of the map and identification of artifacts.

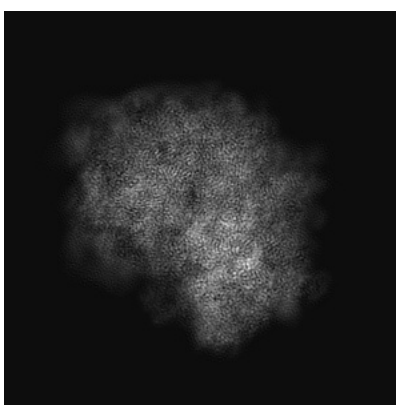
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

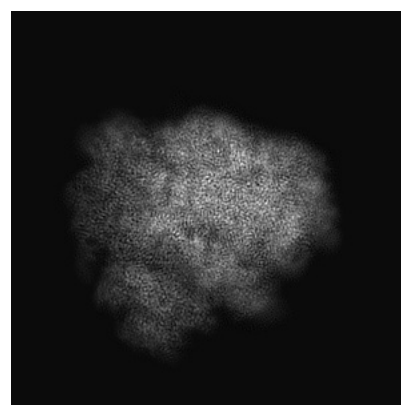
#### 6.1.1 Primary map



X



Y

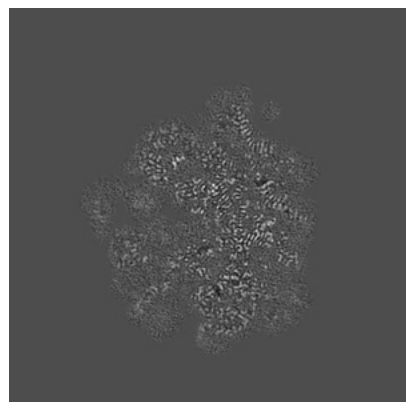


Z

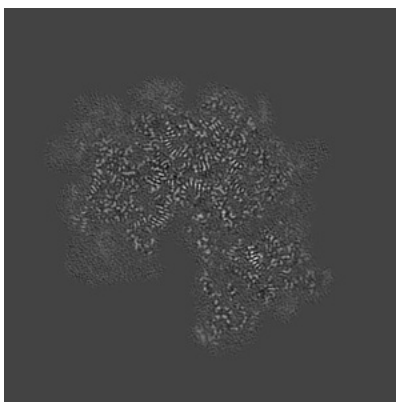
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

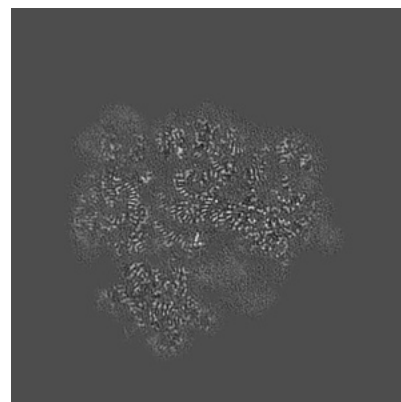
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

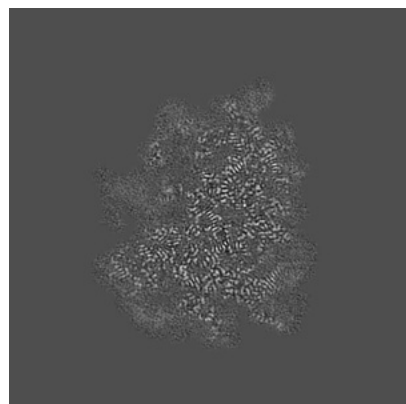


Z Index: 240

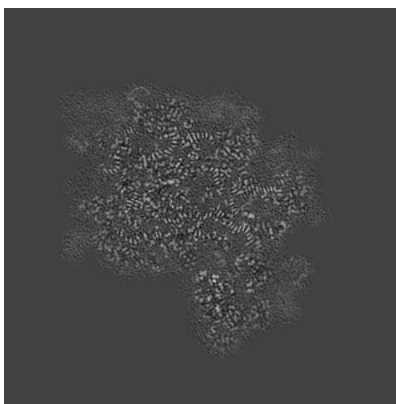
The images above show central slices of the map in three orthogonal directions.

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

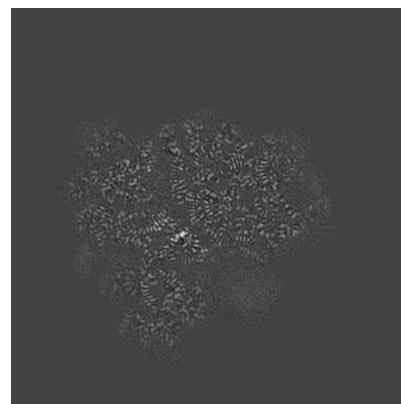
### 6.3.1 Primary map



X Index: 265



Y Index: 271

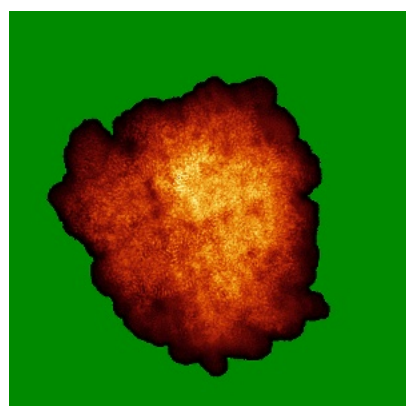


Z Index: 265

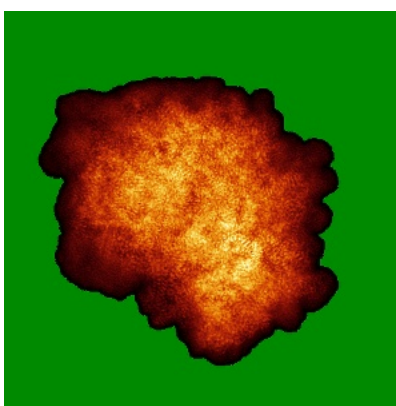
The images above show the largest variance slices of the map in three orthogonal directions.

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

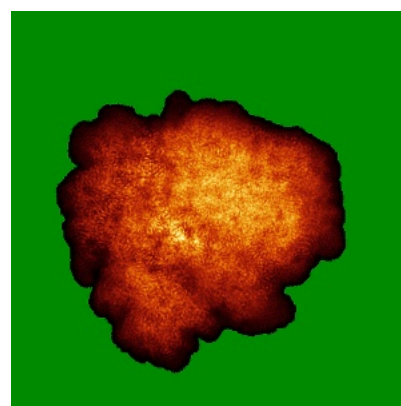
### 6.4.1 Primary map



X



Y

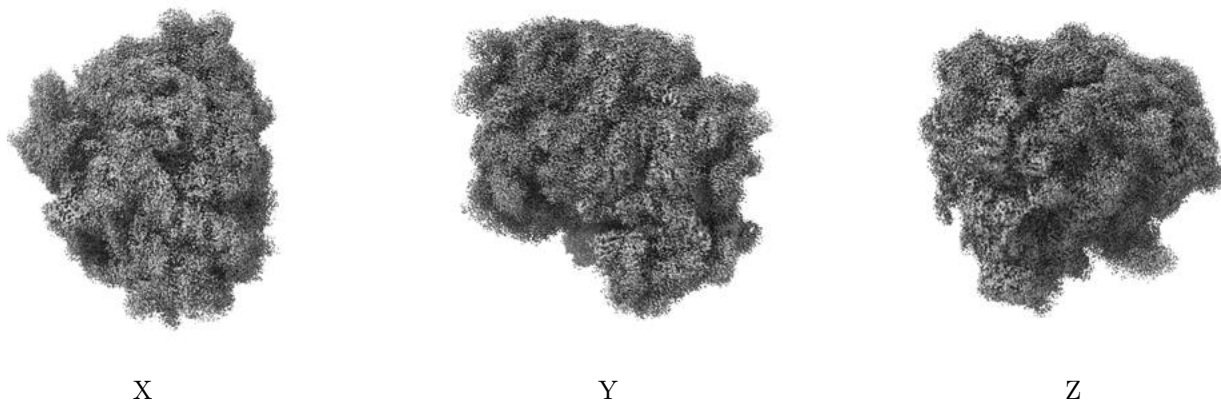


Z

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

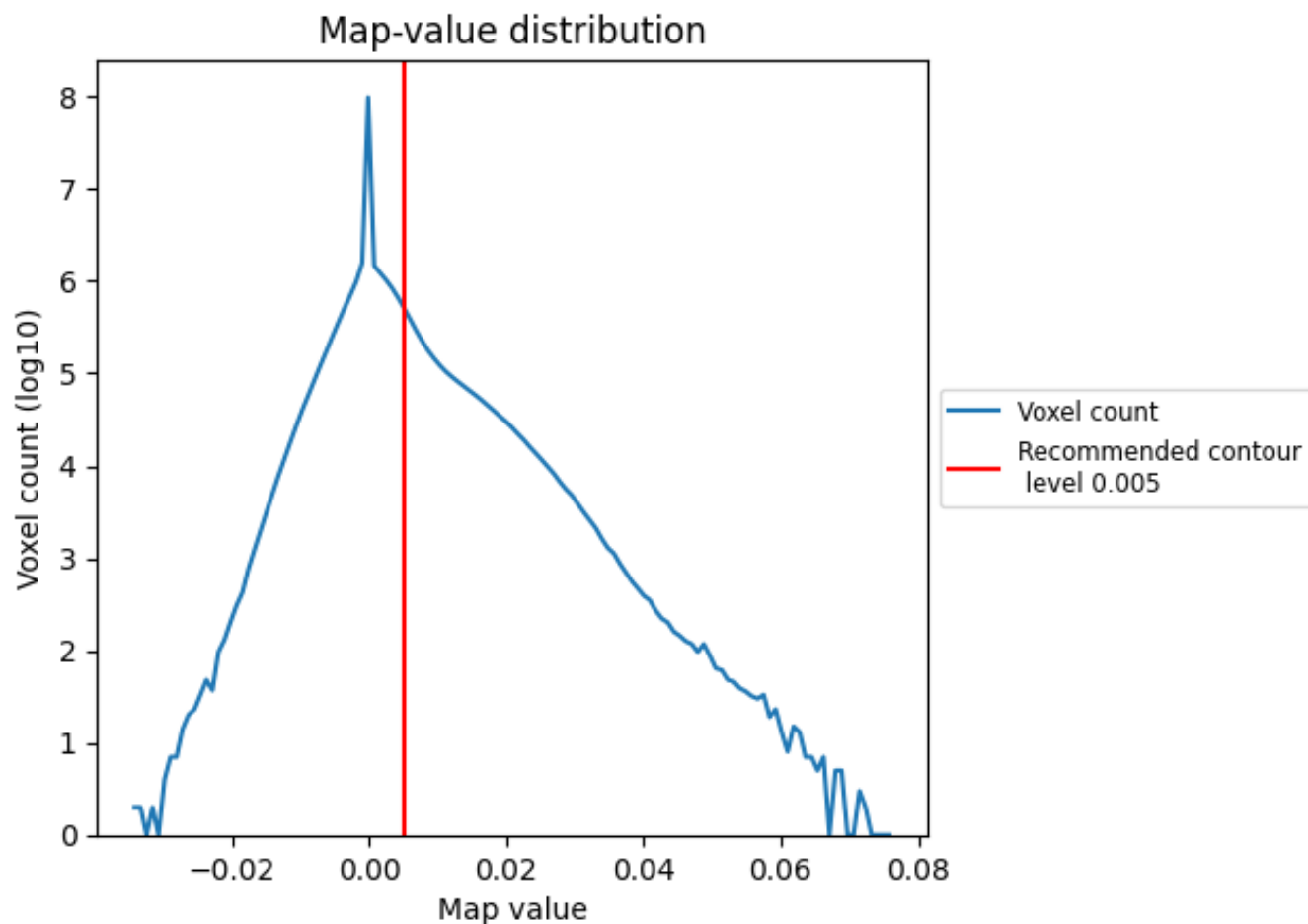
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

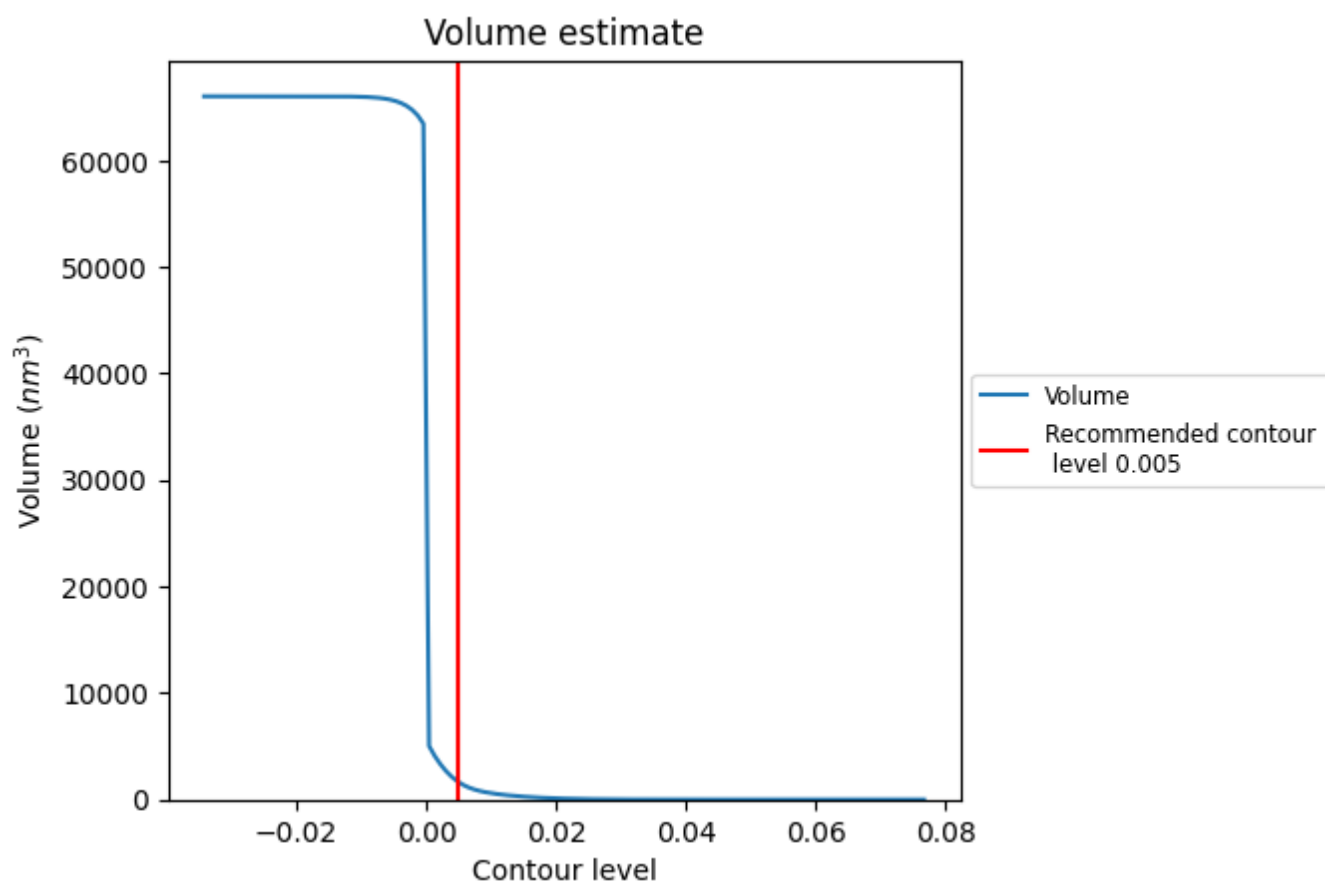
This section contains the results of statistical analysis of the map.

### 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](#)

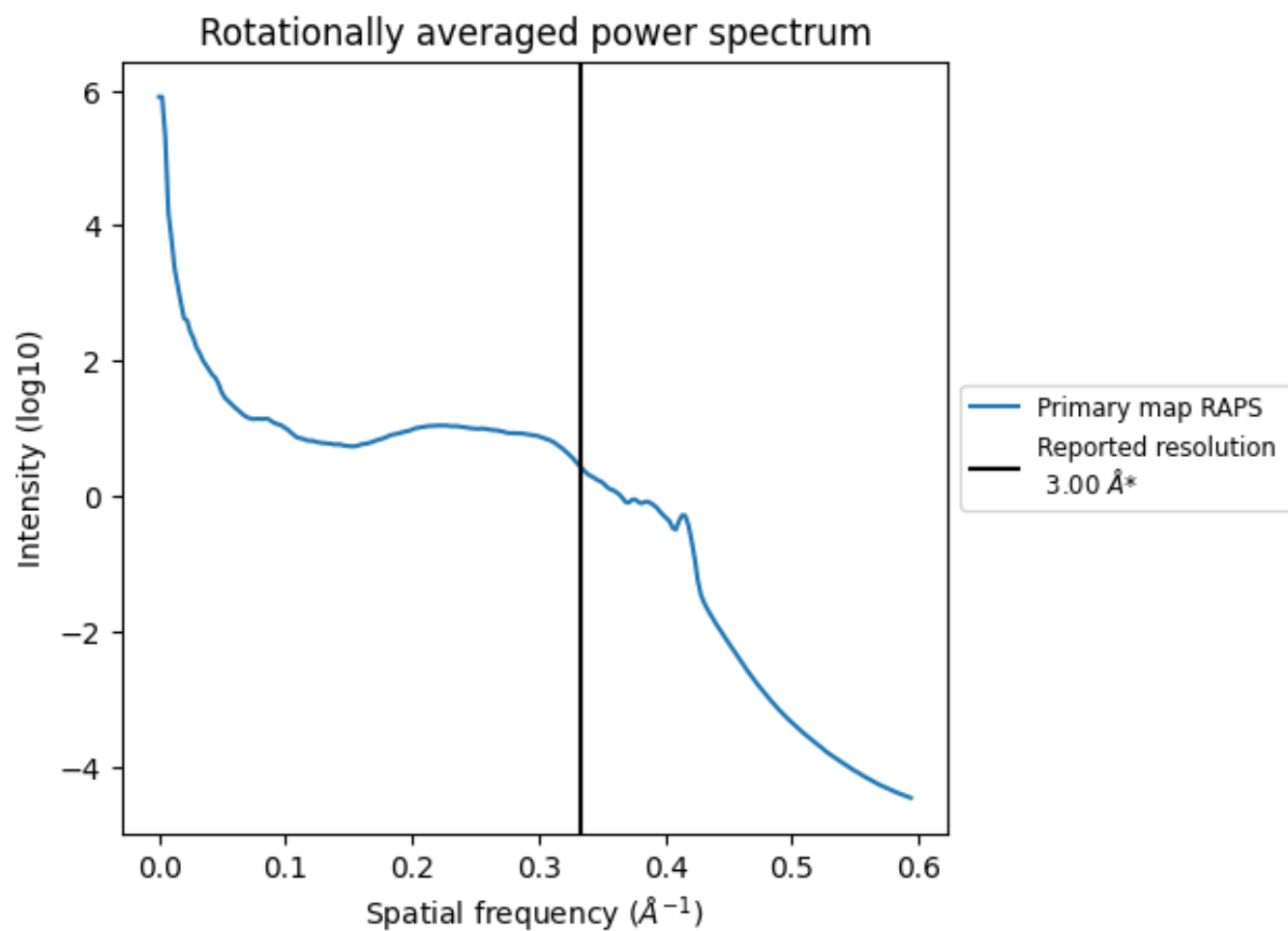


The volume at the recommended contour level is 1649 nm<sup>3</sup>; this corresponds to an approximate mass of 1489 kDa.

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 0.333 Å<sup>-1</sup>

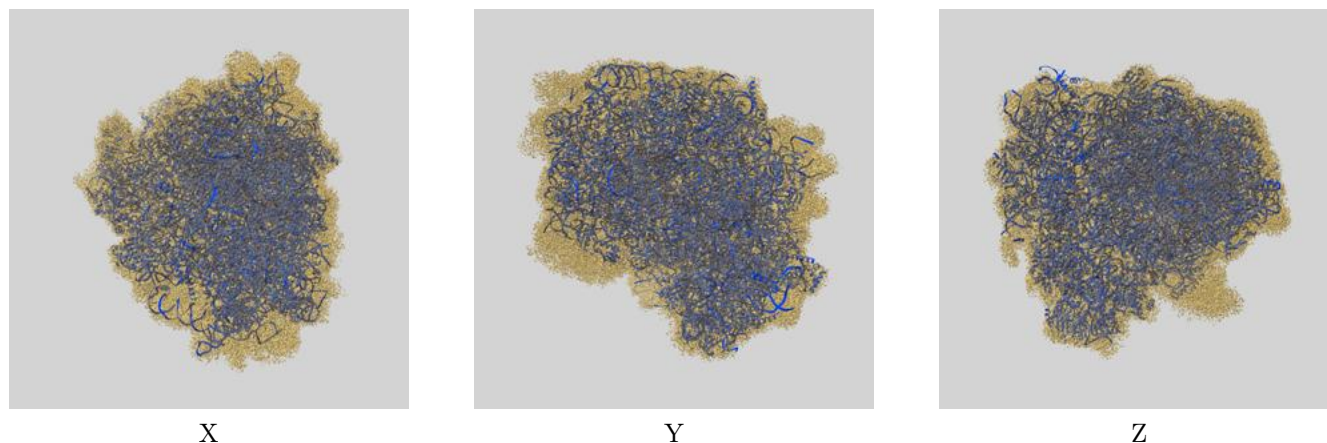
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

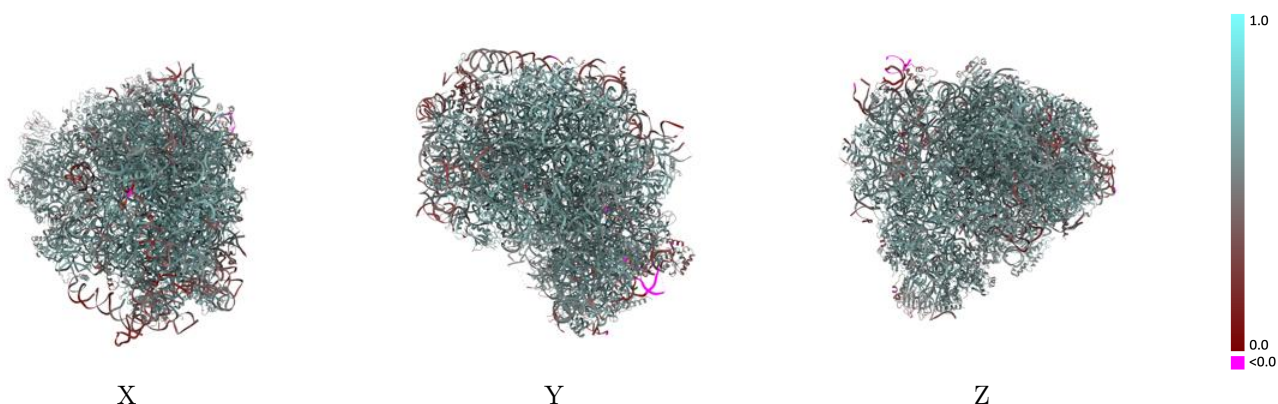
This section contains information regarding the fit between EMDB map EMD-54266 and PDB model 9RU8. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

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



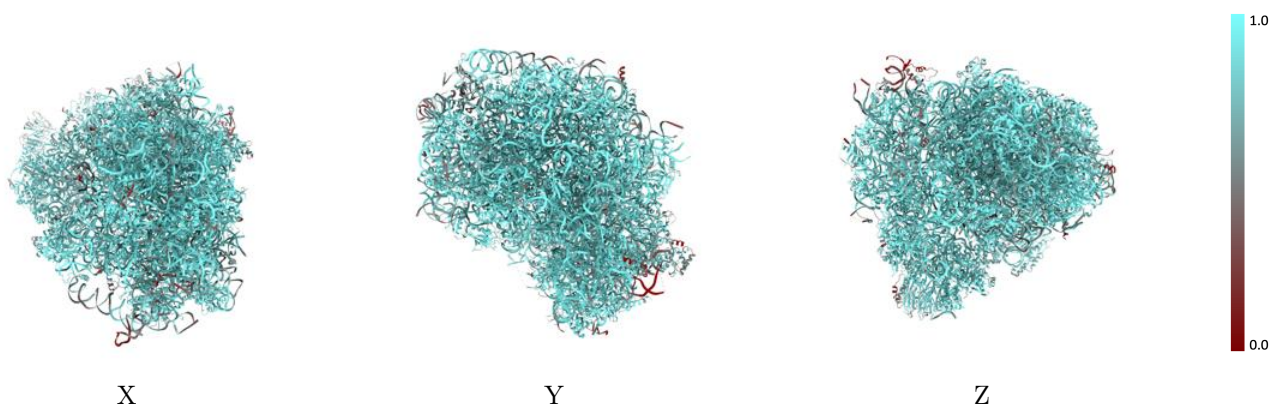
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



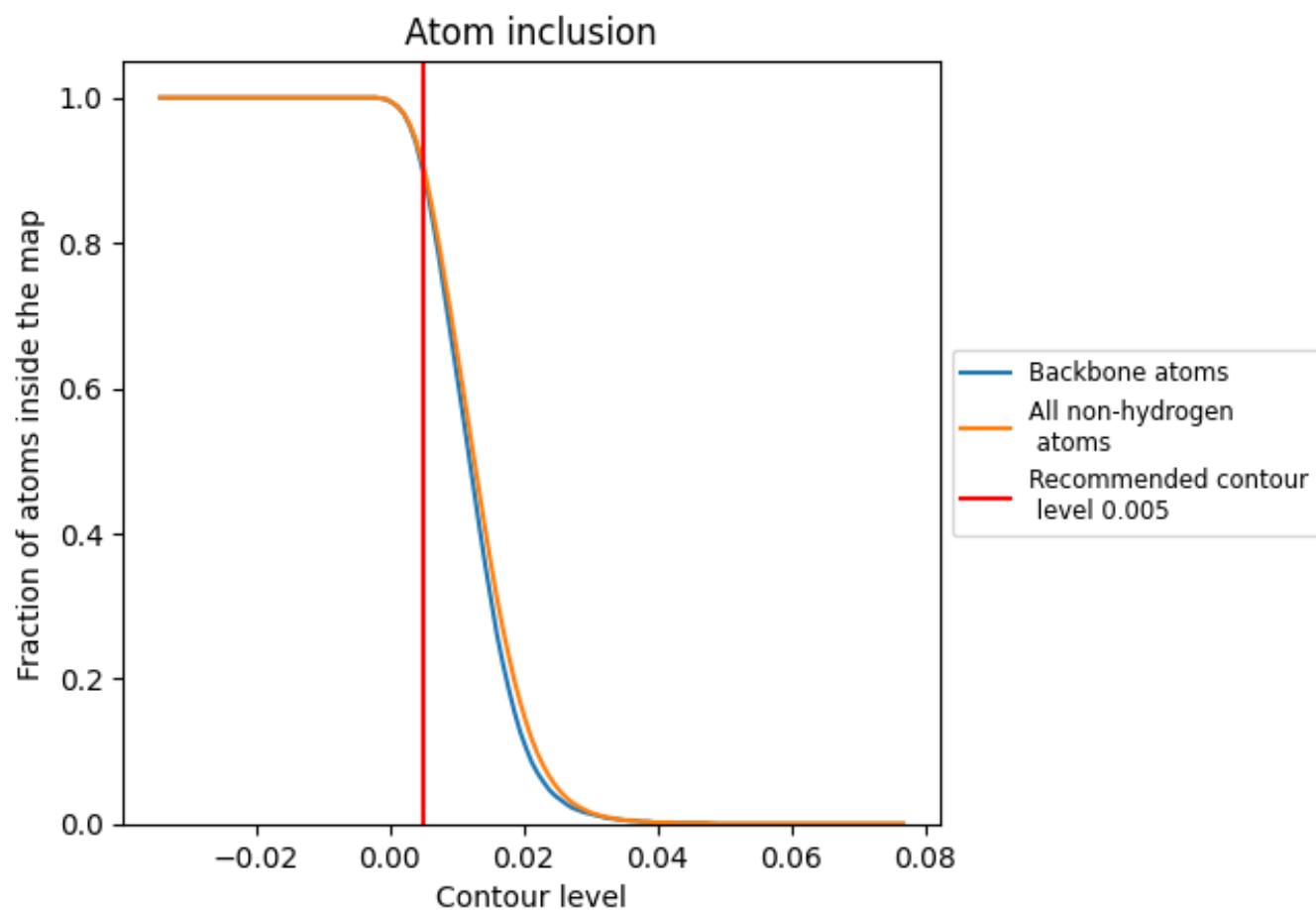
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.5780
L5	 0.9140	 0.5720
L7	 0.9750	 0.6100
L8	 0.9410	 0.5860
LA	 0.9690	 0.6410
LB	 0.9470	 0.6230
LC	 0.9460	 0.6210
LD	 0.8770	 0.5690
LE	 0.8870	 0.5750
LF	 0.9540	 0.6310
LG	 0.8670	 0.5620
LH	 0.9040	 0.5880
LI	 0.9310	 0.6130
LJ	 0.8270	 0.5380
LL	 0.9120	 0.5950
LM	 0.9200	 0.6000
LN	 0.9780	 0.6450
LO	 0.9600	 0.6320
LP	 0.9670	 0.6320
LQ	 0.9540	 0.6300
LR	 0.8940	 0.5860
LS	 0.9510	 0.6290
LT	 0.8990	 0.5950
LU	 0.7430	 0.4810
LV	 0.9320	 0.6190
LW	 0.9400	 0.6140
LX	 0.9000	 0.5840
LY	 0.9510	 0.6130
LZ	 0.9180	 0.5850
La	 0.9560	 0.6310
Lb	 0.8280	 0.5510
Lc	 0.9270	 0.5910
Ld	 0.9330	 0.5980
Le	 0.9540	 0.6350
Lf	 0.9650	 0.6410











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Chain	Atom inclusion	Q-score
Lg	 0.9490	 0.6180
Lh	 0.9300	 0.5980
Li	 0.8900	 0.5760
Lj	 0.9640	 0.6400
Lk	 0.8590	 0.5500
Ll	 0.9450	 0.6250
Lm	 0.9470	 0.6170
Ln	 0.9200	 0.6000
Lo	 0.9170	 0.6130
Lp	 0.9560	 0.6190
Lr	 0.9470	 0.6180
Pt	 0.7240	 0.4580
S2	 0.9220	 0.5740
S6	 0.6020	 0.3170
SA	 0.9020	 0.5890
SB	 0.9210	 0.5860
SC	 0.8860	 0.5890
SD	 0.8630	 0.5640
SE	 0.9090	 0.5910
SF	 0.9030	 0.5740
SG	 0.7860	 0.5220
SH	 0.7330	 0.4950
SI	 0.8250	 0.5530
SJ	 0.9020	 0.5850
SK	 0.8710	 0.5440
SL	 0.9020	 0.6060
SN	 0.9250	 0.5940
SO	 0.9260	 0.5980
SP	 0.8690	 0.5390
SQ	 0.9140	 0.5910
SR	 0.7880	 0.5280
SS	 0.9210	 0.5730
ST	 0.9280	 0.5890
SU	 0.6930	 0.5030
SV	 0.8800	 0.5800
SW	 0.9510	 0.6230
SX	 0.9320	 0.6060
SY	 0.9000	 0.5760
SZ	 0.8630	 0.5290
Sa	 0.9390	 0.5950
Sb	 0.8410	 0.5560
Sc	 0.8740	 0.5630

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Chain	Atom inclusion	Q-score
Sd	 0.9590	 0.6120
Se	 0.8520	 0.5610
Sg	 0.7270	 0.4590
mR	 0.7960	 0.4980