



wwPDB EM Validation Summary Report ⓘ

May 28, 2026 – 11:31 am BST

PDB ID : 9RU9 / pdb_00009ru9
EMDB ID : EMD-54267
Title : RPS26dC HEK mutant 80S ribosome bound to Kozak mRNA (RPS26dC-Kozak)
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.
Deposited on : 2025-07-03
Resolution : 2.97 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

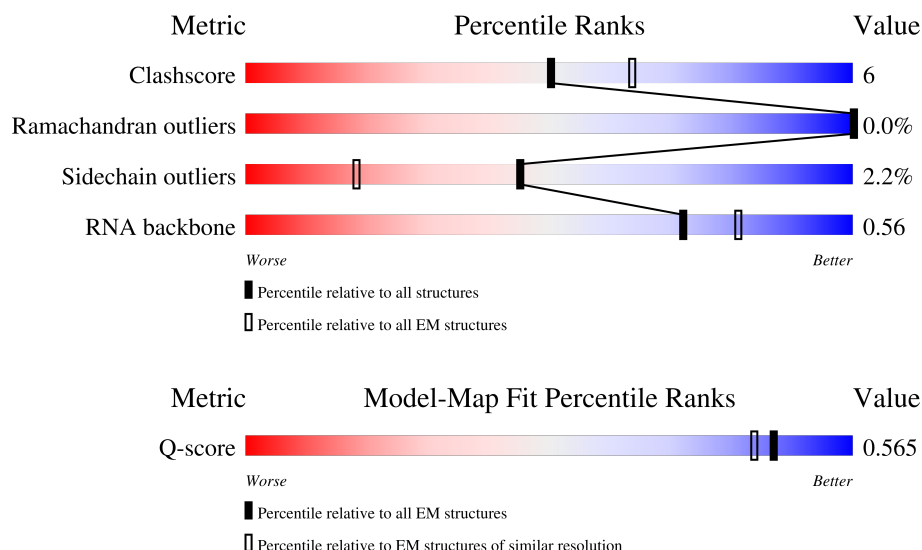
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.97 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	13205 (2.47 - 3.47)

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

Mol	Chain	Length	Quality of chain
1	LA	257	
2	SA	294	
3	LB	403	




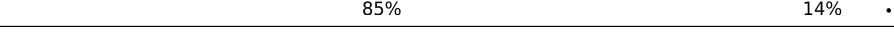

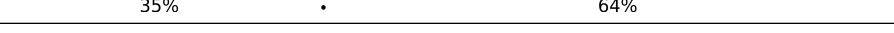



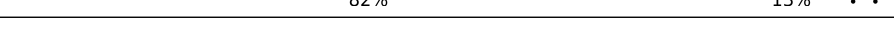















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Mol	Chain	Length	Quality of chain
4	SB	264	
5	L8	156	
6	L7	120	
7	SD	243	
8	SJ	194	
9	SE	263	
10	SC	293	
11	SF	204	
12	SH	194	
13	SW	130	
14	SI	208	
15	SQ	146	
16	SU	119	
17	SK	165	
18	SO	151	
19	SX	143	
20	SM	132	
21	SS	152	
22	Sd	56	
23	SN	151	
24	SL	158	
25	SR	135	
26	SP	145	
27	ST	145	
28	SV	82	

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Mol	Chain	Length	Quality of chain
29	SY	133	
30	SZ	125	
31	Sa	115	
32	Sb	84	
33	Sc	69	
34	Se	133	
35	Sf	156	
36	Sg	317	
37	LC	427	
38	LJ	178	
39	LH	192	
40	LE	288	
41	LG	266	
42	LO	203	
43	LL	211	
44	LV	140	
45	LM	215	
46	La	148	
47	LN	204	
48	LI	214	
49	LD	297	
50	LQ	188	
51	LR	196	
52	LS	176	
53	LT	160	

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Mol	Chain	Length	Quality of chain
54	LP	184	
55	LU	128	
56	LX	156	
57	LY	145	
58	LZ	136	
59	Lr	136	
60	Lh	123	
61	Lb	159	
62	LF	248	
63	Lc	115	
64	Ld	125	
65	Le	135	
66	Lf	110	
67	Lg	117	
68	Li	105	
69	Lj	97	
70	Lk	70	
71	Ll	51	
72	Lm	128	
73	Ln	25	
74	Lo	106	
75	Lp	92	
76	Pt	77	
77	mR	27	
78	S2	1869	

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Mol	Chain	Length	Quality of chain
79	L5	5069	<div><div></div><div>44%</div><div>22%</div><div>.</div><div>30%</div></div>
80	Et	75	<div><div></div><div>56%</div><div>36%</div><div>8%</div></div>
81	LW	157	<div><div></div><div>35%</div><div>..</div><div>61%</div></div>
82	SG	249	<div><div></div><div>71%</div><div>17%</div><div>12%</div></div>

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 209052 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 Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LA	250	Total	C	N	O	S	1	0
			1921	1203	395	317	6		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SA	217	Total	C	N	O	S	0	0
			1692	1077	297	310	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	2	MET	-	initiating methionine	UNP P08865

- Molecule 3 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LB	394	Total	C	N	O	S	0	0
			3068	1956	583	515	14		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SB	221	Total	C	N	O	S	0	0
			1761	1118	319	310	14		

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SD	224	Total	C	N	O	S	0	0
			1642	1049	293	293	7		

- Molecule 8 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SJ	179	Total	C	N	O	S	0	0
			1477	944	298	233	2		

- Molecule 9 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SE	258	Total	C	N	O	S	0	0
			2044	1308	378	350	8		

- Molecule 10 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SC	220	Total	C	N	O	S	1	0
			1685	1093	293	289	10		

- Molecule 11 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SF	182	Total	C	N	O	S	0	0
			1434	898	270	259	7		

- Molecule 12 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SH	183	Total	C	N	O	S	0	0
			1409	903	262	243	1		

- Molecule 13 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SW	129	Total	C	N	O	S	0	0
			1030	657	193	174	6		

- Molecule 14 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SI	206	Total	C	N	O	S	0	0
			1652	1036	328	283	5		

- Molecule 15 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SQ	140	Total	C	N	O	S	0	0
			1109	707	210	189	3		

- Molecule 16 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SU	101	Total	C	N	O		0	0
			519	313	101	105			

- Molecule 17 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SK	96	Total	C	N	O	S	0	0
			678	437	122	114	5		

- Molecule 18 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SO	134	Total	C	N	O	S	0	0
			990	607	197	180	6		

- Molecule 19 is a protein called 40S ribosomal protein S23.

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

- Molecule 20 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	SM	44	Total	C	N	O	0	0
			218	130	44	44		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	105	GLY	GLN	conflict	UNP P25398
SM	106	CYS	ILE	conflict	UNP P25398
SM	107	SER	ASN	conflict	UNP P25398
SM	108	CYS	LEU	conflict	UNP P25398
SM	109	VAL	ILE	conflict	UNP P25398
SM	110	VAL	LYS	conflict	UNP P25398

- Molecule 21 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SS	148	Total	C	N	O	S	0	0
			1184	746	244	193	1		

- Molecule 22 is a protein called 40S ribosomal protein S29.

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

- Molecule 23 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SN	150	Total	C	N	O	S	1	0
			1214	778	231	204	1		

- Molecule 24 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SL	142	Total	C	N	O	S	0	0
			1148	731	215	196	6		

- Molecule 25 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SR	132	Total	C	N	O	S	0	0
			1038	653	195	186	4		

- Molecule 26 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SP	128	Total	C	N	O	S	0	0
			1049	665	198	179	7		

- Molecule 27 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	ST	141	Total	C	N	O	S	1	0
			1010	637	193	178	2		

- Molecule 28 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SV	82	Total	C	N	O	S	0	0
			628	388	116	120	4		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SY	122	Total	C	N	O	S	0	0
			972	617	193	157	5		

- Molecule 30 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SZ	77	Total	C	N	O	S	0	0
			592	382	109	100	1		

- Molecule 31 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Sa	98	Total	C	N	O	S	1	0
			782	488	164	125	5		

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sb	83	Total	C	N	O	S	0	0
			642	403	118	114	7		

- Molecule 33 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sc	58	Total	C	N	O	S	0	0
			449	274	86	87	2		

- Molecule 34 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Se	48	Total	C	N	O	S	0	0
			373	227	84	61	1		

- Molecule 35 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sf	35	Total	C	N	O	S	0	0
			194	116	37	38	3		

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sg	311	Total	C	N	O	S	0	0
			2387	1508	417	451	11		

- Molecule 37 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LC	366	Total	C	N	O	S	0	0
			2914	1832	581	487	14		

- Molecule 38 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LJ	170	Total	C	N	O	S	0	0
			1354	857	253	238	6		

- Molecule 39 is a protein called 60S ribosomal protein L9.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LE	223	Total	C	N	O	S	0	0
			1786	1150	339	293	4		

- Molecule 41 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LG	232	Total	C	N	O	S	0	0
			1856	1182	359	311	4		

- Molecule 42 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LO	202	Total	C	N	O	S	0	0
			1642	1058	320	259	5		

- Molecule 43 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LL	206	Total	C	N	O	S	1	0
			1662	1041	348	269	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LL	112	ALA	THR	conflict	UNP A0A6V7HLS0

- Molecule 44 is a protein called 60S ribosomal protein L23.

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

- Molecule 45 is a protein called 60S ribosomal protein L14.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	La	147	Total	C	N	O	S	0	0
			1152	729	235	185	3		

- Molecule 47 is a protein called 60S ribosomal protein L15.

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

- 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
			1645	1045	317	270	13		

- Molecule 49 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 50 is a protein called 60S ribosomal protein L18.

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

- Molecule 51 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LR	187	Total	C	N	O	S	0	0
			1476	914	317	236	9		

- Molecule 52 is a protein called 60S ribosomal protein L18a.

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

- Molecule 53 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LT	159	Total	C	N	O	S	2	0
			1311	833	256	216	6		

- Molecule 54 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LP	153	Total	C	N	O	S	1	0
			1249	781	243	216	9		

- Molecule 55 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LU	99	Total	C	N	O	S	0	0
			804	515	140	147	2		

- Molecule 56 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LX	118	Total	C	N	O	S	0	0
			966	618	181	166	1		

- Molecule 57 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LY	133	Total	C	N	O	S	0	0
			1102	691	223	185	3		

- Molecule 58 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LZ	135	Total	C	N	O	S	1	0
			1115	719	211	182	3		

- Molecule 59 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Lr	124	Total	C	N	O	S	1	0
			1002	624	207	166	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lr	2	MET	-	initiating methionine	UNP P46779

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

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

- Molecule 61 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Lb	111	Total	C	N	O	S	0	0
			898	560	195	139	4		

- Molecule 62 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LF	225	Total	C	N	O	S	2	0
			1885	1212	364	300	9		

- Molecule 63 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Lc	99	Total	C	N	O	S	0	0
			770	488	136	140	6		

- Molecule 64 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Ld	107	Total	C	N	O	S	0	0
			589	361	112	116			

- Molecule 65 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Le	128	Total	C	N	O	S	1	0
			1061	672	219	165	5		

- Molecule 66 is a protein called 60S ribosomal protein L35a.

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

- Molecule 67 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lg	112	Total	C	N	O	S	0	0
			875	548	180	141	6		

- Molecule 68 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Li	102	Total	C	N	O	S	0	0
			821	513	174	129	5		

- Molecule 69 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Lj	86	Total	C	N	O	S	1	0
			712	439	157	111	5		

- Molecule 70 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Lk	69	Total	C	N	O	S	0	0
			568	366	103	98	1		

- Molecule 71 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ll	50	Total	C	N	O	S	0	0
			437	278	95	63	1		

- Molecule 72 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

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

- Molecule 73 is a protein called 60S ribosomal protein L41.

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

- Molecule 74 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Lo	105	Total	C	N	O	S	1	0
			870	548	177	139	6		

- Molecule 75 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Lp	91	Total	C	N	O	S	1	0
			715	450	139	119	7		

- Molecule 76 is a RNA chain called P site tRNA.

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

- Molecule 77 is a RNA chain called Kozak mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	mR	7	Total	C	N	O	P	0	0
			156	69	32	48	7		

- Molecule 78 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	S2	1635	Total	C	N	O	P	0	0
			34940	15627	6260	11419	1634		

- Molecule 79 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	L5	3523	Total	C	N	O	P	1	0
			75626	33716	13837	24550	3523		

- Molecule 80 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Et	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 81 is a protein called 60S ribosomal protein L24.

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

- Molecule 82 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	SG	220	Total	C	N	O	S	0	0
			1683	1053	337	286	7		

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K).

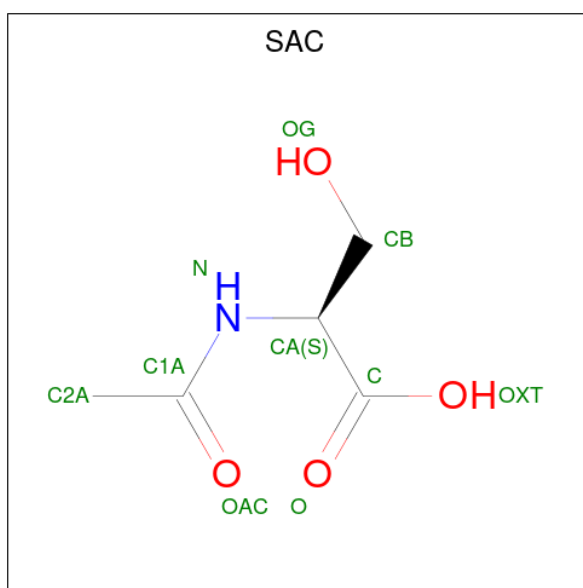
Mol	Chain	Residues	Atoms		AltConf
83	LA	3	Total	K	0
			3	3	
83	L8	3	Total	K	0
			3	3	
83	L7	4	Total	K	0
			4	4	
83	SO	1	Total	K	0
			1	1	
83	SL	1	Total	K	0
			1	1	
83	Sa	1	Total	K	0
			1	1	
83	LH	1	Total	K	0
			1	1	
83	LL	1	Total	K	0
			1	1	
83	LN	1	Total	K	0
			1	1	
83	LI	1	Total	K	0
			1	1	
83	LQ	1	Total	K	0
			1	1	
83	Lb	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
83	Le	1	Total	K	0
			1	1	
83	Lf	1	Total	K	0
			1	1	
83	Ll	1	Total	K	0
			1	1	
83	mR	1	Total	K	0
			1	1	
83	A	14	Total	K	0
			14	14	

- Molecule 84 is N-ACETYL-SERINE (CCD ID: SAC) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				AltConf
84	SA	1	Total	C	N	O	0
			9	5	1	3	
84	Lr	1	Total	C	N	O	0
			9	5	1	3	

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	LB	1	Total	Mg	0
			1	1	
85	L8	16	Total	Mg	0
			16	16	

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Mol	Chain	Residues	Atoms		AltConf
85	L7	15	Total 15	Mg 15	0
85	SX	1	Total 1	Mg 1	0
85	SS	2	Total 2	Mg 2	0
85	Sd	1	Total 1	Mg 1	0
85	SN	1	Total 1	Mg 1	0
85	ST	1	Total 1	Mg 1	0
85	LC	1	Total 1	Mg 1	0
85	LH	1	Total 1	Mg 1	0
85	LG	1	Total 1	Mg 1	0
85	LO	2	Total 2	Mg 2	0
85	LL	1	Total 1	Mg 1	0
85	LV	1	Total 1	Mg 1	0
85	La	1	Total 1	Mg 1	0
85	LN	3	Total 3	Mg 3	0
85	LD	1	Total 1	Mg 1	0
85	LQ	2	Total 2	Mg 2	0
85	LR	1	Total 1	Mg 1	0
85	LS	1	Total 1	Mg 1	0
85	LP	2	Total 2	Mg 2	0
85	Lr	3	Total 3	Mg 3	0
85	LF	1	Total 1	Mg 1	0

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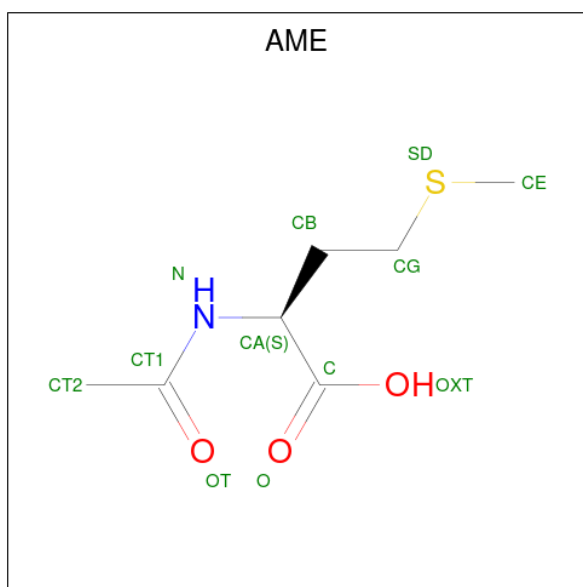
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Mol	Chain	Residues	Atoms		AltConf
85	Lc	1	Total 1	Mg 1	0
85	Lf	1	Total 1	Mg 1	0
85	Lg	1	Total 1	Mg 1	0
85	Lj	2	Total 2	Mg 2	0
85	Lo	1	Total 1	Mg 1	0
85	Lp	2	Total 2	Mg 2	0
85	Pt	1	Total 1	Mg 1	0
85	Et	1	Total 1	Mg 1	0
85	D	12	Total 12	Mg 12	0

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

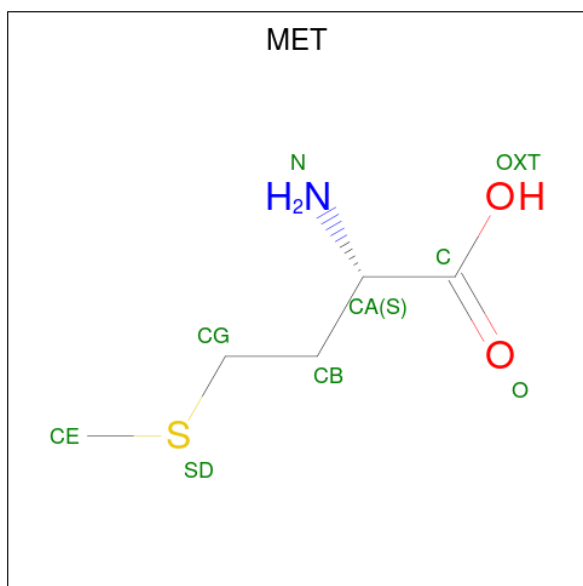
Mol	Chain	Residues	Atoms		AltConf
86	Sd	1	Total 1	Zn 1	0
86	Sa	1	Total 1	Zn 1	0
86	Sf	1	Total 1	Zn 1	0
86	Lg	1	Total 1	Zn 1	0
86	Lj	1	Total 1	Zn 1	0
86	Lm	1	Total 1	Zn 1	0
86	Lo	1	Total 1	Zn 1	0
86	Lp	1	Total 1	Zn 1	0

- Molecule 87 is N-ACETYLMETHIONINE (CCD ID: AME) (formula: C₇H₁₃NO₃S).



Mol	Chain	Residues	Atoms					AltConf
87	SV	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 88 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
88	Pt	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 89 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



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

- Molecule 90 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



Mol	Chain	Residues	Atoms				AltConf
90	L5	1	Total	C	N	O	0
			19	14	1	4	

- Molecule 91 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
91	C	7	Total	Na	0
			7	7	

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	LA	48	Total	O	0
			48	48	
92	LB	42	Total	O	0
			42	42	
92	L8	67	Total	O	0
			67	67	
92	L7	38	Total	O	0
			38	38	
92	SE	1	Total	O	0
			1	1	
92	SO	2	Total	O	0
			2	2	
92	SN	1	Total	O	0
			1	1	
92	SL	1	Total	O	0
			1	1	
92	Sa	2	Total	O	0
			2	2	
92	LC	59	Total	O	0
			59	59	
92	LJ	1	Total	O	0
			1	1	
92	LH	3	Total	O	0
			3	3	
92	LE	6	Total	O	0
			6	6	
92	LG	7	Total	O	0
			7	7	
92	LO	29	Total	O	0
			29	29	
92	LL	26	Total	O	0
			26	26	
92	LV	10	Total	O	0
			10	10	
92	LM	2	Total	O	0
			2	2	
92	La	26	Total	O	0
			26	26	

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Mol	Chain	Residues	Atoms		AltConf
92	LN	40	Total 40	O 40	0
92	LI	11	Total 11	O 11	0
92	LD	11	Total 11	O 11	0
92	LQ	36	Total 36	O 36	0
92	LR	17	Total 17	O 17	0
92	LS	14	Total 14	O 14	0
92	LT	18	Total 18	O 18	0
92	LP	17	Total 17	O 17	0
92	LU	1	Total 1	O 1	0
92	LX	7	Total 7	O 7	0
92	LY	10	Total 10	O 10	0
92	LZ	5	Total 5	O 5	0
92	Lr	12	Total 12	O 12	0
92	Lh	5	Total 5	O 5	0
92	Lb	10	Total 10	O 10	0
92	LF	30	Total 30	O 30	0
92	Lc	4	Total 4	O 4	0
92	Ld	9	Total 9	O 9	0
92	Le	28	Total 28	O 28	0
92	Lf	16	Total 16	O 16	0
92	Lg	22	Total 22	O 22	0

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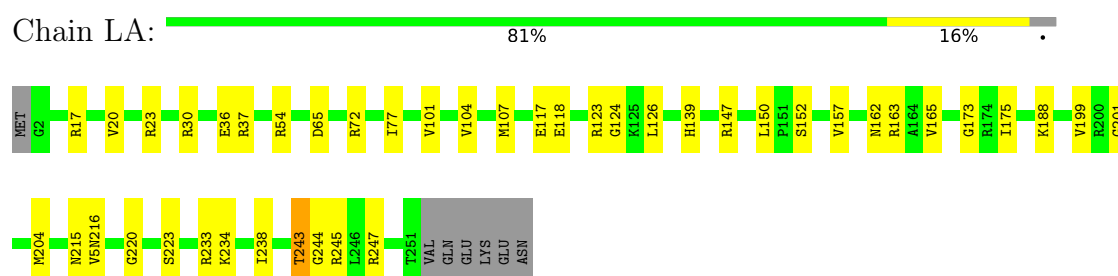
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Mol	Chain	Residues	Atoms		AltConf
92	Li	2	Total 2	O 2	0
92	Lj	19	Total 19	O 19	0
92	Lk	2	Total 2	O 2	0
92	Ll	8	Total 8	O 8	0
92	Lm	2	Total 2	O 2	0
92	Ln	1	Total 1	O 1	0
92	Lo	12	Total 12	O 12	0
92	Lp	14	Total 14	O 14	0
92	Pt	1	Total 1	O 1	0
92	B	18	Total 18	O 18	0

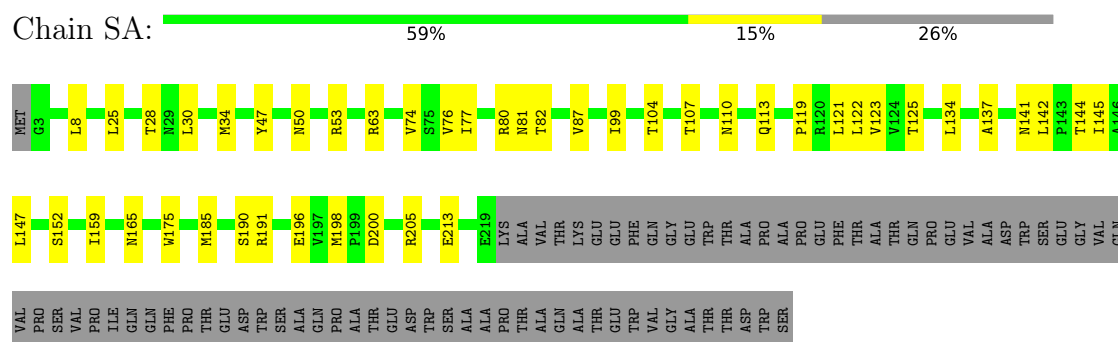
3 Residue-property plots [i](#)

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: Large ribosomal subunit protein uL2



- Molecule 2: Small ribosomal subunit protein uS2

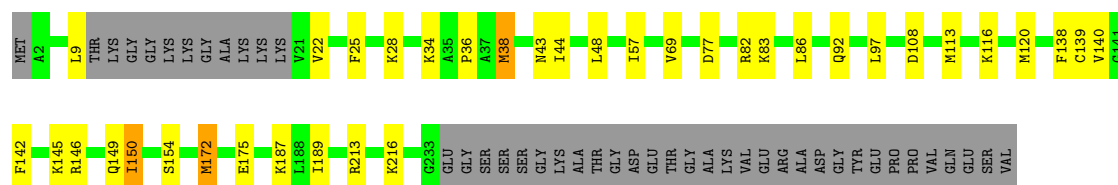


- Molecule 3: Large ribosomal subunit protein uL3



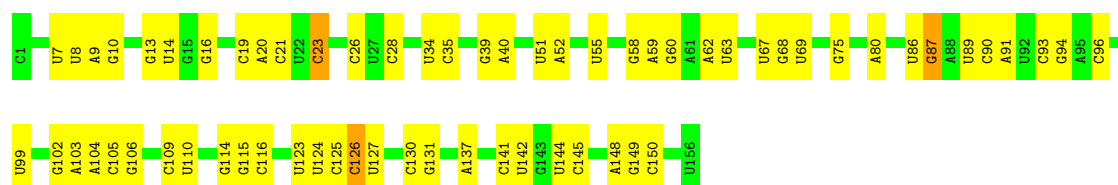
- Molecule 4: 40S ribosomal protein S3a

Chain SB:  70% 13% 16%



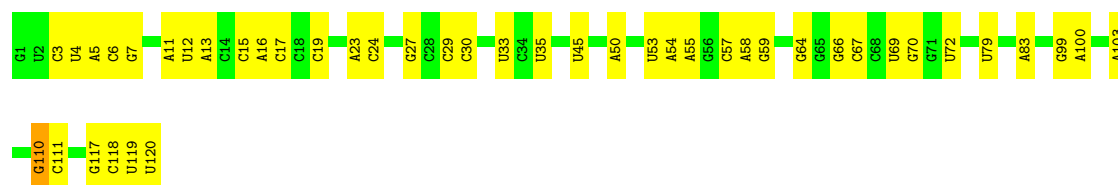
• Molecule 5: 5.8S rRNA

Chain L8:  59% 39%




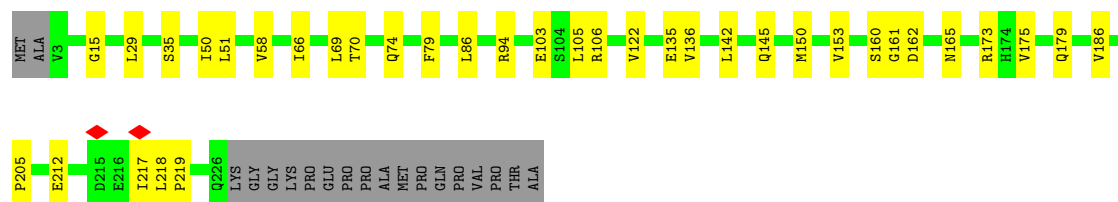
• Molecule 6: 5S rRNA

Chain L7:  63% 36%




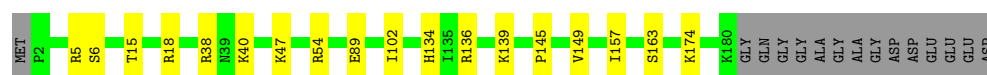
• Molecule 7: 40S ribosomal protein S3

Chain SD:  77% 15% 8%




• Molecule 8: 40S ribosomal protein S9

Chain SJ:  83% 9% 8%

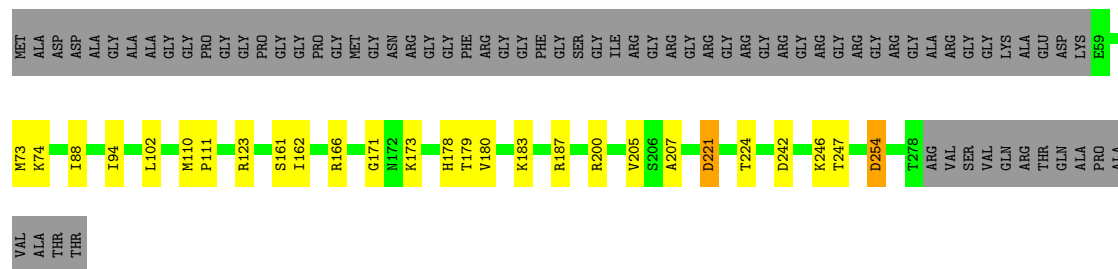


• Molecule 9: Small ribosomal subunit protein eS4, X isoform


Chain SE:  81% 17%

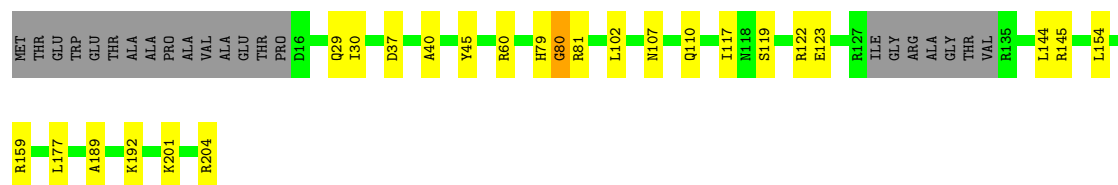
- Molecule 10: 40S ribosomal protein S2

Chain SC:  66% 9% 25%




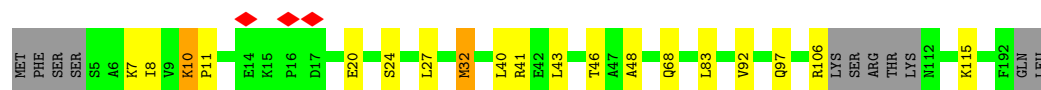
- Molecule 11: 40S ribosomal protein S5

Chain SF: 




- Molecule 12: 40S ribosomal protein S7

Chain SH:  85% 9% • 6%




- Molecule 13: 40S ribosomal protein S15a

Chain SW:  82% 17%



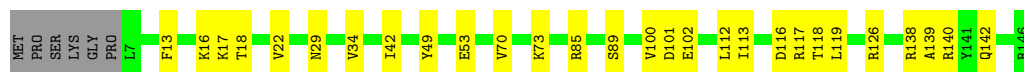
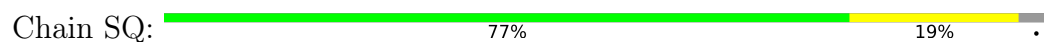
- Molecule 14: 40S ribosomal protein S8

Chain SI:  80% 19%

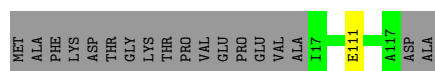




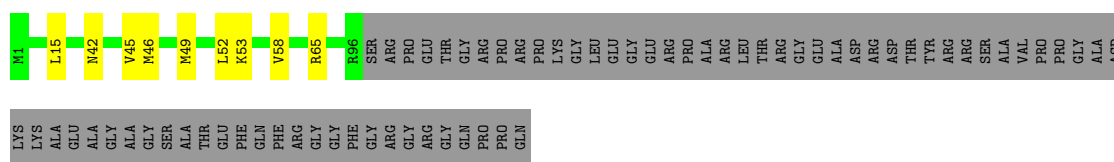
- Molecule 15: 40S ribosomal protein S16



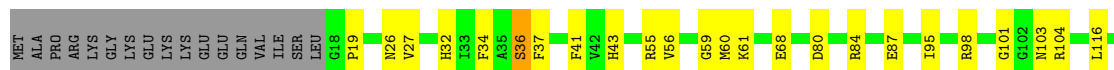
- Molecule 16: 40S ribosomal protein S20



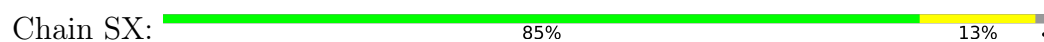
- Molecule 17: 40S ribosomal protein S10



- Molecule 18: 40S ribosomal protein S14

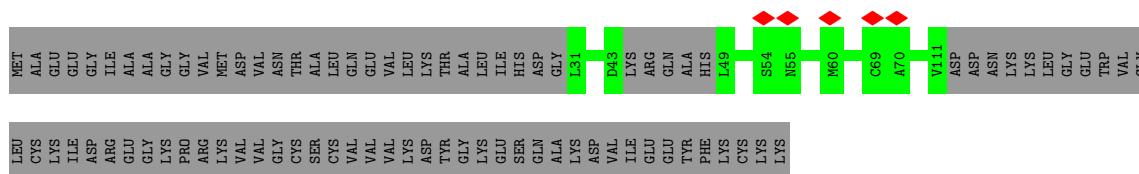


- Molecule 19: 40S ribosomal protein S23



- Molecule 20: Small ribosomal subunit protein eS12





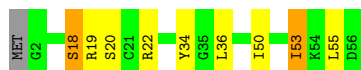
- Molecule 21: 40S ribosomal protein S18

Chain SS: 71% 26% .



- Molecule 22: 40S ribosomal protein S29

Chain Sd: 82% 12% . .



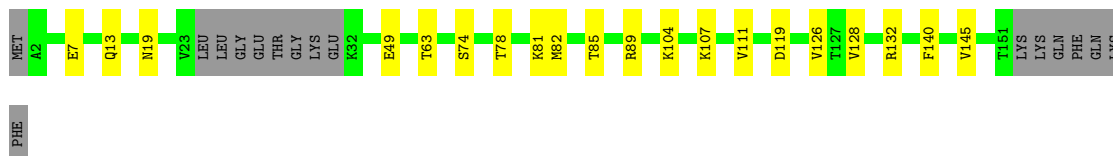
- Molecule 23: 40S ribosomal protein S13

Chain SN: 80% 19% .



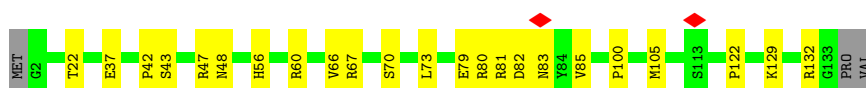
- Molecule 24: 40S ribosomal protein S11

Chain SL: 77% 13% 10%



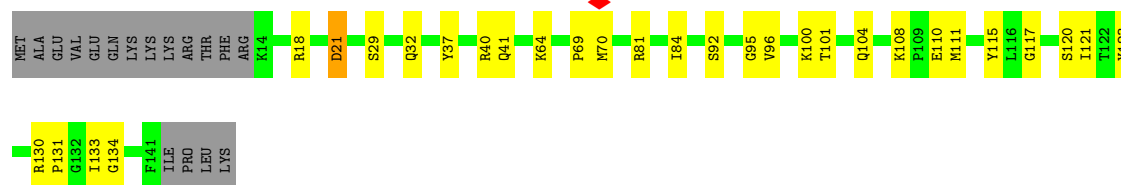
- Molecule 25: 40S ribosomal protein S17

Chain SR: 81% 17% .




- Molecule 26: 40S ribosomal protein S15

Chain SP:  68% 20% 12%




- Molecule 27: 40S ribosomal protein S19

Chain ST:  80% 17%




- Molecule 28: Small ribosomal subunit protein eS21

Chain SV:  89% 11%



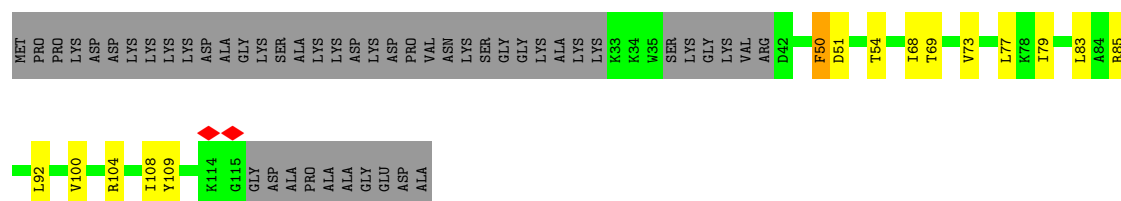
- Molecule 29: 40S ribosomal protein S24

Chain SY:  78% 14% 8%




- Molecule 30: 40S ribosomal protein S25

Chain SZ:  50% 11% 38%




- Molecule 31: 40S ribosomal protein S26

Chain Sa:  76% 10% 15%



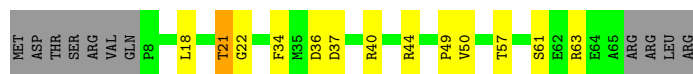
- Molecule 32: 40S ribosomal protein S27

Chain Sb:  85% 14%



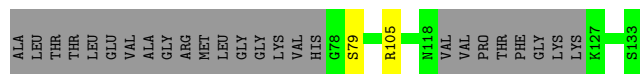
- Molecule 33: 40S ribosomal protein S28

Chain Sc:  65% 17% 16%



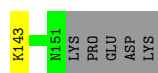
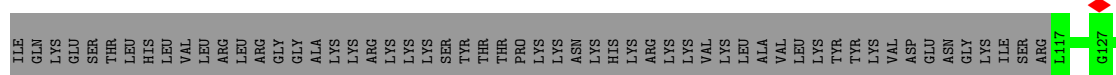
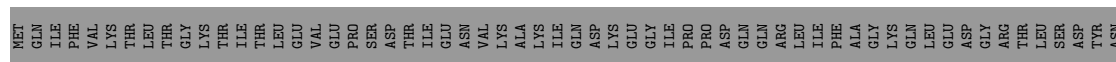
- Molecule 34: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se:  35% 64%




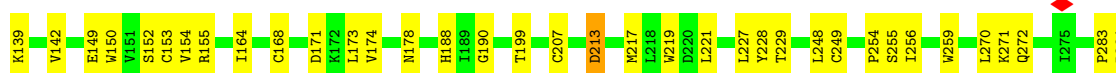
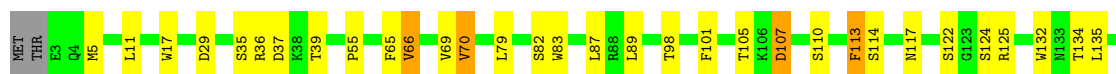
- Molecule 35: Ubiquitin

Chain Sf:  22% 78%

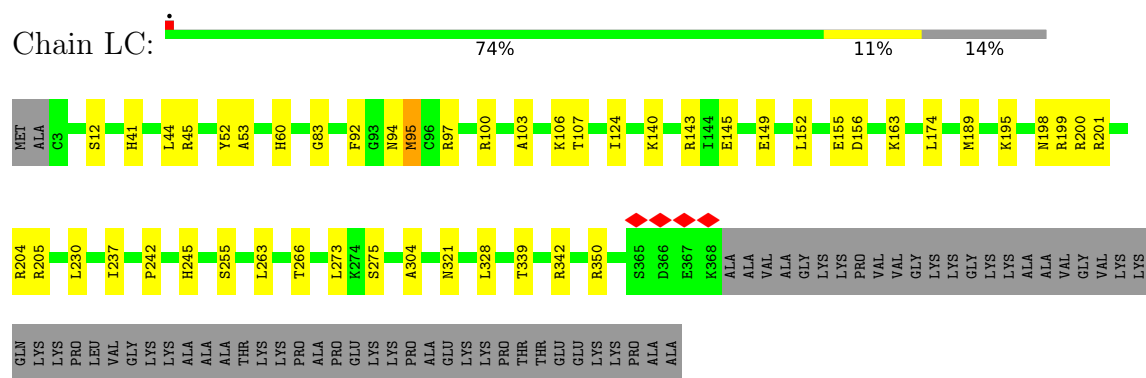


- Molecule 36: Receptor of activated protein C kinase 1

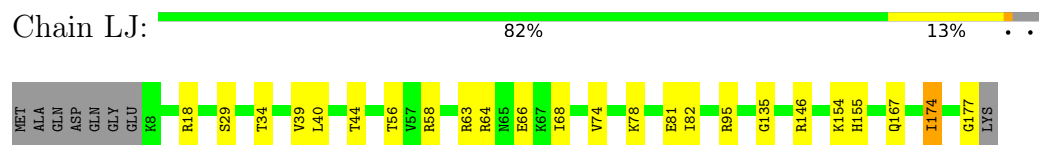
Chain Sg:  74% 23%



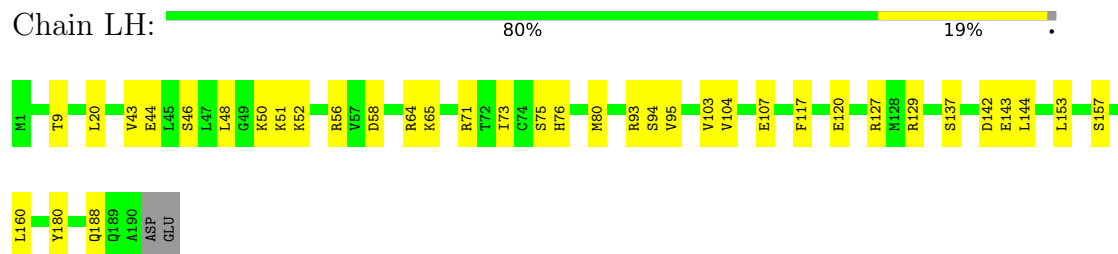
- Molecule 37: 60S ribosomal protein L4



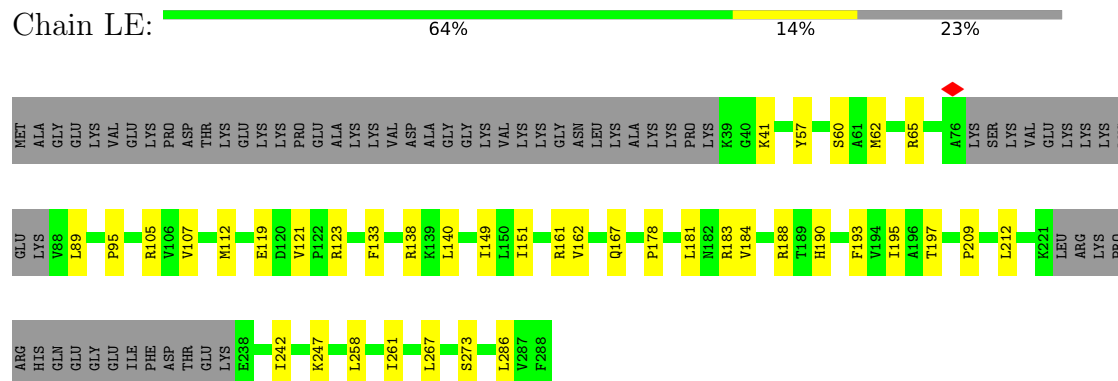
- Molecule 38: 60S ribosomal protein L11



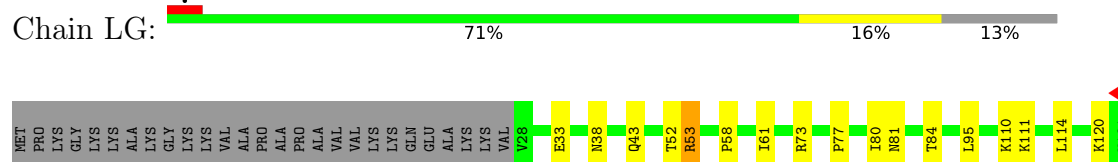
- Molecule 39: 60S ribosomal protein L9



- Molecule 40: Large ribosomal subunit protein eL6




- Molecule 41: 60S ribosomal protein L7a

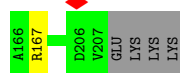




- Chain LO: 80% 19%



- Chain LL:  82% 16%




- Chain LV:  70% 22% 7%

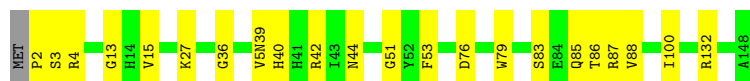


- Chain LM: 




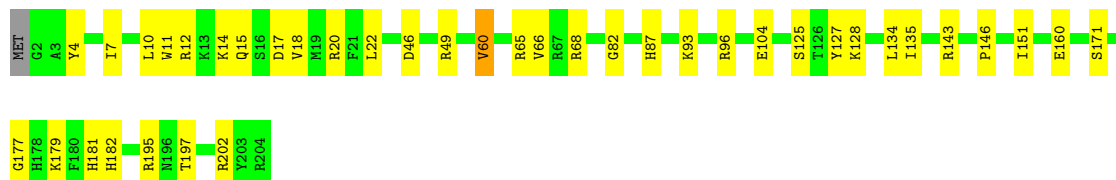
- 

Chain La:  84% 15%




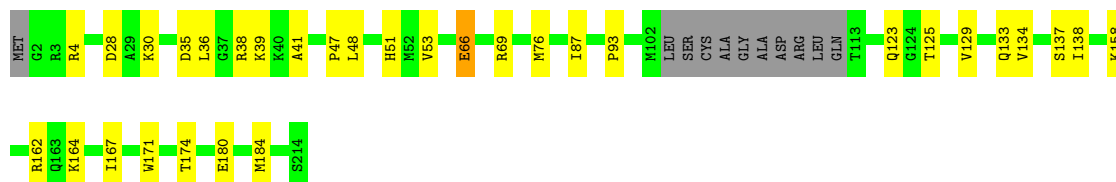
- Molecule 47: 60S ribosomal protein L15

Chain LN:  80% 19%




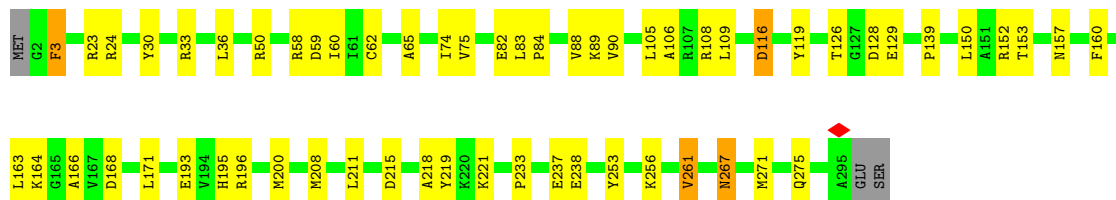
- Molecule 48: 60S ribosomal protein L10

Chain LI:  80% 14% 5%




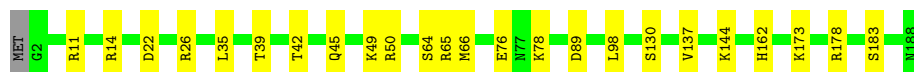
- Molecule 49: 60S ribosomal protein L5

Chain LD:  79% 19%




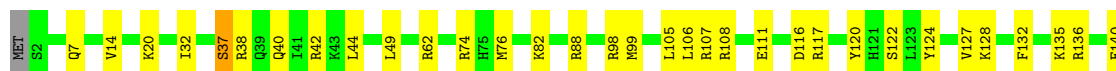
- Molecule 50: 60S ribosomal protein L18

Chain LQ:  87% 13%



- Molecule 51: 60S ribosomal protein L19

Chain LR:  78% 17% 5%



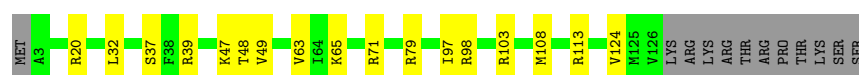
- Molecule 58: 60S ribosomal protein L27

Chain LZ: 82% 15% 3%



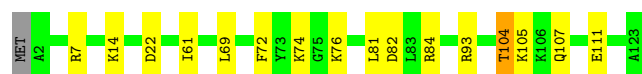
- Molecule 59: Large ribosomal subunit protein eL28

Chain Lr:



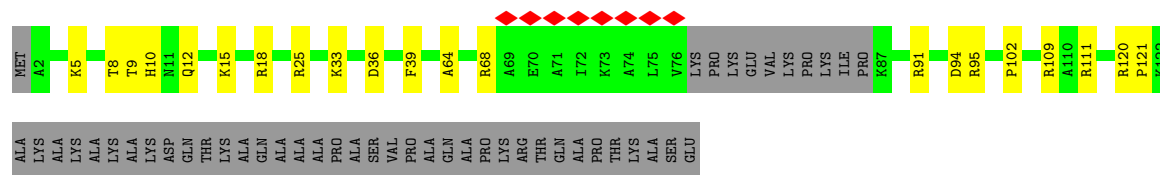
- Molecule 60: 60S ribosomal protein L35

Chain Lh: 86% 12% ..



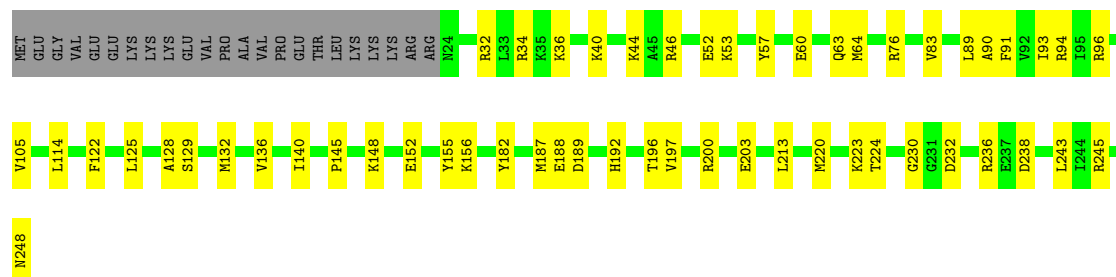
- Molecule 61: Large ribosomal subunit protein eL29

Chain Lb: 



- Molecule 62: Large ribosomal subunit protein uL30

Chain LF: 



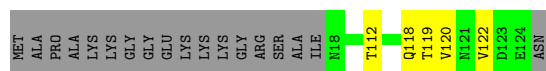
- Molecule 63: 60S ribosomal protein L30

Chain Lc:  73% 13% 14%




- Molecule 64: 60S ribosomal protein L31

Chain Ld:  82% 14%




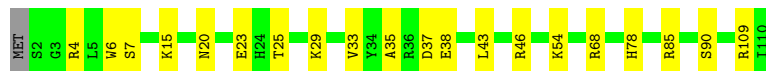
- Molecule 65: 60S ribosomal protein L32

Chain Le:  77% 18% 5%




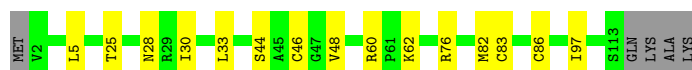
- Molecule 66: 60S ribosomal protein L35a

Chain Lf:  81% 18%



- Molecule 67: 60S ribosomal protein L34

Chain Lg:  83% 13%



- Molecule 68: 60S ribosomal protein L36

Chain Li:  86% 10%



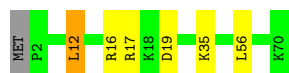
- Molecule 69: Large ribosomal subunit protein eL37

Chain Lj:  74% 14% 11%




- Molecule 70: 60S ribosomal protein L38

Chain Lk:  90% 7% ..




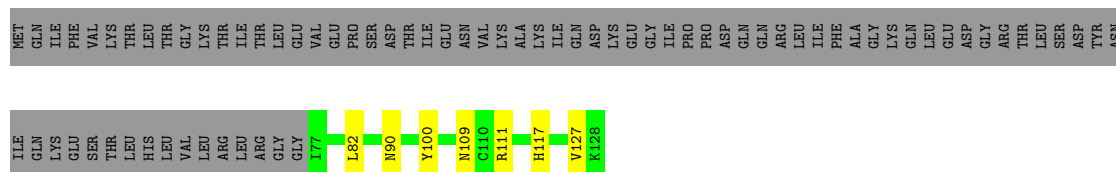
- Molecule 71: 60S ribosomal protein L39

Chain Ll:  76% 22% .




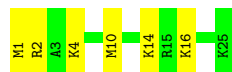
- Molecule 72: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:  35% 5% 59%



- Molecule 73: 60S ribosomal protein L41

Chain Ln:  76% 24%



- Molecule 74: Large ribosomal subunit protein eL42

Chain Lo:  90% 9% .



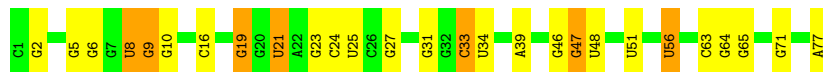
- Molecule 75: 60S ribosomal protein L37a

Chain Lp:  92% 7% .



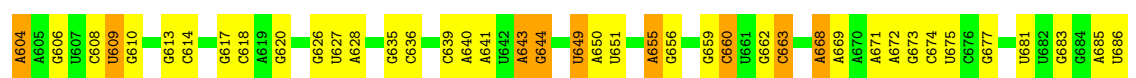
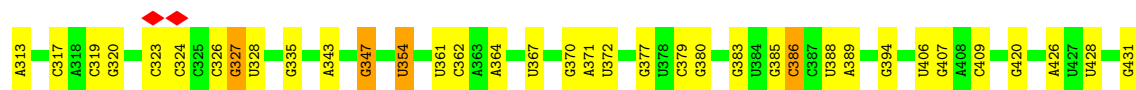
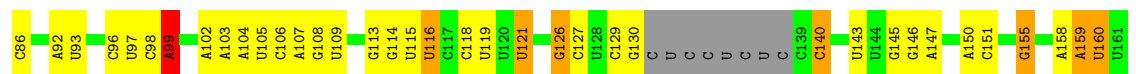
- Molecule 76: P site tRNA

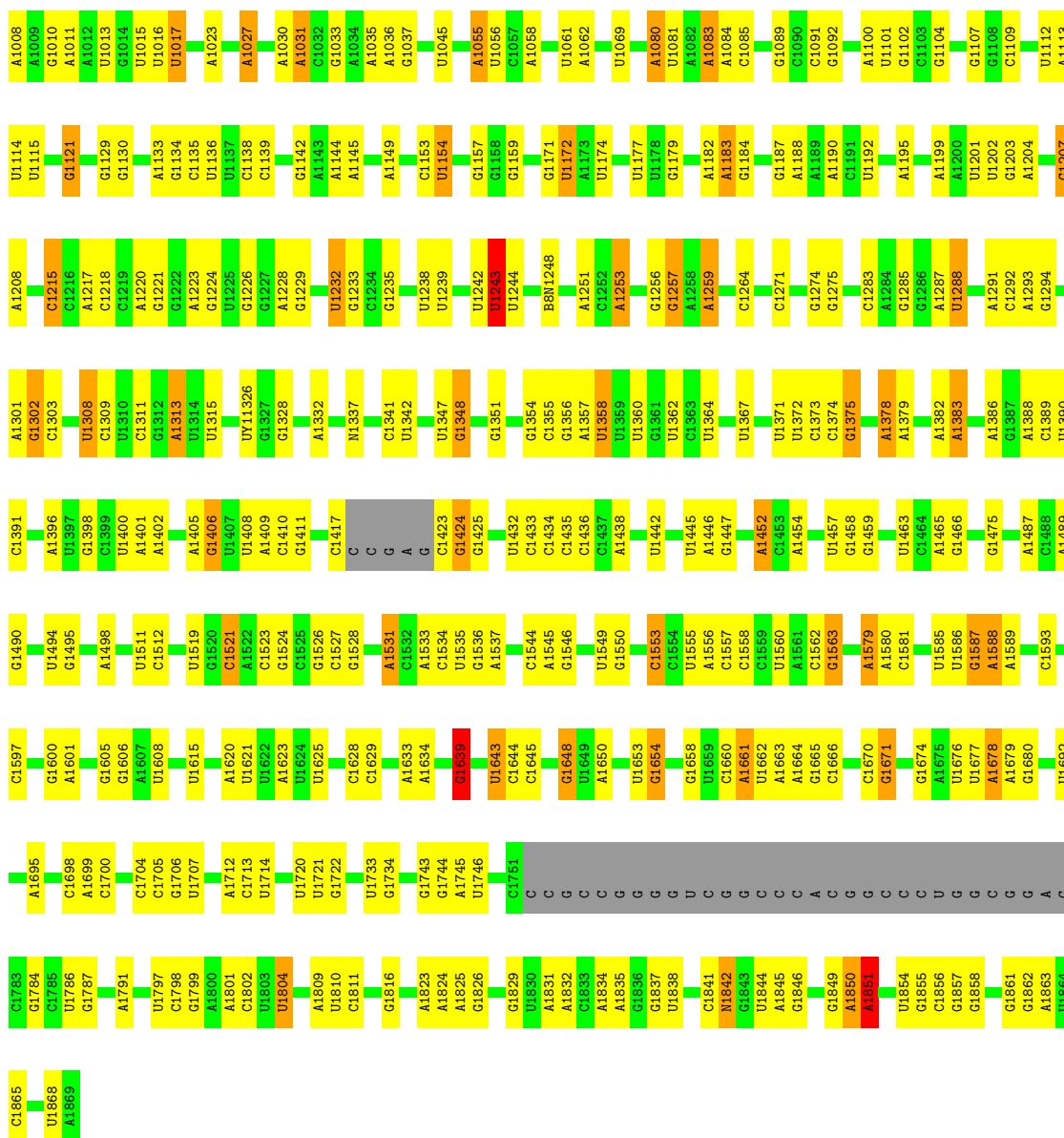
Chain Pt:  65% 26% 9%



A	G	A	U	C	C	G	C	U	A	C	C	G33	G34	G35	A36	A37	U38	G39	U	G	G	A	G	A	G	A
---	---	---	---	---	---	---	---	---	---	---	---	-----	-----	-----	-----	-----	-----	-----	---	---	---	---	---	---	---	---

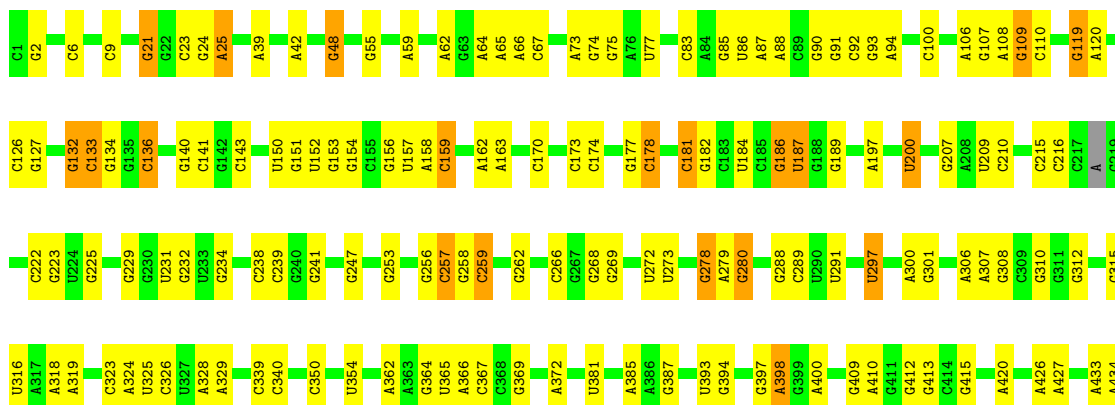
Category	Count
U1	10
A2	10
C3	10
C4	10
U5	10
C6	10
U12	10
C13	10
C14	10
U15	10
C16	10
C17	10
A27	10
U28	10
C29	10
C30	10
C33	10
U34	10
C35	10
U36	10
C37	10
A38	10
C41	10
A42	10
U43	10
U44	10
A45	10
A46	10
U51	10
C52	10
C56	10
U57	10
C58	10
U59	10
C62	10
C63	10
A64	10
C65	10
C66	10
C67	10
A68	10
C73	10
C74	0
C75	0
U76	10
A77	10
C78	10
A79	10
C80	10
A84	10
A85	10

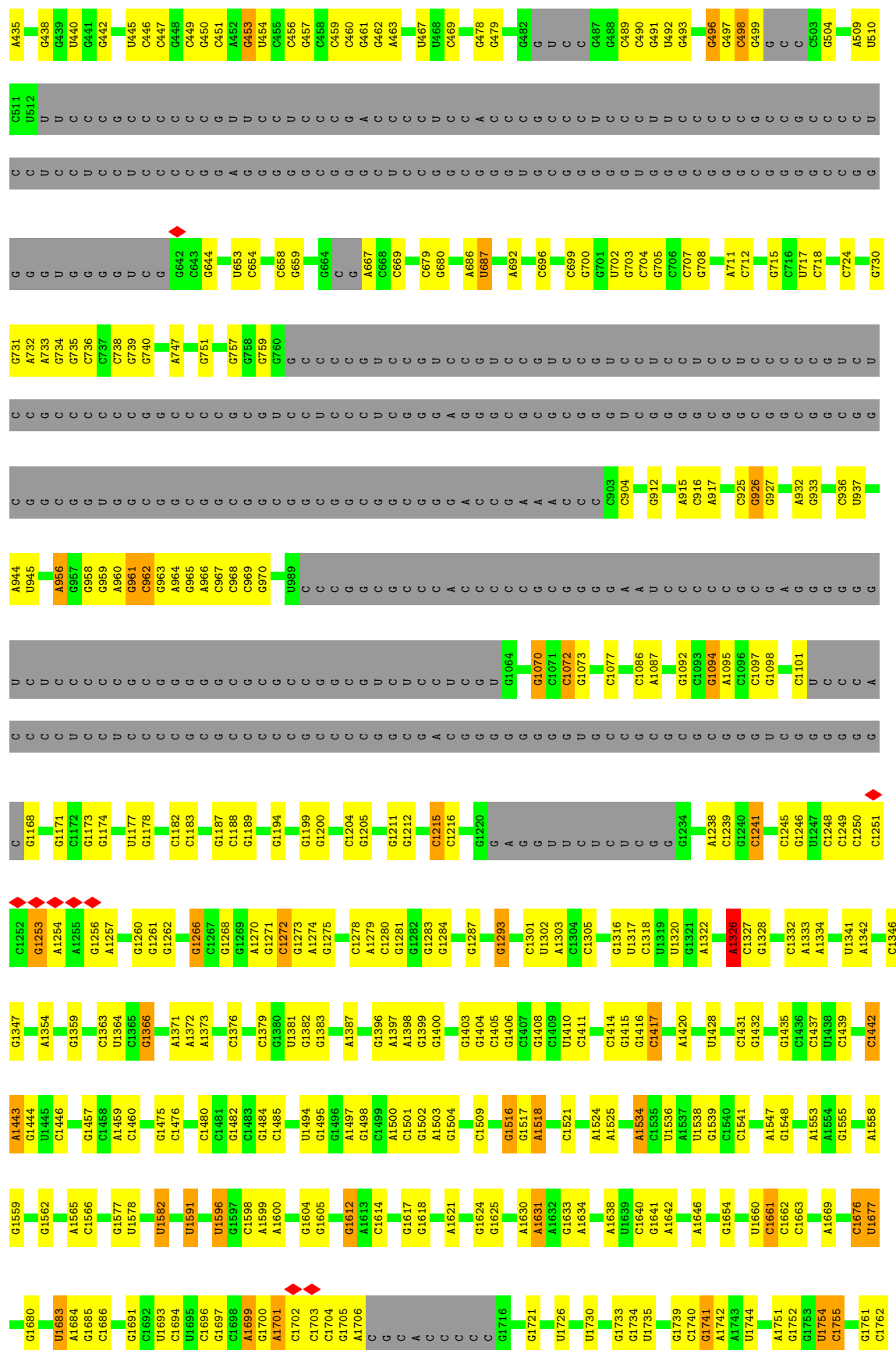




• Molecule 79: 23S rRNA

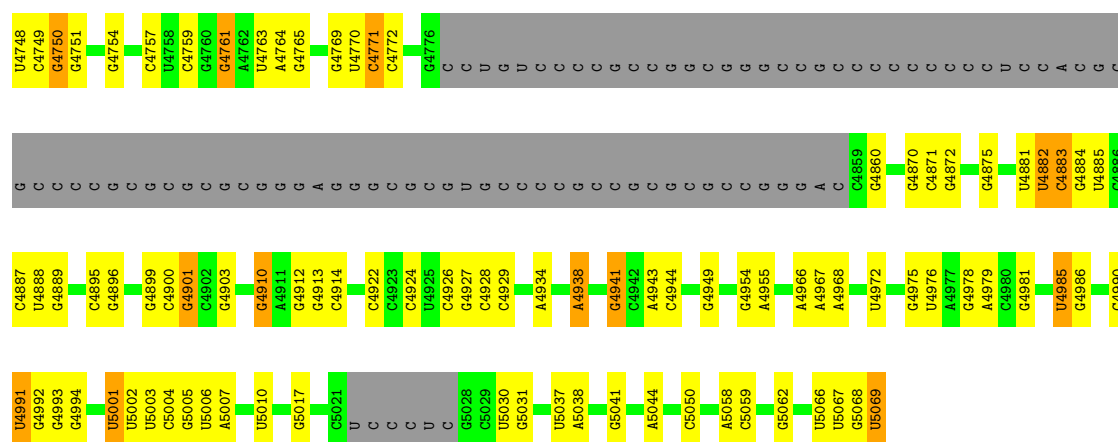
Chain L5: 44% 22% 2% 30%











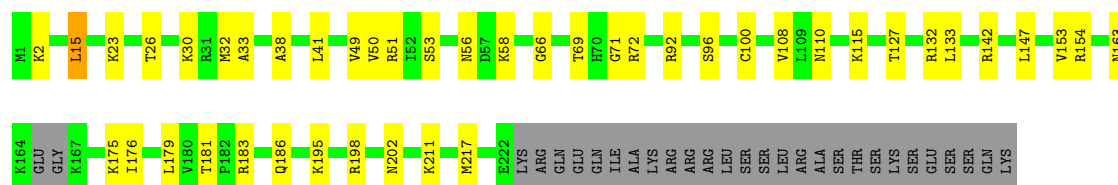
• Molecule 80: E site tRNA



• Molecule 81: 60S ribosomal protein L24



• Molecule 82: 40S ribosomal protein S6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59189	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	0.124	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ANM, NA, UY1, AME, MG, H2U, 5MC, B8N, A2M, HIC, OMG, G7M, V5N, HY3, HYG, SAC, 4SU, UR3, OMC, 4AC, MA6, M3L, PSU, 6MZ, 1MA, OMU, MLZ, K, 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	LA	0.16	0/1949	0.29	0/2610
2	SA	0.13	0/1728	0.27	0/2350
3	LB	0.16	0/3122	0.30	0/4191
4	SB	0.13	0/1787	0.31	1/2394 (0.0%)
5	L8	0.16	0/3631	0.28	0/5657
6	L7	0.16	0/2858	0.25	0/4455
7	SD	0.12	0/1667	0.31	0/2256
8	SJ	0.13	0/1502	0.29	0/2008
9	SE	0.13	0/2086	0.29	0/2809
10	SC	0.13	0/1721	0.29	0/2329
11	SF	0.12	0/1454	0.29	0/1956
12	SH	0.15	0/1429	0.37	0/1920
13	SW	0.15	0/1047	0.30	0/1401
14	SI	0.14	0/1680	0.30	0/2244
15	SQ	0.13	0/1126	0.30	0/1508
16	SU	0.09	0/519	0.28	0/722
17	SK	0.10	0/694	0.29	0/945
18	SO	0.13	0/1003	0.29	0/1347
19	SX	0.13	0/1096	0.28	0/1461
20	SM	0.06	0/215	0.19	0/295
21	SS	0.12	0/1202	0.30	0/1614
22	Sd	0.14	0/469	0.28	0/623
23	SN	0.13	0/1242	0.30	0/1671
24	SL	0.15	0/1168	0.27	0/1565
25	SR	0.13	0/1052	0.36	0/1413
26	SP	0.15	0/1070	0.40	0/1430
27	ST	0.15	0/1035	0.29	0/1402
28	SV	0.12	0/635	0.27	0/850
29	SY	0.13	0/988	0.28	0/1316
30	SZ	0.12	0/599	0.30	0/808
31	Sa	0.13	0/798	0.30	0/1070

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sb	0.13	0/655	0.28	0/878
33	Sc	0.13	0/451	0.28	0/604
34	Se	0.11	0/375	0.26	0/491
35	Sf	0.11	0/194	0.36	0/265
36	Sg	0.15	0/2444	0.40	0/3332
37	LC	0.16	0/2968	0.30	0/3985
38	LJ	0.13	0/1377	0.28	0/1842
39	LH	0.15	0/1537	0.30	0/2066
40	LE	0.15	0/1820	0.31	0/2442
41	LG	0.15	0/1889	0.32	0/2545
42	LO	0.17	0/1674	0.32	0/2244
43	LL	0.16	0/1696	0.34	0/2271
44	LV	0.16	0/986	0.29	0/1324
45	LM	0.15	0/1138	0.31	0/1523
46	La	0.16	0/1168	0.30	0/1562
47	LN	0.17	0/1745	0.30	0/2338
48	LI	0.14	0/1683	0.27	0/2247
49	LD	0.15	0/2437	0.33	0/3263
50	LQ	0.16	0/1536	0.29	0/2052
51	LR	0.15	0/1492	0.27	0/1985
52	LS	0.16	0/1500	0.30	1/2013 (0.0%)
53	LT	0.17	0/1345	0.35	0/1795
54	LP	0.16	0/1279	0.29	0/1716
55	LU	0.15	0/818	0.36	0/1099
56	LX	0.14	0/983	0.27	0/1323
57	LY	0.14	0/1119	0.30	0/1489
58	LZ	0.15	0/1141	0.29	0/1521
59	Lr	0.14	0/1020	0.27	0/1367
60	Lh	0.13	0/1022	0.27	0/1351
61	Lb	0.13	0/900	0.30	0/1187
62	LF	0.16	0/1926	0.32	0/2567
63	Lc	0.14	0/780	0.27	0/1046
64	Ld	0.12	0/591	0.29	0/822
65	Le	0.16	0/1082	0.29	0/1443
66	Lf	0.16	0/894	0.27	0/1198
67	Lg	0.15	0/885	0.29	0/1182
68	Li	0.12	0/832	0.32	0/1101
69	Lj	0.16	0/731	0.31	0/967
70	Lk	0.15	0/574	0.29	0/761
71	Ll	0.13	0/447	0.24	0/592
72	Lm	0.15	0/433	0.31	0/575
73	Ln	0.18	0/240	0.36	0/305
74	Lo	0.14	0/877	0.25	0/1156

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lp	0.16	0/728	0.34	0/967
76	Pt	0.20	1/1721 (0.1%)	0.23	0/2679
77	mR	0.10	0/175	0.20	0/272
78	S2	0.18	0/37093	0.26	0/57803
79	L5	0.18	0/81582	0.27	0/127262
80	Et	0.11	0/1795	0.23	0/2798
81	LW	0.14	0/532	0.27	0/708
82	SG	0.12	0/1703	0.31	0/2285
All	All	0.17	1/218585 (0.0%)	0.28	2/321229 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	Pt	47	G7M	O3'-P	5.04	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	SB	150	ILE	N-CA-C	-5.14	107.40	113.42
52	LS	142	VAL	N-CA-C	-5.04	107.92	112.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	LA	1921	0	2014	32	0
2	SA	1692	0	1689	27	0
3	LB	3068	0	3103	63	0
4	SB	1761	0	1816	25	0
5	L8	3315	0	1685	38	0
6	L7	2558	0	1294	31	0
7	SD	1642	0	1635	21	0
8	SJ	1477	0	1592	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	SE	2044	0	2145	27	0
10	SC	1685	0	1754	19	0
11	SF	1434	0	1471	17	0
12	SH	1409	0	1467	13	0
13	SW	1030	0	1076	17	0
14	SI	1652	0	1703	32	0
15	SQ	1109	0	1177	19	0
16	SU	519	0	254	0	0
17	SK	678	0	569	6	0
18	SO	990	0	1013	21	0
19	SX	1088	0	1149	9	0
20	SM	218	0	107	0	0
21	SS	1184	0	1240	27	0
22	Sd	458	0	448	8	0
23	SN	1214	0	1301	20	0
24	SL	1148	0	1194	13	0
25	SR	1038	0	1065	16	0
26	SP	1049	0	1092	22	0
27	ST	1010	0	935	17	0
28	SV	628	0	625	6	0
29	SY	972	0	1019	15	0
30	SZ	592	0	624	11	0
31	Sa	782	0	835	8	0
32	Sb	642	0	661	8	0
33	Sc	449	0	470	6	0
34	Se	373	0	401	1	0
35	Sf	194	0	121	1	0
36	Sg	2387	0	2316	45	0
37	LC	2914	0	3087	38	0
38	LJ	1354	0	1389	14	0
39	LH	1518	0	1600	24	0
40	LE	1786	0	1945	27	0
41	LG	1856	0	1985	31	0
42	LO	1642	0	1773	28	0
43	LL	1662	0	1773	26	0
44	LV	972	0	1034	18	0
45	LM	1116	0	1176	15	0
46	La	1152	0	1179	18	0
47	LN	1700	0	1749	30	0
48	LI	1645	0	1694	18	0
49	LD	2391	0	2425	40	0
50	LQ	1512	0	1628	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	LR	1476	0	1548	23	0
52	LS	1460	0	1502	18	0
53	LT	1311	0	1392	18	0
54	LP	1249	0	1276	22	0
55	LU	804	0	820	11	0
56	LX	966	0	1040	7	0
57	LY	1102	0	1181	23	0
58	LZ	1115	0	1195	16	0
59	Lr	1002	0	1076	13	0
60	Lh	1014	0	1148	13	0
61	Lb	898	0	983	15	0
62	LF	1885	0	2022	39	0
63	Lc	770	0	809	8	0
64	Ld	589	0	356	0	0
65	Le	1061	0	1160	18	0
66	Lf	875	0	911	11	0
67	Lg	875	0	951	10	0
68	Li	821	0	890	9	0
69	Lj	712	0	744	14	0
70	Lk	568	0	637	6	0
71	Ll	437	0	471	9	0
72	Lm	436	0	476	5	0
73	Ln	239	0	289	8	0
74	Lo	870	0	936	6	0
75	Lp	715	0	768	5	0
76	Pt	1645	0	844	16	0
77	mR	156	0	77	4	0
78	S2	34940	0	17689	363	0
79	L5	75626	0	38304	680	0
80	Et	1604	0	815	18	0
81	LW	519	0	533	4	0
82	SG	1683	0	1735	32	0
83	A	14	0	0	0	0
83	L7	4	0	0	0	0
83	L8	3	0	0	0	0
83	LA	3	0	0	0	0
83	LH	1	0	0	0	0
83	LI	1	0	0	0	0
83	LL	1	0	0	0	0
83	LN	1	0	0	0	0
83	LQ	1	0	0	0	0
83	Lb	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	Le	1	0	0	0	0
83	Lf	1	0	0	0	0
83	Ll	1	0	0	0	0
83	SL	1	0	0	0	0
83	SO	1	0	0	0	0
83	Sa	1	0	0	0	0
83	mR	1	0	0	0	0
84	Lr	9	0	8	0	0
84	SA	9	0	8	0	0
85	D	12	0	0	0	0
85	Et	1	0	0	0	0
85	L7	15	0	0	0	0
85	L8	16	0	0	0	0
85	LB	1	0	0	0	0
85	LC	1	0	0	0	0
85	LD	1	0	0	0	0
85	LF	1	0	0	0	0
85	LG	1	0	0	0	0
85	LH	1	0	0	0	0
85	LL	1	0	0	0	0
85	LN	3	0	0	0	0
85	LO	2	0	0	0	0
85	LP	2	0	0	0	0
85	LQ	2	0	0	0	0
85	LR	1	0	0	0	0
85	LS	1	0	0	0	0
85	LV	1	0	0	0	0
85	La	1	0	0	0	0
85	Lc	1	0	0	0	0
85	Lf	1	0	0	0	0
85	Lg	1	0	0	0	0
85	Lj	2	0	0	0	0
85	Lo	1	0	0	0	0
85	Lp	2	0	0	0	0
85	Lr	3	0	0	0	0
85	Pt	1	0	0	0	0
85	SN	1	0	0	0	0
85	SS	2	0	0	0	0
85	ST	1	0	0	0	0
85	SX	1	0	0	0	0
85	Sd	1	0	0	0	0
86	Lg	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Lj	1	0	0	0	0
86	Lm	1	0	0	0	0
86	Lo	1	0	0	0	0
86	Lp	1	0	0	0	0
86	Sa	1	0	0	0	0
86	Sd	1	0	0	0	0
86	Sf	1	0	0	0	0
87	SV	11	0	12	0	0
88	Pt	8	0	8	0	0
89	S2	36	0	37	0	0
90	L5	19	0	18	1	0
91	C	7	0	0	0	0
92	B	18	0	0	0	0
92	L7	38	0	0	1	0
92	L8	67	0	0	1	0
92	LA	48	0	0	0	0
92	LB	42	0	0	2	0
92	LC	59	0	0	3	0
92	LD	11	0	0	0	0
92	LE	6	0	0	0	0
92	LF	30	0	0	1	0
92	LG	7	0	0	0	0
92	LH	3	0	0	0	0
92	LI	11	0	0	0	0
92	LJ	1	0	0	0	0
92	LL	26	0	0	2	0
92	LM	2	0	0	0	0
92	LN	40	0	0	2	0
92	LO	29	0	0	1	0
92	LP	17	0	0	1	0
92	LQ	36	0	0	1	0
92	LR	17	0	0	1	0
92	LS	14	0	0	0	0
92	LT	18	0	0	0	0
92	LU	1	0	0	0	0
92	LV	10	0	0	0	0
92	LX	7	0	0	1	0
92	LY	10	0	0	0	0
92	LZ	5	0	0	1	0
92	La	26	0	0	1	0
92	Lb	10	0	0	0	0
92	Lc	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	Ld	9	0	0	0	0
92	Le	28	0	0	1	0
92	Lf	16	0	0	1	0
92	Lg	22	0	0	0	0
92	Lh	5	0	0	0	0
92	Li	2	0	0	0	0
92	Lj	19	0	0	3	0
92	Lk	2	0	0	0	0
92	Ll	8	0	0	0	0
92	Lm	2	0	0	0	0
92	Ln	1	0	0	1	0
92	Lo	12	0	0	0	0
92	Lp	14	0	0	0	0
92	Lr	12	0	0	1	0
92	Pt	1	0	0	0	0
92	SE	1	0	0	0	0
92	SL	1	0	0	0	0
92	SN	1	0	0	0	0
92	SO	2	0	0	0	0
92	Sa	2	0	0	0	0
All	All	209052	0	152166	2016	0

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

The worst 5 of 2016 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)
26:SP:29:SER:HB3	26:SP:32:GLN:HE22	1.46	0.80
67:Lg:83:CYS:SG	67:Lg:86:CYS:HB2	2.22	0.80
38:LJ:95:ARG:HE	38:LJ:177:GLY:HA2	1.49	0.77
79:L5:2786:C:H5''	79:L5:2787:A:H5'	1.66	0.77
36:Sg:217:MET:HG2	36:Sg:229:THR:HG23	1.66	0.76

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LA	248/257 (96%)	238 (96%)	10 (4%)	0	100	100
2	SA	215/294 (73%)	211 (98%)	4 (2%)	0	100	100
3	LB	391/403 (97%)	383 (98%)	8 (2%)	0	100	100
4	SB	217/264 (82%)	212 (98%)	5 (2%)	0	100	100
7	SD	222/243 (91%)	211 (95%)	11 (5%)	0	100	100
8	SJ	177/194 (91%)	170 (96%)	7 (4%)	0	100	100
9	SE	256/263 (97%)	253 (99%)	3 (1%)	0	100	100
10	SC	219/293 (75%)	211 (96%)	8 (4%)	0	100	100
11	SF	178/204 (87%)	174 (98%)	3 (2%)	1 (1%)	21	53
12	SH	179/194 (92%)	171 (96%)	8 (4%)	0	100	100
13	SW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
14	SI	204/208 (98%)	196 (96%)	8 (4%)	0	100	100
15	SQ	138/146 (94%)	134 (97%)	4 (3%)	0	100	100
16	SU	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
17	SK	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
18	SO	132/151 (87%)	125 (95%)	7 (5%)	0	100	100
19	SX	137/143 (96%)	131 (96%)	6 (4%)	0	100	100
20	SM	38/132 (29%)	37 (97%)	1 (3%)	0	100	100
21	SS	146/152 (96%)	141 (97%)	5 (3%)	0	100	100
22	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
23	SN	149/151 (99%)	144 (97%)	5 (3%)	0	100	100
24	SL	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
25	SR	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
26	SP	126/145 (87%)	120 (95%)	6 (5%)	0	100	100
27	ST	141/145 (97%)	135 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	SV	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
29	SY	120/133 (90%)	119 (99%)	1 (1%)	0	100	100
30	SZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
31	Sa	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
32	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
33	Sc	56/69 (81%)	54 (96%)	2 (4%)	0	100	100
34	Se	44/133 (33%)	42 (96%)	2 (4%)	0	100	100
35	Sf	33/156 (21%)	30 (91%)	3 (9%)	0	100	100
36	Sg	309/317 (98%)	282 (91%)	27 (9%)	0	100	100
37	LC	364/427 (85%)	357 (98%)	7 (2%)	0	100	100
38	LJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
39	LH	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
40	LE	217/288 (75%)	207 (95%)	10 (5%)	0	100	100
41	LG	230/266 (86%)	223 (97%)	7 (3%)	0	100	100
42	LO	200/203 (98%)	199 (100%)	0	1 (0%)	24	58
43	LL	205/211 (97%)	201 (98%)	4 (2%)	0	100	100
44	LV	128/140 (91%)	126 (98%)	2 (2%)	0	100	100
45	LM	134/215 (62%)	128 (96%)	6 (4%)	0	100	100
46	La	144/148 (97%)	136 (94%)	8 (6%)	0	100	100
47	LN	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
48	LI	199/214 (93%)	196 (98%)	3 (2%)	0	100	100
49	LD	292/297 (98%)	285 (98%)	7 (2%)	0	100	100
50	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
51	LR	185/196 (94%)	181 (98%)	4 (2%)	0	100	100
52	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
53	LT	159/160 (99%)	155 (98%)	4 (2%)	0	100	100
54	LP	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
55	LU	97/128 (76%)	93 (96%)	4 (4%)	0	100	100
56	LX	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
57	LY	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
58	LZ	134/136 (98%)	129 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	Lr	123/136 (90%)	121 (98%)	2 (2%)	0	100	100
60	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
61	Lb	106/159 (67%)	104 (98%)	2 (2%)	0	100	100
62	LF	225/248 (91%)	218 (97%)	6 (3%)	1 (0%)	30	62
63	Lc	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
64	Ld	105/125 (84%)	105 (100%)	0	0	100	100
65	Le	127/135 (94%)	125 (98%)	2 (2%)	0	100	100
66	Lf	107/110 (97%)	107 (100%)	0	0	100	100
67	Lg	110/117 (94%)	109 (99%)	1 (1%)	0	100	100
68	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
69	Lj	85/97 (88%)	85 (100%)	0	0	100	100
70	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
71	Ll	48/51 (94%)	48 (100%)	0	0	100	100
72	Lm	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
73	Ln	23/25 (92%)	23 (100%)	0	0	100	100
74	Lo	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
75	Lp	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
81	LW	60/157 (38%)	60 (100%)	0	0	100	100
82	SG	216/249 (87%)	211 (98%)	5 (2%)	0	100	100
All	All	11012/12759 (86%)	10698 (97%)	311 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	LO	186	GLU
11	SF	80	GLY
62	LF	197	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LA	191/198 (96%)	188 (98%)	3 (2%)	55	78
2	SA	175/242 (72%)	171 (98%)	4 (2%)	44	72
3	LB	309/348 (89%)	306 (99%)	3 (1%)	68	83
4	SB	192/231 (83%)	186 (97%)	6 (3%)	35	66
7	SD	160/202 (79%)	157 (98%)	3 (2%)	50	75
8	SJ	155/168 (92%)	154 (99%)	1 (1%)	78	88
9	SE	220/225 (98%)	218 (99%)	2 (1%)	70	85
10	SC	177/225 (79%)	174 (98%)	3 (2%)	53	77
11	SF	152/170 (89%)	151 (99%)	1 (1%)	76	87
12	SH	147/174 (84%)	144 (98%)	3 (2%)	48	75
13	SW	111/113 (98%)	110 (99%)	1 (1%)	70	85
14	SI	168/180 (93%)	168 (100%)	0	100	100
15	SQ	114/121 (94%)	112 (98%)	2 (2%)	51	76
16	SU	7/107 (6%)	6 (86%)	1 (14%)	3	14
17	SK	51/136 (38%)	51 (100%)	0	100	100
18	SO	101/119 (85%)	100 (99%)	1 (1%)	68	83
19	SX	111/114 (97%)	109 (98%)	2 (2%)	51	76
21	SS	120/132 (91%)	117 (98%)	3 (2%)	42	71
22	Sd	48/49 (98%)	45 (94%)	3 (6%)	16	46
23	SN	131/131 (100%)	127 (97%)	4 (3%)	35	66
24	SL	124/142 (87%)	121 (98%)	3 (2%)	43	72
25	SR	109/122 (89%)	105 (96%)	4 (4%)	30	62
26	SP	114/130 (88%)	112 (98%)	2 (2%)	51	76
27	ST	84/115 (73%)	82 (98%)	2 (2%)	43	72
28	SV	66/66 (100%)	65 (98%)	1 (2%)	57	79
29	SY	98/115 (85%)	97 (99%)	1 (1%)	68	83
30	SZ	61/103 (59%)	59 (97%)	2 (3%)	33	65
31	Sa	84/98 (86%)	82 (98%)	2 (2%)	43	72
32	Sb	73/76 (96%)	71 (97%)	2 (3%)	39	70
33	Sc	51/62 (82%)	47 (92%)	4 (8%)	11	37
34	Se	36/104 (35%)	35 (97%)	1 (3%)	38	69
35	Sf	8/140 (6%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Sg	260/275 (94%)	247 (95%)	13 (5%)	22	54
37	LC	305/348 (88%)	299 (98%)	6 (2%)	48	75
38	LJ	141/149 (95%)	136 (96%)	5 (4%)	32	63
39	LH	169/171 (99%)	165 (98%)	4 (2%)	43	72
40	LE	196/252 (78%)	194 (99%)	2 (1%)	68	83
41	LG	195/223 (87%)	186 (95%)	9 (5%)	24	57
42	LO	170/174 (98%)	168 (99%)	2 (1%)	63	82
43	LL	170/177 (96%)	168 (99%)	2 (1%)	63	82
44	LV	100/107 (94%)	98 (98%)	2 (2%)	48	75
45	LM	115/161 (71%)	110 (96%)	5 (4%)	26	58
46	La	116/120 (97%)	115 (99%)	1 (1%)	70	85
47	LN	171/172 (99%)	167 (98%)	4 (2%)	44	72
48	LI	173/181 (96%)	170 (98%)	3 (2%)	53	77
49	LD	247/250 (99%)	239 (97%)	8 (3%)	34	65
50	LQ	164/165 (99%)	161 (98%)	3 (2%)	51	76
51	LR	144/175 (82%)	142 (99%)	2 (1%)	59	80
52	LS	157/157 (100%)	151 (96%)	6 (4%)	29	61
53	LT	141/140 (101%)	136 (96%)	5 (4%)	32	63
54	LP	135/163 (83%)	134 (99%)	1 (1%)	76	87
55	LU	88/115 (76%)	84 (96%)	4 (4%)	24	57
56	LX	106/133 (80%)	104 (98%)	2 (2%)	50	75
57	LY	122/135 (90%)	118 (97%)	4 (3%)	33	65
58	LZ	118/118 (100%)	115 (98%)	3 (2%)	42	71
59	Lr	109/120 (91%)	107 (98%)	2 (2%)	51	76
60	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	85
61	Lb	90/125 (72%)	89 (99%)	1 (1%)	65	82
62	LF	196/215 (91%)	196 (100%)	0	100	100
63	Lc	84/97 (87%)	82 (98%)	2 (2%)	43	72
64	Ld	20/110 (18%)	15 (75%)	5 (25%)	0	3
65	Le	115/121 (95%)	113 (98%)	2 (2%)	53	77
66	Lf	88/89 (99%)	84 (96%)	4 (4%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	Lg	92/100 (92%)	89 (97%)	3 (3%)	33	65
68	Li	83/89 (93%)	82 (99%)	1 (1%)	63	82
69	Lj	74/80 (92%)	72 (97%)	2 (3%)	39	70
70	Lk	64/65 (98%)	62 (97%)	2 (3%)	35	66
71	Ll	46/48 (96%)	44 (96%)	2 (4%)	26	58
72	Lm	48/115 (42%)	47 (98%)	1 (2%)	47	74
73	Ln	24/24 (100%)	24 (100%)	0	100	100
74	Lo	93/93 (100%)	92 (99%)	1 (1%)	65	82
75	Lp	75/75 (100%)	75 (100%)	0	100	100
81	LW	54/126 (43%)	52 (96%)	2 (4%)	30	62
82	SG	167/218 (77%)	161 (96%)	6 (4%)	31	63
All	All	9082/10739 (85%)	8879 (98%)	203 (2%)	45	73

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	LM	28	VAL
52	LS	75	VAL
82	SG	163	ASN
45	LM	125	ASN
49	LD	75	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
47	LN	15	GLN
64	Ld	118	GLN
47	LN	99	GLN
56	LX	107	HIS
66	Lf	99	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L8	155/156 (99%)	22 (14%)	0
6	L7	119/120 (99%)	7 (5%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
76	Pt	76/77 (98%)	8 (10%)	0
77	mR	6/27 (22%)	3 (50%)	0
78	S2	1627/1869 (87%)	264 (16%)	0
79	L5	3504/5069 (69%)	531 (15%)	5 (0%)
80	Et	74/75 (98%)	17 (22%)	0
All	All	5561/7393 (75%)	852 (15%)	5 (0%)

5 of 852 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	L8	16	G
5	L8	23	C
5	L8	34	U
5	L8	35	C
5	L8	51	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
79	L5	132	G
79	L5	1633	G
79	L5	1754	U
79	L5	1765	A
79	L5	4699	U

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

225 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
78	A2M	S2	1678	-	22,25,26	3.94	10 (45%)	31,36,39	3.82	14 (45%)
79	PSU	L5	4579	-	18,21,22	1.03	1 (5%)	22,30,33	1.70	4 (18%)
78	OMG	S2	644	-	23,26,27	0.49	0	33,38,41	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
78	OMU	S2	428	-	19,22,23	3.05	8 (42%)	26,31,34	1.71	4 (15%)
78	PSU	S2	1232	-	18,21,22	1.11	1 (5%)	22,30,33	1.77	4 (18%)
79	PSU	L5	1782	-	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
79	PSU	L5	4576	-	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
78	PSU	S2	1367	-	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
78	PSU	S2	1239	-	18,21,22	1.09	1 (5%)	22,30,33	1.73	4 (18%)
78	PSU	S2	36	-	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
78	PSU	S2	573	-	18,21,22	1.11	1 (5%)	22,30,33	1.75	4 (18%)
78	OMU	S2	1288	-	19,22,23	3.02	8 (42%)	26,31,34	1.65	4 (15%)
79	OMG	L5	1625	-	23,26,27	0.54	0	33,38,41	0.54	0
79	A2M	L5	3718	-	22,25,26	3.90	11 (50%)	31,36,39	3.66	14 (45%)
76	4SU	Pt	8	-	18,21,22	3.74	8 (44%)	26,30,33	2.22	4 (15%)
79	OMU	L5	2415	-	19,22,23	3.00	8 (42%)	26,31,34	1.70	4 (15%)
79	A2M	L5	4523	-	22,25,26	3.91	11 (50%)	31,36,39	3.70	15 (48%)
79	A2M	L5	1524	-	22,25,26	3.97	9 (40%)	31,36,39	3.94	14 (45%)
78	OMC	S2	517	-	19,22,23	0.54	0	26,31,34	0.64	0
79	OMU	L5	4620	-	19,22,23	2.94	8 (42%)	26,31,34	1.69	5 (19%)
78	PSU	S2	109	-	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
78	PSU	S2	649	-	18,21,22	1.08	1 (5%)	22,30,33	1.76	4 (18%)
79	PSU	L5	3639	-	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
79	OMU	L5	4498	-	19,22,23	2.99	8 (42%)	26,31,34	1.71	5 (19%)
79	5MC	L5	4447	-	18,22,23	0.73	0	26,32,35	0.67	0
79	OMG	L5	4618	-	23,26,27	0.50	0	33,38,41	0.54	0
79	A2M	L5	1326	-	22,25,26	3.92	10 (45%)	31,36,39	3.69	14 (45%)
79	PSU	L5	3729	-	18,21,22	1.07	1 (5%)	22,30,33	1.71	4 (18%)
79	PSU	L5	4636	-	18,21,22	1.04	1 (5%)	22,30,33	1.71	5 (22%)
78	PSU	S2	1244	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
78	A2M	S2	27	-	22,25,26	3.91	10 (45%)	31,36,39	3.68	13 (41%)
79	PSU	L5	3762	-	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
78	OMC	S2	462	-	19,22,23	0.53	0	26,31,34	0.68	0
78	MA6	S2	1851	-	23,26,27	1.46	4 (17%)	34,38,41	3.48	12 (35%)
79	PSU	L5	4972	-	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
78	PSU	S2	1136	-	18,21,22	1.05	1 (5%)	22,30,33	1.83	5 (22%)
79	OMC	L5	3701	-	19,22,23	0.53	0	26,31,34	0.57	0
79	OMU	L5	2837	-	19,22,23	3.01	8 (42%)	26,31,34	1.77	5 (19%)
78	PSU	S2	681	-	18,21,22	1.05	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
79	OMG	L5	3944	-	23,26,27	0.49	0	33,38,41	0.55	0
78	OMU	S2	172	-	19,22,23	3.02	8 (42%)	26,31,34	1.76	5 (19%)
79	A2M	L5	2815	-	22,25,26	3.93	10 (45%)	31,36,39	3.78	14 (45%)
79	PSU	L5	4689	-	18,21,22	1.04	1 (5%)	22,30,33	1.71	4 (18%)
79	A2M	L5	1534	-	22,25,26	3.93	11 (50%)	31,36,39	3.81	15 (48%)
79	PSU	L5	2839	-	18,21,22	1.09	1 (5%)	22,30,33	1.73	4 (18%)
79	PSU	L5	5001	-	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
78	PSU	S2	1643	-	18,21,22	1.07	1 (5%)	22,30,33	1.78	6 (27%)
79	PSU	L5	3637	-	18,21,22	1.04	1 (5%)	22,30,33	1.83	4 (18%)
79	A2M	L5	2401	-	22,25,26	3.94	10 (45%)	31,36,39	3.74	16 (51%)
78	PSU	S2	1174	-	18,21,22	1.09	1 (5%)	22,30,33	1.74	4 (18%)
79	OMG	L5	1316	-	23,26,27	0.54	0	33,38,41	0.58	0
79	A2M	L5	2363	-	22,25,26	3.93	10 (45%)	31,36,39	3.73	14 (45%)
79	PSU	L5	3695	-	18,21,22	1.09	1 (5%)	22,30,33	1.80	4 (18%)
79	PSU	L5	4493	-	18,21,22	1.05	1 (5%)	22,30,33	1.71	4 (18%)
78	PSU	S2	1445	-	18,21,22	1.06	1 (5%)	22,30,33	1.78	5 (22%)
78	PSU	S2	1243	-	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
79	OMG	L5	3627	-	23,26,27	0.52	0	33,38,41	0.64	0
78	PSU	S2	814	-	18,21,22	1.03	1 (5%)	22,30,33	1.69	4 (18%)
79	PSU	L5	4673	-	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
79	A2M	L5	4571	-	22,25,26	3.93	10 (45%)	31,36,39	3.74	14 (45%)
78	PSU	S2	918	-	18,21,22	1.09	2 (11%)	22,30,33	1.79	5 (22%)
79	PSU	L5	3758	-	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
78	A2M	S2	99	-	22,25,26	3.93	11 (50%)	31,36,39	3.70	15 (48%)
79	PSU	L5	1536	-	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
79	PSU	L5	4420	-	18,21,22	1.06	1 (5%)	22,30,33	1.60	5 (22%)
78	PSU	S2	572	-	18,21,22	1.03	1 (5%)	22,30,33	1.71	4 (18%)
79	OMC	L5	2804	-	19,22,23	0.55	0	26,31,34	0.71	0
78	PSU	S2	966	-	18,21,22	1.01	1 (5%)	22,30,33	1.67	4 (18%)
79	PSU	L5	3853	-	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
79	A2M	L5	1871	-	22,25,26	3.93	10 (45%)	31,36,39	3.67	15 (48%)
78	A2M	S2	590	-	22,25,26	3.97	9 (40%)	31,36,39	3.93	13 (41%)
79	OMC	L5	2824	-	19,22,23	0.56	0	26,31,34	0.75	1 (3%)
79	PSU	L5	4552	-	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
79	PSU	L5	3715	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
79	PSU	L5	4293	-	18,21,22	1.08	1 (5%)	22,30,33	1.79	4 (18%)
79	PSU	L5	3844	-	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
79	PSU	L5	4569	-	18,21,22	1.06	1 (5%)	22,30,33	1.66	4 (18%)
79	OMG	L5	3899	-	23,26,27	0.56	0	33,38,41	0.60	0
76	G7M	Pt	47	-	23,26,27	2.79	8 (34%)	35,39,42	2.29	10 (28%)
78	OMG	S2	1328	-	23,26,27	0.49	0	33,38,41	0.48	0
79	OMC	L5	1881	-	19,22,23	0.57	0	26,31,34	0.67	0
79	PSU	L5	3920	-	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
46	V5N	La	39	-	9,11,12	2.66	2 (22%)	9,14,16	1.23	1 (11%)
78	PSU	S2	651	-	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
79	OMC	L5	1340	-	19,22,23	0.56	0	26,31,34	0.66	0
79	PSU	L5	1779	-	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
78	A2M	S2	1383	-	22,25,26	3.95	10 (45%)	31,36,39	3.69	15 (48%)
79	PSU	L5	1860	-	18,21,22	1.03	1 (5%)	22,30,33	1.74	4 (18%)
78	PSU	S2	863	-	18,21,22	1.10	1 (5%)	22,30,33	1.72	4 (18%)
78	A2M	S2	166	-	22,25,26	3.93	9 (40%)	31,36,39	3.74	16 (51%)
79	OMG	L5	2876	-	23,26,27	0.57	0	33,38,41	0.74	1 (3%)
79	OMG	L5	3744	-	23,26,27	0.50	0	33,38,41	0.48	0
1	V5N	LA	216	-	9,11,12	2.71	2 (22%)	9,14,16	1.25	1 (11%)
74	MLZ	Lo	53	-	8,9,10	0.75	0	4,9,11	0.61	0
79	OMG	L5	4370	-	23,26,27	0.51	0	33,38,41	0.51	0
78	OMG	S2	1447	-	23,26,27	0.48	0	33,38,41	0.50	0
79	OMU	L5	3925	-	19,22,23	2.99	8 (42%)	26,31,34	1.74	5 (19%)
78	PSU	S2	406	-	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
78	PSU	S2	815	-	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
78	PSU	S2	1347	-	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
78	A2M	S2	468	-	22,25,26	3.92	11 (50%)	31,36,39	3.65	15 (48%)
78	OMC	S2	174	-	19,22,23	0.52	0	26,31,34	0.65	0
78	PSU	S2	1004	-	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
79	PSU	L5	1792	-	18,21,22	1.01	1 (5%)	22,30,33	1.70	4 (18%)
79	OMC	L5	2365	-	19,22,23	0.56	0	26,31,34	0.65	0
79	A2M	L5	3825	-	22,25,26	3.92	10 (45%)	31,36,39	3.65	14 (45%)
78	A2M	S2	576	-	22,25,26	3.93	11 (50%)	31,36,39	3.71	15 (48%)
78	PSU	S2	119	-	18,21,22	1.05	1 (5%)	22,30,33	1.61	4 (18%)
78	4AC	S2	1842	-	21,24,25	3.45	10 (47%)	29,34,37	1.11	4 (13%)
78	6MZ	S2	1832	-	22,25,26	2.54	3 (13%)	30,36,39	3.51	12 (40%)
78	MA6	S2	1850	-	23,26,27	1.48	4 (17%)	34,38,41	3.28	11 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
79	PSU	L5	4442	-	18,21,22	1.07	1 (5%)	22,30,33	1.77	5 (22%)
79	PSU	L5	1744	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
78	OMG	S2	436	-	23,26,27	0.53	0	33,38,41	0.54	0
78	PSU	S2	822	-	18,21,22	1.04	1 (5%)	22,30,33	1.76	5 (22%)
79	OMC	L5	4456	-	19,22,23	0.60	0	26,31,34	0.79	1 (3%)
78	PSU	S2	1081	-	18,21,22	1.02	1 (5%)	22,30,33	1.70	5 (22%)
76	OMC	Pt	33	-	19,22,23	0.57	0	26,31,34	1.01	2 (7%)
76	PSU	Pt	56	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
78	PSU	S2	105	-	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
78	PSU	S2	1177	-	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
78	OMU	S2	116	-	19,22,23	2.97	8 (42%)	26,31,34	1.64	5 (19%)
78	PSU	S2	1238	-	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
79	PSU	L5	4353	-	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
76	H2U	Pt	21	-	18,21,22	0.45	0	21,30,33	1.02	1 (4%)
79	OMU	L5	4227	-	19,22,23	2.99	8 (42%)	26,31,34	1.73	5 (19%)
79	A2M	L5	3724	-	22,25,26	3.94	11 (50%)	31,36,39	3.72	14 (45%)
79	A2M	L5	3830	-	22,25,26	3.92	10 (45%)	31,36,39	3.63	14 (45%)
79	5MC	L5	3782	-	18,22,23	0.57	0	26,32,35	0.72	0
79	OMG	L5	4637	-	23,26,27	0.53	0	33,38,41	0.50	0
78	PSU	S2	866	-	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
79	OMC	L5	4536	-	19,22,23	0.57	0	26,31,34	0.76	0
79	PSU	L5	3851	-	18,21,22	1.04	1 (5%)	22,30,33	1.79	4 (18%)
79	PSU	L5	4628	-	18,21,22	1.05	1 (5%)	22,30,33	1.88	5 (22%)
79	UR3	L5	4530	-	19,22,23	2.76	8 (42%)	26,32,35	1.29	2 (7%)
78	PSU	S2	686	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
79	A2M	L5	4590	-	22,25,26	3.94	9 (40%)	31,36,39	3.76	16 (51%)
79	OMG	L5	2424	-	23,26,27	0.52	0	33,38,41	0.44	0
78	A2M	S2	1031	-	22,25,26	3.92	10 (45%)	31,36,39	3.71	15 (48%)
78	OMG	S2	509	-	23,26,27	0.51	0	33,38,41	0.53	0
79	OMG	L5	3792	-	23,26,27	0.51	0	33,38,41	0.47	0
78	PSU	S2	1625	-	18,21,22	1.10	1 (5%)	22,30,33	1.71	4 (18%)
79	PSU	L5	2508	-	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
79	1MA	L5	1322	-	21,25,26	0.51	0	31,37,40	0.76	1 (3%)
79	PSU	L5	1677	-	18,21,22	1.13	1 (5%)	22,30,33	1.79	5 (22%)
79	PSU	L5	4361	-	18,21,22	1.06	1 (5%)	22,30,33	1.72	4 (18%)
3	HIC	LB	245	-	10,11,12	0.53	0	8,14,16	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
79	OMC	L5	2351	-	19,22,23	0.59	0	26,31,34	1.23	2 (7%)
78	A2M	S2	512	-	22,25,26	3.92	10 (45%)	31,36,39	3.70	15 (48%)
79	PSU	L5	4312	-	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
79	OMC	L5	3887	-	19,22,23	0.56	0	26,31,34	0.66	0
78	UY1	S2	1326	-	19,22,23	4.20	8 (42%)	22,31,34	1.81	5 (22%)
78	OMU	S2	1804	-	19,22,23	2.99	8 (42%)	26,31,34	1.77	5 (19%)
79	OMC	L5	3869	-	19,22,23	0.58	0	26,31,34	0.74	0
61	MLZ	Lb	5	-	8,9,10	0.78	0	4,9,11	0.68	0
72	M3L	Lm	98	-	10,11,12	0.40	0	9,14,16	0.28	0
78	OMG	S2	1490	-	23,26,27	0.54	0	33,38,41	0.51	0
79	PSU	L5	2632	-	18,21,22	1.05	1 (5%)	22,30,33	1.66	4 (18%)
79	OMG	L5	4499	-	23,26,27	0.52	0	33,38,41	0.47	0
79	OMG	L5	1522	-	23,26,27	0.51	0	33,38,41	0.61	0
78	A2M	S2	159	-	22,25,26	3.89	10 (45%)	31,36,39	3.69	13 (41%)
79	PSU	L5	4299	-	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
79	OMG	L5	4623	-	23,26,27	0.53	0	33,38,41	0.59	0
78	PSU	S2	609	-	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)
78	OMC	S2	1391	-	19,22,23	0.53	0	26,31,34	0.65	0
79	PSU	L5	4521	-	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
79	PSU	L5	3734	-	18,21,22	1.01	1 (5%)	22,30,33	1.63	4 (18%)
79	PSU	L5	5010	-	18,21,22	1.06	1 (5%)	22,30,33	1.69	4 (18%)
78	G7M	S2	1639	-	23,26,27	2.76	8 (34%)	35,39,42	2.32	10 (28%)
79	PSU	L5	4403	-	18,21,22	1.00	1 (5%)	22,30,33	1.82	5 (22%)
79	OMC	L5	2861	-	19,22,23	0.58	0	26,31,34	0.83	1 (3%)
79	A2M	L5	3867	-	22,25,26	3.94	10 (45%)	31,36,39	3.75	14 (45%)
79	PSU	L5	3768	-	18,21,22	1.06	1 (5%)	22,30,33	1.69	4 (18%)
79	PSU	L5	4531	-	18,21,22	1.08	1 (5%)	22,30,33	1.81	5 (22%)
78	OMG	S2	601	-	23,26,27	0.49	0	33,38,41	0.46	0
79	PSU	L5	3770	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
78	OMU	S2	627	-	19,22,23	3.04	8 (42%)	26,31,34	1.67	4 (15%)
79	OMC	L5	3841	-	19,22,23	0.57	0	26,31,34	0.65	0
79	OMG	L5	4392	-	23,26,27	0.50	0	33,38,41	0.45	0
79	6MZ	L5	4220	-	22,25,26	2.61	3 (13%)	30,36,39	3.46	9 (30%)
79	OMG	L5	4494	-	23,26,27	0.53	0	33,38,41	0.49	0
79	PSU	L5	2843	-	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
79	PSU	L5	4471	-	18,21,22	1.06	1 (5%)	22,30,33	1.67	4 (18%)
78	OMC	S2	1703	-	19,22,23	0.55	0	26,31,34	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
79	PSU	L5	4296	-	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
78	PSU	S2	1692	-	18,21,22	1.06	1 (5%)	22,30,33	1.72	4 (18%)
79	PSU	L5	4532	-	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
79	OMC	L5	2422	-	19,22,23	0.58	0	26,31,34	0.77	1 (3%)
79	OMC	L5	3808	-	19,22,23	0.64	0	26,31,34	0.90	2 (7%)
79	PSU	L5	1862	-	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
79	A2M	L5	3785	-	22,25,26	3.94	11 (50%)	31,36,39	3.76	14 (45%)
78	PSU	S2	34	-	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
78	A2M	S2	668	-	22,25,26	3.91	11 (50%)	31,36,39	3.63	14 (45%)
79	OMG	L5	2364	-	23,26,27	0.51	0	33,38,41	0.47	0
78	B8N	S2	1248	-	24,29,30	3.02	6 (25%)	29,42,45	1.75	5 (17%)
79	UY1	L5	3818	-	19,22,23	4.18	8 (42%)	22,31,34	1.80	5 (22%)
79	PSU	L5	4423	-	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
19	HY3	SX	62	-	6,8,9	7.80	3 (50%)	5,10,12	0.98	0
78	OMU	S2	121	-	19,22,23	2.99	8 (42%)	26,31,34	1.66	5 (19%)
78	OMU	S2	354	-	19,22,23	2.96	8 (42%)	26,31,34	1.71	5 (19%)
79	PSU	L5	4457	-	18,21,22	1.04	1 (5%)	22,30,33	1.80	5 (22%)
5	PSU	L8	55	-	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
79	A2M	L5	3723	-	22,25,26	3.93	10 (45%)	31,36,39	3.74	14 (45%)
78	4AC	S2	1337	-	21,24,25	3.46	10 (47%)	29,34,37	1.09	3 (10%)
78	OMG	S2	683	-	23,26,27	0.51	0	33,38,41	0.57	0
79	A2M	L5	398	-	22,25,26	3.88	10 (45%)	31,36,39	3.69	13 (41%)
79	PSU	L5	1781	-	18,21,22	1.08	1 (5%)	22,30,33	1.65	4 (18%)
79	PSU	L5	4500	-	18,21,22	1.03	1 (5%)	22,30,33	1.87	5 (22%)
79	PSU	L5	3764	-	18,21,22	1.06	1 (5%)	22,30,33	1.74	5 (22%)
78	PSU	S2	218	-	18,21,22	1.06	1 (5%)	22,30,33	1.69	5 (22%)
78	PSU	S2	296	-	18,21,22	1.03	1 (5%)	22,30,33	1.68	4 (18%)
78	PSU	S2	1056	-	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
5	PSU	L8	69	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	5 (22%)
79	A2M	L5	400	-	22,25,26	3.93	10 (45%)	31,36,39	3.71	14 (45%)
79	OMU	L5	4306	-	19,22,23	2.99	8 (42%)	26,31,34	1.70	5 (19%)
78	A2M	S2	484	-	22,25,26	3.85	11 (50%)	31,36,39	3.68	13 (41%)
79	OMG	L5	4228	-	23,26,27	0.50	0	33,38,41	0.55	0
78	PSU	S2	93	-	18,21,22	1.05	1 (5%)	22,30,33	1.65	4 (18%)
79	PSU	L5	4431	-	18,21,22	1.05	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
79	PSU	L5	1582	-	18,21,22	1.07	1 (5%)	22,30,33	1.70	4 (18%)
78	PSU	S2	801	-	18,21,22	1.09	1 (5%)	22,30,33	1.74	4 (18%)
79	PSU	L5	1683	-	18,21,22	1.07	1 (5%)	22,30,33	1.71	4 (18%)
5	OMG	L8	75	-	23,26,27	0.49	0	33,38,41	0.49	0
79	PSU	L5	3884	-	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
79	OMG	L5	4196	-	23,26,27	0.52	0	33,38,41	0.54	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
78	A2M	S2	1678	-	-	1/9/27/28	0/3/3/3
79	PSU	L5	4579	-	-	0/7/25/26	0/2/2/2
78	OMG	S2	644	-	-	3/9/27/28	0/3/3/3
78	OMU	S2	428	-	-	6/9/27/28	0/2/2/2
78	PSU	S2	1232	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	1782	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4576	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1367	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1239	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	36	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	573	-	-	0/7/25/26	0/2/2/2
78	OMU	S2	1288	-	-	0/9/27/28	0/2/2/2
79	OMG	L5	1625	-	-	1/9/27/28	0/3/3/3
79	A2M	L5	3718	-	-	0/9/27/28	0/3/3/3
76	4SU	Pt	8	-	-	0/7/25/26	0/2/2/2
79	OMU	L5	2415	-	-	1/9/27/28	0/2/2/2
79	A2M	L5	4523	-	-	2/9/27/28	0/3/3/3
79	A2M	L5	1524	-	-	2/9/27/28	0/3/3/3
78	OMC	S2	517	-	-	0/9/27/28	0/2/2/2
79	OMU	L5	4620	-	-	1/9/27/28	0/2/2/2
78	PSU	S2	109	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	649	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3639	-	-	0/7/25/26	0/2/2/2
79	OMU	L5	4498	-	-	0/9/27/28	0/2/2/2
79	5MC	L5	4447	-	-	4/7/25/26	0/2/2/2
79	OMG	L5	4618	-	-	0/9/27/28	0/3/3/3
79	A2M	L5	1326	-	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	PSU	L5	3729	-	-	2/7/25/26	0/2/2/2
79	PSU	L5	4636	-	-	2/7/25/26	0/2/2/2
78	PSU	S2	1244	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	27	-	-	2/9/27/28	0/3/3/3
79	PSU	L5	3762	-	-	0/7/25/26	0/2/2/2
78	OMC	S2	462	-	-	0/9/27/28	0/2/2/2
78	MA6	S2	1851	-	-	3/11/29/30	0/3/3/3
79	PSU	L5	4972	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1136	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	3701	-	-	4/9/27/28	0/2/2/2
79	OMU	L5	2837	-	-	0/9/27/28	0/2/2/2
78	PSU	S2	681	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	3944	-	-	0/9/27/28	0/3/3/3
78	OMU	S2	172	-	-	0/9/27/28	0/2/2/2
79	A2M	L5	2815	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	4689	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	1534	-	-	2/9/27/28	0/3/3/3
79	PSU	L5	2839	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	5001	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1643	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3637	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	2401	-	-	0/9/27/28	0/3/3/3
78	PSU	S2	1174	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	1316	-	-	1/9/27/28	0/3/3/3
79	A2M	L5	2363	-	-	0/9/27/28	0/3/3/3
79	PSU	L5	3695	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4493	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1445	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1243	-	-	2/7/25/26	0/2/2/2
79	OMG	L5	3627	-	-	0/9/27/28	0/3/3/3
78	PSU	S2	814	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4673	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	4571	-	-	1/9/27/28	0/3/3/3
78	PSU	S2	918	-	-	2/7/25/26	0/2/2/2
79	PSU	L5	3758	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	99	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	1536	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4420	-	-	4/7/25/26	0/2/2/2
78	PSU	S2	572	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	2804	-	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
78	PSU	S2	966	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3853	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	1871	-	-	0/9/27/28	0/3/3/3
78	A2M	S2	590	-	-	6/9/27/28	0/3/3/3
79	OMC	L5	2824	-	-	1/9/27/28	0/2/2/2
79	PSU	L5	4552	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3715	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4293	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3844	-	-	1/7/25/26	0/2/2/2
79	PSU	L5	4569	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	3899	-	-	0/9/27/28	0/3/3/3
76	G7M	Pt	47	-	-	2/7/25/26	0/3/3/3
78	OMG	S2	1328	-	-	1/9/27/28	0/3/3/3
79	OMC	L5	1881	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	3920	-	-	0/7/25/26	0/2/2/2
46	V5N	La	39	-	-	1/9/10/12	0/1/1/1
78	PSU	S2	651	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	1340	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	1779	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	1383	-	-	1/9/27/28	0/3/3/3
79	PSU	L5	1860	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	863	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	166	-	-	1/9/27/28	0/3/3/3
79	OMG	L5	2876	-	-	3/9/27/28	0/3/3/3
79	OMG	L5	3744	-	-	0/9/27/28	0/3/3/3
1	V5N	LA	216	-	-	1/9/10/12	0/1/1/1
74	MLZ	Lo	53	-	-	2/7/8/10	-
79	OMG	L5	4370	-	-	2/9/27/28	0/3/3/3
78	OMG	S2	1447	-	-	2/9/27/28	0/3/3/3
79	OMU	L5	3925	-	-	1/9/27/28	0/2/2/2
78	PSU	S2	406	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	815	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1347	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	468	-	-	2/9/27/28	0/3/3/3
78	OMC	S2	174	-	-	0/9/27/28	0/2/2/2
78	PSU	S2	1004	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	1792	-	-	2/7/25/26	0/2/2/2
79	OMC	L5	2365	-	-	0/9/27/28	0/2/2/2
79	A2M	L5	3825	-	-	1/9/27/28	0/3/3/3
78	A2M	S2	576	-	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
78	PSU	S2	119	-	-	1/7/25/26	0/2/2/2
78	4AC	S2	1842	-	-	0/11/29/30	0/2/2/2
78	6MZ	S2	1832	-	-	0/9/27/28	0/3/3/3
78	MA6	S2	1850	-	-	0/11/29/30	0/3/3/3
79	PSU	L5	4442	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	1744	-	-	0/7/25/26	0/2/2/2
78	OMG	S2	436	-	-	2/9/27/28	0/3/3/3
78	PSU	S2	822	-	-	2/7/25/26	0/2/2/2
79	OMC	L5	4456	-	-	0/9/27/28	0/2/2/2
78	PSU	S2	1081	-	-	0/7/25/26	0/2/2/2
76	OMC	Pt	33	-	-	1/9/27/28	0/2/2/2
76	PSU	Pt	56	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	105	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1177	-	-	0/7/25/26	0/2/2/2
78	OMU	S2	116	-	-	1/9/27/28	0/2/2/2
78	PSU	S2	1238	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4353	-	-	0/7/25/26	0/2/2/2
76	H2U	Pt	21	-	-	6/7/38/39	0/2/2/2
79	OMU	L5	4227	-	-	0/9/27/28	0/2/2/2
79	A2M	L5	3724	-	-	1/9/27/28	0/3/3/3
79	A2M	L5	3830	-	-	0/9/27/28	0/3/3/3
79	5MC	L5	3782	-	-	1/7/25/26	0/2/2/2
79	OMG	L5	4637	-	-	3/9/27/28	0/3/3/3
78	PSU	S2	866	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	4536	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	3851	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4628	-	-	0/7/25/26	0/2/2/2
79	UR3	L5	4530	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	686	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	4590	-	-	1/9/27/28	0/3/3/3
79	OMG	L5	2424	-	-	0/9/27/28	0/3/3/3
78	A2M	S2	1031	-	-	0/9/27/28	0/3/3/3
78	OMG	S2	509	-	-	2/9/27/28	0/3/3/3
79	OMG	L5	3792	-	-	0/9/27/28	0/3/3/3
78	PSU	S2	1625	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	2508	-	-	0/7/25/26	0/2/2/2
79	1MA	L5	1322	-	-	2/7/25/26	0/3/3/3
79	PSU	L5	1677	-	-	1/7/25/26	0/2/2/2
79	PSU	L5	4361	-	-	1/7/25/26	0/2/2/2
3	HIC	LB	245	-	-	0/5/6/8	0/1/1/1
79	OMC	L5	2351	-	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
78	A2M	S2	512	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	4312	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	3887	-	-	1/9/27/28	0/2/2/2
78	UY1	S2	1326	-	-	2/9/27/28	0/2/2/2
78	OMU	S2	1804	-	-	1/9/27/28	0/2/2/2
79	OMC	L5	3869	-	-	0/9/27/28	0/2/2/2
61	MLZ	Lb	5	-	-	4/7/8/10	-
72	M3L	Lm	98	-	-	0/9/10/12	-
78	OMG	S2	1490	-	-	2/9/27/28	0/3/3/3
79	PSU	L5	2632	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	4499	-	-	0/9/27/28	0/3/3/3
79	OMG	L5	1522	-	-	0/9/27/28	0/3/3/3
78	A2M	S2	159	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	4299	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	4623	-	-	0/9/27/28	0/3/3/3
78	PSU	S2	609	-	-	0/7/25/26	0/2/2/2
78	OMC	S2	1391	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	4521	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3734	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	5010	-	-	0/7/25/26	0/2/2/2
78	G7M	S2	1639	-	-	2/7/25/26	0/3/3/3
79	PSU	L5	4403	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	2861	-	-	0/9/27/28	0/2/2/2
79	A2M	L5	3867	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	3768	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4531	-	-	0/7/25/26	0/2/2/2
78	OMG	S2	601	-	-	1/9/27/28	0/3/3/3
79	PSU	L5	3770	-	-	0/7/25/26	0/2/2/2
78	OMU	S2	627	-	-	0/9/27/28	0/2/2/2
79	OMC	L5	3841	-	-	0/9/27/28	0/2/2/2
79	OMG	L5	4392	-	-	0/9/27/28	0/3/3/3
79	6MZ	L5	4220	-	-	2/9/27/28	0/3/3/3
79	OMG	L5	4494	-	-	1/9/27/28	0/3/3/3
79	PSU	L5	2843	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4471	-	-	0/7/25/26	0/2/2/2
78	OMC	S2	1703	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	4296	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1692	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4532	-	-	2/7/25/26	0/2/2/2
79	OMC	L5	2422	-	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	OMC	L5	3808	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	1862	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	3785	-	-	4/9/27/28	0/3/3/3
78	PSU	S2	34	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	668	-	-	2/9/27/28	0/3/3/3
79	OMG	L5	2364	-	-	2/9/27/28	0/3/3/3
78	B8N	S2	1248	-	-	6/16/34/35	0/2/2/2
79	UY1	L5	3818	-	-	3/9/27/28	0/2/2/2
79	PSU	L5	4423	-	-	0/7/25/26	0/2/2/2
19	HY3	SX	62	-	-	0/1/12/14	0/1/1/1
78	OMU	S2	121	-	-	0/9/27/28	0/2/2/2
78	OMU	S2	354	-	-	1/9/27/28	0/2/2/2
79	PSU	L5	4457	-	-	0/7/25/26	0/2/2/2
5	PSU	L8	55	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	3723	-	-	1/9/27/28	0/3/3/3
78	4AC	S2	1337	-	-	0/11/29/30	0/2/2/2
78	OMG	S2	683	-	-	2/9/27/28	0/3/3/3
79	A2M	L5	398	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	1781	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4500	-	-	1/7/25/26	0/2/2/2
79	PSU	L5	3764	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	218	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	296	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1056	-	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	400	-	-	0/9/27/28	0/3/3/3
79	OMU	L5	4306	-	-	0/9/27/28	0/2/2/2
78	A2M	S2	484	-	-	1/9/27/28	0/3/3/3
79	OMG	L5	4228	-	-	2/9/27/28	0/3/3/3
78	PSU	S2	93	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4431	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	1582	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	801	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	1683	-	-	0/7/25/26	0/2/2/2
5	OMG	L8	75	-	-	0/9/27/28	0/3/3/3
79	PSU	L5	3884	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	4196	-	-	1/9/27/28	0/3/3/3

The worst 5 of 646 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	SX	62	HY3	C3-CA	-17.99	1.37	1.55
78	S2	590	A2M	C3'-C2'	-12.71	1.24	1.52
78	S2	1383	A2M	C3'-C2'	-12.67	1.24	1.52
79	L5	4590	A2M	C3'-C2'	-12.67	1.24	1.52
79	L5	3785	A2M	C3'-C2'	-12.67	1.24	1.52

The worst 5 of 1072 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	1851	MA6	N1-C6-N6	-14.02	101.76	117.08
78	S2	1850	MA6	N1-C6-N6	-12.80	103.09	117.08
79	L5	1524	A2M	C1'-N9-C8	-12.49	98.93	127.14
78	S2	590	A2M	C1'-N9-C8	-12.39	99.15	127.14
78	S2	1678	A2M	C1'-N9-C8	-11.53	101.09	127.14

There are no chirality outliers.

5 of 173 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	LA	216	V5N	O-C-CA-CB
46	La	39	V5N	O2-CB-CG-CD2
61	Lb	5	MLZ	N-CA-CB-CG
61	Lb	5	MLZ	C-CA-CB-CG
74	Lo	53	MLZ	O-C-CA-CB

There are no ring outliers.

76 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
78	S2	1678	A2M	1	0
79	L5	4579	PSU	2	0
78	S2	644	OMG	1	0
78	S2	1232	PSU	2	0
78	S2	1288	OMU	1	0
79	L5	3718	A2M	3	0
79	L5	2415	OMU	2	0
79	L5	4523	A2M	1	0
79	L5	4620	OMU	4	0
78	S2	649	PSU	1	0
79	L5	1326	A2M	1	0
78	S2	1851	MA6	1	0
79	L5	5001	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
78	S2	1643	PSU	1	0
79	L5	1316	OMG	1	0
79	L5	2363	A2M	1	0
78	S2	1243	PSU	1	0
79	L5	3627	OMG	1	0
79	L5	4571	A2M	1	0
78	S2	99	A2M	1	0
78	S2	572	PSU	1	0
79	L5	1871	A2M	1	0
79	L5	3715	PSU	1	0
76	Pt	47	G7M	2	0
78	S2	1328	OMG	1	0
78	S2	1383	A2M	1	0
78	S2	863	PSU	1	0
79	L5	2876	OMG	1	0
78	S2	1447	OMG	2	0
79	L5	3925	OMU	1	0
78	S2	576	A2M	1	0
78	S2	1842	4AC	3	0
78	S2	1850	MA6	1	0
79	L5	4442	PSU	2	0
78	S2	436	OMG	1	0
79	L5	4456	OMC	2	0
76	Pt	33	OMC	1	0
76	Pt	56	PSU	1	0
78	S2	116	OMU	3	0
79	L5	4353	PSU	1	0
79	L5	3724	A2M	1	0
79	L5	4637	OMG	1	0
79	L5	4536	OMC	1	0
79	L5	2424	OMG	1	0
78	S2	1031	A2M	1	0
78	S2	509	OMG	2	0
79	L5	2508	PSU	2	0
3	LB	245	HIC	1	0
78	S2	512	A2M	1	0
78	S2	1804	OMU	1	0
61	Lb	5	MLZ	1	0
79	L5	4499	OMG	1	0
78	S2	159	A2M	1	0
79	L5	4299	PSU	1	0
78	S2	609	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
78	S2	1391	OMC	1	0
78	S2	1639	G7M	1	0
79	L5	3867	A2M	1	0
78	S2	601	OMG	1	0
79	L5	3770	PSU	1	0
79	L5	3785	A2M	1	0
78	S2	121	OMU	1	0
78	S2	354	OMU	2	0
79	L5	4457	PSU	1	0
79	L5	3723	A2M	2	0
79	L5	1781	PSU	1	0
79	L5	4500	PSU	1	0
79	L5	3764	PSU	1	0
78	S2	484	A2M	1	0
79	L5	4228	OMG	1	0
79	L5	1582	PSU	1	0
78	S2	801	PSU	1	0
79	L5	1683	PSU	2	0
5	L8	75	OMG	1	0
79	L5	3884	PSU	1	0
79	L5	4196	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 140 ligands modelled in this entry, 134 are monoatomic - leaving 6 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	$\# Z > 2$
89	HYG	S2	1901	-	35,39,39	3.09	11 (31%)	43,60,60	1.51	7 (16%)
88	MET	Pt	78	-	6,7,8	0.46	0	2,7,9	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	SAC	SA	2	-	7,8,9	0.41	0	8,9,11	1.66	1 (12%)
84	SAC	Lr	2	-	7,8,9	0.36	0	8,9,11	1.14	1 (12%)
90	ANM	L5	5101	-	20,20,20	4.06	10 (50%)	22,27,27	1.53	4 (18%)
87	AME	SV	1	-	9,10,11	1.44	1 (11%)	9,11,13	1.53	2 (22%)

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
89	HYG	S2	1901	-	-	4/12/87/87	0/4/4/4
88	MET	Pt	78	-	-	1/5/6/8	-
84	SAC	SA	2	-	-	3/7/8/10	-
84	SAC	Lr	2	-	-	2/7/8/10	-
90	ANM	L5	5101	-	-	4/10/23/23	0/2/2/2
87	AME	SV	1	-	-	3/9/10/12	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	L5	5101	ANM	C2-C16	-11.68	1.30	1.53
89	S2	1901	HYG	O29-C12	10.88	1.61	1.43
90	L5	5101	ANM	C16-N1	8.95	1.67	1.48
89	S2	1901	HYG	O22-C17	6.61	1.53	1.43
89	S2	1901	HYG	O14-C13	6.55	1.58	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	L5	5101	ANM	O2-C5-C6	5.02	120.32	111.09
89	S2	1901	HYG	O29-C12-C13	4.74	123.29	110.86
89	S2	1901	HYG	O22-C17-C16	4.15	121.33	111.22
84	SA	2	SAC	CA-N-C1A	4.08	130.68	123.15
89	S2	1901	HYG	O28-C27-C26	3.12	112.95	108.52

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	SA	2	SAC	CB-CA-N-C1A
84	SA	2	SAC	C-CA-CB-OG
87	SV	1	AME	O-C-CA-CB
88	Pt	78	MET	N-CA-CB-CG
89	S2	1901	HYG	C27-C33-C34-O35

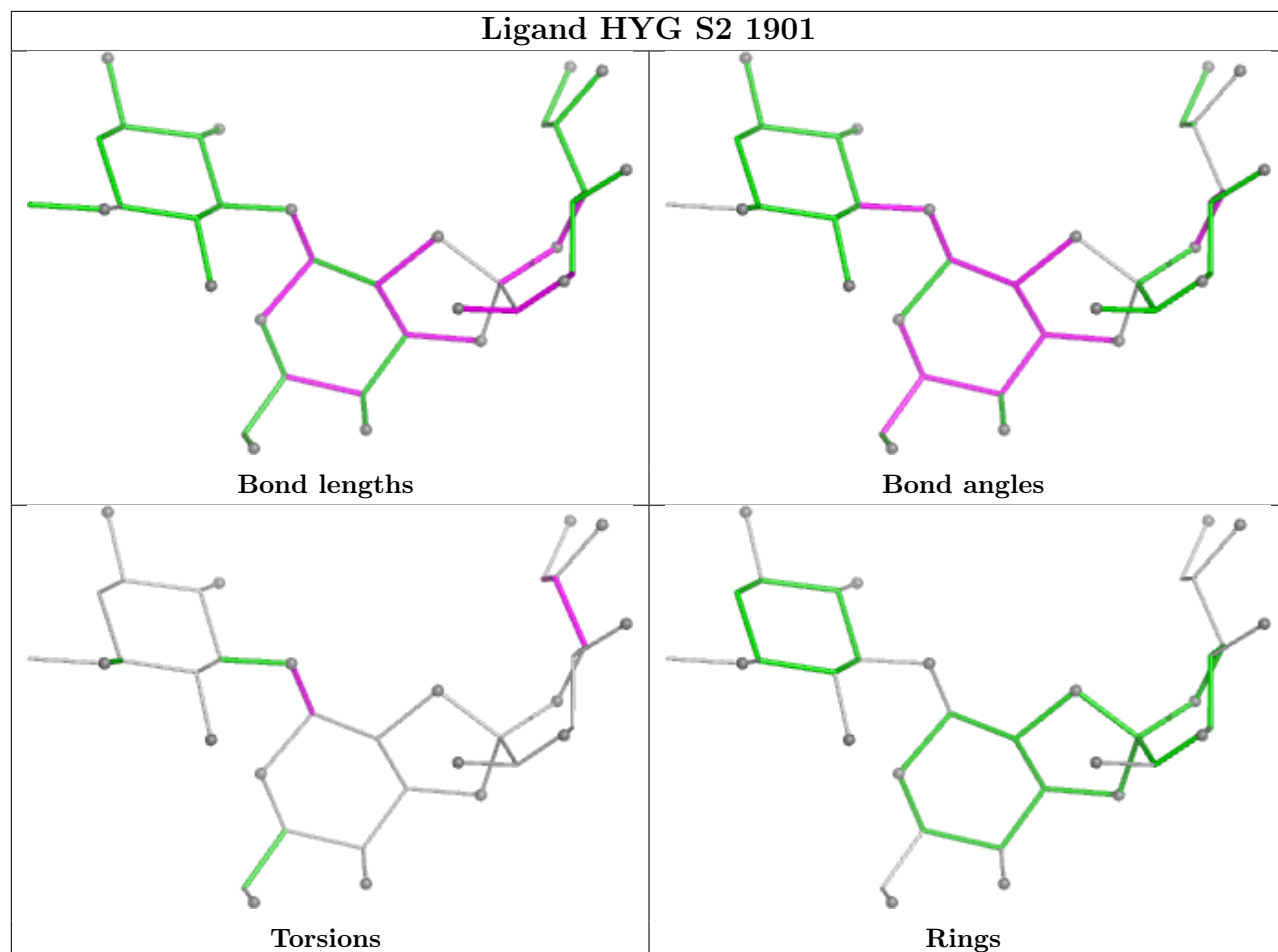
There are no ring outliers.

1 monomer is involved in 1 short contact:

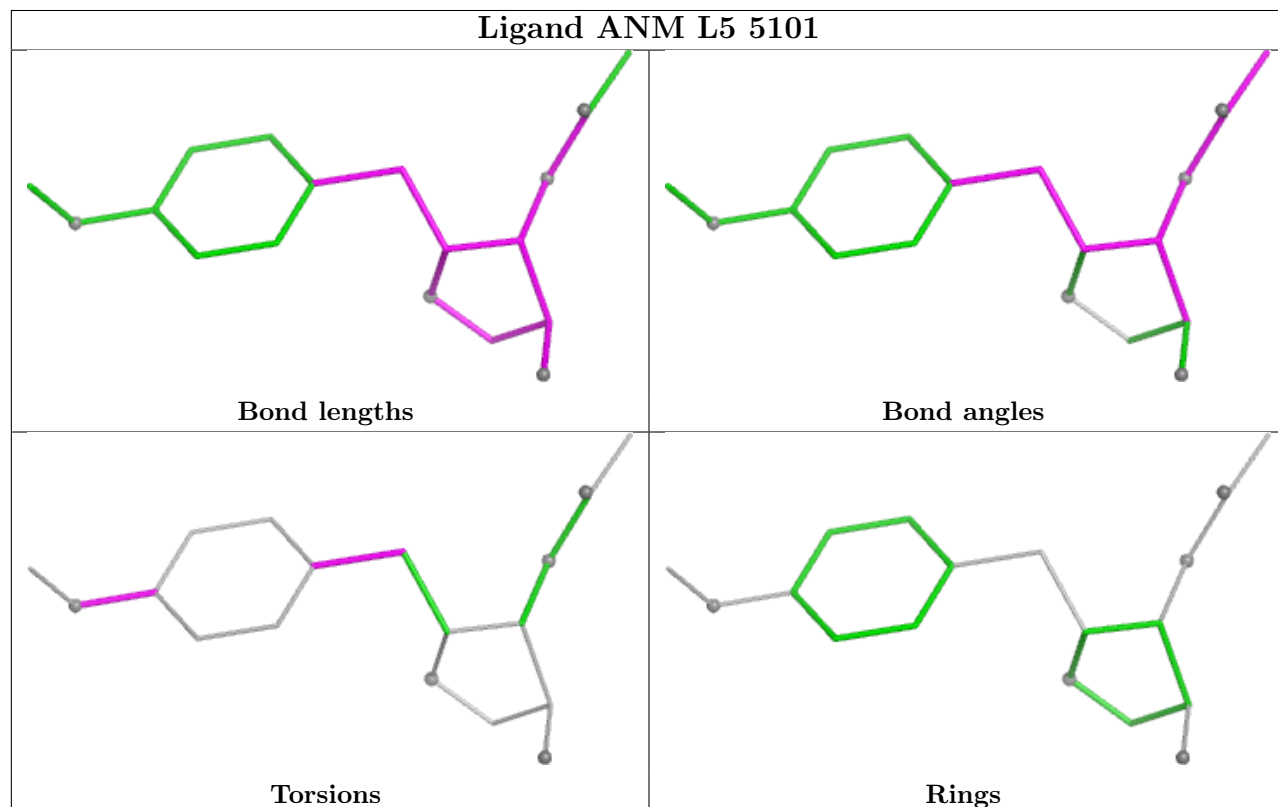
Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	L5	5101	ANM	1	0

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

Ligand HYG S2 1901



Ligand ANM L5 5101



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
20	SM	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SM	72:HIS	C	105:GLY	N	25.35

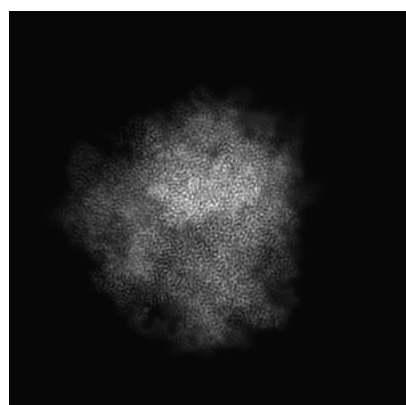
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54267. These allow visual inspection of the internal detail of the map and identification of artifacts.

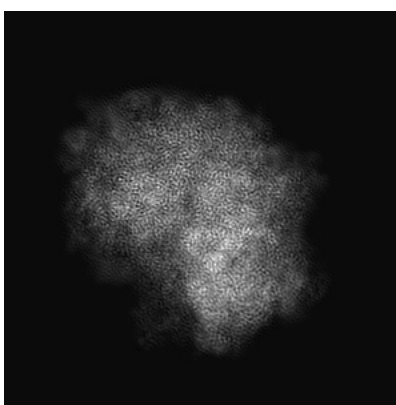
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

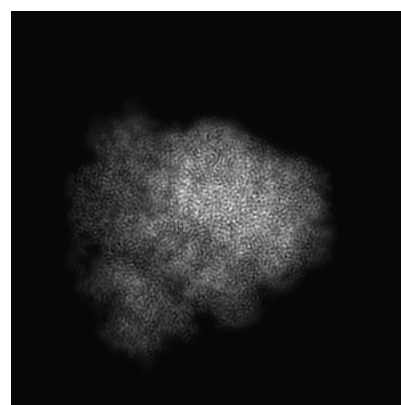
6.1.1 Primary map



X



Y

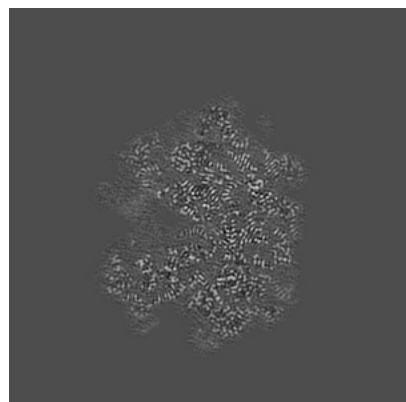


Z

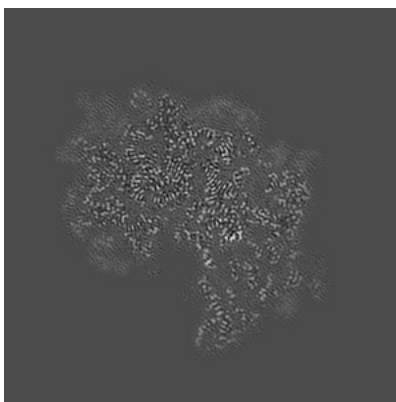
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

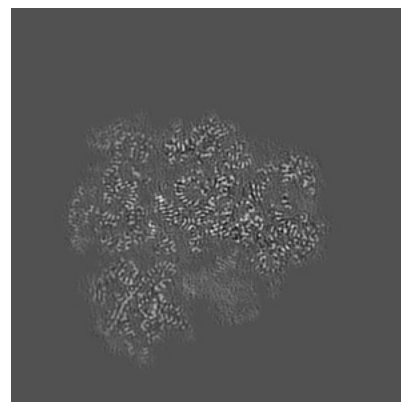
6.2.1 Primary map



X Index: 240



Y Index: 240

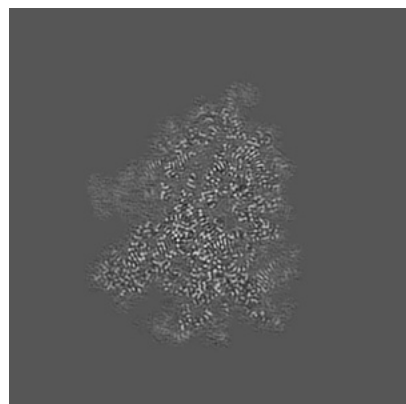


Z Index: 240

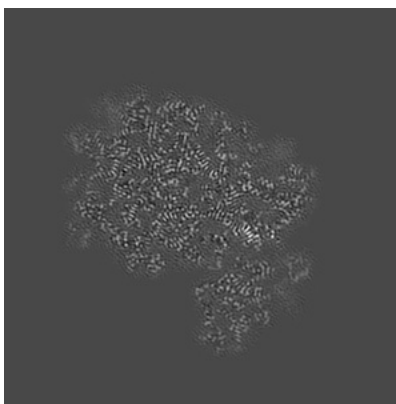
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

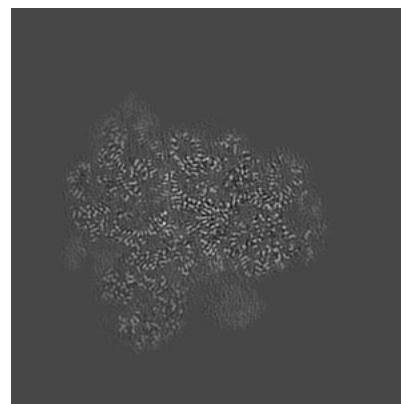
6.3.1 Primary map



X Index: 272



Y Index: 258

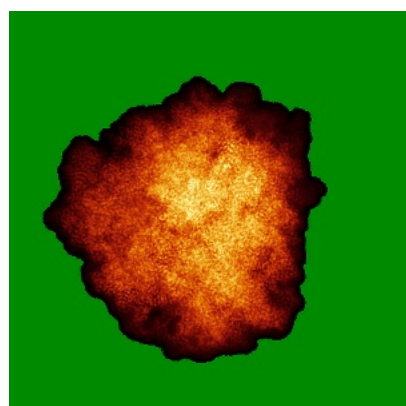


Z Index: 261

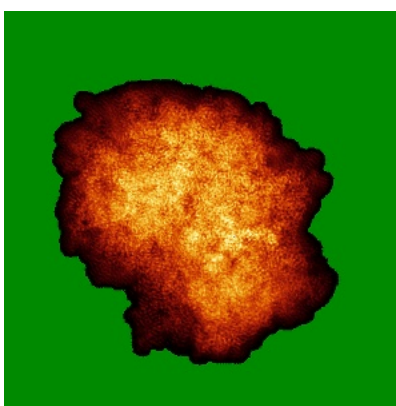
The images above show the largest variance slices of the map in three orthogonal directions.

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

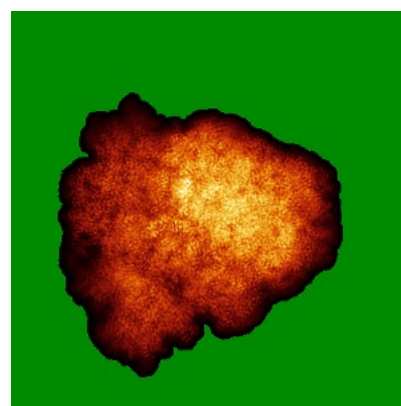
6.4.1 Primary map



X



Y

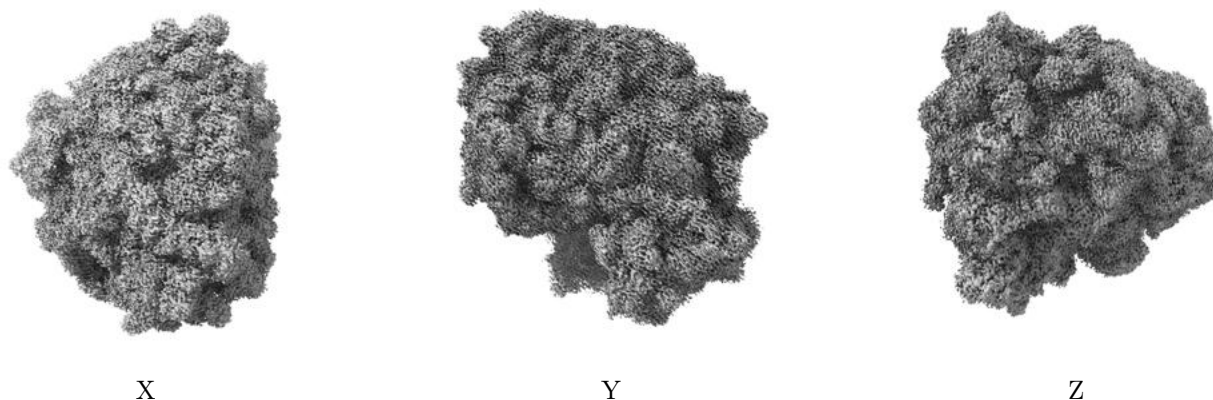


Z

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.

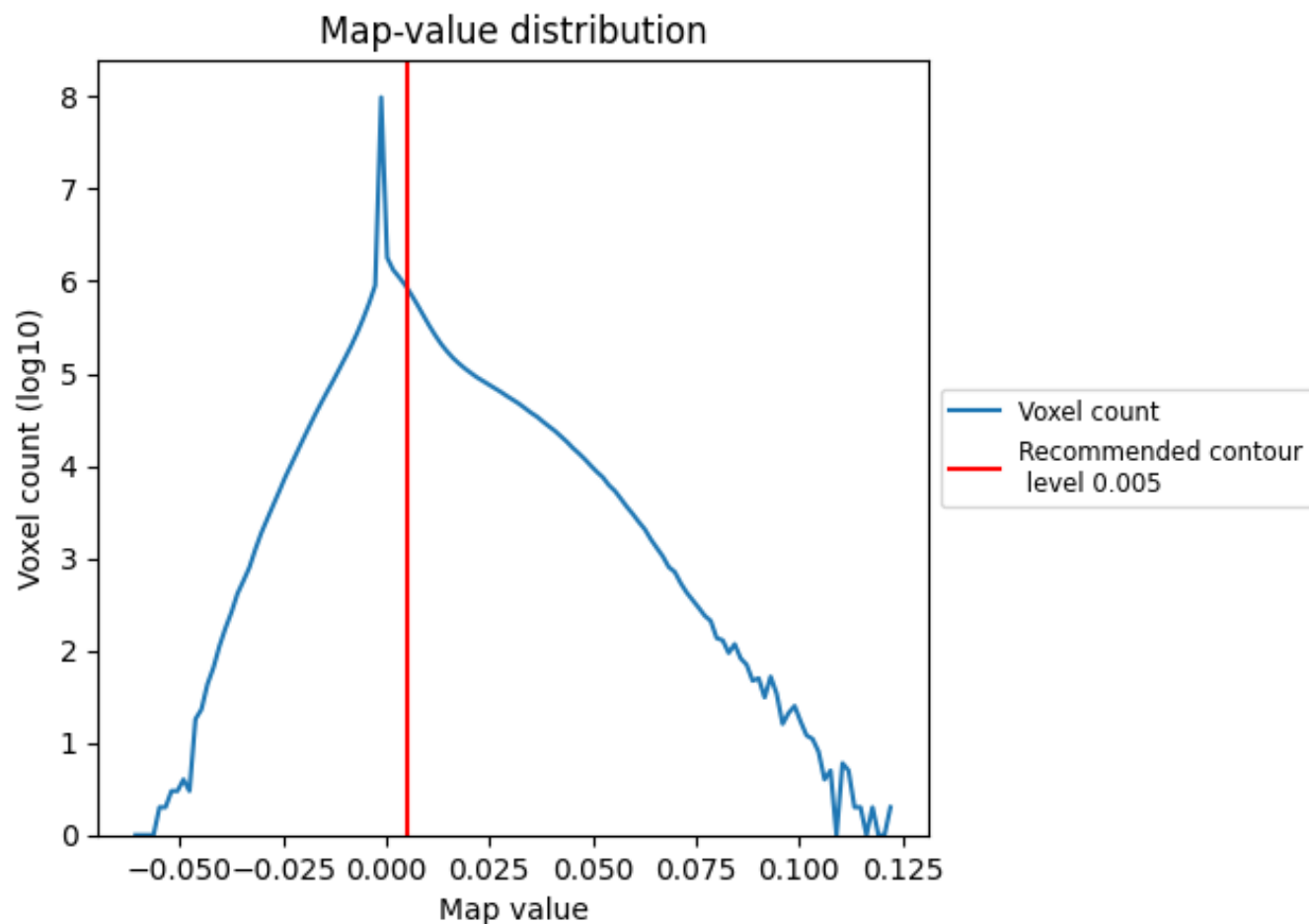
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

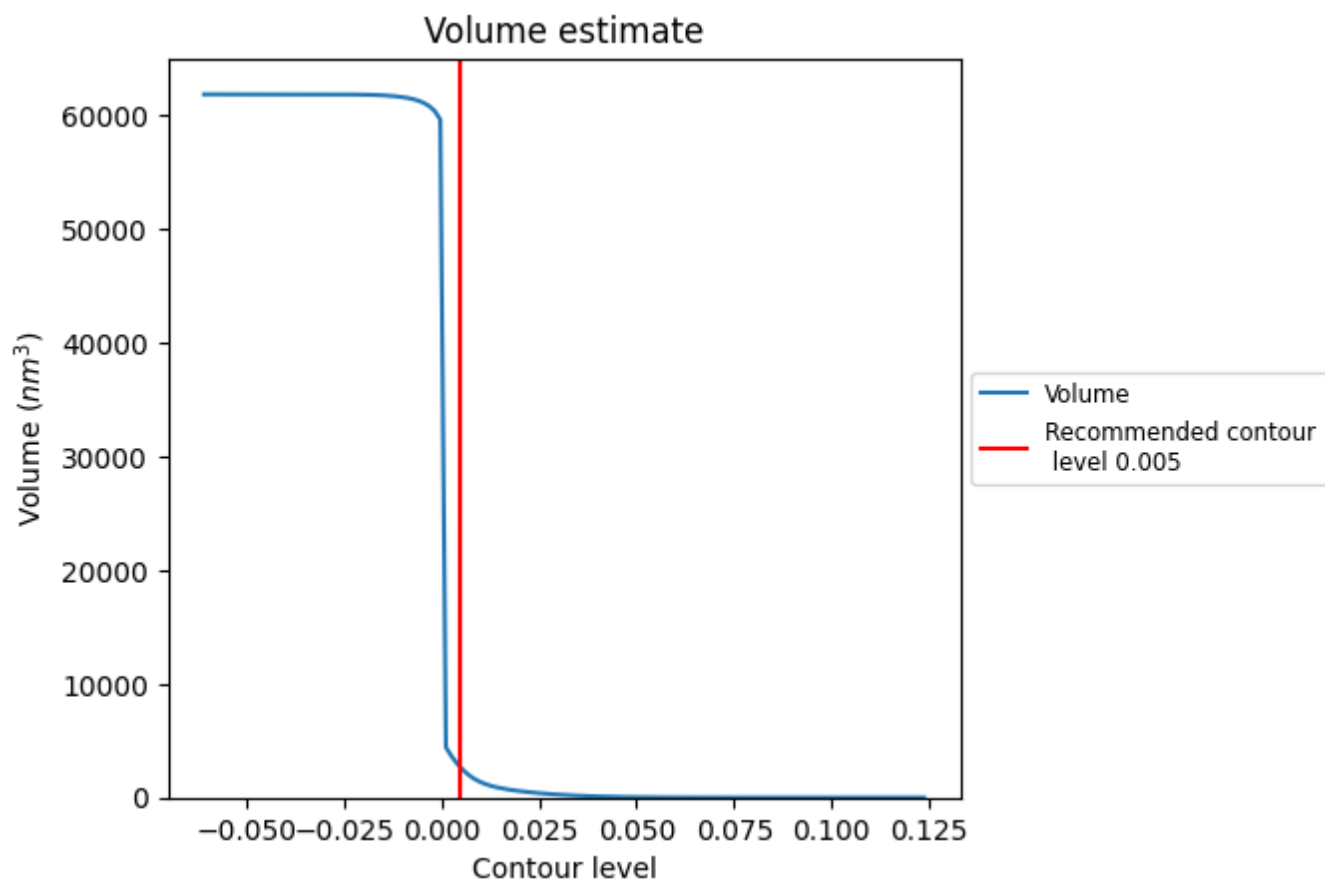
This section contains the results of statistical analysis of the map.

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.

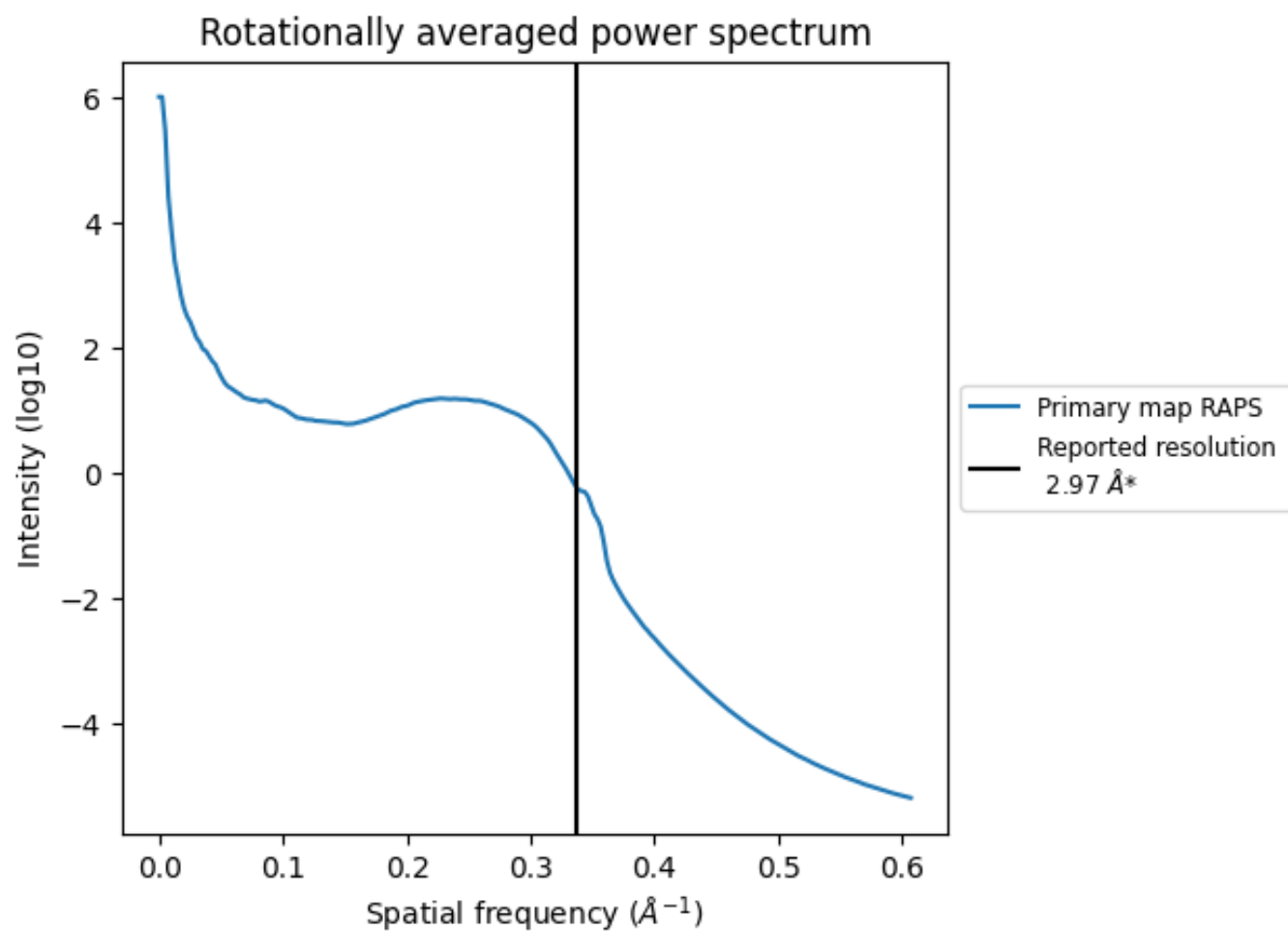
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2631 nm^3 ; this corresponds to an approximate mass of 2376 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 0.337 Å⁻¹

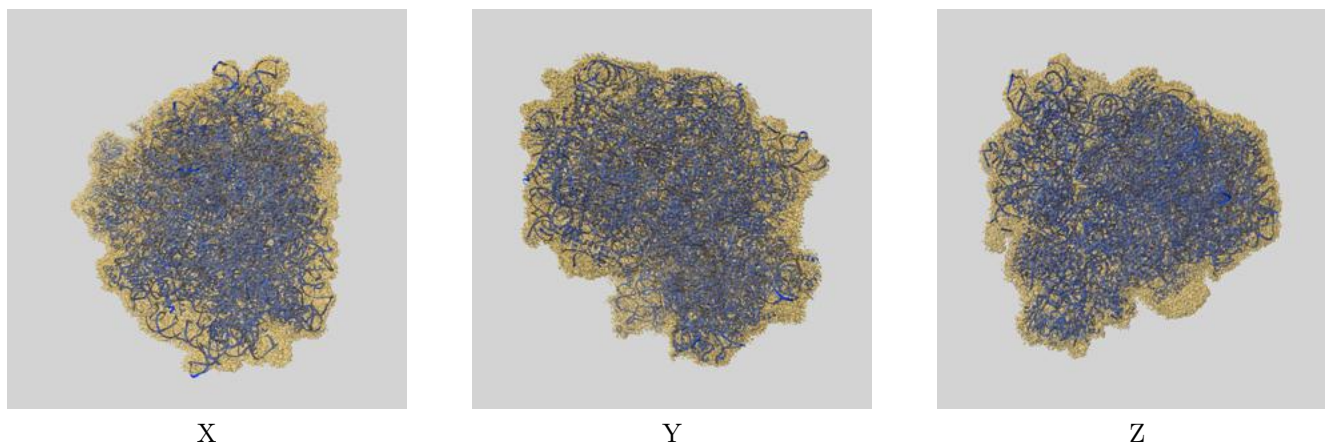
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

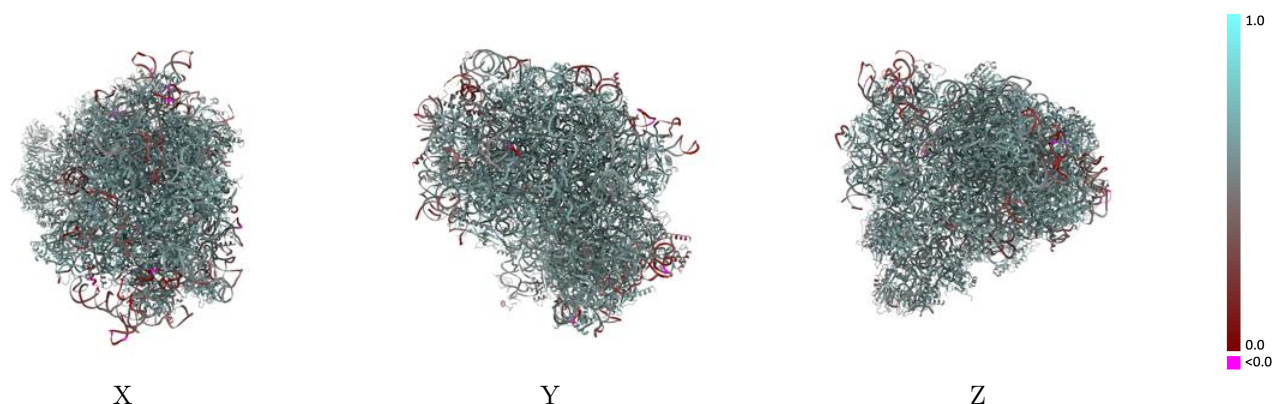
This section contains information regarding the fit between EMDB map EMD-54267 and PDB model 9RU9. Per-residue inclusion information can be found in section [3](#) on page [28](#).

9.1 Map-model overlay [i](#)



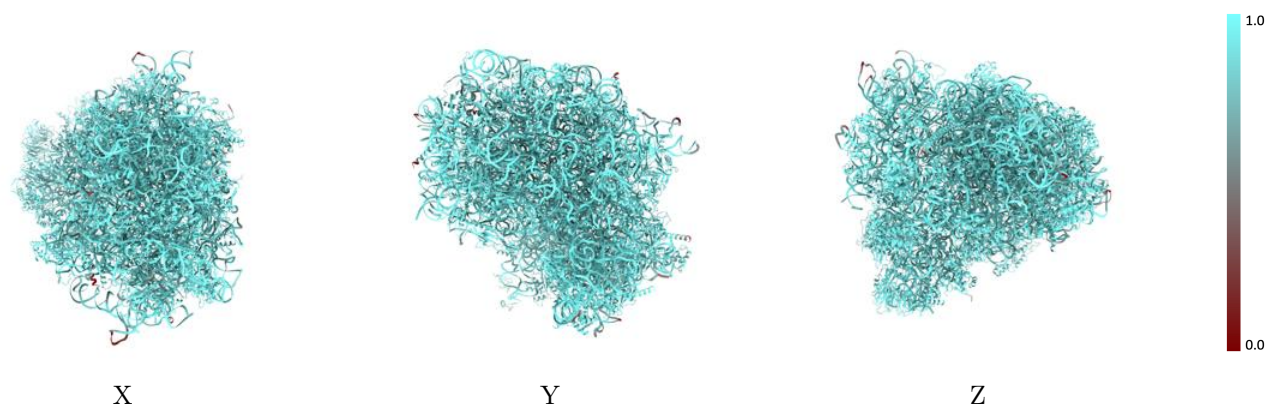
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



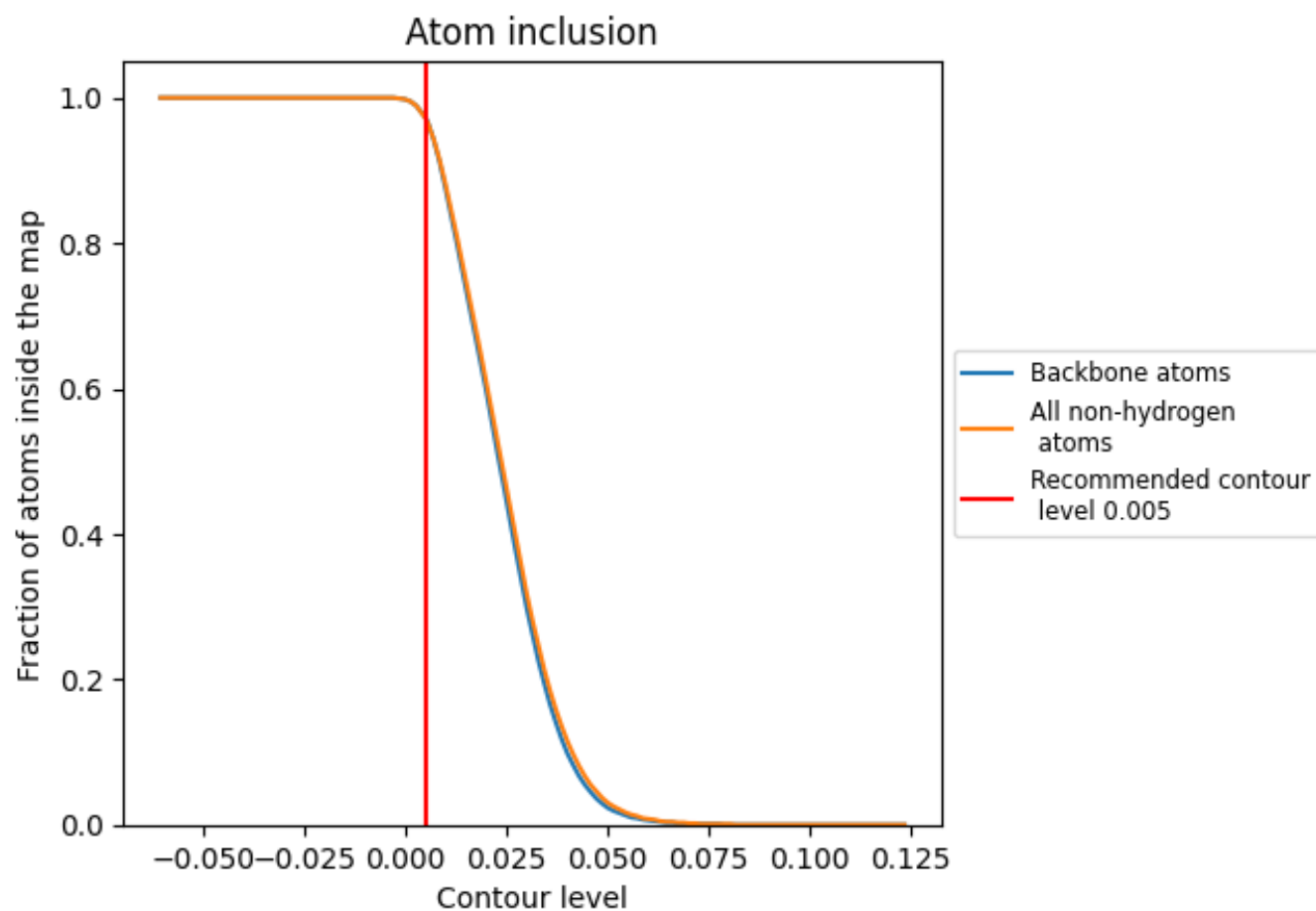
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 97% of all backbone atoms, 97% 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	 0.9710	 0.5650
A	 1.0000	 0.7620
C	 1.0000	 0.7760
D	 1.0000	 0.7260
Et	 0.8770	 0.2960
L5	 0.9710	 0.5520
L7	 0.9930	 0.5930
L8	 0.9860	 0.5690
LA	 0.9960	 0.6190
LB	 0.9900	 0.6130
LC	 0.9720	 0.6010
LD	 0.9710	 0.5870
LE	 0.9720	 0.5740
LF	 0.9890	 0.6070
LG	 0.9380	 0.5550
LH	 0.9830	 0.6030
LI	 0.9830	 0.6100
LJ	 0.9750	 0.5830
LL	 0.9750	 0.5850
LM	 0.9800	 0.5940
LN	 0.9960	 0.6230
LO	 0.9880	 0.6100
LP	 0.9880	 0.6080
LQ	 0.9910	 0.6150
LR	 0.9650	 0.5760
LS	 0.9940	 0.6160
LT	 0.9870	 0.5970
LU	 0.9710	 0.5460
LV	 0.9960	 0.6130
LW	 0.9960	 0.6150
LX	 0.9900	 0.5990
LY	 0.9890	 0.6130
LZ	 0.9830	 0.5910
La	 0.9940	 0.6180
Lb	 0.9070	 0.5270





















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Chain	Atom inclusion	Q-score
Lc	 0.9920	 0.5940
Ld	 0.9920	 0.5840
Le	 0.9940	 0.6150
Lf	 0.9940	 0.6240
Lg	 0.9920	 0.6000
Lh	 0.9790	 0.6020
Li	 0.9710	 0.5820
Lj	 0.9970	 0.6150
Lk	 0.9780	 0.5700
Ll	 0.9950	 0.6080
Lm	 0.9860	 0.5940
Ln	 0.9950	 0.5800
Lo	 0.9860	 0.6070
Lp	 0.9930	 0.6040
Lr	 0.9850	 0.6100
Pt	 0.9200	 0.4720
S2	 0.9700	 0.5510
SA	 0.9720	 0.5860
SB	 0.9830	 0.5870
SC	 0.9770	 0.5950
SD	 0.9400	 0.5480
SE	 0.9780	 0.5930
SF	 0.9740	 0.5790
SG	 0.9640	 0.5490
SH	 0.9310	 0.5370
SI	 0.9660	 0.5680
SJ	 0.9660	 0.5880
SK	 0.9430	 0.5400
SL	 0.9830	 0.5990
SM	 0.7800	 0.3940
SN	 0.9860	 0.5910
SO	 0.9810	 0.5920
SP	 0.9500	 0.5460
SQ	 0.9710	 0.5830
SR	 0.9200	 0.5470
SS	 0.9680	 0.5670
ST	 0.9780	 0.5800
SU	 0.9440	 0.5380
SV	 0.9660	 0.5820
SW	 0.9800	 0.6030
SX	 0.9900	 0.5990
SY	 0.9750	 0.5790

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Chain	Atom inclusion	Q-score
SZ	 0.9520	 0.5560
Sa	 0.9770	 0.5840
Sb	 0.9590	 0.5620
Sc	 0.9660	 0.5780
Sd	 0.9860	 0.5980
Se	 0.9750	 0.5780
Sf	 0.8510	 0.4260
Sg	 0.9150	 0.5300
mR	 0.8790	 0.4760