



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2026 – 10:17 AM JST

PDB ID : 9VXN / pdb_00009vxn
EMDB ID : EMD-65434
Title : Human cytosolic ribosome in a rotated state, with multiple neomycin molecules bound, featuring A/P-site and P/E-site tRNAs
Authors : Zhu, L.; Jia, C.; Wu, M.; Li, W.
Deposited on : 2025-07-19
Resolution : 2.51 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:

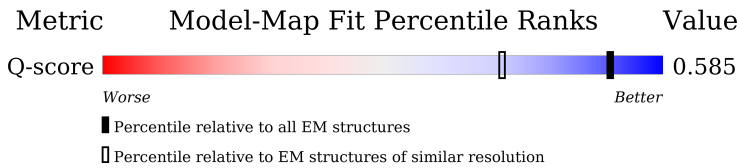
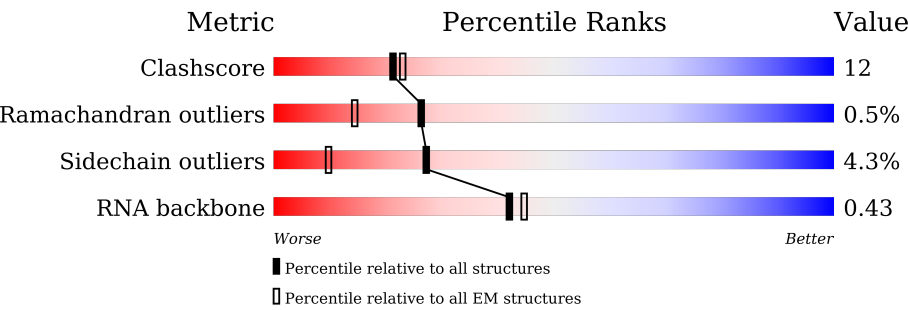
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.51 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.



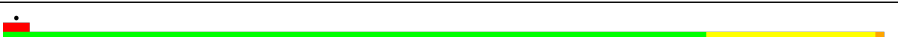
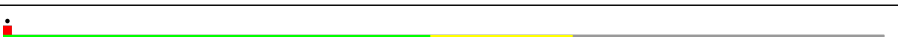
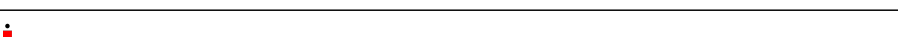
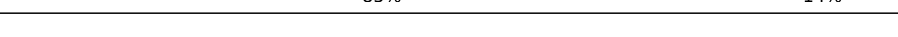
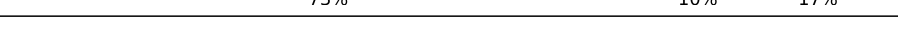
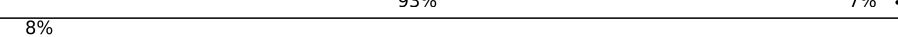
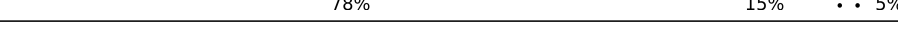
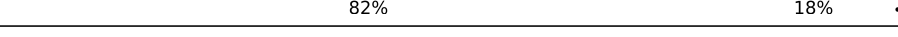
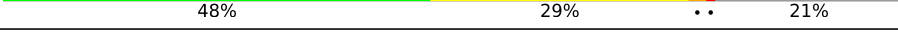
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7159 (2.01 - 3.01)

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	L5	5069	5% 37% 24% 10% 28%
2	L7	120	74% 22%
3	L8	157	57% 32% 11%

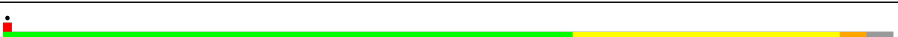
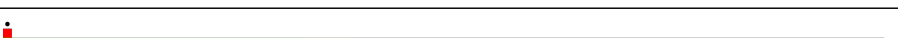
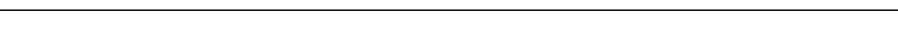
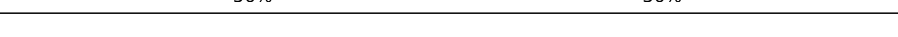
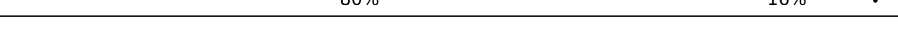
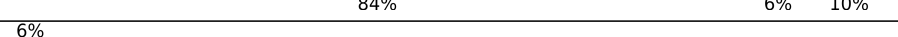
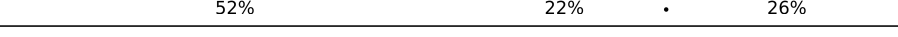
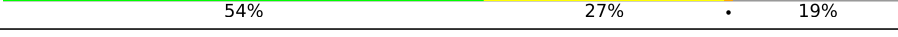
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Mol	Chain	Length	Quality of chain
4	LA	257	
5	LB	403	
6	LC	368	
7	LD	294	
8	LE	288	
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	

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Mol	Chain	Length	Quality of chain
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	S2	1869	
47	SA	295	
48	SB	264	
49	SC	293	
50	SD	243	
51	SE	263	
52	SF	204	
53	SG	249	

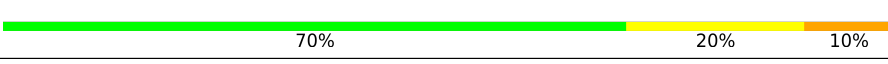
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Mol	Chain	Length	Quality of chain
54	SH	194	
55	SI	208	
56	SJ	194	
57	SK	165	
58	SL	158	
59	SM	132	
60	SN	151	
61	SO	151	
62	SP	145	
63	SQ	146	
64	SR	135	
65	SS	152	
66	ST	145	
67	SU	119	
68	SV	83	
69	SW	130	
70	SX	143	
71	SY	133	
72	SZ	125	
73	Sa	115	
74	Sb	84	
75	Sc	69	
76	Sd	56	
77	Se	133	
78	Sf	156	

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Mol	Chain	Length	Quality of chain
79	Sg	317	
80	u	76	
81	v	76	
82	w	10	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 217115 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3651	Total	C	N	O	P	0	0
			78335	34920	14322	25443	3650		

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L8	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 9 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 10 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 12 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	213	Total	C	N	O	S	0	0
			1713	1083	329	285	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	49	CYS	GLY	conflict	UNP Q96L21

- Molecule 13 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 17 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 22 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	100	Total	C	N	O	S	0	0
			813	510	163	136	4		

- Molecule 26 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 27 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	132	Total	C	N	O	S	0	0
			1102	692	223	184	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	La	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	99	Total	C	N	O	S	0	0
			808	502	177	125	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ld	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 33 is a protein called Large ribosomal subunit protein eL32.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lg	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Li	99	Total	C	N	O	S	0	0
			813	509	173	126	5		

- Molecule 38 is a protein called Large ribosomal subunit protein eL37.

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

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

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 41 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	51	Total	C	N	O	S	0	0
			419	260	88	65	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 43 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	102	Total	C	N	O	S	1	0
			842	527	174	135	6		

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

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

- Molecule 45 is a protein called Large ribosomal subunit protein eL28.

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

- Molecule 46 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S2	1705	Total	C	N	O	P	0	0
			36324	16236	6498	11886	1704		

- Molecule 47 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SA	219	Total	C	N	O	S	0	0
			1727	1096	302	320	9		

- Molecule 48 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SB	215	Total	C	N	O	S	0	0
			1747	1109	312	312	14		

- Molecule 49 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SC	221	Total	C	N	O	S	1	0
			1724	1115	298	301	10		

- Molecule 50 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 51 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 52 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 53 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SG	234	Total	C	N	O	S	0	0
			1903	1188	384	324	7		

- Molecule 54 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 55 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 56 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SJ	182	Total	C	N	O	S	1	0
			1520	967	306	245	2		

- Molecule 57 is a protein called Small ribosomal subunit protein eS10.

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

- Molecule 58 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SL	154	Total	C	N	O	S	0	0
			1258	802	235	215	6		

- Molecule 59 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SM	118	Total	C	N	O	S	0	0
			906	568	158	172	8		

- Molecule 60 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 61 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SO	135	Total	C	N	O	S	0	0
			1008	617	198	187	6		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 62 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SP	125	Total	C	N	O	S	0	0
			1027	653	193	174	7		

- Molecule 63 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 64 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 65 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 66 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	ST	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 67 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SU	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 68 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 69 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 70 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 71 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SY	128	Total	C	N	O	S	1	0
			1048	661	207	175	5		

- Molecule 72 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 73 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sa	102	Total	C	N	O	S	1	0
			829	517	174	133	5		

- Molecule 74 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 75 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 76 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 77 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 78 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 79 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 80 is a RNA chain called A/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	u	76	Total	C	N	O	P	0	0
			1613	720	283	535	75		

- Molecule 81 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	v	76	Total	C	N	O	P	0	0
			1618	721	287	534	76		

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	w	10	Total	C	N	O	P	0	0
			213	95	37	72	9		

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

Mol	Chain	Residues	Atoms		AltConf
83	L5	198	Total	Mg	0
			198	198	
83	L7	1	Total	Mg	0
			1	1	
83	L8	5	Total	Mg	0
			5	5	
83	LI	1	Total	Mg	0
			1	1	
83	LN	1	Total	Mg	0
			1	1	
83	LP	1	Total	Mg	0
			1	1	
83	LV	1	Total	Mg	0
			1	1	
83	S2	83	Total	Mg	0
			83	83	
83	ST	1	Total	Mg	0
			1	1	

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

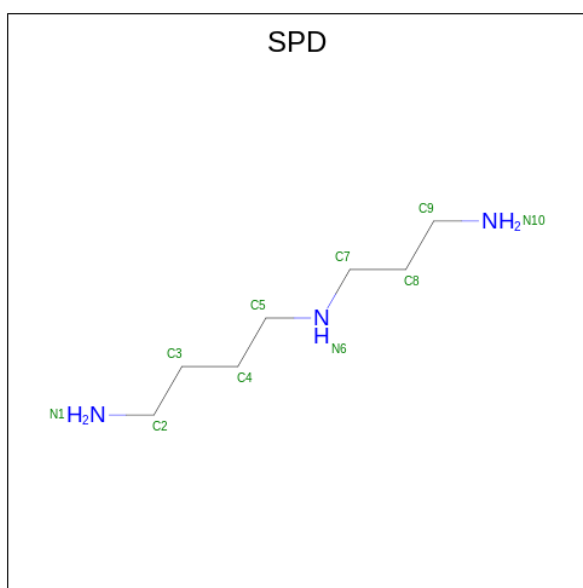
Mol	Chain	Residues	Atoms		AltConf
84	L5	78	Total	K	0
			78	78	
84	L7	1	Total	K	0
			1	1	
84	LA	1	Total	K	0
			1	1	
84	LI	1	Total	K	0
			1	1	
84	Le	1	Total	K	0
			1	1	
84	Lf	1	Total	K	0
			1	1	
84	Lg	1	Total	K	0
			1	1	
84	Lo	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
84	S2	19	Total	K	0
			19	19	
84	SO	1	Total	K	0
			1	1	
84	SS	1	Total	K	0
			1	1	
84	SX	1	Total	K	0
			1	1	
84	Sd	1	Total	K	0
			1	1	

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

- Molecule 86 is NEOMYCIN (CCD ID: NMY) (formula: $C_{23}H_{46}N_6O_{13}$) (labeled as "Ligand of Interest" by depositor).



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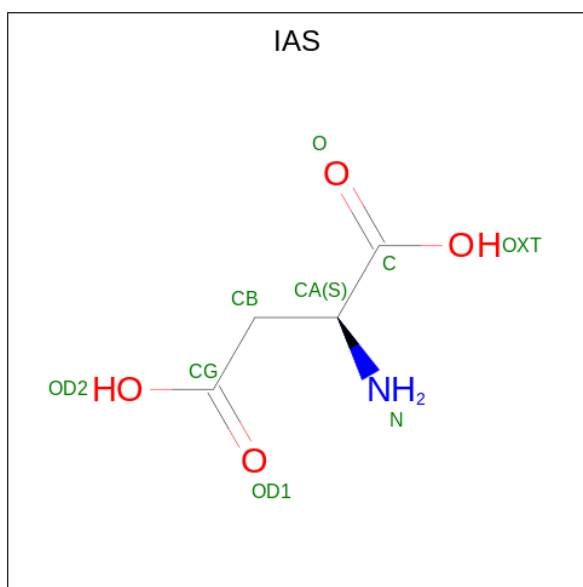
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Mol	Chain	Residues	Atoms				AltConf
86	S2	1	Total	C	N	O	0
			42	23	6	13	
86	S2	1	Total	C	N	O	0
			42	23	6	13	
86	S2	1	Total	C	N	O	0
			42	23	6	13	

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

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

- Molecule 88 is BETA-L-ASPARTIC ACID (CCD ID: IAS) (formula: C₄H₇NO₄).

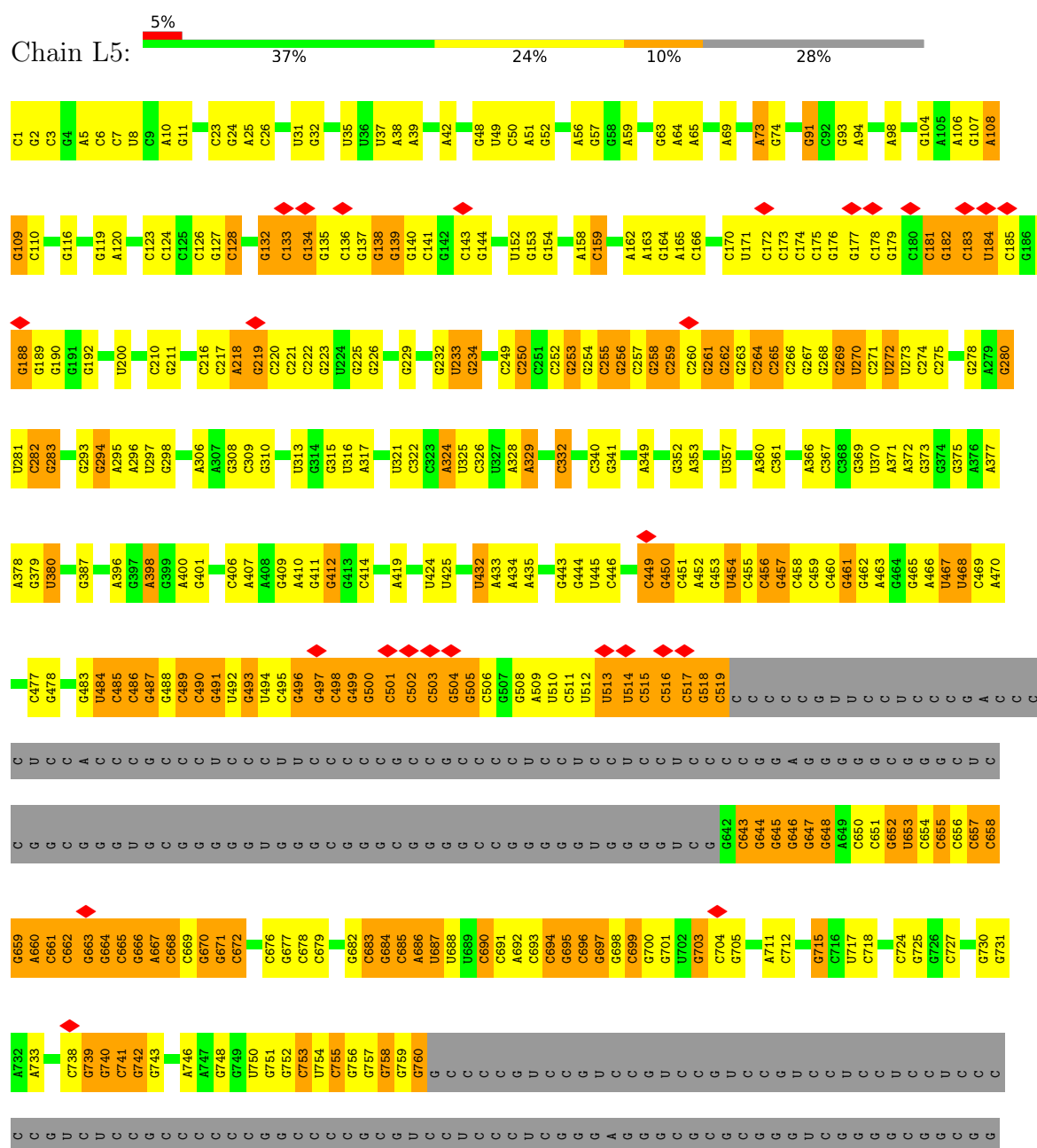


Mol	Chain	Residues	Atoms				AltConf
88	SO	1	Total	C	N	O	0
			8	4	1	3	

3 Residue-property plots

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

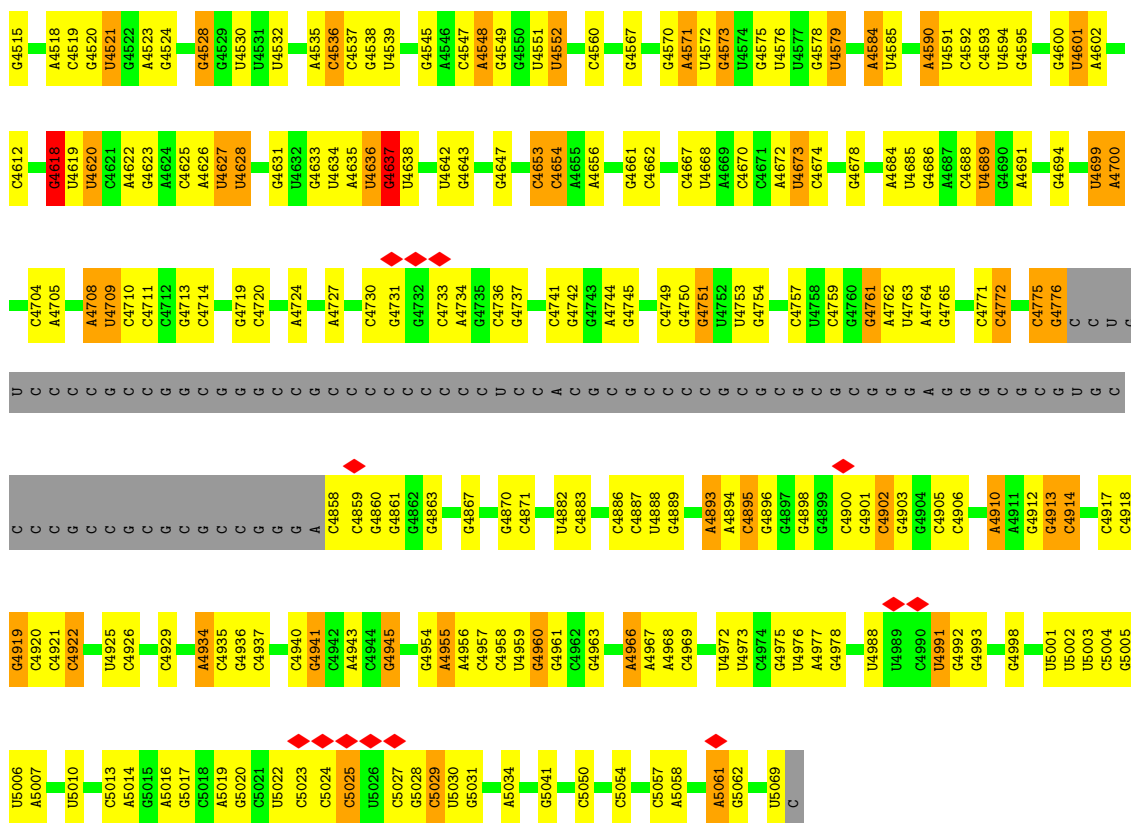
• Molecule 1: 28S rRNA



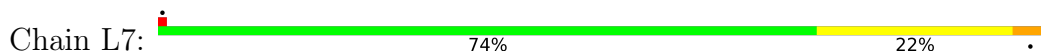




C4421	U4312	U4229	G4135	C	G3929	U3838	A3759	A3683	G
A4422	A4313	U4232	G4136	C	U3930	G3839	A3760	G3664	C
U4423	C4314	C4233	C4137	C	C3931	U3840	U3762	G3665	C
U4431	G4320	A4234	C4138	C	G3934	C3841	U3763	C3670	U
C4434	U4321	G4235	A4139	A	C3935	U3844	U3764	G3584	
U4442	G4328	G4236	C4140	G		A3845	G3765	G3585	
C4443	G4330	G4237	U4141	G	G3944	C3846	A3766	G3586	
C4444	G4331	A4239	U4142	G	A	U3847	C3767	C3587	
U4445	G4332	G4241	C4143	G	G	U3848	U3768	C3588	
U4446	C4332	C4242	C4144	C	C	A3849	C3769	G3589	
C4447	G4338	U4243	C4145	C	A	U3850	U3770	G3590	
G4448	A4339	C4244	U4146	C	U	C3851	C3771	C3591	
A4449	U4342	A4244	C4147	G	G	A3852	U3772	C3592	
U4452	U4343	G4245	C4148	G	A	U3853	U3773	C3593	
C4453	U4344	U4250	C4149	G	G	A3855	A3774	G3594	
G4454	C4345	G4251	G4150	G	A	C3857	G3775	U3595	
G4455	U4346	G4252	G4151	C	G	A3861	G3777	A3596	
U4456	U4347	G4253	C4152	G	U	A3862	C3782	C3597	
U4457	A4348	G4254	C4153	G	G	A3867	A3783	A3604	
C4458	C4349	C4255	U4163	U	A	A3868	A3784	U3709	
U4459	G4350	G4256	G4169	C	G	C3869	U3785	G3710	
U4460	U4353	C4261	A4170	G	A	G3873	C3787	A3711	
C4461	U4354	C4262	C4171	G	A	G3874	C3788	A3712	
U4463	U4355	G4263	G4172	C	U	G3875	U3789	U3713	
A4464	U4361	A4268	G4173	C	A	A3877	U3790	A3611	
U4465	G4370	U4273	U4174	C	G	C3878	G3792	C3716	
C4466	U4371	A4274	A4178	C	U	G3879	U3793	A3717	
A4467	G4373	G4275	G4179	C	G	G3880	C3794	G3614	
U4471	A4376	G4277	C4100	U	G	G3881	A3795	U3616	
G4472	G4377	U4281	C4101	C	A	U3884	U3798	G3617	
A4473	A4378	A4282	C4102	C	G	C3887	A3799	C3618	
G4475	U4379	U4283	C4103	G	C	G3888	U3801	G3619	
A4484	A4387	G4287	U4104	G	C	G3897	U3802	G3626	
U4493	C4388	U4288	A4105	C	C	G3898	A3803	G3627	
G4494	A4389	C4289	C4106	C	C	G3899	C3808	A3635	
U4498	G4391	A4292	U4107	G	G	G3900	G3809	C3636	
G4499	U4392	U4293	C4108	C	C	A3901	C3810	U3637	
U4500	C4393	G4296	G4109	C	G	A3906	G3811	G3638	
U4501	A4394	C4297	C4110	G	G	A3907	A3814	U3639	
C4502	G4400	U4298	U4111	U	C	A3908	U3815	U3640	
A4503	U4403	U4299	C4112	A	C	U3915	A3817	U3641	
C4504	U4404	A4303	U4113	A	C	U3920	U3822	A3642	
C4505	G4405	C4304	C4114	U	C	U3921	G3823	U3644	
A4507	U4507	G4305	C4115	A	C	G3922	A3824	U3645	
C4508	C4413	U4306	C4119	C	G	C3924	A3825	A3646	
U4512	A4414	G4309	G4122	A	U	U3925	A3830	A3647	
A4513	G4416	U4227	A4127	C	U	A3928		A3648	
G4514		G4228	C4130	C	C			A3652	
			C4131	C				A3653	
			C4132	C				A3656	
			C4133	C				U3657	
			C4134	C				A3662	



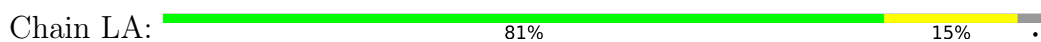
• Molecule 2: 5S rRNA

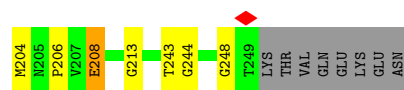


• Molecule 3: 5.8S rRNA



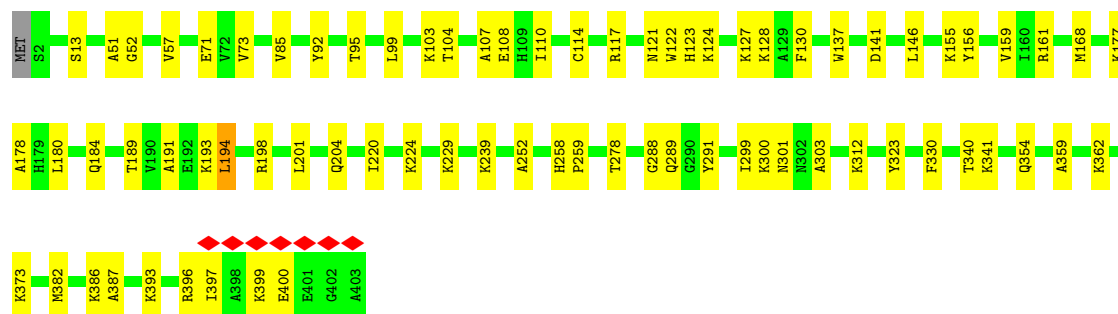
• Molecule 4: Large ribosomal subunit protein uL2





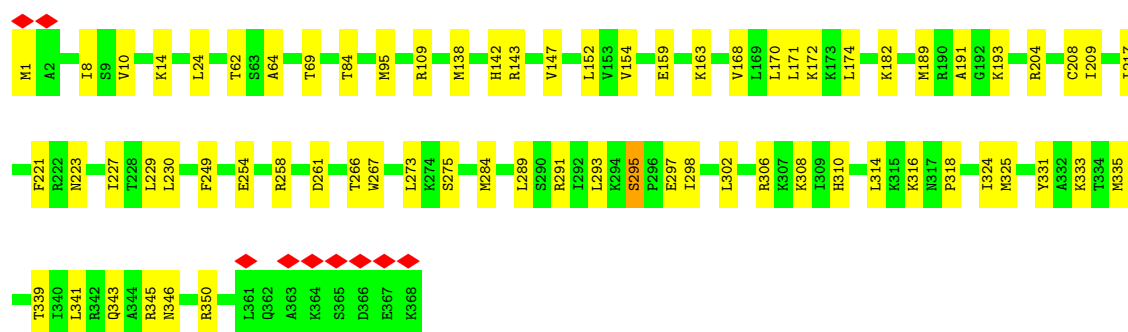
- Molecule 5: Large ribosomal subunit protein uL3

Chain LB: 81% 18%



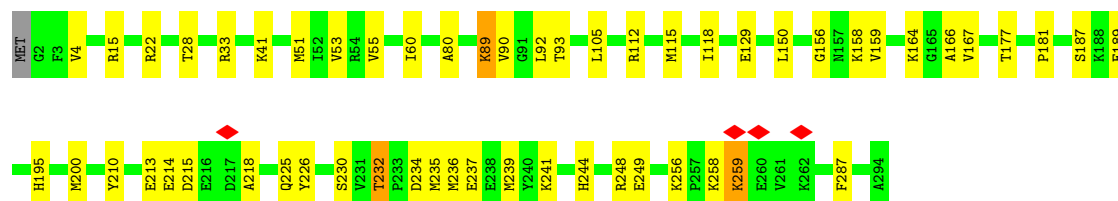
- Molecule 6: Large ribosomal subunit protein uL4

Chain LC: 81% 19%



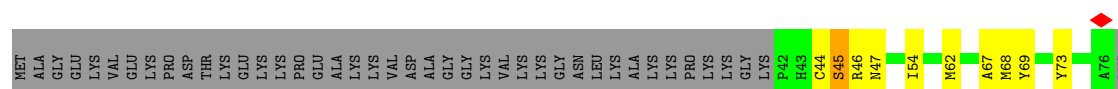
- Molecule 7: Large ribosomal subunit protein uL18

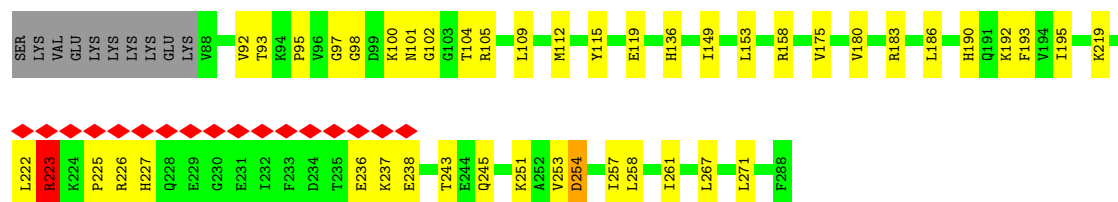
Chain LD: 81% 18%



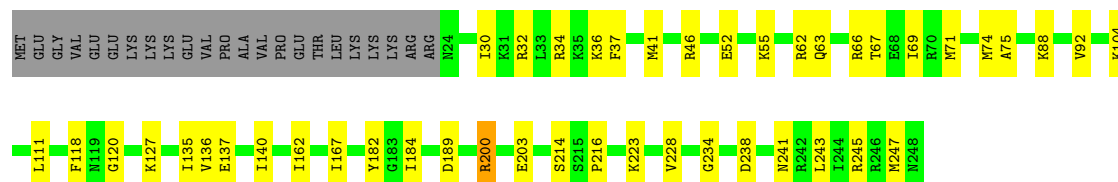
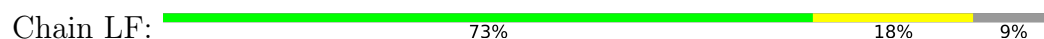
- Molecule 8: Large ribosomal subunit protein eL6

Chain LE: 6% 63% 18% 18%

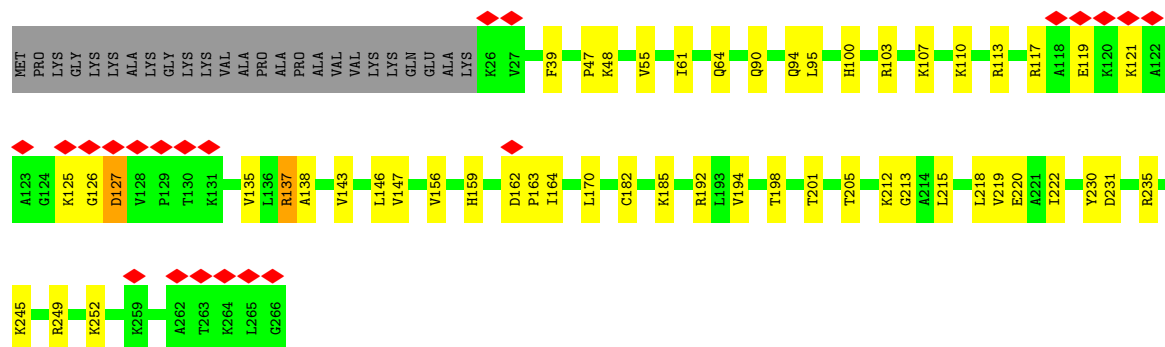




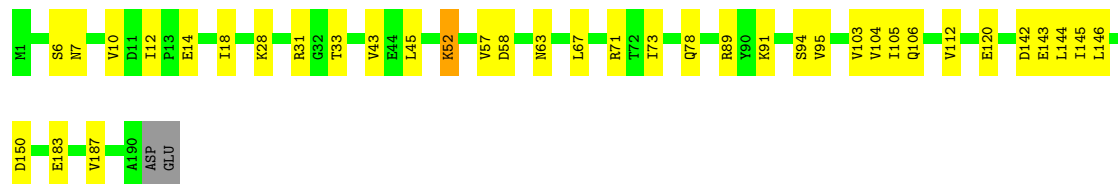
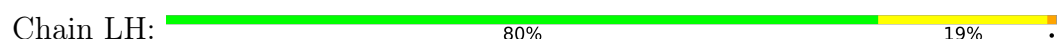
- Molecule 9: Large ribosomal subunit protein uL30



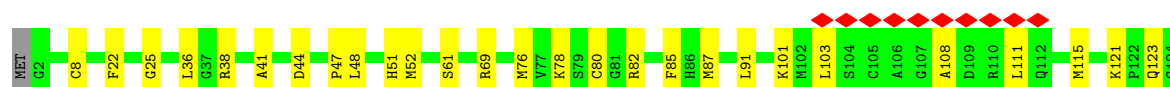
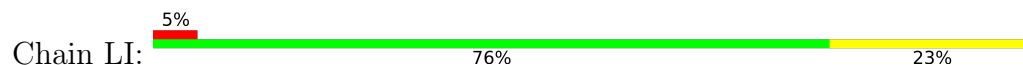
- Molecule 10: Large ribosomal subunit protein eL8

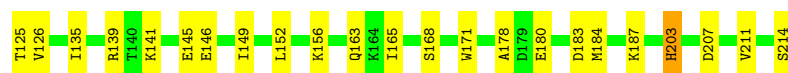


- Molecule 11: Large ribosomal subunit protein uL6

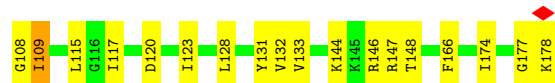
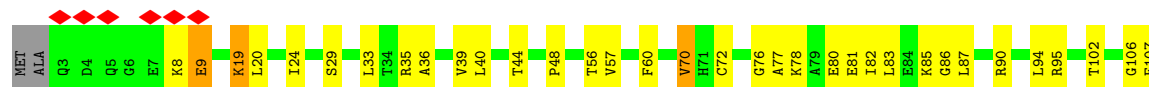


- Molecule 12: Ribosomal protein uL16-like

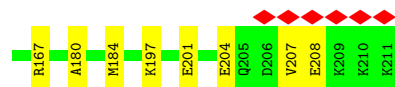
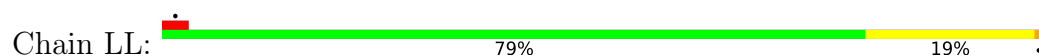




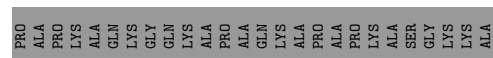
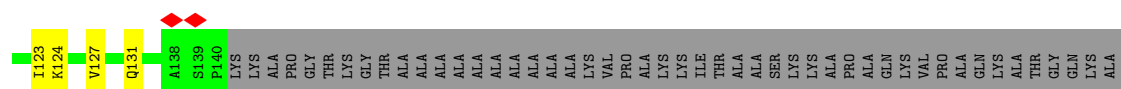
- Molecule 13: Large ribosomal subunit protein uL5



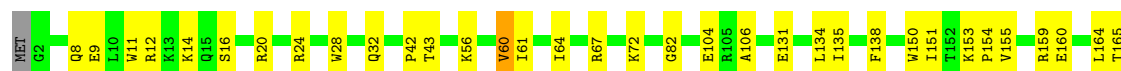
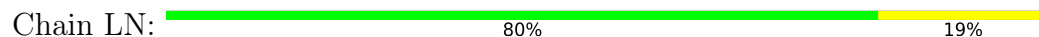
- Molecule 14: Large ribosomal subunit protein eL13



- Molecule 15: Large ribosomal subunit protein eL14



- Molecule 16: Large ribosomal subunit protein eL15



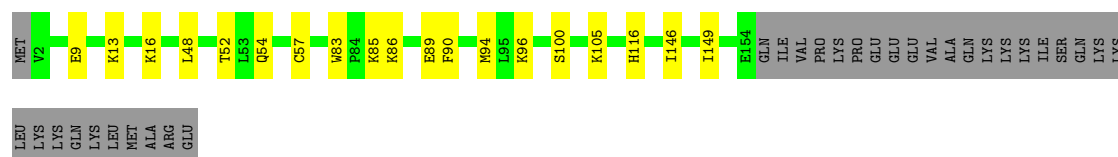
- Molecule 17: Large ribosomal subunit protein uL13

Chain LO:  85% 14%



- Molecule 18: Large ribosomal subunit protein uL22

Chain LP:  73% 10% 17%



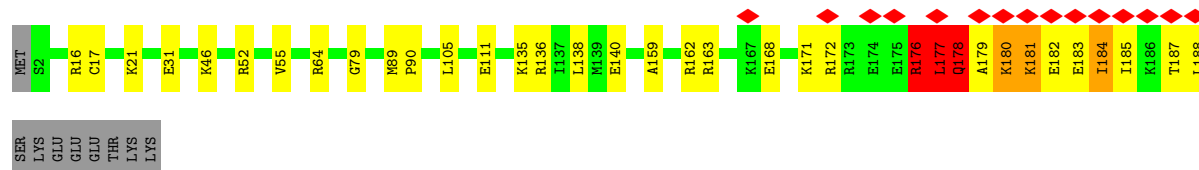
- Molecule 19: Large ribosomal subunit protein eL18

Chain LQ:  93% 7%



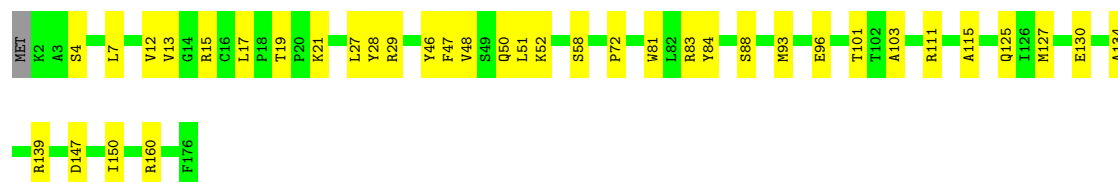
- Molecule 20: Large ribosomal subunit protein eL19

Chain LR:  8% 78% 15% 5%



- Molecule 21: Large ribosomal subunit protein eL20

Chain LS:  78% 21%



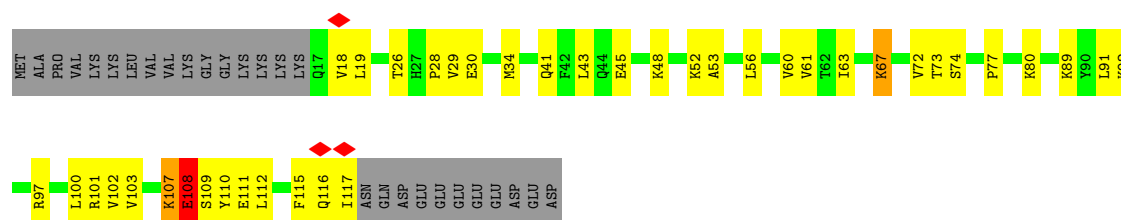
- Molecule 22: Large ribosomal subunit protein eL21

Chain LT:  82% 18%



- Molecule 23: Large ribosomal subunit protein eL22

Chain LU: 

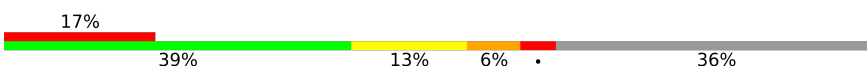


- Molecule 24: Large ribosomal subunit protein uL14

Chain LV: 



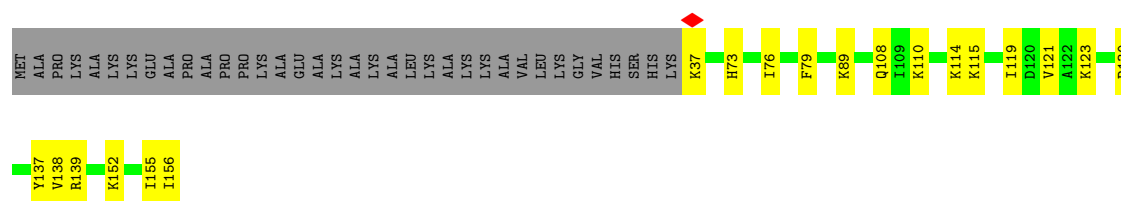
- Molecule 25: Large ribosomal subunit protein eL24

Chain LW: 



- Molecule 26: Large ribosomal subunit protein uL23

Chain LX: 



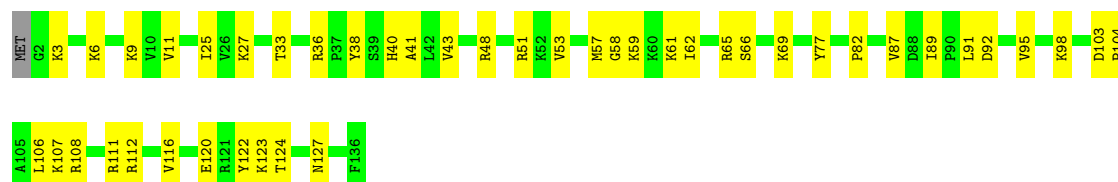
- Molecule 27: Large ribosomal subunit protein uL24

Chain LY: 



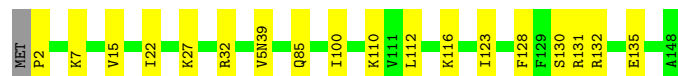
- Molecule 28: Large ribosomal subunit protein eL27

Chain LZ: 



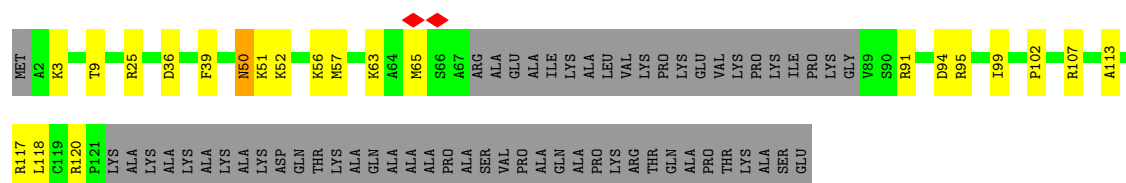
- Molecule 29: Large ribosomal subunit protein uL15

Chain La: 87% 12%



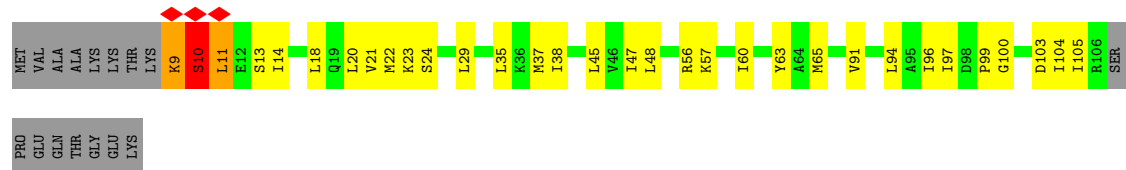
- Molecule 30: Large ribosomal subunit protein eL29

Chain Lb: 48% 13% 38%



- Molecule 31: Large ribosomal subunit protein eL30

Chain Lc: 57% 25% 15%



- Molecule 32: Large ribosomal subunit protein eL31

Chain Ld: 74% 10% 15%



- Molecule 33: Large ribosomal subunit protein eL32

Chain Le: 87% 7% 5%



- Molecule 34: Large ribosomal subunit protein eL33

Chain Lf:  89% 10%



- Molecule 35: Large ribosomal subunit protein eL34

Chain Lg:  83% 10% 7%



- Molecule 36: Large ribosomal subunit protein uL29

Chain Lh:  82% 17%



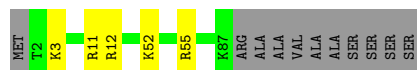
- Molecule 37: Large ribosomal subunit protein eL36

Chain Li:  80% 13% 6%



- Molecule 38: Large ribosomal subunit protein eL37

Chain Lj:  84% 5% 11%



- Molecule 39: Large ribosomal subunit protein eL38

Chain Lk:  64% 30%

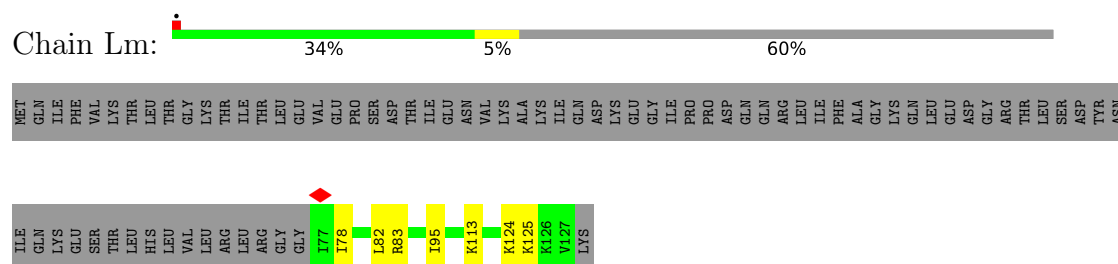


- Molecule 40: Large ribosomal subunit protein eL39

Chain Ll:  80% 18%



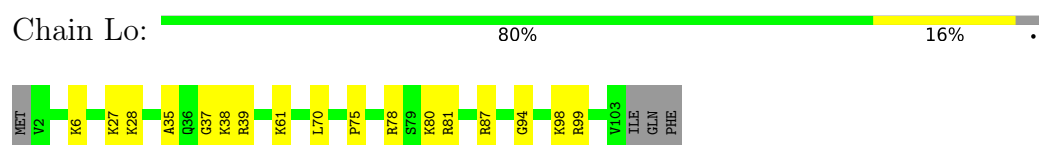
- Molecule 41: Ubiquitin-ribosomal protein eL40 fusion protein



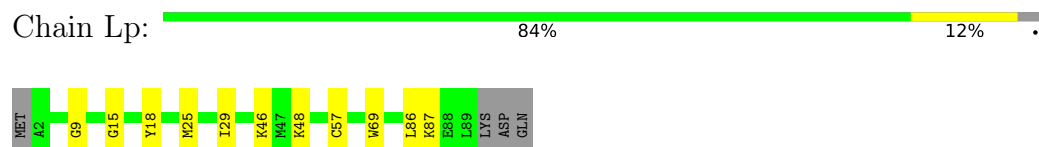
- Molecule 42: Small ribosomal subunit protein eS32



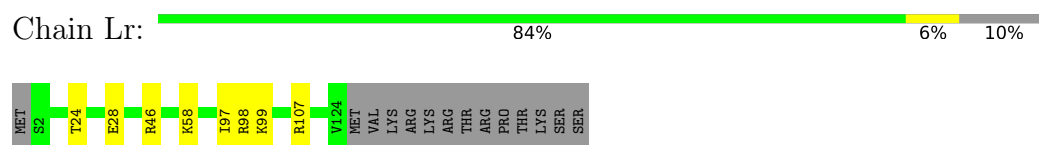
- Molecule 43: Large ribosomal subunit protein eL42



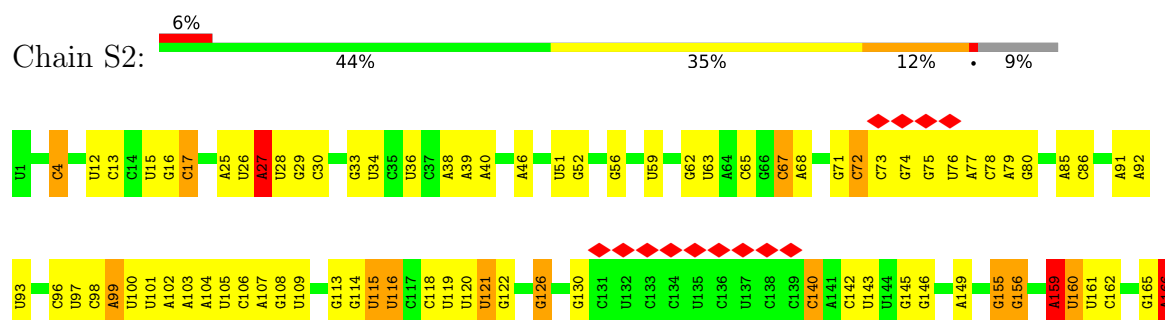
- Molecule 44: Large ribosomal subunit protein eL43

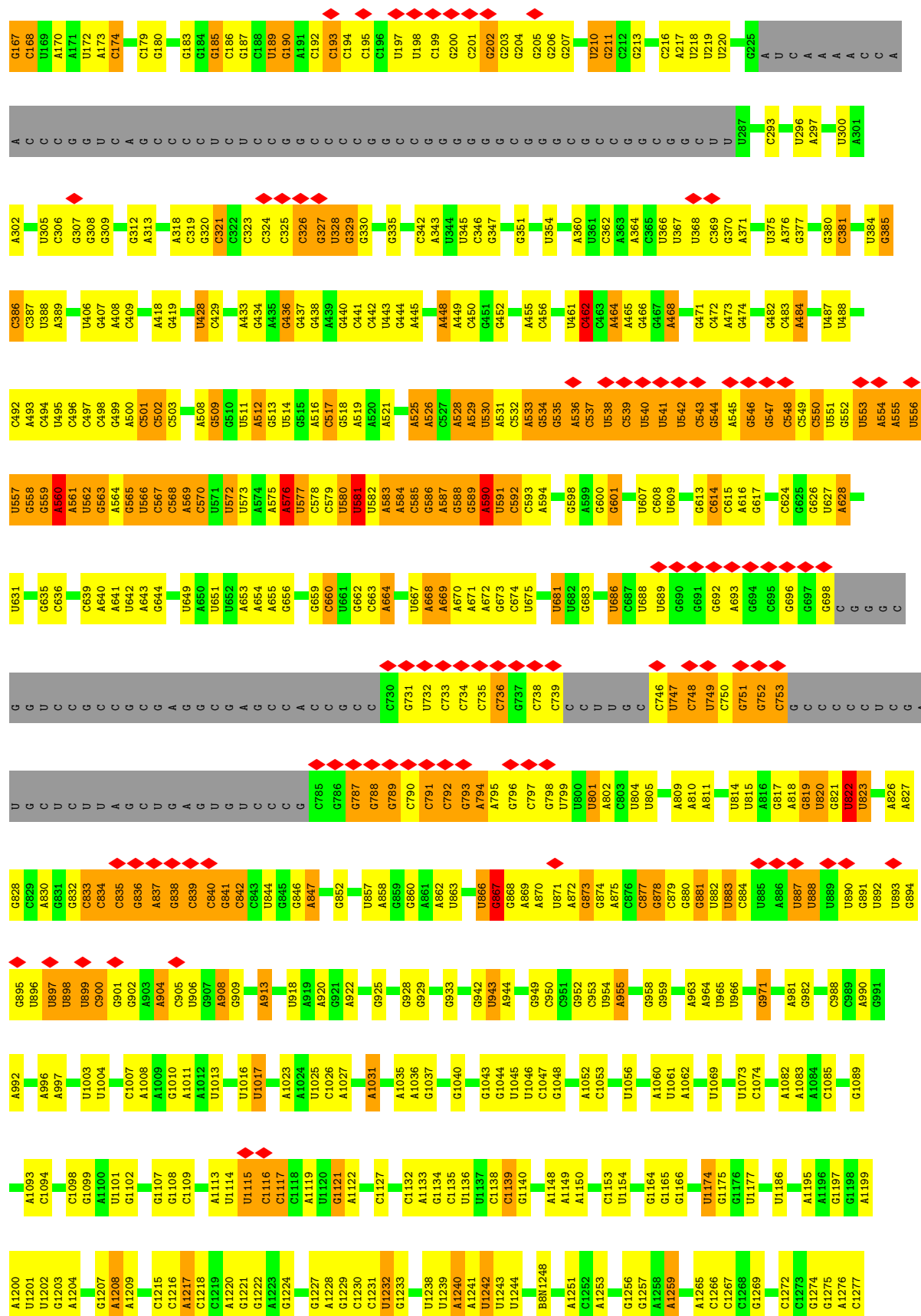


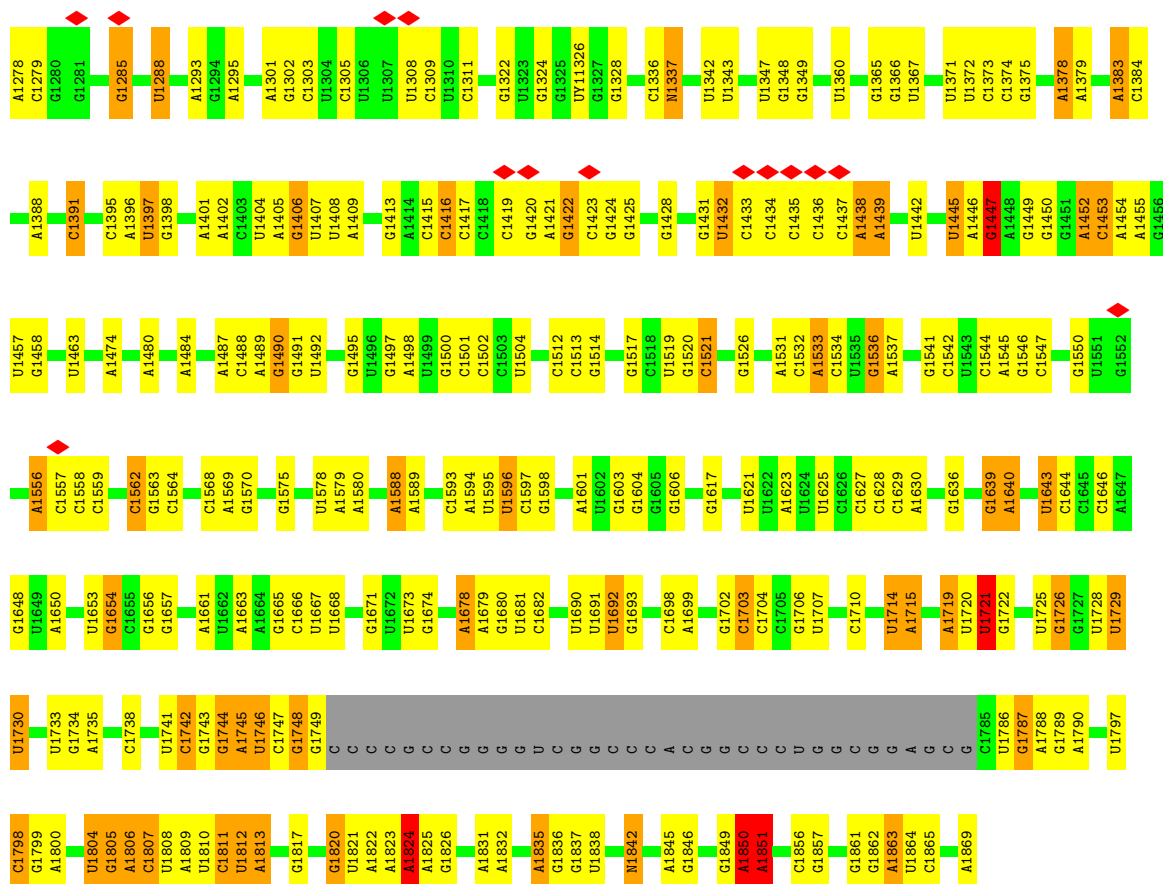
- Molecule 45: Large ribosomal subunit protein eL28



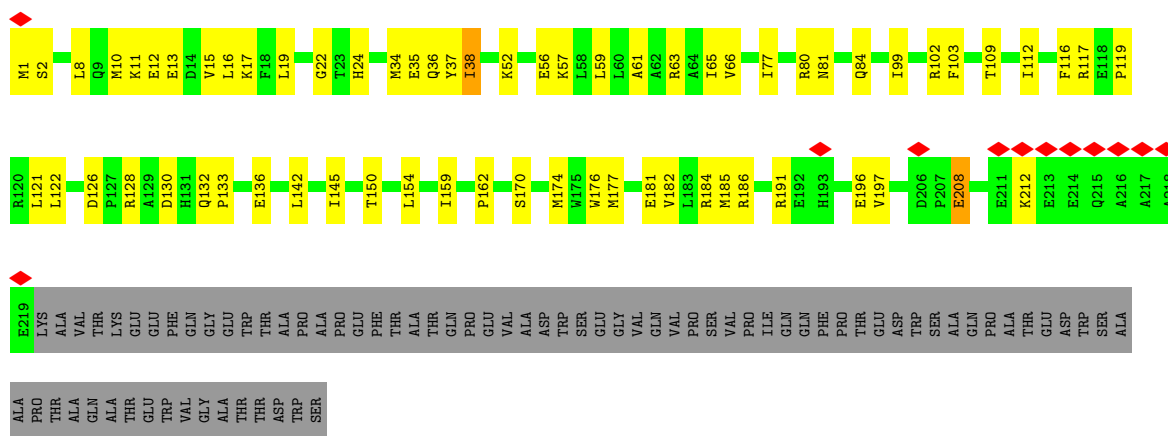
- Molecule 46: 18S rRNA





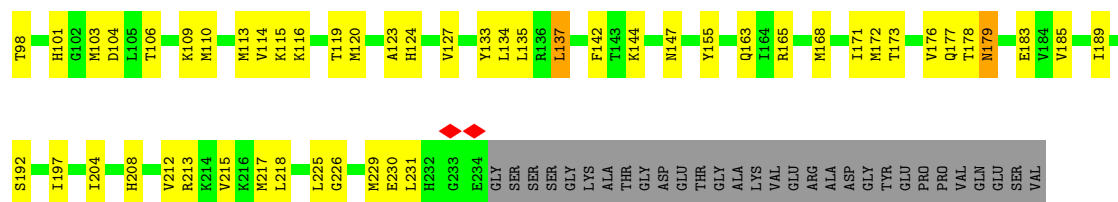


• Molecule 47: Small ribosomal subunit protein uS2

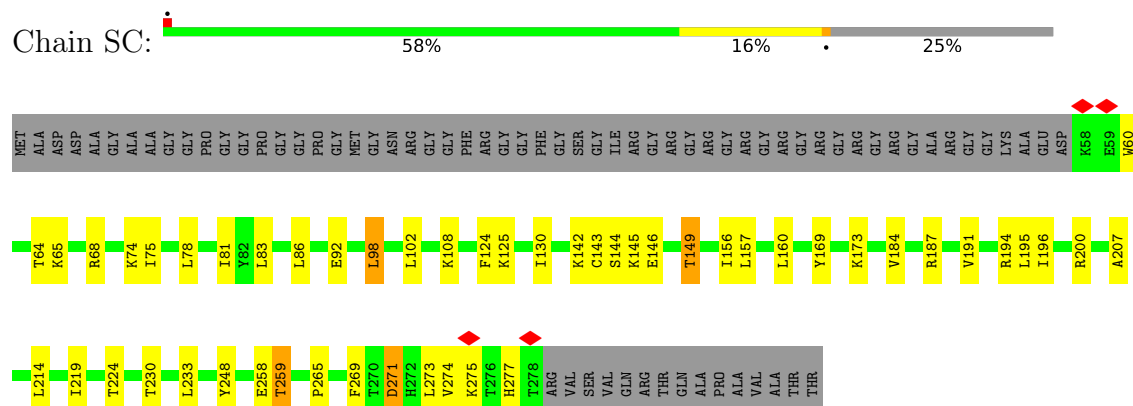


• Molecule 48: Small ribosomal subunit protein eS1

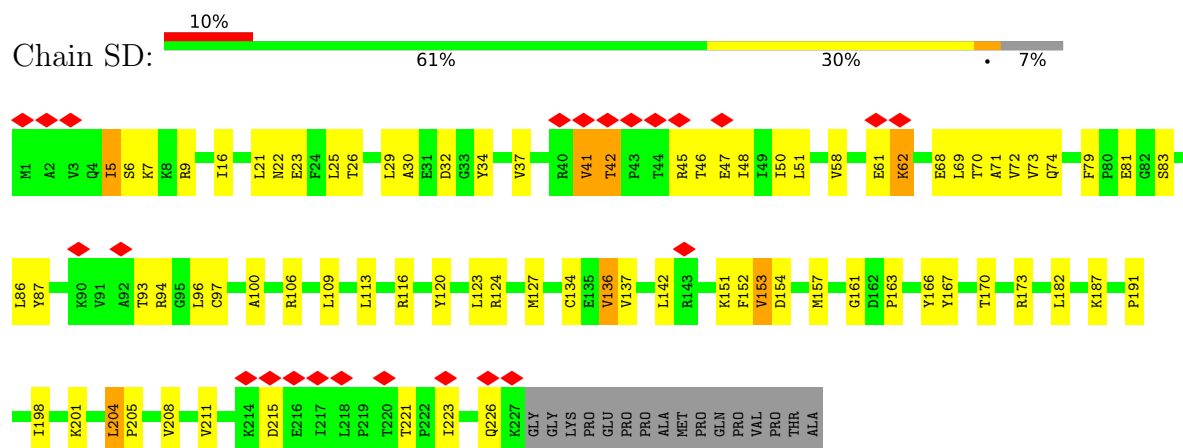




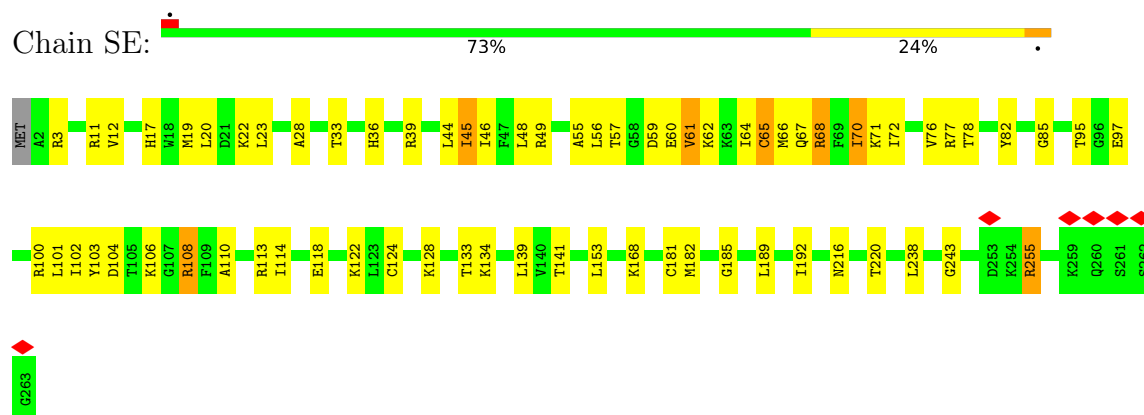
- Molecule 49: Small ribosomal subunit protein uS5



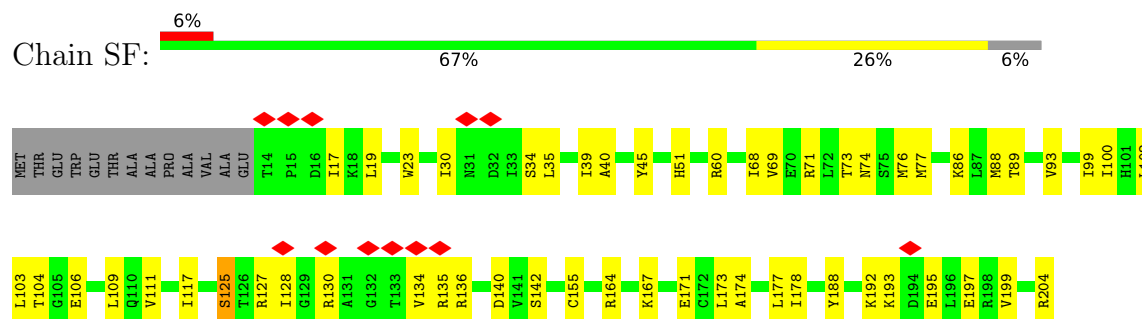
- Molecule 50: Small ribosomal subunit protein uS3



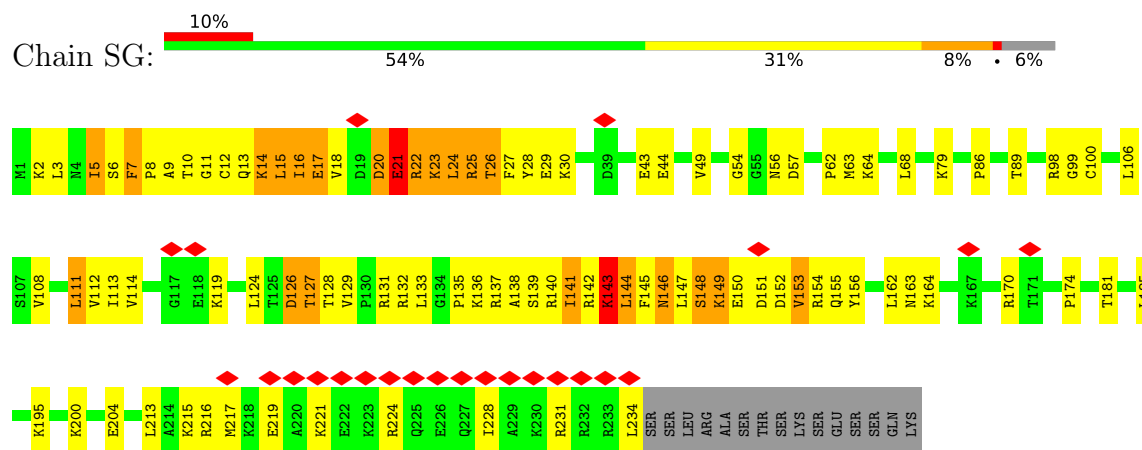
- Molecule 51: Small ribosomal subunit protein eS4, X isoform



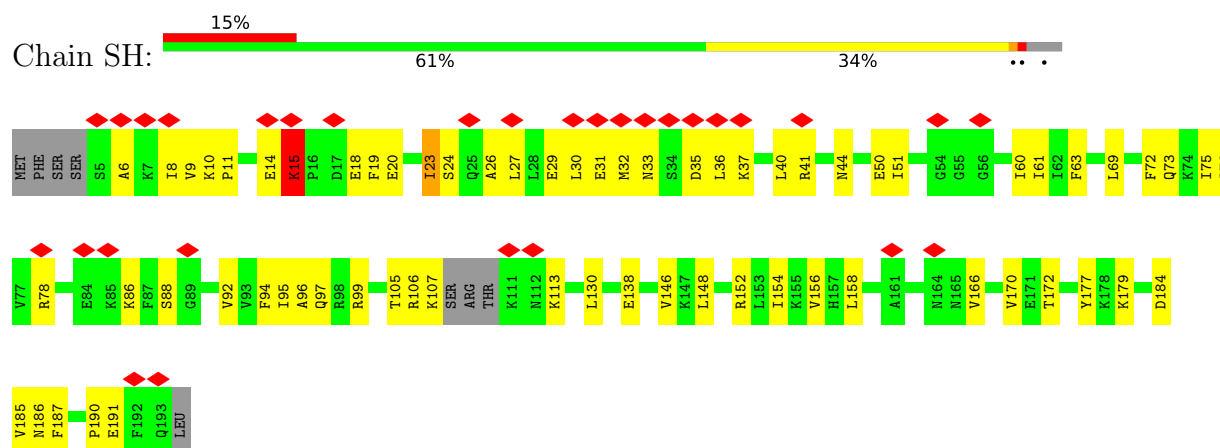
- Molecule 52: Small ribosomal subunit protein uS7



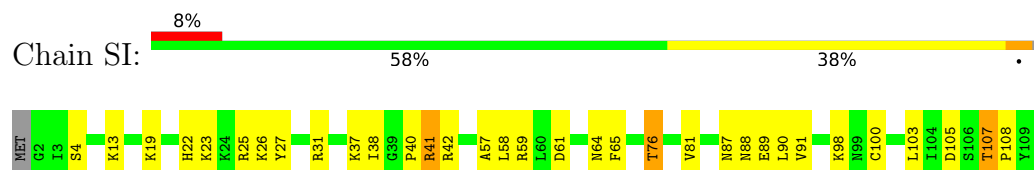
- Molecule 53: Small ribosomal subunit protein eS6

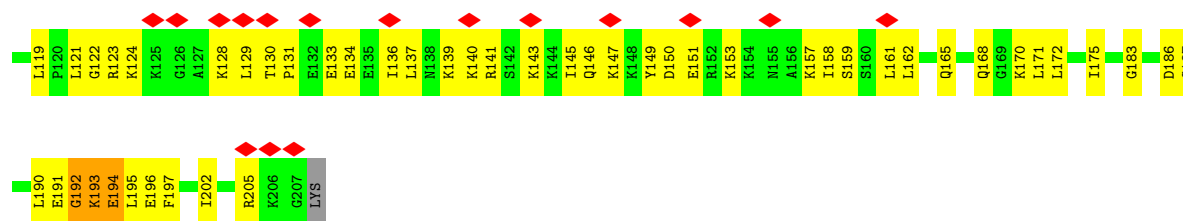


- Molecule 54: Small ribosomal subunit protein eS7

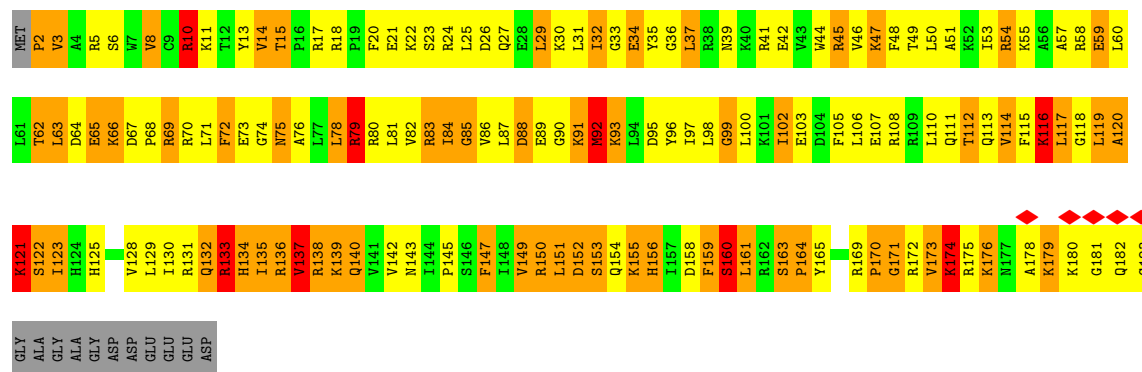
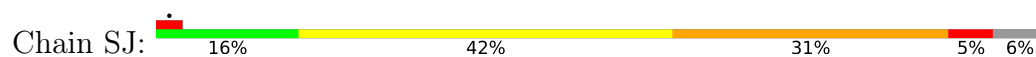


- Molecule 55: Small ribosomal subunit protein eS8

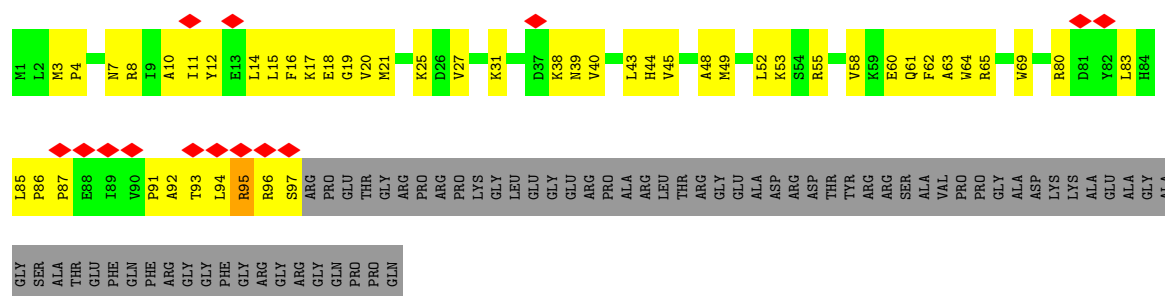
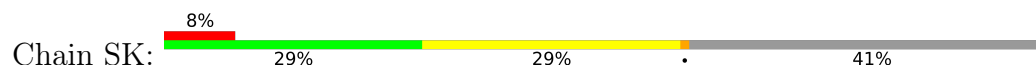




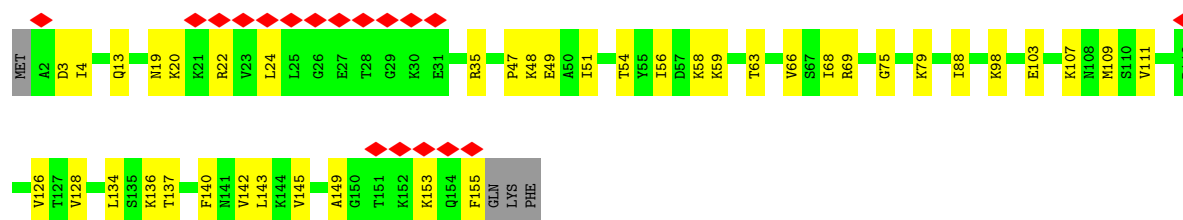
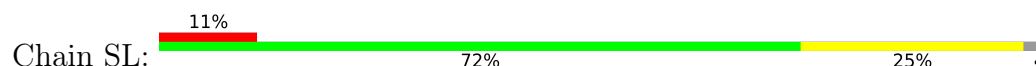
• Molecule 56: Small ribosomal subunit protein uS4



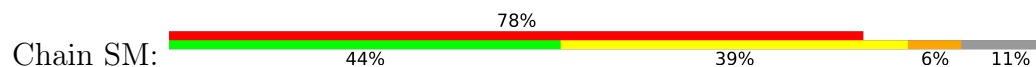
• Molecule 57: Small ribosomal subunit protein eS10



• Molecule 58: Small ribosomal subunit protein uS17

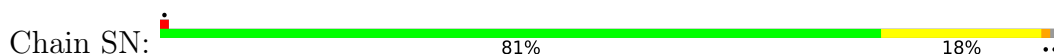


• Molecule 59: Small ribosomal subunit protein eS12

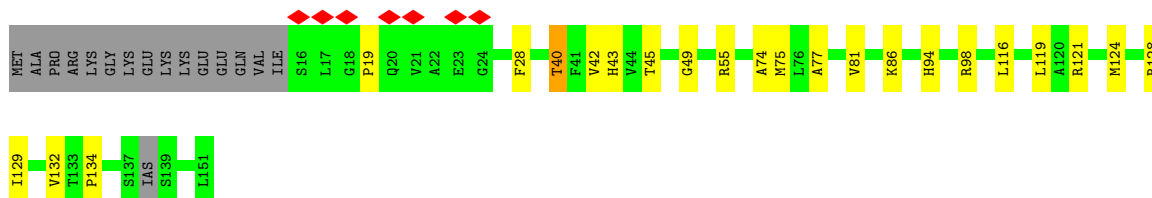
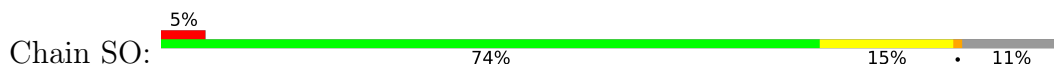




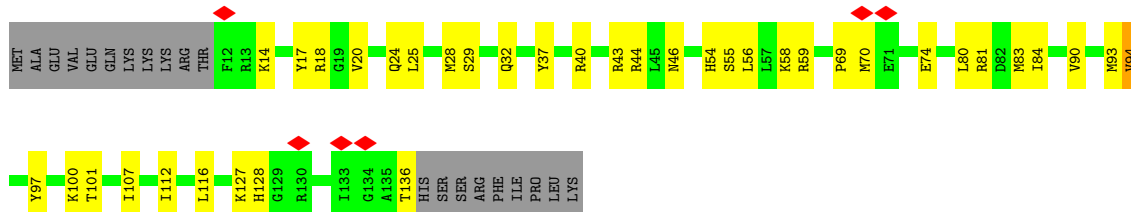
- Molecule 60: Small ribosomal subunit protein uS15



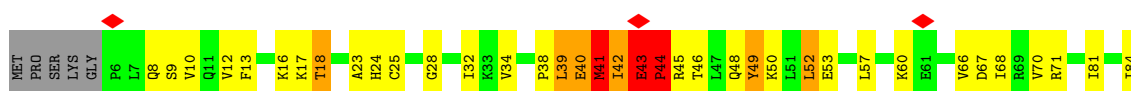
- Molecule 61: Small ribosomal subunit protein uS11

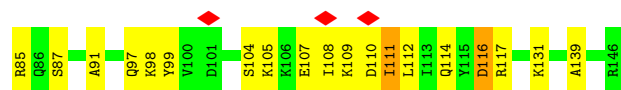


- Molecule 62: Small ribosomal subunit protein uS19

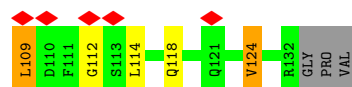


- Molecule 63: Small ribosomal subunit protein uS9

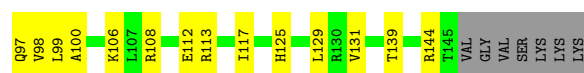




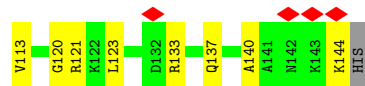
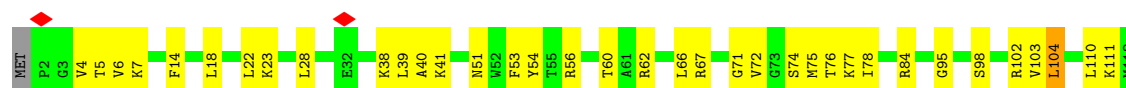
- Molecule 64: Small ribosomal subunit protein eS17



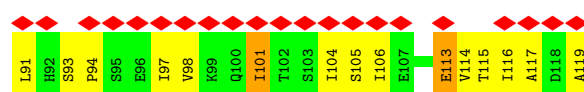
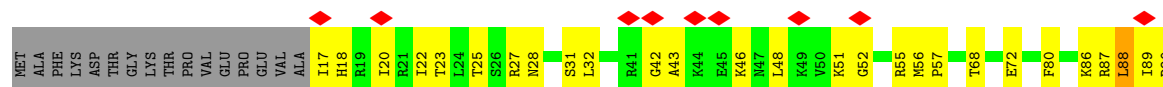
- Molecule 65: Small ribosomal subunit protein uS13



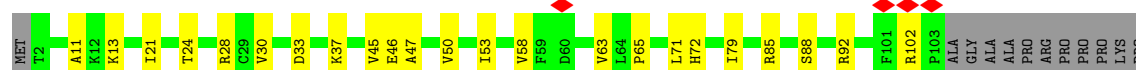
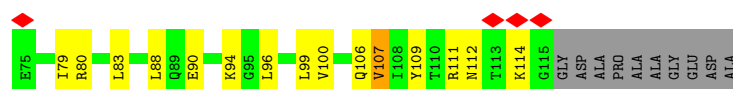
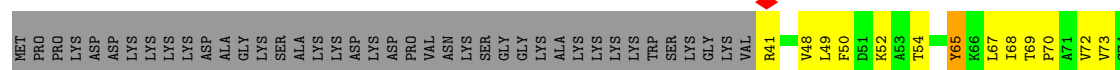
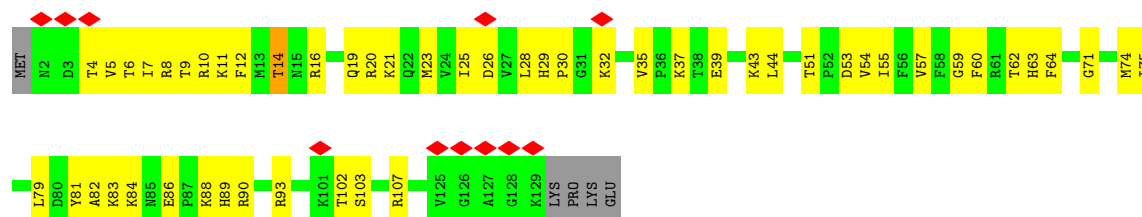
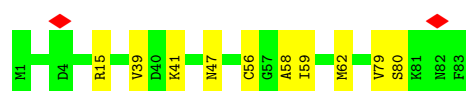
- Molecule 66: Small ribosomal subunit protein eS19



- Molecule 67: Small ribosomal subunit protein uS10



- Molecule 68: Small ribosomal subunit protein eS21



MET

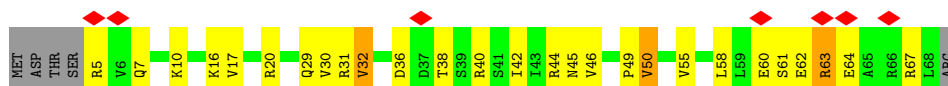
- Molecule 74: Small ribosomal subunit protein eS27

Chain Sb: 



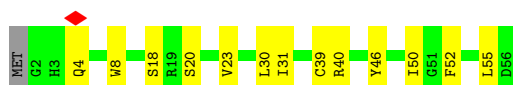
- Molecule 75: Small ribosomal subunit protein eS28

Chain Sc: 



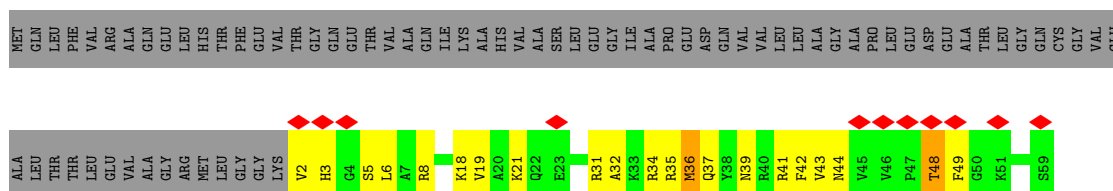
- Molecule 76: Small ribosomal subunit protein uS14

Chain Sd: 



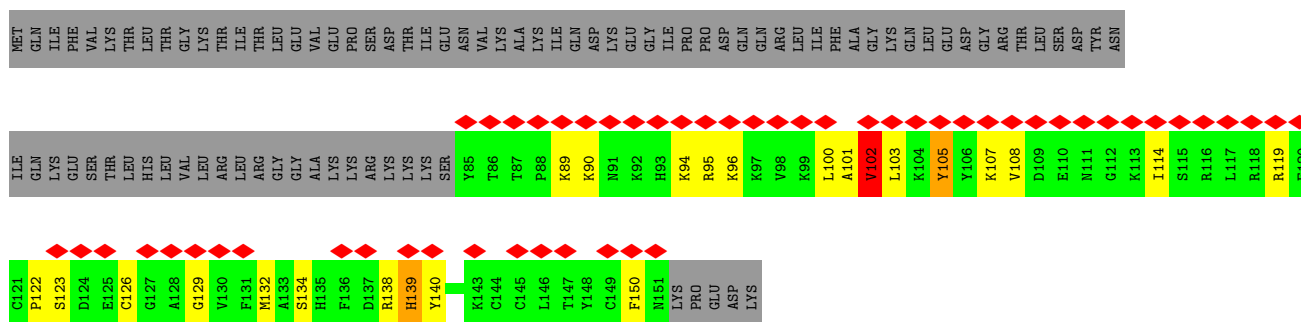
- Molecule 77: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se: 

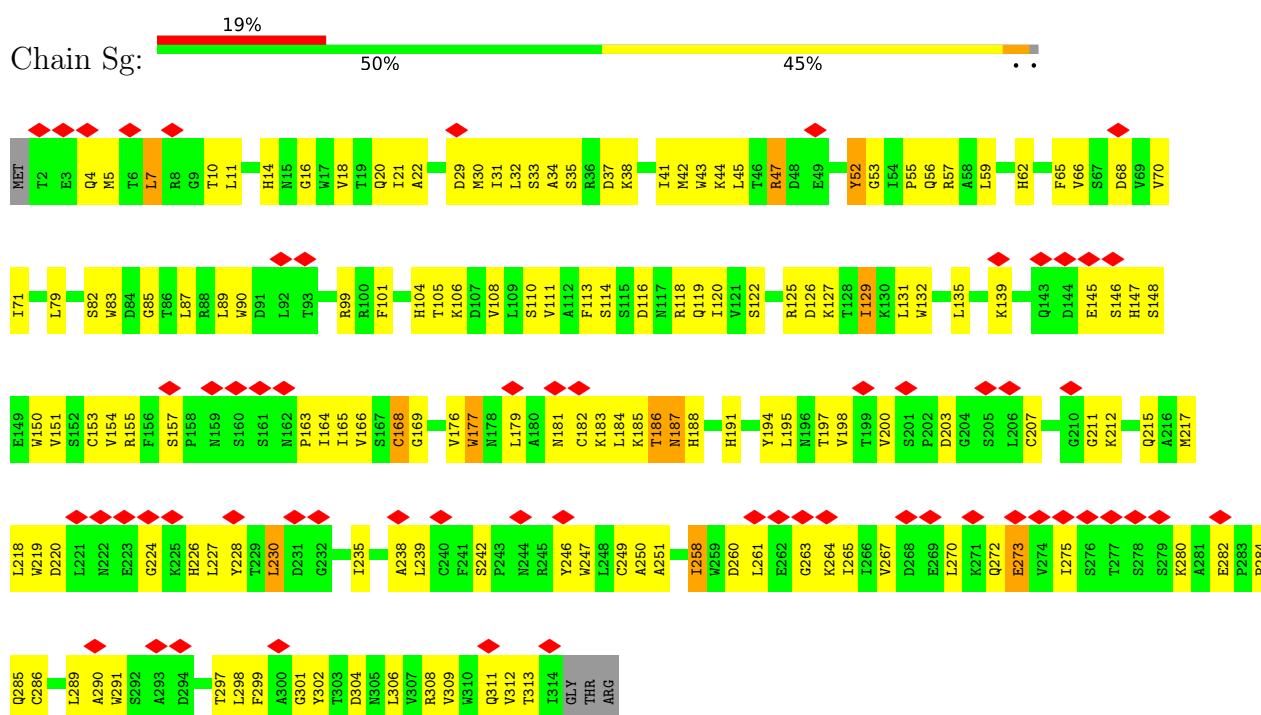


- Molecule 78: Ubiquitin

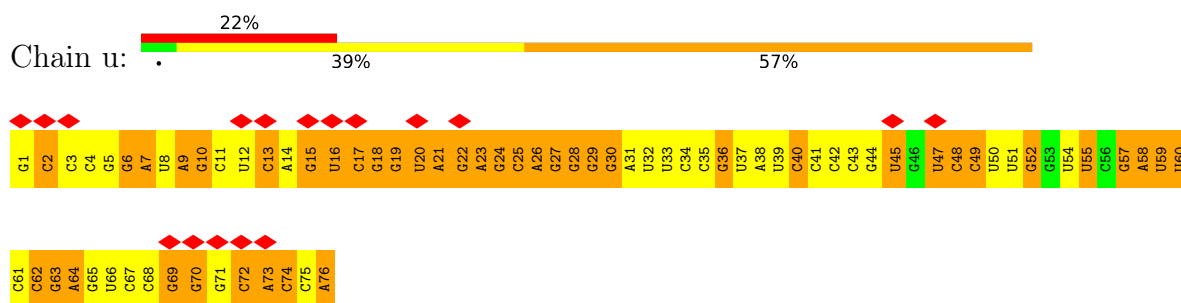
Chain Sf: 



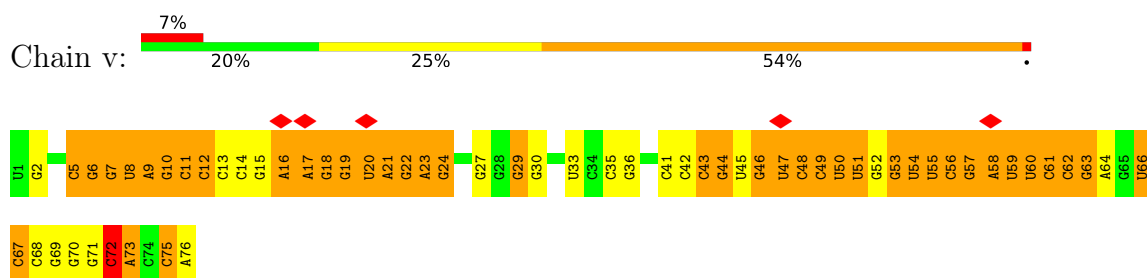
- Molecule 79: Small ribosomal subunit protein RACK1



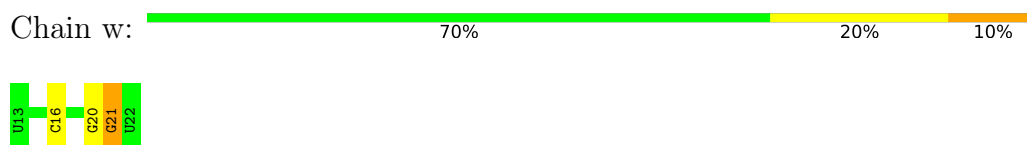
• Molecule 80: A/P-tRNA



• Molecule 81: P/E-tRNA



• Molecule 82: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104519	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	5.343	Depositor
Minimum map value	-2.542	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.136	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	552.16, 552.16, 552.16	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.812, 0.812, 0.812	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UY1, MG, HIC, 1MA, K, UR3, 6MZ, OMC, OMG, 4AC, A2M, PSU, OMU, ZN, NMY, B8N, SPD, V5N, 5MC, NMM, MA6, IAS

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	L5	0.39	1/84680 (0.0%)	0.49	15/132111 (0.0%)
2	L7	0.25	0/2858	0.27	0/4455
3	L8	0.29	0/3609	0.34	0/5623
4	LA	0.26	0/1936	0.47	0/2596
5	LB	0.24	0/3294	0.42	1/4406 (0.0%)
6	LC	0.35	1/2981 (0.0%)	0.45	0/4002
7	LD	0.23	0/2428	0.44	0/3252
8	LE	0.22	0/1942	0.45	0/2606
9	LF	0.25	0/1916	0.41	0/2553
10	LG	0.23	0/1971	0.52	0/2651
11	LH	0.22	0/1537	0.39	0/2066
12	LI	0.24	0/1753	0.48	0/2343
13	LJ	0.25	0/1433	0.53	0/1915
14	LL	0.23	0/1732	0.48	0/2315
15	LM	0.21	0/1161	0.40	0/1554
16	LN	0.30	1/1746 (0.1%)	0.42	0/2338
17	LO	0.25	0/1682	0.47	0/2250
18	LP	0.25	0/1268	0.42	0/1701
19	LQ	0.27	0/1537	0.45	0/2052
20	LR	0.30	0/1582	0.53	2/2091 (0.1%)
21	LS	0.26	0/1493	0.44	0/2003
22	LT	0.25	0/1326	0.44	0/1770
23	LU	0.31	0/839	0.68	2/1126 (0.2%)
24	LV	0.25	0/993	0.39	0/1332
25	LW	0.67	3/826 (0.4%)	0.95	6/1095 (0.5%)
26	LX	0.22	0/1002	0.38	0/1345
27	LY	0.23	0/1119	0.43	0/1488
28	LZ	0.21	0/1130	0.42	0/1507
29	La	0.27	0/1179	0.43	0/1573
30	Lb	0.36	0/821	0.61	1/1084 (0.1%)
31	Lc	0.45	1/774 (0.1%)	0.64	2/1038 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.23	0/894	0.46	0/1204
33	Le	0.25	0/1071	0.38	0/1429
34	Lf	0.26	0/895	0.36	0/1198
35	Lg	0.23	0/878	0.39	0/1170
36	Lh	0.21	0/1023	0.41	0/1351
37	Li	0.21	0/824	0.52	0/1090
38	Lj	0.27	0/720	0.47	0/952
39	Lk	0.21	0/565	0.44	0/750
40	Ll	0.24	0/454	0.36	0/599
41	Lm	0.23	0/425	0.49	0/564
42	Ln	1.15	2/231 (0.9%)	0.81	1/294 (0.3%)
43	Lo	0.25	0/858	0.36	0/1131
44	Lp	0.26	0/691	0.45	0/919
45	Lr	0.25	0/1002	0.40	0/1344
46	S2	0.29	0/38456	0.42	5/59926 (0.0%)
47	SA	0.23	0/1764	0.51	0/2396
48	SB	0.23	0/1774	0.51	0/2373
49	SC	0.23	0/1764	0.48	0/2382
50	SD	0.23	0/1793	0.59	0/2414
51	SE	0.47	1/2118 (0.0%)	0.55	2/2849 (0.1%)
52	SF	0.22	0/1531	0.53	0/2059
53	SG	0.69	2/1926 (0.1%)	0.81	5/2563 (0.2%)
54	SH	0.27	0/1519	0.66	0/2033
55	SI	0.45	1/1715 (0.1%)	0.61	3/2287 (0.1%)
56	SJ	1.77	21/1548 (1.4%)	1.53	39/2066 (1.9%)
57	SK	0.24	0/840	0.59	0/1133
58	SL	0.23	0/1280	0.47	0/1712
59	SM	0.27	0/916	0.79	0/1233
60	SN	0.23	0/1232	0.53	2/1656 (0.1%)
61	SO	0.21	0/1020	0.40	0/1366
62	SP	0.21	0/1047	0.49	0/1399
63	SQ	0.53	1/1142 (0.1%)	0.83	4/1528 (0.3%)
64	SR	0.42	0/1078	0.60	2/1447 (0.1%)
65	SS	0.22	0/1216	0.54	1/1628 (0.1%)
66	ST	0.20	0/1119	0.52	0/1498
67	SU	0.24	0/827	0.62	0/1110
68	SV	0.21	0/643	0.46	0/860
69	SW	0.25	0/1051	0.42	0/1406
70	SX	0.22	0/1116	0.43	0/1490
71	SY	0.20	0/1068	0.54	0/1418
72	SZ	0.20	0/604	0.58	0/810
73	Sa	0.25	0/847	0.44	0/1135
74	Sb	0.23	0/665	0.53	0/891

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sc	0.24	0/508	0.58	0/680
76	Sd	0.26	0/470	0.52	0/623
77	Se	0.48	0/465	0.61	0/612
78	Sf	0.20	0/560	0.64	0/745
79	Sg	0.24	0/2493	0.71	1/3394 (0.0%)
80	u	0.45	0/1800	0.77	0/2804
81	v	0.48	0/1806	0.80	1/2813 (0.0%)
82	w	0.23	0/235	0.42	0/365
All	All	0.37	35/227035 (0.0%)	0.51	95/333340 (0.0%)

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Ln	2	ARG	CA-C	-8.12	1.41	1.53
53	SG	141	ILE	CA-C	-7.71	1.43	1.52
31	Lc	13	SER	CA-C	-7.04	1.44	1.52
6	LC	295	SER	CA-C	-7.03	1.44	1.53
56	SJ	62	THR	CA-C	-6.50	1.44	1.52

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	SJ	123	ILE	N-CA-C	-13.34	97.24	110.72
63	SQ	44	PRO	N-CA-C	-10.52	90.80	112.47
53	SG	141	ILE	N-CA-C	-9.71	101.40	110.53
53	SG	24	LEU	N-CA-C	-9.35	102.69	114.56
25	LW	104	GLN	N-CA-C	-8.97	102.74	114.31

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	L5	78335	0	39651	1590	0
2	L7	2558	0	1295	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L8	3316	0	1687	45	0
4	LA	1898	0	1993	26	0
5	LB	3239	0	3376	48	0
6	LC	2927	0	3104	48	0
7	LD	2382	0	2410	35	0
8	LE	1904	0	2055	42	0
9	LF	1878	0	2009	39	0
10	LG	1935	0	2087	32	0
11	LH	1518	0	1601	21	0
12	LI	1713	0	1751	34	0
13	LJ	1410	0	1441	33	0
14	LL	1701	0	1818	30	0
15	LM	1138	0	1204	19	0
16	LN	1701	0	1749	26	0
17	LO	1650	0	1794	19	0
18	LP	1242	0	1269	12	0
19	LQ	1513	0	1628	10	0
20	LR	1566	0	1729	27	0
21	LS	1453	0	1490	23	0
22	LT	1298	0	1366	18	0
23	LU	825	0	850	22	0
24	LV	979	0	1039	12	0
25	LW	813	0	853	82	0
26	LX	985	0	1066	12	0
27	LY	1102	0	1189	15	0
28	LZ	1107	0	1182	27	0
29	La	1163	0	1206	13	0
30	Lb	808	0	875	15	0
31	Lc	764	0	804	29	0
32	Ld	879	0	924	9	0
33	Le	1053	0	1147	5	0
34	Lf	876	0	912	6	0
35	Lg	868	0	959	8	0
36	Lh	1015	0	1148	17	0
37	Li	813	0	894	9	0
38	Lj	705	0	737	3	0
39	Lk	559	0	624	12	0
40	Ll	444	0	483	7	0
41	Lm	419	0	452	5	0
42	Ln	230	0	276	6	0
43	Lo	842	0	914	10	0
44	Lp	681	0	731	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Lr	987	0	1050	7	0
46	S2	36324	0	18361	692	0
47	SA	1727	0	1729	59	0
48	SB	1747	0	1822	46	0
49	SC	1724	0	1817	35	0
50	SD	1765	0	1865	58	0
51	SE	2076	0	2177	52	0
52	SF	1509	0	1563	49	0
53	SG	1903	0	2068	100	0
54	SH	1497	0	1590	44	0
55	SI	1686	0	1772	61	0
56	SJ	1520	0	1642	136	0
57	SK	816	0	841	39	0
58	SL	1258	0	1332	29	0
59	SM	906	0	921	53	0
60	SN	1208	0	1293	20	0
61	SO	1008	0	1034	19	0
62	SP	1027	0	1075	25	0
63	SQ	1124	0	1193	44	0
64	SR	1064	0	1118	31	0
65	SS	1198	0	1261	33	0
66	ST	1113	0	1145	28	0
67	SU	817	0	882	38	0
68	SV	636	0	637	9	0
69	SW	1034	0	1080	19	0
70	SX	1098	0	1167	20	0
71	SY	1048	0	1122	36	0
72	SZ	598	0	656	29	0
73	Sa	829	0	883	17	0
74	Sb	651	0	672	11	0
75	Sc	506	0	536	18	0
76	Sd	459	0	448	12	0
77	Se	459	0	503	20	0
78	Sf	548	0	552	29	0
79	Sg	2436	0	2393	119	0
80	u	1613	0	821	112	0
81	v	1618	0	822	116	0
82	w	213	0	109	3	0
83	L5	198	0	0	0	0
83	L7	1	0	0	0	0
83	L8	5	0	0	0	0
83	LI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	LN	1	0	0	0	0
83	LP	1	0	0	0	0
83	LV	1	0	0	0	0
83	S2	83	0	0	0	0
83	ST	1	0	0	0	0
84	L5	78	0	0	0	0
84	L7	1	0	0	0	0
84	LA	1	0	0	0	0
84	LI	1	0	0	0	0
84	Le	1	0	0	0	0
84	Lf	1	0	0	0	0
84	Lg	1	0	0	0	0
84	Lo	1	0	0	0	0
84	S2	19	0	0	0	0
84	SO	1	0	0	0	0
84	SS	1	0	0	0	0
84	SX	1	0	0	0	0
84	Sd	1	0	0	0	0
85	L5	30	0	57	3	0
86	L5	504	0	552	28	0
86	L7	42	0	46	4	0
86	S2	168	0	183	6	0
87	Lg	1	0	0	0	0
87	Lj	1	0	0	0	0
87	Lm	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
87	Sa	1	0	0	0	0
87	Sd	1	0	0	0	0
87	Sf	1	0	0	0	0
88	SO	8	0	4	0	0
All	All	217115	0	160566	4413	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 12.

The worst 5 of 4413 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)
1:L5:497:G:C1'	1:L5:498:C:H5'	1.32	1.55
1:L5:497:G:H1'	1:L5:498:C:C5'	1.37	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:255:C:H2'	1:L5:256:G:C8	1.60	1.35
1:L5:741:C:C3'	1:L5:742:G:H5''	1.60	1.28
1:L5:741:C:H3'	1:L5:742:G:C5'	1.63	1.26

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	236 (96%)	10 (4%)	0	100	100
5	LB	399/403 (99%)	387 (97%)	11 (3%)	1 (0%)	36	55
6	LC	366/368 (100%)	357 (98%)	9 (2%)	0	100	100
7	LD	291/294 (99%)	281 (97%)	9 (3%)	1 (0%)	36	55
8	LE	232/288 (81%)	213 (92%)	18 (8%)	1 (0%)	30	49
9	LF	224/248 (90%)	218 (97%)	6 (3%)	0	100	100
10	LG	240/266 (90%)	227 (95%)	12 (5%)	1 (0%)	30	49
11	LH	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
12	LI	211/214 (99%)	201 (95%)	9 (4%)	1 (0%)	24	43
13	LJ	174/178 (98%)	163 (94%)	9 (5%)	2 (1%)	11	22
14	LL	208/211 (99%)	194 (93%)	12 (6%)	2 (1%)	12	24
15	LM	137/215 (64%)	132 (96%)	5 (4%)	0	100	100
16	LN	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
17	LO	199/203 (98%)	191 (96%)	7 (4%)	1 (0%)	24	43
18	LP	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
19	LQ	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
20	LR	185/196 (94%)	176 (95%)	7 (4%)	2 (1%)	11	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	LS	173/176 (98%)	169 (98%)	4 (2%)	0	100	100
22	LT	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
23	LU	99/128 (77%)	91 (92%)	6 (6%)	2 (2%)	6	10
24	LV	129/140 (92%)	127 (98%)	2 (2%)	0	100	100
25	LW	96/157 (61%)	78 (81%)	8 (8%)	10 (10%)	0	0
26	LX	118/156 (76%)	116 (98%)	2 (2%)	0	100	100
27	LY	130/145 (90%)	128 (98%)	2 (2%)	0	100	100
28	LZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
29	La	144/148 (97%)	137 (95%)	6 (4%)	1 (1%)	18	34
30	Lb	95/159 (60%)	92 (97%)	3 (3%)	0	100	100
31	Lc	96/115 (84%)	88 (92%)	7 (7%)	1 (1%)	12	24
32	Ld	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
33	Le	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
34	Lf	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
35	Lg	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
36	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
37	Li	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
38	Lj	84/97 (87%)	84 (100%)	0	0	100	100
39	Lk	66/70 (94%)	63 (96%)	3 (4%)	0	100	100
40	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
41	Lm	49/128 (38%)	49 (100%)	0	0	100	100
42	Ln	22/25 (88%)	20 (91%)	2 (9%)	0	100	100
43	Lo	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
44	Lp	86/92 (94%)	81 (94%)	5 (6%)	0	100	100
45	Lr	121/137 (88%)	120 (99%)	1 (1%)	0	100	100
47	SA	217/295 (74%)	208 (96%)	9 (4%)	0	100	100
48	SB	213/264 (81%)	207 (97%)	5 (2%)	1 (0%)	24	43
49	SC	220/293 (75%)	209 (95%)	11 (5%)	0	100	100
50	SD	225/243 (93%)	203 (90%)	18 (8%)	4 (2%)	6	12
51	SE	260/263 (99%)	245 (94%)	14 (5%)	1 (0%)	30	49
52	SF	189/204 (93%)	176 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	SG	232/249 (93%)	200 (86%)	26 (11%)	6 (3%)	4	7
54	SH	182/194 (94%)	167 (92%)	13 (7%)	2 (1%)	11	22
55	SI	204/208 (98%)	187 (92%)	17 (8%)	0	100	100
56	SJ	181/194 (93%)	134 (74%)	37 (20%)	10 (6%)	1	1
57	SK	95/165 (58%)	86 (90%)	8 (8%)	1 (1%)	11	22
58	SL	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
59	SM	116/132 (88%)	96 (83%)	19 (16%)	1 (1%)	14	27
60	SN	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
61	SO	131/151 (87%)	126 (96%)	5 (4%)	0	100	100
62	SP	123/145 (85%)	119 (97%)	3 (2%)	1 (1%)	16	31
63	SQ	139/146 (95%)	126 (91%)	9 (6%)	4 (3%)	3	5
64	SR	129/135 (96%)	120 (93%)	9 (7%)	0	100	100
65	SS	143/152 (94%)	137 (96%)	6 (4%)	0	100	100
66	ST	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
67	SU	101/119 (85%)	92 (91%)	9 (9%)	0	100	100
68	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
69	SW	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
70	SX	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
71	SY	127/133 (96%)	119 (94%)	8 (6%)	0	100	100
72	SZ	73/125 (58%)	65 (89%)	8 (11%)	0	100	100
73	Sa	101/115 (88%)	99 (98%)	2 (2%)	0	100	100
74	Sb	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
75	Sc	62/69 (90%)	54 (87%)	7 (11%)	1 (2%)	7	14
76	Sd	53/56 (95%)	53 (100%)	0	0	100	100
77	Se	56/133 (42%)	48 (86%)	8 (14%)	0	100	100
78	Sf	65/156 (42%)	58 (89%)	6 (9%)	1 (2%)	8	16
79	Sg	311/317 (98%)	265 (85%)	46 (15%)	0	100	100
All	All	11261/12700 (89%)	10639 (94%)	563 (5%)	59 (0%)	26	43

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	LB	191	ALA

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Mol	Chain	Res	Type
7	LD	259	LYS
8	LE	223	ARG
13	LJ	9	GLU
13	LJ	117	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/199 (96%)	188 (99%)	2 (1%)	65	84
5	LB	347/348 (100%)	343 (99%)	4 (1%)	63	83
6	LC	306/306 (100%)	301 (98%)	5 (2%)	55	79
7	LD	246/248 (99%)	239 (97%)	7 (3%)	38	66
8	LE	209/252 (83%)	202 (97%)	7 (3%)	33	61
9	LF	195/215 (91%)	190 (97%)	5 (3%)	40	68
10	LG	204/223 (92%)	198 (97%)	6 (3%)	37	65
11	LH	169/171 (99%)	164 (97%)	5 (3%)	36	64
12	LI	181/182 (100%)	173 (96%)	8 (4%)	25	50
13	LJ	148/149 (99%)	142 (96%)	6 (4%)	27	53
14	LL	176/177 (99%)	167 (95%)	9 (5%)	21	43
15	LM	118/161 (73%)	114 (97%)	4 (3%)	32	60
16	LN	171/172 (99%)	167 (98%)	4 (2%)	44	72
17	LO	173/174 (99%)	171 (99%)	2 (1%)	63	83
18	LP	134/163 (82%)	129 (96%)	5 (4%)	30	57
19	LQ	164/165 (99%)	163 (99%)	1 (1%)	78	91
20	LR	166/175 (95%)	158 (95%)	8 (5%)	23	46
21	LS	156/157 (99%)	151 (97%)	5 (3%)	34	62
22	LT	139/140 (99%)	136 (98%)	3 (2%)	45	73
23	LU	91/115 (79%)	83 (91%)	8 (9%)	9	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	LV	101/107 (94%)	99 (98%)	2 (2%)	48	75
25	LW	82/126 (65%)	69 (84%)	13 (16%)	2	5
26	LX	108/133 (81%)	107 (99%)	1 (1%)	70	87
27	LY	123/135 (91%)	122 (99%)	1 (1%)	73	88
28	LZ	117/118 (99%)	114 (97%)	3 (3%)	40	68
29	La	119/120 (99%)	119 (100%)	0	100	100
30	Lb	83/126 (66%)	79 (95%)	4 (5%)	23	46
31	Lc	83/97 (86%)	78 (94%)	5 (6%)	17	36
32	Ld	97/110 (88%)	96 (99%)	1 (1%)	68	86
33	Le	114/121 (94%)	111 (97%)	3 (3%)	40	68
34	Lf	88/89 (99%)	87 (99%)	1 (1%)	65	84
35	Lg	94/100 (94%)	93 (99%)	1 (1%)	65	84
36	Lh	109/110 (99%)	107 (98%)	2 (2%)	51	77
37	Li	85/89 (96%)	82 (96%)	3 (4%)	32	58
38	Lj	73/80 (91%)	72 (99%)	1 (1%)	59	81
39	Lk	63/65 (97%)	55 (87%)	8 (13%)	4	9
40	Ll	47/48 (98%)	45 (96%)	2 (4%)	26	51
41	Lm	47/116 (40%)	46 (98%)	1 (2%)	47	74
42	Ln	23/24 (96%)	22 (96%)	1 (4%)	26	51
43	Lo	91/94 (97%)	89 (98%)	2 (2%)	45	73
44	Lp	71/75 (95%)	71 (100%)	0	100	100
45	Lr	107/121 (88%)	105 (98%)	2 (2%)	50	76
47	SA	182/243 (75%)	175 (96%)	7 (4%)	29	56
48	SB	196/231 (85%)	187 (95%)	9 (5%)	24	48
49	SC	188/225 (84%)	180 (96%)	8 (4%)	26	51
50	SD	190/202 (94%)	180 (95%)	10 (5%)	20	42
51	SE	224/225 (100%)	208 (93%)	16 (7%)	13	29
52	SF	161/170 (95%)	157 (98%)	4 (2%)	42	69
53	SG	204/218 (94%)	176 (86%)	28 (14%)	3	7
54	SH	166/174 (95%)	152 (92%)	14 (8%)	10	22
55	SI	178/180 (99%)	168 (94%)	10 (6%)	19	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	SJ	162/168 (96%)	112 (69%)	50 (31%)	0	0
57	SK	88/136 (65%)	87 (99%)	1 (1%)	65	84
58	SL	138/142 (97%)	133 (96%)	5 (4%)	31	58
59	SM	98/108 (91%)	89 (91%)	9 (9%)	8	19
60	SN	130/131 (99%)	130 (100%)	0	100	100
61	SO	105/118 (89%)	104 (99%)	1 (1%)	68	86
62	SP	111/130 (85%)	108 (97%)	3 (3%)	39	67
63	SQ	117/121 (97%)	108 (92%)	9 (8%)	12	25
64	SR	119/122 (98%)	115 (97%)	4 (3%)	32	60
65	SS	126/132 (96%)	122 (97%)	4 (3%)	34	62
66	ST	112/114 (98%)	109 (97%)	3 (3%)	39	67
67	SU	94/107 (88%)	88 (94%)	6 (6%)	16	33
68	SV	67/67 (100%)	65 (97%)	2 (3%)	36	64
69	SW	112/113 (99%)	109 (97%)	3 (3%)	39	67
70	SX	113/115 (98%)	108 (96%)	5 (4%)	25	50
71	SY	111/115 (96%)	105 (95%)	6 (5%)	20	41
72	SZ	66/103 (64%)	63 (96%)	3 (4%)	24	49
73	Sa	90/98 (92%)	86 (96%)	4 (4%)	25	50
74	Sb	75/76 (99%)	71 (95%)	4 (5%)	20	42
75	Sc	57/62 (92%)	49 (86%)	8 (14%)	3	7
76	Sd	48/49 (98%)	46 (96%)	2 (4%)	26	52
77	Se	47/104 (45%)	43 (92%)	4 (8%)	10	22
78	Sf	60/140 (43%)	56 (93%)	4 (7%)	15	31
79	Sg	272/275 (99%)	251 (92%)	21 (8%)	12	25
All	All	9815/10810 (91%)	9387 (96%)	428 (4%)	27	50

5 of 428 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	SG	128	THR
56	SJ	78	LEU
77	Se	3	HIS
53	SG	152	ASP
55	SI	76	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
57	SK	28	HIS
65	SS	105	ASN
59	SM	15	ASN
61	SO	103	ASN
69	SW	5	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3640/5069 (71%)	961 (26%)	73 (2%)
2	L7	119/120 (99%)	13 (10%)	0
3	L8	155/157 (98%)	32 (20%)	2 (1%)
46	S2	1689/1869 (90%)	433 (25%)	31 (1%)
80	u	75/76 (98%)	49 (65%)	0
81	v	75/76 (98%)	48 (64%)	0
82	w	9/10 (90%)	1 (11%)	0
All	All	5762/7377 (78%)	1537 (26%)	106 (1%)

5 of 1537 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	39	A
1	L5	42	A
1	L5	48	G
1	L5	56	A
1	L5	57	G

5 of 106 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	2488	C
1	L5	4699	U
46	S2	1520	G
1	L5	2492	C
1	L5	3673	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PSU	L5	5001	1	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
46	OMC	S2	517	46	19,22,23	2.95	8 (42%)	26,31,34	0.73	0
1	A2M	L5	398	1	22,25,26	1.50	4 (18%)	31,36,39	2.04	9 (29%)
1	OMG	L5	4499	1	23,26,27	3.01	10 (43%)	33,38,41	2.52	13 (39%)
1	A2M	L5	2787	1,83	22,25,26	1.62	4 (18%)	31,36,39	2.18	9 (29%)
1	OMU	L5	2415	1	19,22,23	2.94	8 (42%)	26,31,34	1.66	5 (19%)
3	PSU	L8	55	3	18,21,22	1.07	1 (5%)	22,30,33	1.81	4 (18%)
1	OMG	L5	4228	1	23,26,27	2.92	10 (43%)	33,38,41	2.39	13 (39%)
46	PSU	S2	609	46	18,21,22	1.13	1 (5%)	22,30,33	1.70	4 (18%)
1	PSU	L5	3844	1	18,21,22	1.01	1 (5%)	22,30,33	1.76	4 (18%)
46	A2M	S2	166	46	22,25,26	1.46	4 (18%)	31,36,39	2.10	7 (22%)
1	A2M	L5	1534	1,83	22,25,26	1.62	5 (22%)	31,36,39	2.24	9 (29%)
1	A2M	L5	4590	1	22,25,26	1.55	4 (18%)	31,36,39	2.14	11 (35%)
1	A2M	L5	1871	1,83	22,25,26	1.56	4 (18%)	31,36,39	2.28	11 (35%)
46	PSU	S2	1186	46	18,21,22	1.01	1 (5%)	22,30,33	1.80	4 (18%)
46	PSU	S2	366	46	18,21,22	1.04	1 (5%)	22,30,33	1.89	5 (22%)
1	PSU	L5	4636	1	18,21,22	1.05	1 (5%)	22,30,33	2.03	5 (22%)
1	OMG	L5	4392	1	23,26,27	2.92	9 (39%)	33,38,41	2.46	13 (39%)
46	6MZ	S2	1832	84,83,46	22,25,26	3.16	4 (18%)	30,36,39	2.17	9 (30%)
46	OMU	S2	428	46	19,22,23	2.98	8 (42%)	26,31,34	1.77	5 (19%)
1	OMG	L5	4494	1	23,26,27	2.97	9 (39%)	33,38,41	2.50	12 (36%)
46	OMG	S2	1447	46	23,26,27	3.06	10 (43%)	33,38,41	2.63	12 (36%)
46	A2M	S2	1031	46	22,25,26	1.55	4 (18%)	31,36,39	2.18	11 (35%)
1	5MC	L5	4447	1,84	18,22,23	3.67	7 (38%)	26,32,35	1.23	1 (3%)
1	OMC	L5	1881	1,83	19,22,23	2.88	8 (42%)	26,31,34	0.82	0
1	OMC	L5	3808	1	19,22,23	1.27	3 (15%)	26,31,34	1.08	1 (3%)
1	PSU	L5	3822	1	18,21,22	0.99	1 (5%)	22,30,33	1.79	3 (13%)
46	PSU	S2	815	46	18,21,22	1.07	1 (5%)	22,30,33	1.81	5 (22%)
46	PSU	S2	1174	46	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	4628	1	18,21,22	1.05	1 (5%)	22,30,33	1.93	5 (22%)
46	PSU	S2	918	46	18,21,22	1.12	2 (11%)	22,30,33	1.90	6 (27%)
3	PSU	L8	69	3	18,21,22	1.07	1 (5%)	22,30,33	1.83	5 (22%)
1	PSU	L5	3637	1,84	18,21,22	1.01	1 (5%)	22,30,33	1.82	4 (18%)
1	OMC	L5	2824	1	19,22,23	2.95	8 (42%)	26,31,34	0.73	0
1	OMG	L5	4196	1,80,83	23,26,27	2.97	9 (39%)	33,38,41	2.49	12 (36%)
1	A2M	L5	1326	1	22,25,26	1.57	5 (22%)	31,36,39	2.35	11 (35%)
46	PSU	S2	1596	46	18,21,22	1.05	1 (5%)	22,30,33	1.69	4 (18%)
1	UY1	L5	3818	1,84	19,22,23	4.09	9 (47%)	22,31,34	1.97	6 (27%)
46	PSU	S2	966	46	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
46	UY1	S2	1326	83,46	19,22,23	4.20	8 (42%)	22,31,34	1.92	4 (18%)
1	PSU	L5	4579	1	18,21,22	1.04	1 (5%)	22,30,33	1.88	5 (22%)
46	MA6	S2	1850	46	23,26,27	1.61	4 (17%)	34,38,41	2.42	14 (41%)
1	OMC	L5	3887	1	19,22,23	2.93	8 (42%)	26,31,34	0.74	0
46	PSU	S2	1360	84,83,46	18,21,22	1.04	2 (11%)	22,30,33	1.76	5 (22%)
1	PSU	L5	4312	1	18,21,22	1.00	1 (5%)	22,30,33	1.76	4 (18%)
46	PSU	S2	1367	46	18,21,22	1.10	1 (5%)	22,30,33	1.87	5 (22%)
46	PSU	S2	105	46	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
46	OMU	S2	354	46	19,22,23	2.92	8 (42%)	26,31,34	1.72	5 (19%)
46	PSU	S2	686	46	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
1	PSU	L5	4361	1	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
46	A2M	S2	576	46	22,25,26	1.46	5 (22%)	31,36,39	2.37	10 (32%)
46	PSU	S2	801	46	18,21,22	1.10	1 (5%)	22,30,33	1.75	4 (18%)
1	PSU	L5	4431	1	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
1	5MC	L5	3782	1,83	18,22,23	3.68	7 (38%)	26,32,35	1.04	2 (7%)
46	OMU	S2	116	46	19,22,23	2.96	8 (42%)	26,31,34	1.66	5 (19%)
46	A2M	S2	484	46	22,25,26	1.51	5 (22%)	31,36,39	2.12	9 (29%)
46	OMG	S2	683	46	23,26,27	3.03	10 (43%)	33,38,41	2.60	12 (36%)
46	PSU	S2	218	46	18,21,22	1.04	1 (5%)	22,30,33	1.75	4 (18%)
1	PSU	L5	3920	1,83	18,21,22	1.02	1 (5%)	22,30,33	1.74	4 (18%)
1	OMC	L5	1340	1	19,22,23	1.41	4 (21%)	26,31,34	1.01	2 (7%)
46	OMC	S2	1703	46	19,22,23	2.92	8 (42%)	26,31,34	0.74	0
1	PSU	L5	1860	1	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
1	6MZ	L5	4220	1	22,25,26	3.06	4 (18%)	30,36,39	2.24	9 (30%)
1	PSU	L5	4973	1	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	L5	1316	1,84	23,26,27	1.89	6 (26%)	33,38,41	2.20	10 (30%)
46	A2M	S2	27	83,46	22,25,26	1.50	4 (18%)	31,36,39	2.21	11 (35%)
46	OMG	S2	436	46	23,26,27	3.03	10 (43%)	33,38,41	2.54	16 (48%)
46	OMC	S2	1272	46	19,22,23	3.02	8 (42%)	26,31,34	0.70	0
1	OMU	L5	3925	1	19,22,23	2.89	8 (42%)	26,31,34	1.65	4 (15%)
46	PSU	S2	100	83,46	18,21,22	1.01	1 (5%)	22,30,33	1.82	4 (18%)
46	OMG	S2	867	46	23,26,27	3.09	10 (43%)	33,38,41	2.63	11 (33%)
46	OMG	S2	1328	84,46	23,26,27	3.02	10 (43%)	33,38,41	2.59	12 (36%)
46	4AC	S2	1842	46	21,24,25	3.10	10 (47%)	29,34,37	1.03	4 (13%)
1	A2M	L5	2815	1	22,25,26	1.52	4 (18%)	31,36,39	2.23	9 (29%)
46	OMC	S2	1391	46	19,22,23	2.98	8 (42%)	26,31,34	0.73	0
46	4AC	S2	1337	46	21,24,25	3.21	9 (42%)	29,34,37	1.15	3 (10%)
46	PSU	S2	822	46	18,21,22	1.10	1 (5%)	22,30,33	1.85	5 (22%)
1	PSU	L5	1782	1	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
1	OMC	L5	4536	1	19,22,23	2.88	8 (42%)	26,31,34	0.74	0
46	PSU	S2	34	46	18,21,22	1.03	1 (5%)	22,30,33	1.82	5 (22%)
1	PSU	L5	1582	1	18,21,22	1.03	1 (5%)	22,30,33	1.62	4 (18%)
1	OMU	L5	4498	1,83	19,22,23	2.91	8 (42%)	26,31,34	1.75	5 (19%)
1	OMU	L5	4620	1	19,22,23	2.90	8 (42%)	26,31,34	1.66	5 (19%)
46	PSU	S2	651	46	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
46	OMG	S2	601	46	23,26,27	2.92	10 (43%)	33,38,41	2.56	12 (36%)
1	PSU	L5	3851	1	18,21,22	1.05	1 (5%)	22,30,33	1.83	4 (18%)
1	PSU	L5	4299	1	18,21,22	1.05	1 (5%)	22,30,33	1.69	4 (18%)
46	PSU	S2	1643	83,46	18,21,22	1.08	1 (5%)	22,30,33	1.75	5 (22%)
1	PSU	L5	4293	1	18,21,22	1.02	1 (5%)	22,30,33	1.69	3 (13%)
46	PSU	S2	1445	46	18,21,22	1.04	1 (5%)	22,30,33	1.82	5 (22%)
1	PSU	L5	3730	1	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
1	PSU	L5	4353	1	18,21,22	1.06	1 (5%)	22,30,33	1.82	5 (22%)
46	A2M	S2	159	46	22,25,26	1.44	6 (27%)	31,36,39	2.46	11 (35%)
46	PSU	S2	866	46	18,21,22	1.10	1 (5%)	22,30,33	1.84	5 (22%)
46	OMC	S2	462	46	19,22,23	2.95	8 (42%)	26,31,34	0.66	0
1	PSU	L5	2839	1	18,21,22	1.04	1 (5%)	22,30,33	1.71	4 (18%)
1	A2M	L5	3724	1	22,25,26	1.44	5 (22%)	31,36,39	2.20	10 (32%)
46	A2M	S2	1383	46	22,25,26	1.39	4 (18%)	31,36,39	2.24	9 (29%)
1	PSU	L5	1862	1	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	L5	2363	1,83	22,25,26	1.61	4 (18%)	31,36,39	2.20	10 (32%)
1	A2M	L5	4571	1	22,25,26	1.65	4 (18%)	31,36,39	2.04	9 (29%)
1	PSU	L5	1779	1	18,21,22	1.01	1 (5%)	22,30,33	1.80	5 (22%)
1	PSU	L5	1792	1	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
1	PSU	L5	4471	1	18,21,22	1.06	1 (5%)	22,30,33	1.68	4 (18%)
1	PSU	L5	3768	1	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
1	PSU	L5	4521	1,84,83	18,21,22	1.09	1 (5%)	22,30,33	1.88	5 (22%)
1	OMG	L5	1625	1,84	23,26,27	2.98	9 (39%)	33,38,41	2.54	13 (39%)
46	OMU	S2	121	46	19,22,23	2.96	8 (42%)	26,31,34	1.58	4 (15%)
5	HIC	LB	245	5	10,11,12	0.58	0	8,14,16	0.77	0
1	OMG	L5	3627	1	23,26,27	2.94	10 (43%)	33,38,41	2.45	14 (42%)
1	OMC	L5	4456	1	19,22,23	2.87	8 (42%)	26,31,34	0.68	0
46	OMG	S2	1490	83,46	23,26,27	2.99	10 (43%)	33,38,41	2.52	13 (39%)
1	PSU	L5	3884	1	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
1	PSU	L5	4689	1	18,21,22	1.04	1 (5%)	22,30,33	1.66	4 (18%)
46	PSU	S2	406	46	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
46	OMU	S2	1442	83,46	19,22,23	2.99	8 (42%)	26,31,34	1.73	5 (19%)
1	PSU	L5	3695	1	18,21,22	1.06	1 (5%)	22,30,33	1.72	4 (18%)
46	PSU	S2	1003	46	18,21,22	1.10	1 (5%)	22,30,33	1.74	4 (18%)
1	OMC	L5	3869	1	19,22,23	1.12	2 (10%)	26,31,34	0.96	1 (3%)
1	OMU	L5	4227	1	19,22,23	2.96	8 (42%)	26,31,34	1.73	5 (19%)
1	PSU	L5	4500	1	18,21,22	1.07	1 (5%)	22,30,33	1.87	5 (22%)
46	PSU	S2	649	46	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
46	OMG	S2	644	46	23,26,27	2.99	10 (43%)	33,38,41	2.53	13 (39%)
46	PSU	S2	667	46	18,21,22	1.07	2 (11%)	22,30,33	1.79	5 (22%)
46	PSU	S2	1238	46	18,21,22	1.10	2 (11%)	22,30,33	1.78	5 (22%)
1	PSU	L5	4673	1,84	18,21,22	1.03	1 (5%)	22,30,33	1.74	4 (18%)
1	OMG	L5	2364	1	23,26,27	1.53	4 (17%)	33,38,41	2.09	9 (27%)
1	PSU	L5	3770	1	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
1	OMC	L5	2861	1	19,22,23	2.93	8 (42%)	26,31,34	0.76	0
1	PSU	L5	4576	1	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
1	PSU	L5	4493	1,84	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
1	PSU	L5	4972	1	18,21,22	1.02	1 (5%)	22,30,33	1.75	4 (18%)
46	PSU	S2	814	46	18,21,22	1.04	1 (5%)	22,30,33	1.67	4 (18%)
1	1MA	L5	1322	1,83	21,25,26	1.55	6 (28%)	31,37,40	1.91	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	S2	863	46	18,21,22	1.04	1 (5%)	22,30,33	1.77	4 (18%)
46	PSU	S2	1625	46	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
1	PSU	L5	4532	1	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
46	A2M	S2	668	83,46	22,25,26	1.52	4 (18%)	31,36,39	2.09	7 (22%)
46	PSU	S2	1692	46	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
3	OMU	L8	14	1,3	19,22,23	2.94	8 (42%)	26,31,34	1.80	5 (19%)
46	PSU	S2	1232	46	18,21,22	1.01	1 (5%)	22,30,33	1.74	4 (18%)
1	A2M	L5	3867	1	22,25,26	1.69	4 (18%)	31,36,39	2.10	11 (35%)
46	PSU	S2	119	46	18,21,22	1.01	1 (5%)	22,30,33	1.67	4 (18%)
46	PSU	S2	1177	46	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
1	PSU	L5	4403	1	18,21,22	1.09	1 (5%)	22,30,33	1.77	6 (27%)
1	PSU	L5	4457	1	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
46	A2M	S2	512	46	22,25,26	1.47	5 (22%)	31,36,39	2.33	11 (35%)
46	PSU	S2	681	46	18,21,22	1.09	1 (5%)	22,30,33	1.78	4 (18%)
1	OMG	L5	4370	1	23,26,27	2.94	10 (43%)	33,38,41	2.48	14 (42%)
1	UR3	L5	4530	1	19,22,23	2.67	5 (26%)	26,32,35	1.31	3 (11%)
66	NMM	ST	67	66	9,11,12	0.60	0	6,12,14	2.78	2 (33%)
1	PSU	L5	3762	1	18,21,22	1.02	1 (5%)	22,30,33	1.88	4 (18%)
46	PSU	S2	1136	46	18,21,22	1.07	1 (5%)	22,30,33	1.85	5 (22%)
3	OMG	L8	75	3	23,26,27	2.97	10 (43%)	33,38,41	2.44	12 (36%)
1	PSU	L5	2508	1	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
1	OMC	L5	2804	1	19,22,23	2.90	8 (42%)	26,31,34	0.67	0
1	PSU	L5	4296	1	18,21,22	1.08	1 (5%)	22,30,33	1.83	5 (22%)
1	OMU	L5	4306	1	19,22,23	2.88	8 (42%)	26,31,34	1.67	5 (19%)
46	PSU	S2	1046	46	18,21,22	1.04	1 (5%)	22,30,33	1.72	4 (18%)
46	OMU	S2	1288	46	19,22,23	3.03	8 (42%)	26,31,34	1.65	4 (15%)
1	OMG	L5	1522	1	23,26,27	1.60	5 (21%)	33,38,41	2.37	8 (24%)
1	OMG	L5	4637	1,84	23,26,27	2.97	10 (43%)	33,38,41	2.48	13 (39%)
1	A2M	L5	3718	1	22,25,26	1.53	4 (18%)	31,36,39	2.07	9 (29%)
46	A2M	S2	468	46	22,25,26	1.46	5 (22%)	31,36,39	2.36	10 (32%)
46	PSU	S2	109	46	18,21,22	1.04	1 (5%)	22,30,33	1.82	4 (18%)
46	PSU	S2	1347	46	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
46	PSU	S2	1244	46	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
1	PSU	L5	1536	1	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
1	OMC	L5	3701	1,84	19,22,23	2.86	8 (42%)	26,31,34	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	OMU	S2	1804	46	19,22,23	1.57	4 (21%)	26,31,34	1.97	6 (23%)
46	A2M	S2	1678	46	22,25,26	1.52	5 (22%)	31,36,39	2.08	9 (29%)
1	OMC	L5	3841	1	19,22,23	2.91	8 (42%)	26,31,34	0.66	0
46	PSU	S2	93	46	18,21,22	1.09	1 (5%)	22,30,33	1.69	4 (18%)
46	OMU	S2	172	46	19,22,23	3.04	8 (42%)	26,31,34	1.73	5 (19%)
29	V5N	La	39	29	9,11,12	0.96	0	9,14,16	1.42	2 (22%)
1	PSU	L5	3764	1	18,21,22	1.05	1 (5%)	22,30,33	1.87	5 (22%)
46	A2M	S2	590	46	22,25,26	1.48	5 (22%)	31,36,39	2.15	7 (22%)
1	OMC	L5	2365	1,83	19,22,23	1.12	2 (10%)	26,31,34	0.98	1 (3%)
46	B8N	S2	1248	46	24,29,30	3.13	6 (25%)	29,42,45	1.81	6 (20%)
1	OMG	L5	4618	1	23,26,27	2.96	10 (43%)	33,38,41	2.46	14 (42%)
46	PSU	S2	1045	46	18,21,22	1.01	1 (5%)	22,30,33	1.79	3 (13%)
1	OMG	L5	4623	1	23,26,27	2.94	10 (43%)	33,38,41	2.46	14 (42%)
1	PSU	L5	2632	1	18,21,22	1.06	1 (5%)	22,30,33	1.71	4 (18%)
1	OMG	L5	2876	1	23,26,27	3.01	10 (43%)	33,38,41	2.71	12 (36%)
46	OMC	S2	174	46	19,22,23	3.03	8 (42%)	26,31,34	0.74	0
1	PSU	L5	1677	1	18,21,22	1.11	1 (5%)	22,30,33	1.81	6 (27%)
1	OMU	L5	2837	1	19,22,23	2.91	8 (42%)	26,31,34	1.79	5 (19%)
46	MA6	S2	1851	46	23,26,27	1.60	5 (21%)	34,38,41	2.48	11 (32%)
1	PSU	L5	4552	1	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
1	PSU	L5	4423	1	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
1	OMC	L5	2422	1,83	19,22,23	2.92	8 (42%)	26,31,34	0.69	0
46	PSU	S2	1056	46	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
46	PSU	S2	572	46	18,21,22	1.06	1 (5%)	22,30,33	1.72	5 (22%)
1	PSU	L5	1781	1	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
1	PSU	L5	1683	1,84	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
1	OMG	L5	3899	1,83	23,26,27	2.92	9 (39%)	33,38,41	2.39	14 (42%)
1	PSU	L5	2843	1	18,21,22	1.08	1 (5%)	22,30,33	1.82	5 (22%)
1	A2M	L5	2401	1	22,25,26	1.54	4 (18%)	31,36,39	2.23	10 (32%)
1	A2M	L5	3830	1	22,25,26	1.49	4 (18%)	31,36,39	2.25	10 (32%)
46	PSU	S2	296	46	18,21,22	1.07	1 (5%)	22,30,33	1.72	4 (18%)
1	PSU	L5	1744	1	18,21,22	1.04	1 (5%)	22,30,33	1.79	4 (18%)
46	PSU	S2	36	46	18,21,22	1.04	1 (5%)	22,30,33	1.77	4 (18%)
46	OMG	S2	509	83,46	23,26,27	3.03	9 (39%)	33,38,41	2.56	13 (39%)
46	PSU	S2	1004	46	18,21,22	1.03	1 (5%)	22,30,33	1.69	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	5010	1	18,21,22	1.08	1 (5%)	22,30,33	1.81	4 (18%)
46	PSU	S2	63	46	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
1	A2M	L5	3785	1	22,25,26	1.55	5 (22%)	31,36,39	2.52	14 (45%)
1	OMG	L5	3744	1	23,26,27	2.97	10 (43%)	33,38,41	2.47	13 (39%)
1	OMC	L5	2351	1,83	19,22,23	2.80	8 (42%)	26,31,34	0.95	2 (7%)
1	A2M	L5	1524	1	22,25,26	1.56	5 (22%)	31,36,39	2.33	11 (35%)
46	PSU	S2	300	46	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
46	A2M	S2	99	83,46	22,25,26	1.53	4 (18%)	31,36,39	2.24	9 (29%)
1	PSU	L5	3853	1,83	18,21,22	1.05	1 (5%)	22,30,33	1.81	5 (22%)
1	A2M	L5	400	1	22,25,26	1.50	4 (18%)	31,36,39	2.16	10 (32%)
1	PSU	L5	3639	1	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
1	PSU	L5	4442	1	18,21,22	1.08	1 (5%)	22,30,33	1.79	6 (27%)
1	A2M	L5	1323	1	22,25,26	1.57	4 (18%)	31,36,39	2.25	9 (29%)
1	OMG	L5	3792	1	23,26,27	1.65	6 (26%)	33,38,41	2.07	7 (21%)
1	A2M	L5	4523	1,83	22,25,26	1.50	4 (18%)	31,36,39	2.30	10 (32%)
1	A2M	L5	3825	1	22,25,26	1.51	4 (18%)	31,36,39	2.24	10 (32%)
1	PSU	L5	3715	1	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
1	OMG	L5	2424	1	23,26,27	3.03	10 (43%)	33,38,41	2.69	11 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	5001	1	-	0/7/25/26	0/2/2/2
46	OMC	S2	517	46	-	0/9/27/28	0/2/2/2
1	A2M	L5	398	1	-	1/9/27/28	0/3/3/3
1	OMG	L5	4499	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	2787	1,83	-	3/9/27/28	0/3/3/3
1	OMU	L5	2415	1	-	0/9/27/28	0/2/2/2
3	PSU	L8	55	3	-	0/7/25/26	0/2/2/2
1	OMG	L5	4228	1	-	0/9/27/28	0/3/3/3
46	PSU	S2	609	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	3844	1	-	3/7/25/26	0/2/2/2
46	A2M	S2	166	46	-	3/9/27/28	0/3/3/3
1	A2M	L5	1534	1,83	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	L5	4590	1	-	1/9/27/28	0/3/3/3
1	A2M	L5	1871	1,83	-	0/9/27/28	0/3/3/3
46	PSU	S2	1186	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	366	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4636	1	-	4/7/25/26	0/2/2/2
1	OMG	L5	4392	1	-	0/9/27/28	0/3/3/3
46	6MZ	S2	1832	84,83,46	-	2/9/27/28	0/3/3/3
46	OMU	S2	428	46	-	4/9/27/28	0/2/2/2
1	OMG	L5	4494	1	-	0/9/27/28	0/3/3/3
46	OMG	S2	1447	46	-	3/9/27/28	0/3/3/3
46	A2M	S2	1031	46	-	0/9/27/28	0/3/3/3
1	5MC	L5	4447	1,84	-	4/7/25/26	0/2/2/2
1	OMC	L5	1881	1,83	-	0/9/27/28	0/2/2/2
1	OMC	L5	3808	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	3822	1	-	2/7/25/26	0/2/2/2
46	PSU	S2	815	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1174	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4628	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	918	46	-	2/7/25/26	0/2/2/2
3	PSU	L8	69	3	-	0/7/25/26	0/2/2/2
1	PSU	L5	3637	1,84	-	0/7/25/26	0/2/2/2
1	OMC	L5	2824	1	-	1/9/27/28	0/2/2/2
1	OMG	L5	4196	1,80,83	-	1/9/27/28	0/3/3/3
1	A2M	L5	1326	1	-	1/9/27/28	0/3/3/3
46	PSU	S2	1596	46	-	0/7/25/26	0/2/2/2
1	UY1	L5	3818	1,84	-	4/9/27/28	0/2/2/2
46	PSU	S2	966	46	-	1/7/25/26	0/2/2/2
46	UY1	S2	1326	83,46	-	3/9/27/28	0/2/2/2
1	PSU	L5	4579	1	-	0/7/25/26	0/2/2/2
46	MA6	S2	1850	46	-	5/11/29/30	0/3/3/3
1	OMC	L5	3887	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	1360	84,83,46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4312	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1367	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	105	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	354	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	686	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4361	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	576	46	-	3/9/27/28	0/3/3/3
46	PSU	S2	801	46	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	4431	1	-	0/7/25/26	0/2/2/2
1	5MC	L5	3782	1,83	-	0/7/25/26	0/2/2/2
46	OMU	S2	116	46	-	0/9/27/28	0/2/2/2
46	A2M	S2	484	46	-	0/9/27/28	0/3/3/3
46	OMG	S2	683	46	-	3/9/27/28	0/3/3/3
46	PSU	S2	218	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	3920	1,83	-	0/7/25/26	0/2/2/2
1	OMC	L5	1340	1	-	0/9/27/28	0/2/2/2
46	OMC	S2	1703	46	-	3/9/27/28	0/2/2/2
1	PSU	L5	1860	1	-	0/7/25/26	0/2/2/2
1	6MZ	L5	4220	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4973	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	1316	1,84	-	0/9/27/28	0/3/3/3
46	A2M	S2	27	83,46	-	3/9/27/28	0/3/3/3
46	OMG	S2	436	46	-	0/9/27/28	0/3/3/3
46	OMC	S2	1272	46	-	0/9/27/28	0/2/2/2
1	OMU	L5	3925	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	100	83,46	-	2/7/25/26	0/2/2/2
46	OMG	S2	867	46	-	3/9/27/28	0/3/3/3
46	OMG	S2	1328	84,46	-	1/9/27/28	0/3/3/3
46	4AC	S2	1842	46	-	0/11/29/30	0/2/2/2
1	A2M	L5	2815	1	-	3/9/27/28	0/3/3/3
46	OMC	S2	1391	46	-	0/9/27/28	0/2/2/2
46	4AC	S2	1337	46	-	0/11/29/30	0/2/2/2
46	PSU	S2	822	46	-	3/7/25/26	0/2/2/2
1	PSU	L5	1782	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	4536	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	34	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	1582	1	-	3/7/25/26	0/2/2/2
1	OMU	L5	4498	1,83	-	0/9/27/28	0/2/2/2
1	OMU	L5	4620	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	651	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	601	46	-	1/9/27/28	0/3/3/3
1	PSU	L5	3851	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4299	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1643	83,46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4293	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1445	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	3730	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4353	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	A2M	S2	159	46	-	0/9/27/28	0/3/3/3
46	PSU	S2	866	46	-	0/7/25/26	0/2/2/2
46	OMC	S2	462	46	-	1/9/27/28	0/2/2/2
1	PSU	L5	2839	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	3724	1	-	3/9/27/28	0/3/3/3
46	A2M	S2	1383	46	-	1/9/27/28	0/3/3/3
1	PSU	L5	1862	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	2363	1,83	-	0/9/27/28	0/3/3/3
1	A2M	L5	4571	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1779	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1792	1	-	2/7/25/26	0/2/2/2
1	PSU	L5	4471	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3768	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4521	1,84,83	-	0/7/25/26	0/2/2/2
1	OMG	L5	1625	1,84	-	0/9/27/28	0/3/3/3
46	OMU	S2	121	46	-	0/9/27/28	0/2/2/2
5	HIC	LB	245	5	-	0/5/6/8	0/1/1/1
1	OMG	L5	3627	1	-	1/9/27/28	0/3/3/3
1	OMC	L5	4456	1	-	0/9/27/28	0/2/2/2
46	OMG	S2	1490	83,46	-	2/9/27/28	0/3/3/3
1	PSU	L5	3884	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4689	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	406	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	1442	83,46	-	0/9/27/28	0/2/2/2
1	PSU	L5	3695	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1003	46	-	0/7/25/26	0/2/2/2
1	OMC	L5	3869	1	-	0/9/27/28	0/2/2/2
1	OMU	L5	4227	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4500	1	-	3/7/25/26	0/2/2/2
46	PSU	S2	649	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	644	46	-	1/9/27/28	0/3/3/3
46	PSU	S2	667	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1238	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4673	1,84	-	0/7/25/26	0/2/2/2
1	OMG	L5	2364	1	-	2/9/27/28	0/3/3/3
1	PSU	L5	3770	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2861	1	-	1/9/27/28	0/2/2/2
1	PSU	L5	4576	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4493	1,84	-	0/7/25/26	0/2/2/2
1	PSU	L5	4972	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	814	46	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1MA	L5	1322	1,83	-	2/7/25/26	0/3/3/3
46	PSU	S2	863	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1625	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4532	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	668	83,46	-	2/9/27/28	0/3/3/3
46	PSU	S2	1692	46	-	0/7/25/26	0/2/2/2
3	OMU	L8	14	1,3	-	1/9/27/28	0/2/2/2
46	PSU	S2	1232	46	-	0/7/25/26	0/2/2/2
1	A2M	L5	3867	1	-	0/9/27/28	0/3/3/3
46	PSU	S2	119	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1177	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4403	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4457	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	512	46	-	1/9/27/28	0/3/3/3
46	PSU	S2	681	46	-	0/7/25/26	0/2/2/2
1	OMG	L5	4370	1	-	0/9/27/28	0/3/3/3
1	UR3	L5	4530	1	-	0/7/25/26	0/2/2/2
66	NMM	ST	67	66	-	5/9/11/13	-
1	PSU	L5	3762	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1136	46	-	0/7/25/26	0/2/2/2
3	OMG	L8	75	3	-	0/9/27/28	0/3/3/3
1	PSU	L5	2508	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2804	1	-	1/9/27/28	0/2/2/2
1	PSU	L5	4296	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	4306	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	1046	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	1288	46	-	0/9/27/28	0/2/2/2
1	OMG	L5	1522	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	4637	1,84	-	3/9/27/28	0/3/3/3
1	A2M	L5	3718	1	-	0/9/27/28	0/3/3/3
46	A2M	S2	468	46	-	0/9/27/28	0/3/3/3
46	PSU	S2	109	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1347	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1244	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	1536	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	3701	1,84	-	4/9/27/28	0/2/2/2
46	OMU	S2	1804	46	-	0/9/27/28	0/2/2/2
46	A2M	S2	1678	46	-	1/9/27/28	0/3/3/3
1	OMC	L5	3841	1	-	1/9/27/28	0/2/2/2
46	PSU	S2	93	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	172	46	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	V5N	La	39	29	-	0/9/10/12	0/1/1/1
1	PSU	L5	3764	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	590	46	-	4/9/27/28	0/3/3/3
1	OMC	L5	2365	1,83	-	0/9/27/28	0/2/2/2
46	B8N	S2	1248	46	-	8/16/34/35	0/2/2/2
1	OMG	L5	4618	1	-	2/9/27/28	0/3/3/3
46	PSU	S2	1045	46	-	1/7/25/26	0/2/2/2
1	OMG	L5	4623	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	2632	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2876	1	-	0/9/27/28	0/3/3/3
46	OMC	S2	174	46	-	1/9/27/28	0/2/2/2
1	PSU	L5	1677	1	-	1/7/25/26	0/2/2/2
1	OMU	L5	2837	1	-	0/9/27/28	0/2/2/2
46	MA6	S2	1851	46	-	6/11/29/30	0/3/3/3
1	PSU	L5	4552	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4423	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2422	1,83	-	2/9/27/28	0/2/2/2
46	PSU	S2	1056	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	572	46	-	2/7/25/26	0/2/2/2
1	PSU	L5	1781	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1683	1,84	-	0/7/25/26	0/2/2/2
1	OMG	L5	3899	1,83	-	1/9/27/28	0/3/3/3
1	PSU	L5	2843	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	2401	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	3830	1	-	0/9/27/28	0/3/3/3
46	PSU	S2	296	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	1744	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	36	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	509	83,46	-	2/9/27/28	0/3/3/3
46	PSU	S2	1004	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	5010	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	63	46	-	0/7/25/26	0/2/2/2
1	A2M	L5	3785	1	-	2/9/27/28	0/3/3/3
1	OMG	L5	3744	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	2351	1,83	-	3/9/27/28	0/2/2/2
1	A2M	L5	1524	1	-	1/9/27/28	0/3/3/3
46	PSU	S2	300	46	-	0/7/25/26	0/2/2/2
46	A2M	S2	99	83,46	-	2/9/27/28	0/3/3/3
1	PSU	L5	3853	1,83	-	0/7/25/26	0/2/2/2
1	A2M	L5	400	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	3639	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4442	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	1323	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	3792	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	4523	1,83	-	1/9/27/28	0/3/3/3
1	A2M	L5	3825	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	3715	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2424	1	-	1/9/27/28	0/3/3/3

The worst 5 of 876 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1832	6MZ	C6-N6	13.64	1.49	1.34
1	L5	4220	6MZ	C6-N6	13.03	1.48	1.34
46	S2	1326	UY1	C6-C5	10.63	1.47	1.35
1	L5	3818	UY1	C6-C5	10.23	1.47	1.35
46	S2	1326	UY1	C2-N1	10.01	1.50	1.36

The worst 5 of 1305 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2876	OMG	C1'-N9-C8	-9.21	100.48	126.70
1	L5	2424	OMG	C1'-N9-C8	-8.90	101.36	126.70
46	S2	683	OMG	C1'-N9-C8	-8.41	102.76	126.70
46	S2	867	OMG	C1'-N9-C8	-8.33	102.99	126.70
1	L5	1625	OMG	C1'-N9-C8	-8.27	103.14	126.70

There are no chirality outliers.

5 of 158 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L8	14	OMU	C1'-C2'-O2'-CM2
66	ST	67	NMM	O-C-CA-CB
1	L5	1582	PSU	O4'-C1'-C5-C4
1	L5	1582	PSU	O4'-C1'-C5-C6
1	L5	1792	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

93 monomers are involved in 139 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	S2	517	OMC	1	0
1	L5	398	A2M	1	0
1	L5	4499	OMG	1	0
1	L5	2787	A2M	1	0
1	L5	2415	OMU	2	0
1	L5	4228	OMG	1	0
46	S2	166	A2M	4	0
1	L5	1534	A2M	2	0
1	L5	1871	A2M	1	0
1	L5	4392	OMG	2	0
46	S2	428	OMU	1	0
46	S2	1447	OMG	2	0
46	S2	1031	A2M	1	0
1	L5	4447	5MC	2	0
1	L5	1881	OMC	2	0
46	S2	1174	PSU	2	0
1	L5	4628	PSU	1	0
3	L8	69	PSU	1	0
1	L5	2824	OMC	1	0
1	L5	4196	OMG	1	0
1	L5	1326	A2M	2	0
46	S2	1596	PSU	1	0
1	L5	3818	UY1	2	0
1	L5	4579	PSU	2	0
46	S2	1850	MA6	2	0
46	S2	686	PSU	1	0
46	S2	576	A2M	5	0
46	S2	801	PSU	1	0
46	S2	116	OMU	2	0
46	S2	484	A2M	2	0
1	L5	3920	PSU	1	0
1	L5	1340	OMC	2	0
46	S2	1703	OMC	3	0
1	L5	4220	6MZ	3	0
46	S2	27	A2M	1	0
46	S2	436	OMG	1	0
1	L5	3925	OMU	1	0
46	S2	867	OMG	5	0
46	S2	1842	4AC	1	0
46	S2	1391	OMC	1	0
46	S2	1337	4AC	1	0
46	S2	822	PSU	2	0
1	L5	4536	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	4498	OMU	1	0
1	L5	4620	OMU	2	0
46	S2	601	OMG	1	0
1	L5	3851	PSU	1	0
46	S2	1643	PSU	1	0
1	L5	4293	PSU	1	0
46	S2	1445	PSU	1	0
46	S2	159	A2M	1	0
46	S2	462	OMC	2	0
1	L5	3724	A2M	1	0
46	S2	1383	A2M	1	0
1	L5	2363	A2M	3	0
1	L5	4571	A2M	2	0
1	L5	4471	PSU	1	0
1	L5	4521	PSU	1	0
46	S2	121	OMU	1	0
1	L5	4689	PSU	1	0
1	L5	4500	PSU	2	0
1	L5	4673	PSU	2	0
1	L5	2364	OMG	1	0
1	L5	3770	PSU	1	0
46	S2	1692	PSU	1	0
46	S2	1232	PSU	2	0
1	L5	3867	A2M	5	0
1	L5	4457	PSU	1	0
46	S2	512	A2M	2	0
46	S2	681	PSU	1	0
1	L5	2804	OMC	1	0
1	L5	4296	PSU	1	0
46	S2	1288	OMU	1	0
1	L5	4637	OMG	1	0
1	L5	3718	A2M	1	0
46	S2	468	A2M	1	0
1	L5	3701	OMC	1	0
46	S2	1678	A2M	2	0
1	L5	3841	OMC	1	0
46	S2	590	A2M	4	0
1	L5	4618	OMG	1	0
1	L5	2876	OMG	1	0
46	S2	174	OMC	1	0
46	S2	1851	MA6	2	0
1	L5	4552	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	2422	OMC	1	0
46	S2	572	PSU	1	0
1	L5	1781	PSU	1	0
46	S2	509	OMG	1	0
1	L5	3785	A2M	1	0
1	L5	2351	OMC	3	0
1	L5	3792	OMG	1	0
1	L5	2424	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 429 ligands modelled in this entry, 408 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	NMY	L5	5379	-	45,45,45	1.02	2 (4%)	63,67,67	1.13	5 (7%)
86	NMY	L5	5383	-	45,45,45	0.79	1 (2%)	63,67,67	1.48	8 (12%)
86	NMY	L5	5389	-	45,45,45	0.68	1 (2%)	63,67,67	1.36	7 (11%)
86	NMY	L5	5380	-	45,45,45	0.73	1 (2%)	63,67,67	1.04	3 (4%)
86	NMY	L5	5382	-	45,45,45	0.65	0	63,67,67	1.03	2 (3%)
86	NMY	L5	5385	-	45,45,45	0.73	1 (2%)	63,67,67	1.26	5 (7%)
85	SPD	L5	5376	-	9,9,9	0.28	0	8,8,8	0.29	0
86	NMY	L5	5381	-	45,45,45	0.73	0	63,67,67	1.12	4 (6%)
88	IAS	SO	202	-	6,7,8	1.07	0	6,8,10	1.52	1 (16%)
85	SPD	L5	5377	-	9,9,9	0.35	0	8,8,8	0.72	0
86	NMY	S2	1966	-	45,45,45	0.60	0	63,67,67	1.49	11 (17%)
86	NMY	L5	5384	-	45,45,45	0.68	0	63,67,67	1.57	10 (15%)
85	SPD	L5	5375	-	9,9,9	0.25	0	8,8,8	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	NMY	L7	202	-	45,45,45	0.90	1 (2%)	63,67,67	2.18	21 (33%)
86	NMY	L5	5387	-	45,45,45	0.75	2 (4%)	63,67,67	1.57	13 (20%)
86	NMY	L5	5378	-	45,45,45	0.79	1 (2%)	63,67,67	1.24	4 (6%)
86	NMY	L5	5386	-	45,45,45	0.71	0	63,67,67	1.12	6 (9%)
86	NMY	S2	1975	83	45,45,45	0.87	2 (4%)	63,67,67	1.12	5 (7%)
86	NMY	L5	5388	-	45,45,45	0.67	0	63,67,67	1.25	7 (11%)
86	NMY	S2	1902	-	45,45,45	0.68	0	63,67,67	1.17	5 (7%)
86	NMY	S2	1945	-	45,45,45	0.76	1 (2%)	63,67,67	1.04	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	NMY	L5	5379	-	-	5/18/94/94	0/4/4/4
86	NMY	L5	5383	-	-	5/18/94/94	0/4/4/4
86	NMY	L5	5389	-	-	6/18/94/94	0/4/4/4
86	NMY	L5	5380	-	-	10/18/94/94	0/4/4/4
86	NMY	L5	5382	-	-	10/18/94/94	0/4/4/4
86	NMY	L5	5385	-	-	12/18/94/94	0/4/4/4
85	SPD	L5	5376	-	-	4/7/7/7	-
86	NMY	L5	5381	-	-	6/18/94/94	0/4/4/4
88	IAS	SO	202	-	-	0/7/7/8	-
85	SPD	L5	5377	-	-	4/7/7/7	-
86	NMY	S2	1966	-	-	12/18/94/94	0/4/4/4
86	NMY	L5	5384	-	-	8/18/94/94	0/4/4/4
85	SPD	L5	5375	-	-	3/7/7/7	-
86	NMY	L7	202	-	-	7/18/94/94	0/4/4/4
86	NMY	L5	5387	-	-	12/18/94/94	0/4/4/4
86	NMY	L5	5378	-	-	2/18/94/94	0/4/4/4
86	NMY	L5	5386	-	-	9/18/94/94	0/4/4/4
86	NMY	S2	1975	83	-	3/18/94/94	0/4/4/4
86	NMY	L5	5388	-	-	6/18/94/94	0/4/4/4
86	NMY	S2	1902	-	-	9/18/94/94	0/4/4/4
86	NMY	S2	1945	-	-	6/18/94/94	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	L7	202	NMY	C3-C2	-2.90	1.49	1.53
86	L5	5379	NMY	C2-N2	-2.57	1.43	1.47
86	L5	5378	NMY	C2-N2	-2.29	1.43	1.47
86	L5	5385	NMY	C13-C14	-2.26	1.50	1.52
86	L5	5389	NMY	C13-C14	-2.25	1.50	1.52

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	L7	202	NMY	C1-O1-C10	-6.09	102.89	117.96
86	L5	5389	NMY	O11-C13-O16	-5.64	105.33	111.43
86	L7	202	NMY	C8-C7-C12	5.35	118.12	110.04
86	L7	202	NMY	C12-C11-C10	-5.28	99.60	111.66
86	L5	5383	NMY	C8-C7-C12	4.94	117.50	110.04

There are no chirality outliers.

5 of 139 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	L5	5378	NMY	C21-C22-C23-N19
86	L5	5378	NMY	O22-C22-C23-N19
86	L5	5380	NMY	C14-C13-O11-C11
86	L5	5380	NMY	C21-C22-C23-N19
86	L5	5380	NMY	O22-C22-C23-N19

There are no ring outliers.

16 monomers are involved in 41 short contacts:

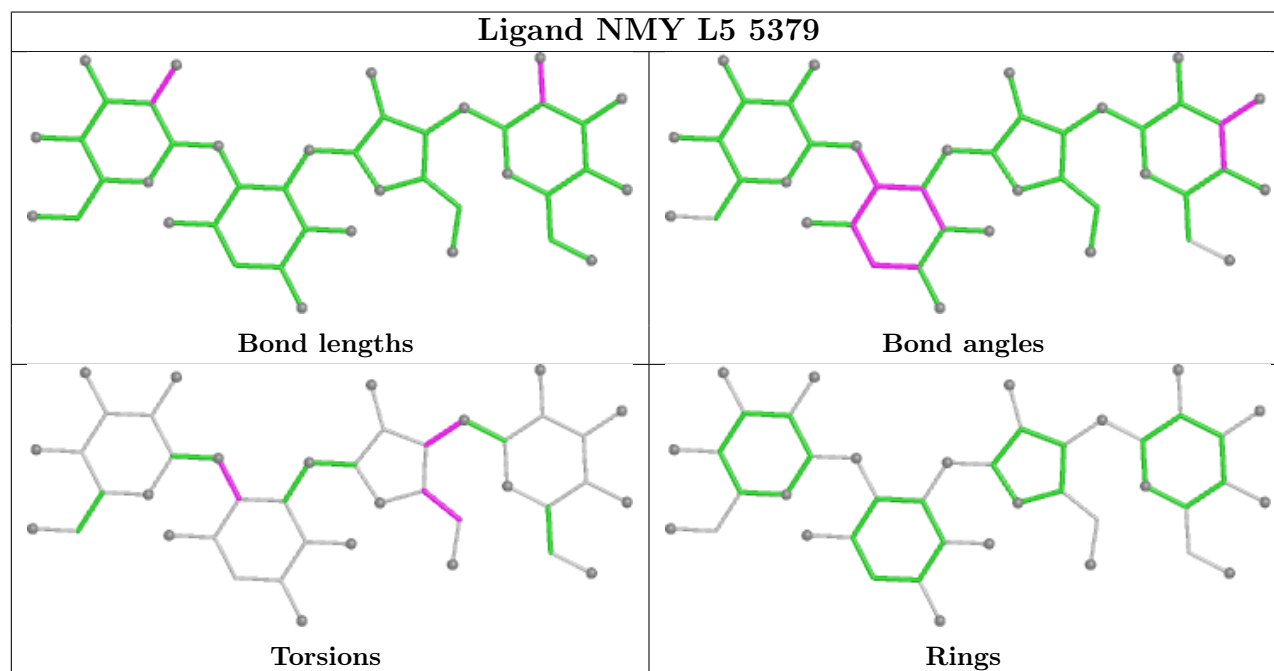
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5379	NMY	1	0
86	L5	5383	NMY	4	0
86	L5	5389	NMY	2	0
86	L5	5380	NMY	1	0
86	L5	5382	NMY	2	0
86	L5	5385	NMY	6	0
85	L5	5376	SPD	2	0
86	L5	5381	NMY	1	0
85	L5	5377	SPD	1	0
86	S2	1966	NMY	5	0
86	L5	5384	NMY	4	0

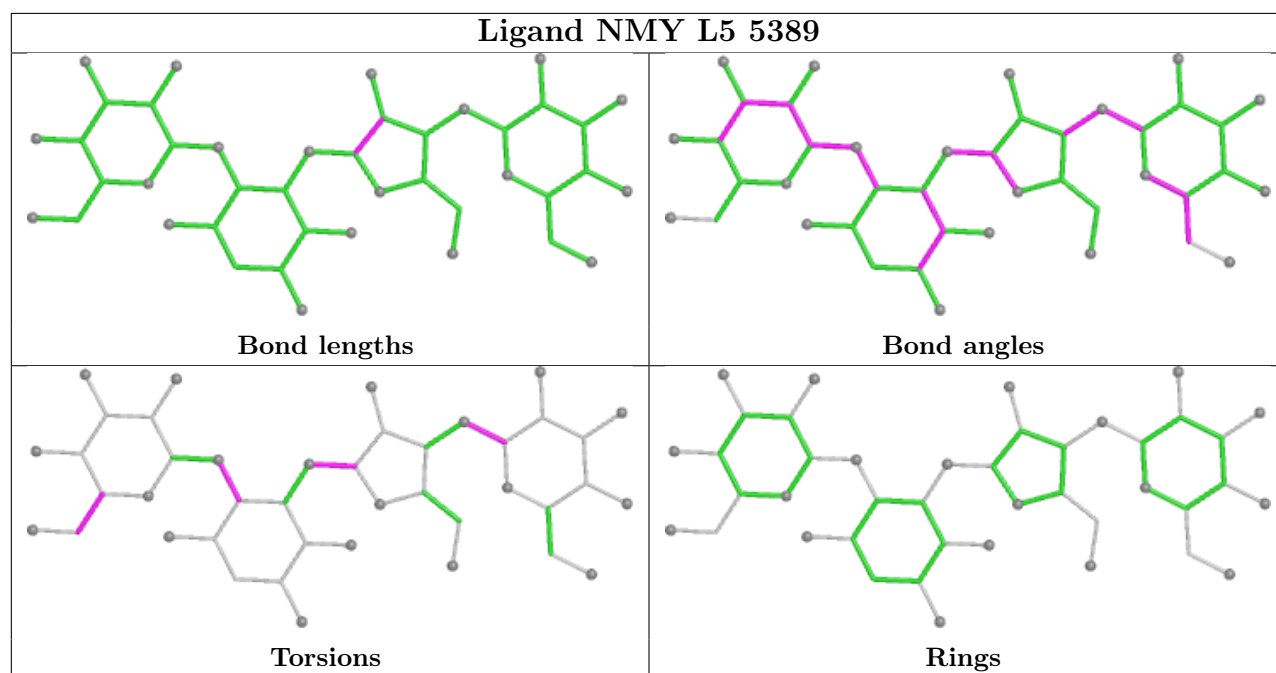
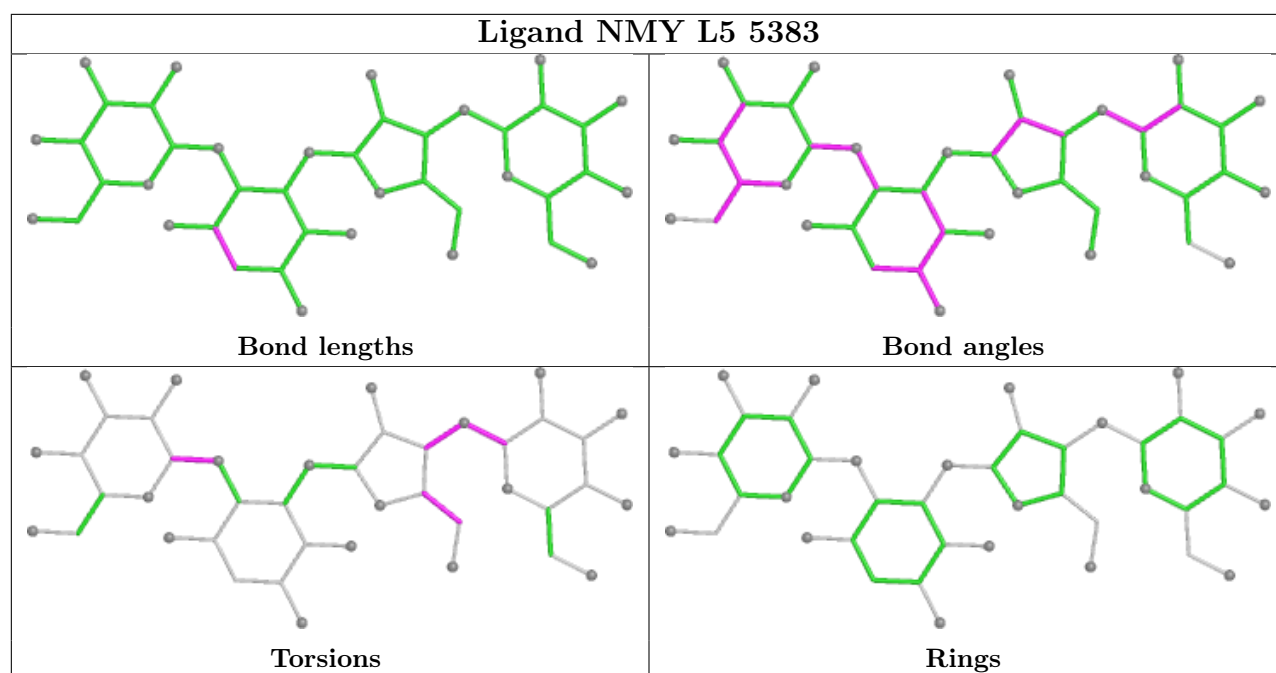
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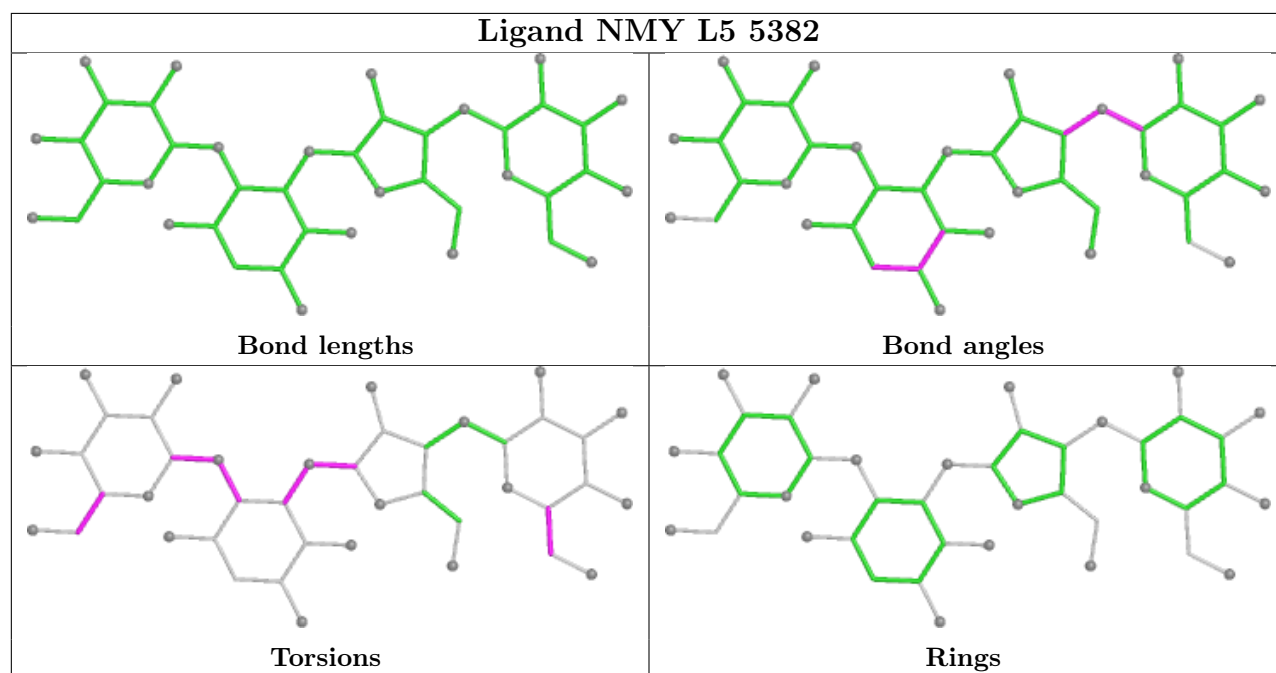
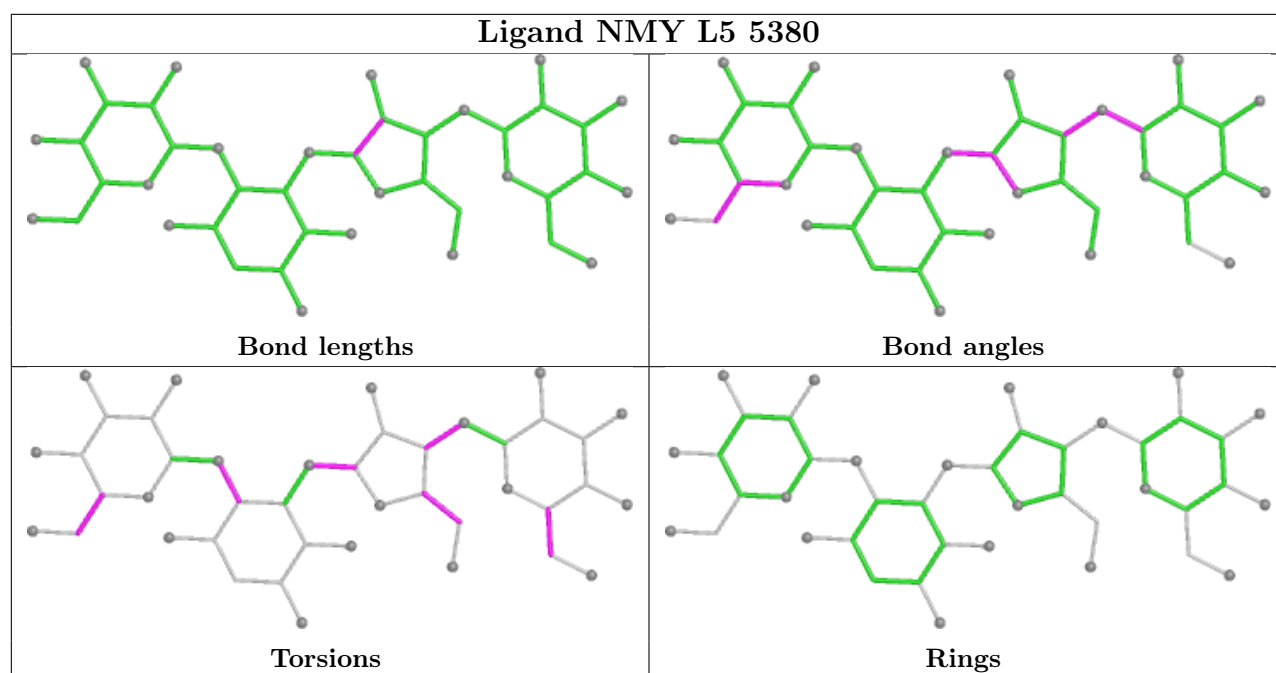
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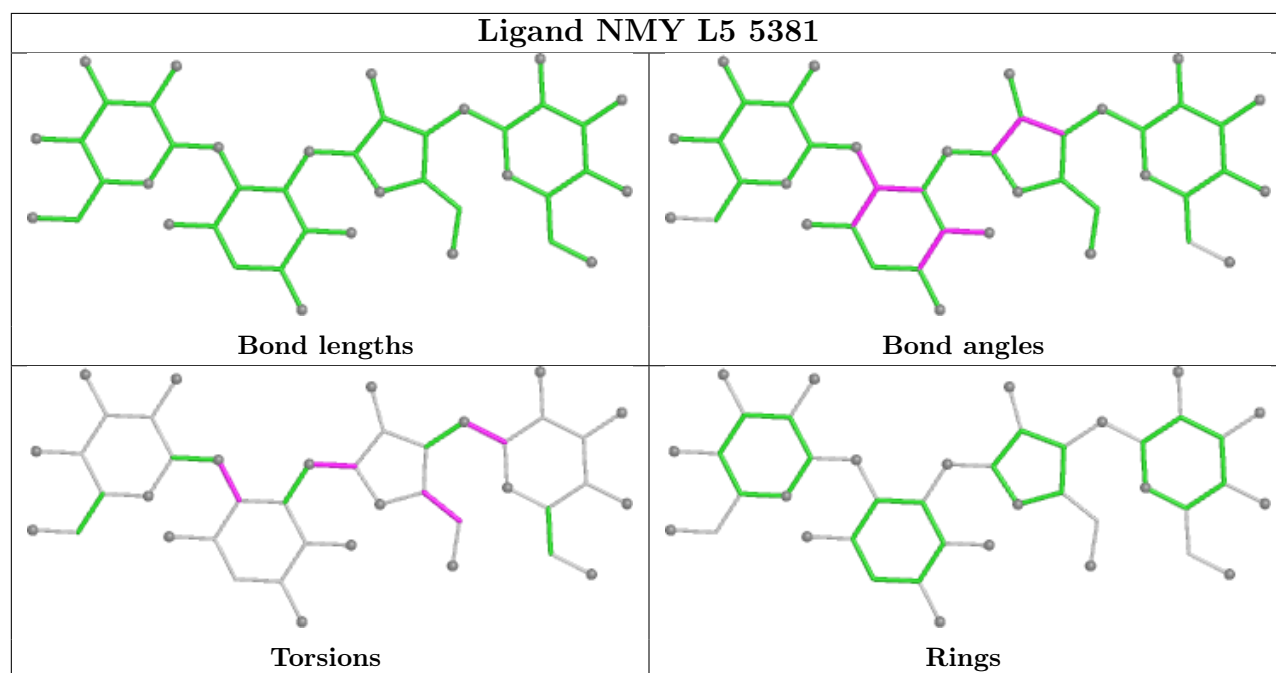
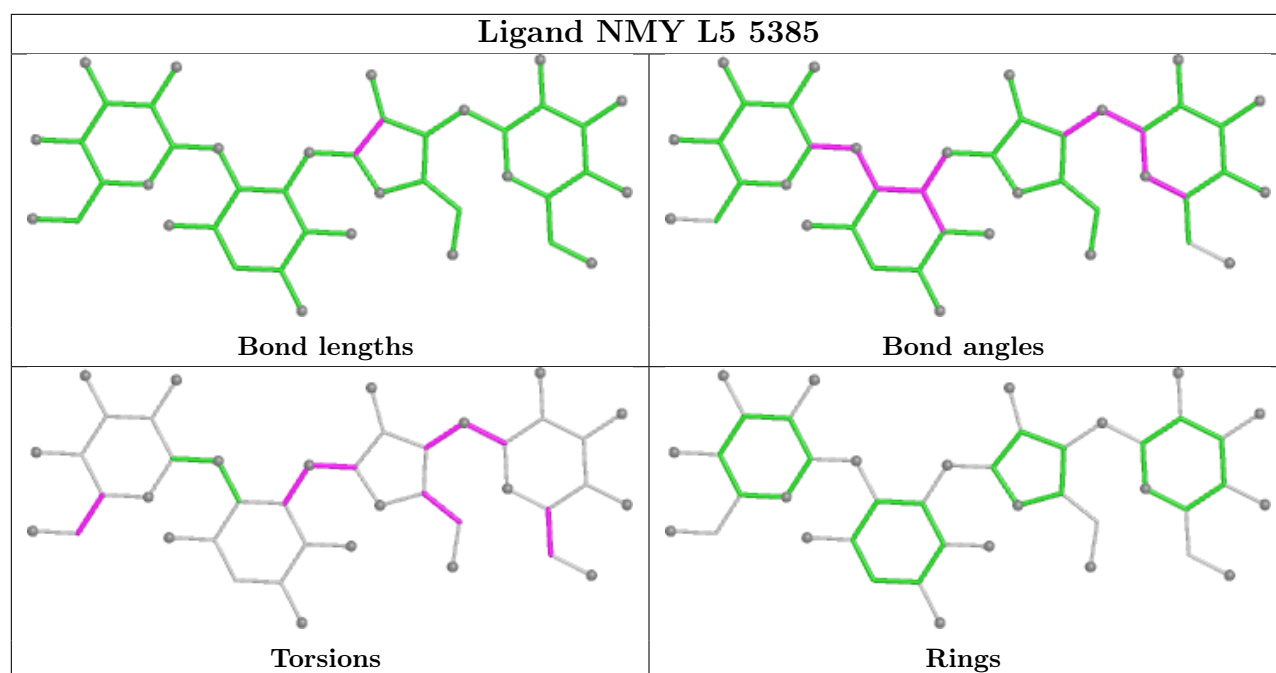
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L7	202	NMY	4	0
86	L5	5387	NMY	5	0
86	L5	5378	NMY	1	0
86	L5	5386	NMY	1	0
86	S2	1902	NMY	1	0

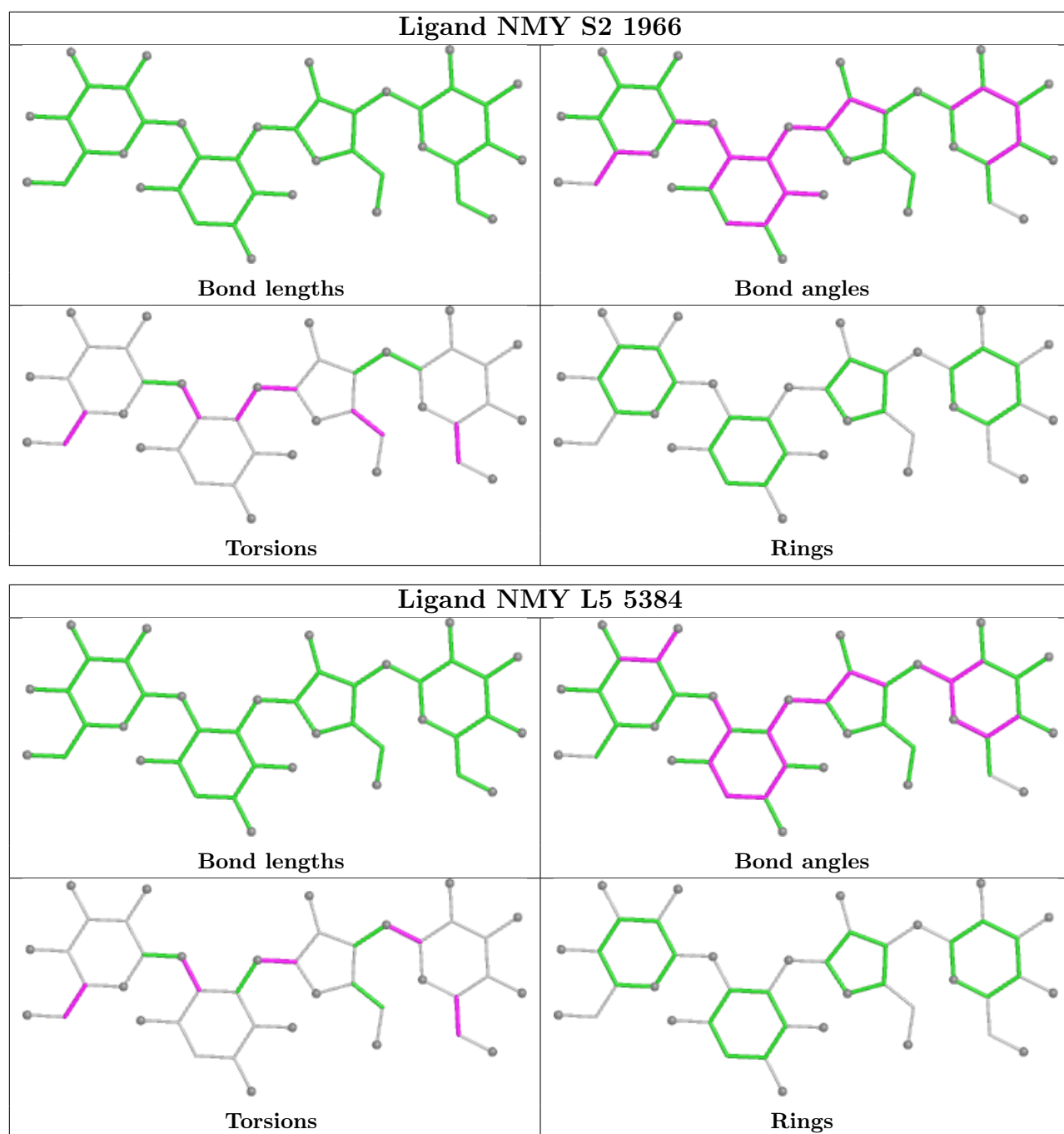
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

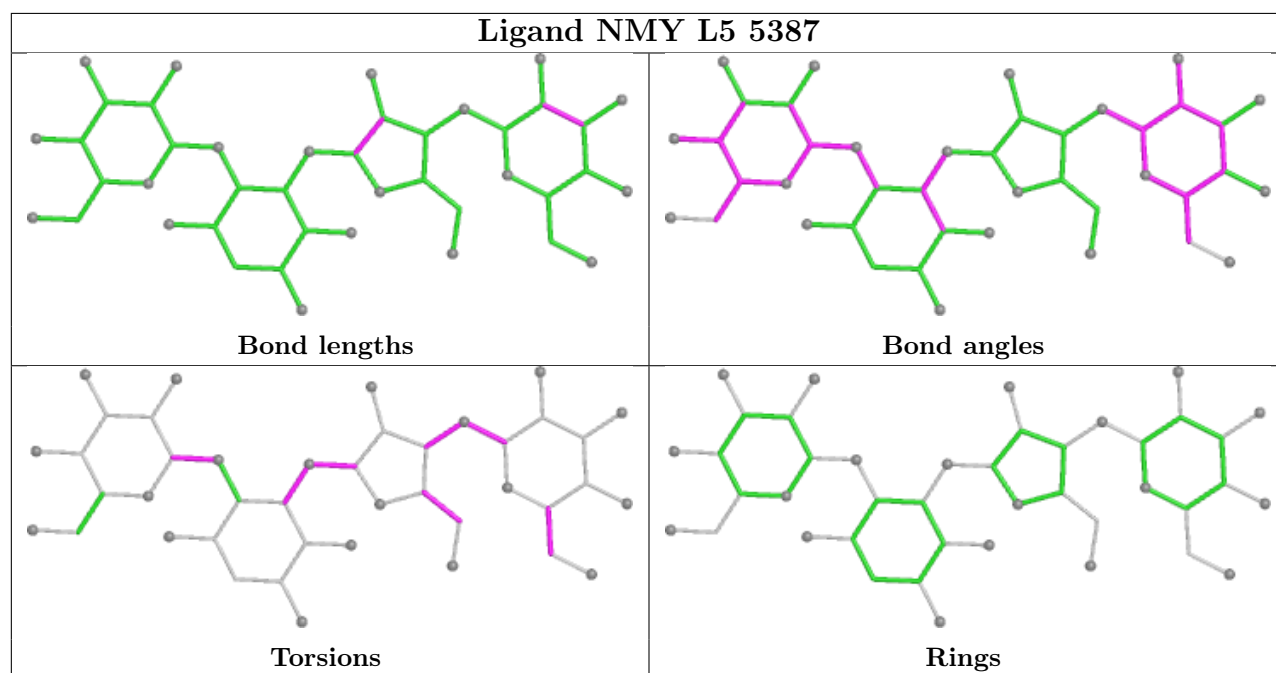
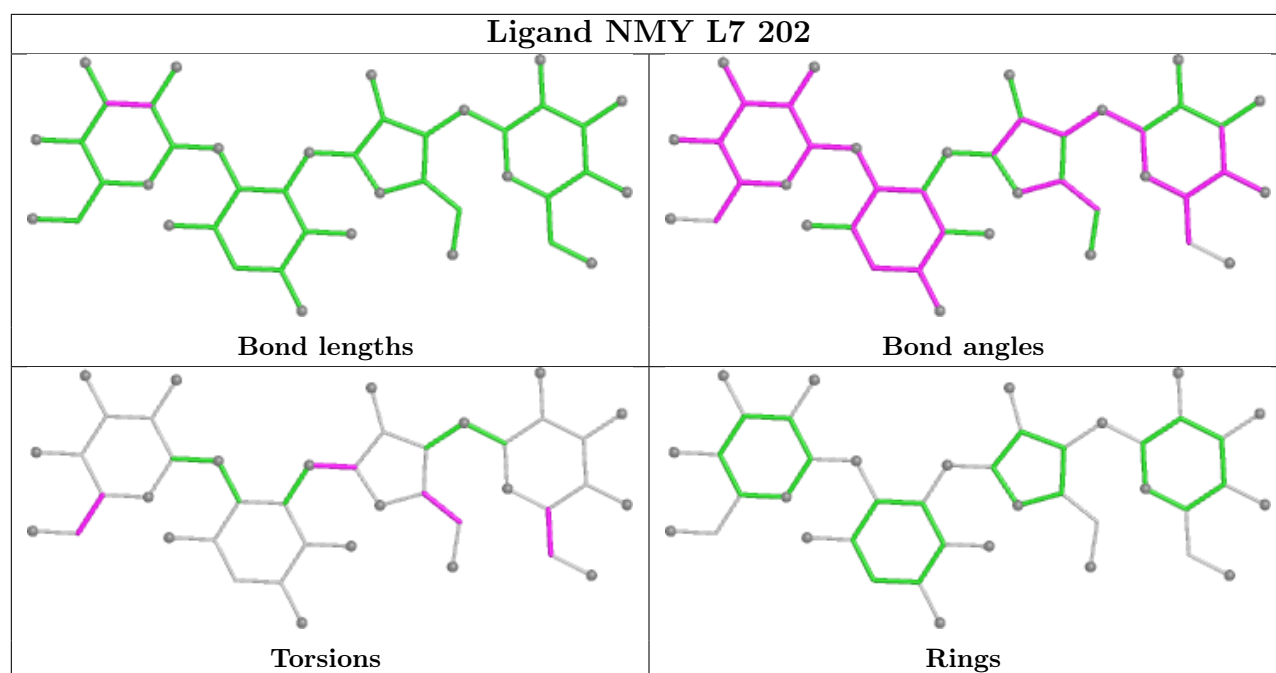


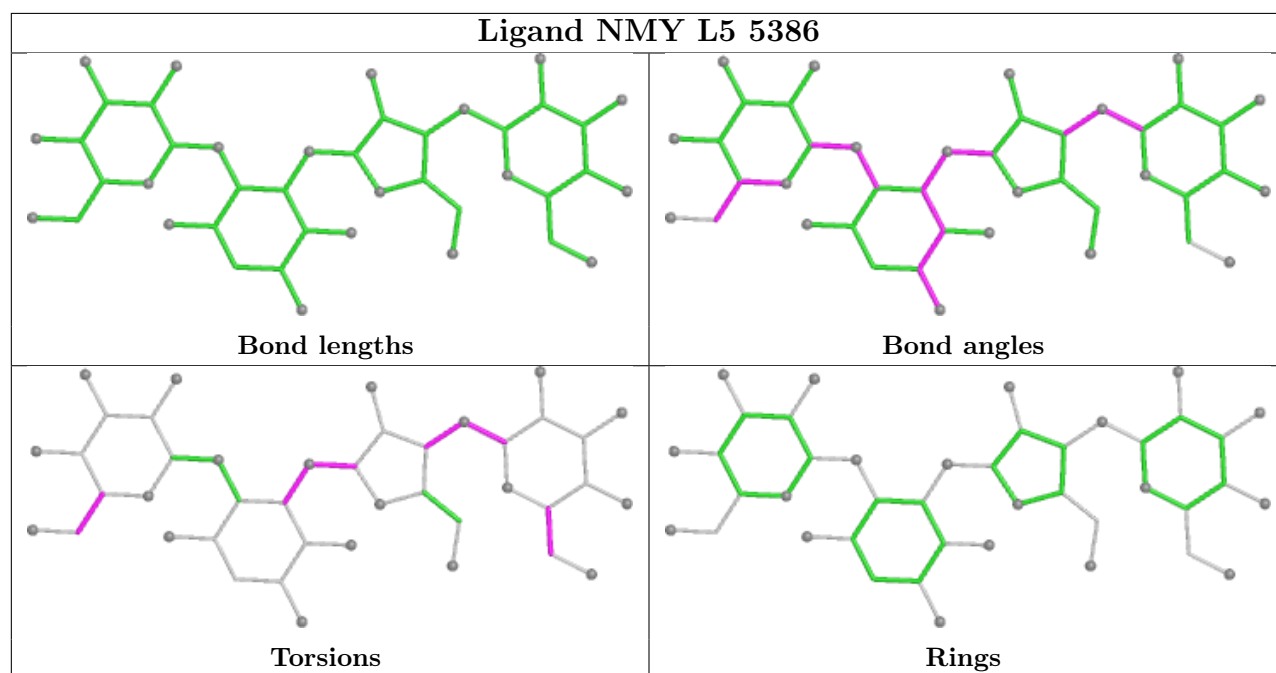
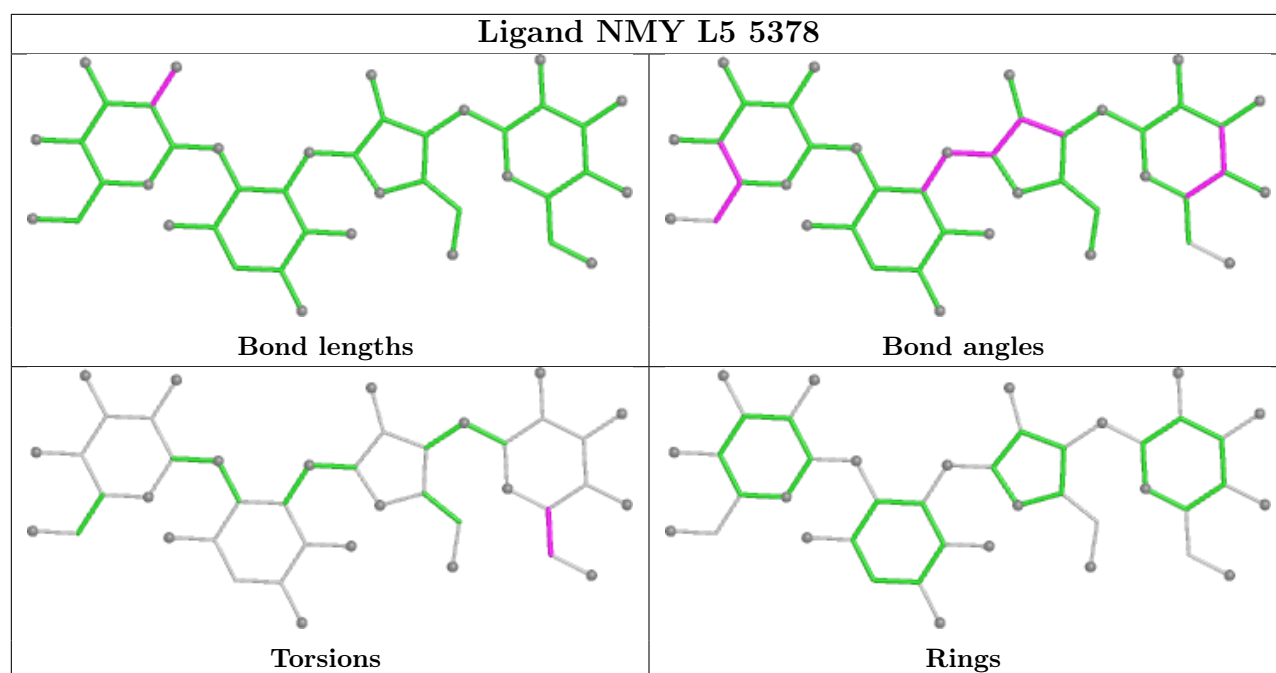


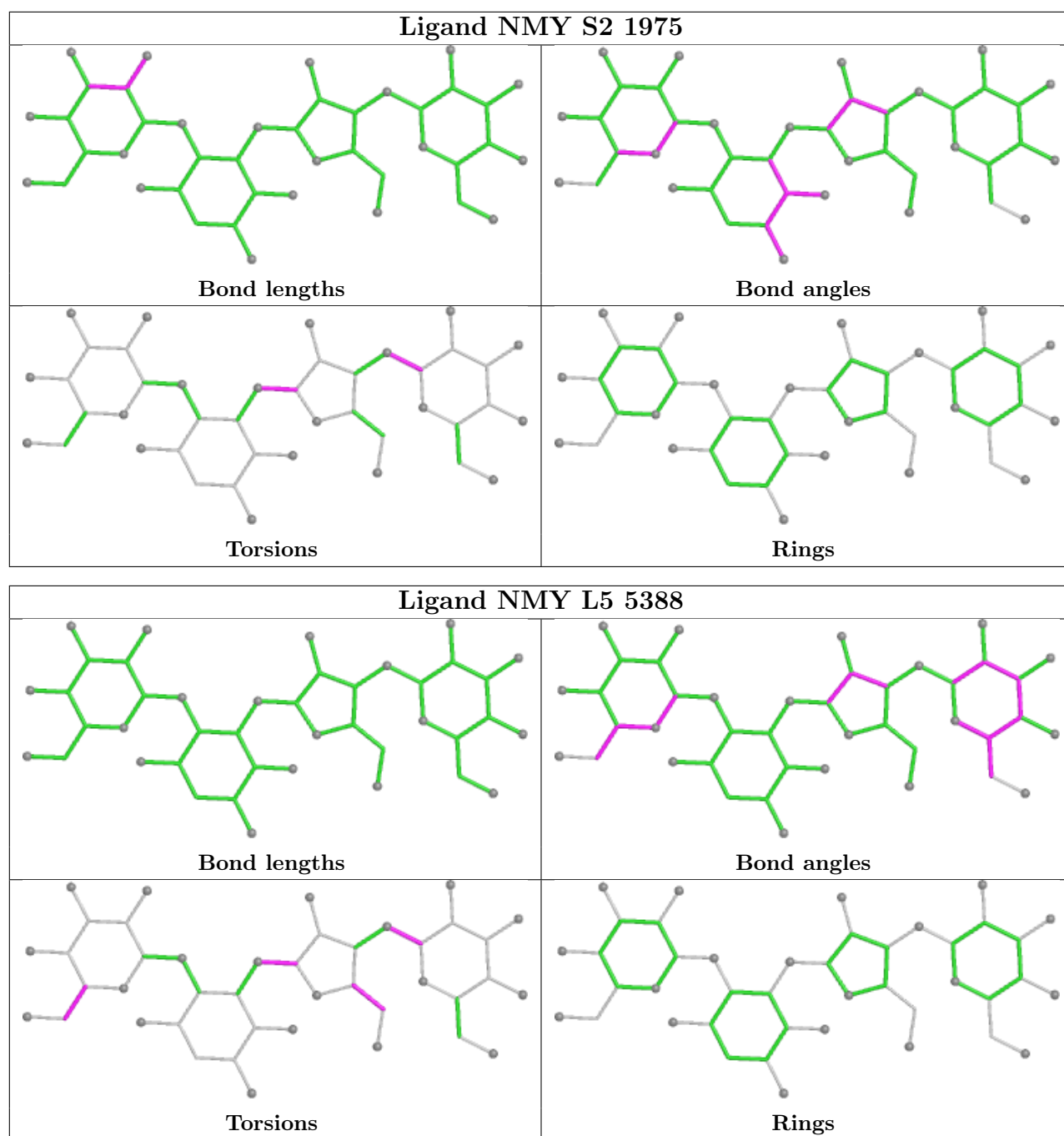


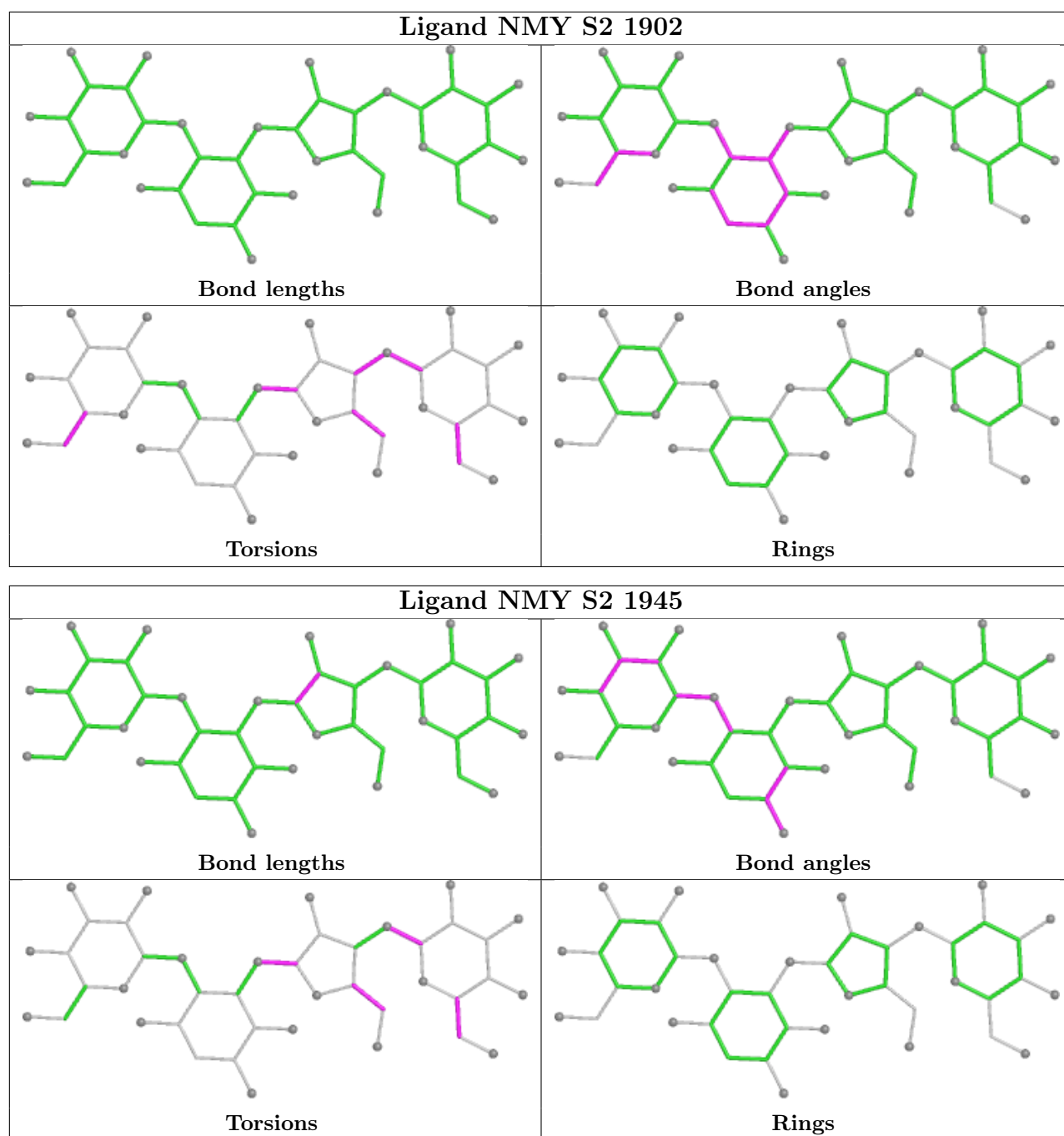












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

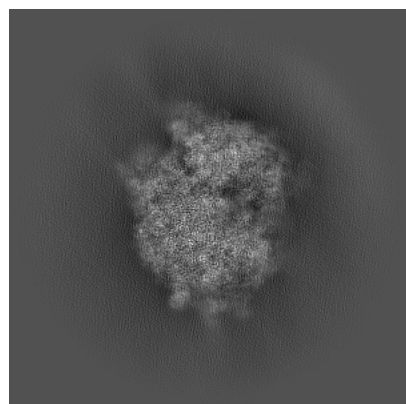
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65434. These allow visual inspection of the internal detail of the map and identification of artifacts.

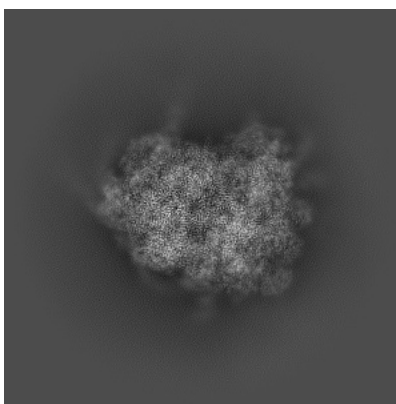
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

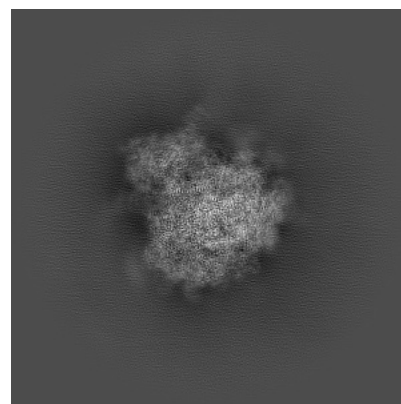
6.1.1 Primary map



X

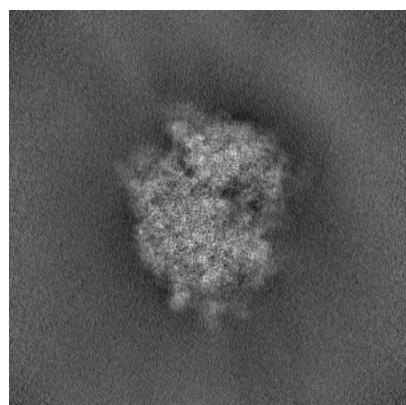


Y

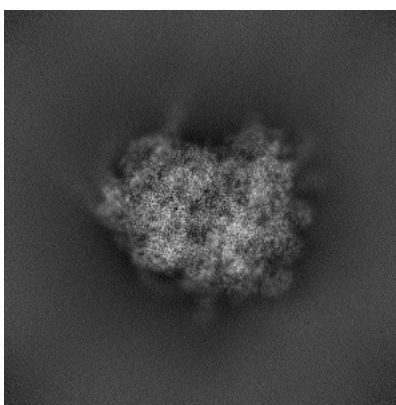


Z

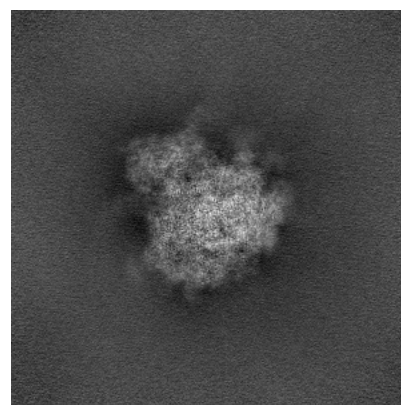
6.1.2 Raw map



X



Y

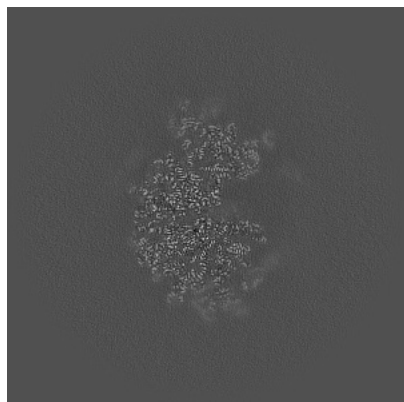


Z

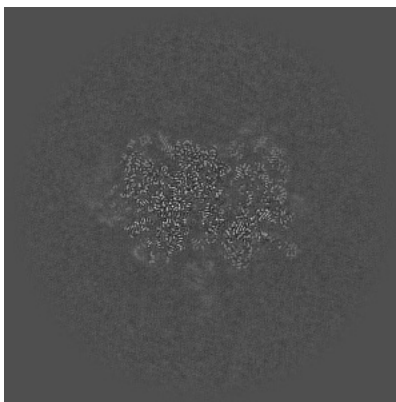
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

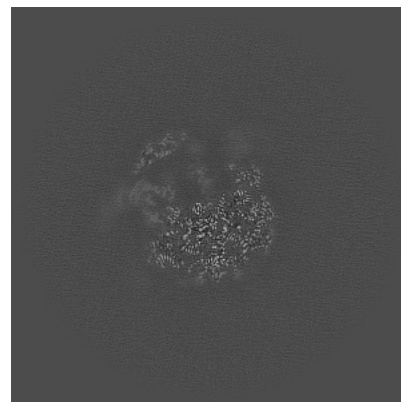
6.2.1 Primary map



X Index: 340

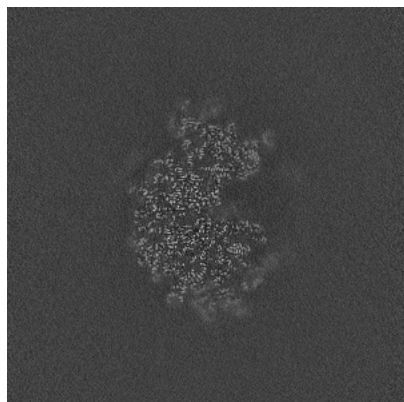


Y Index: 340

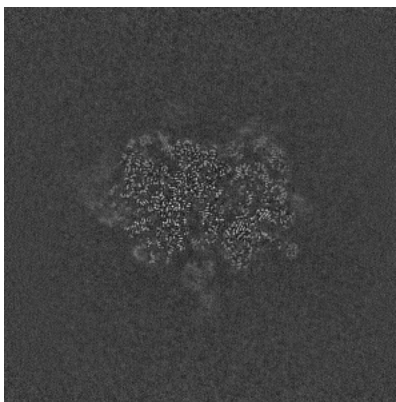


Z Index: 340

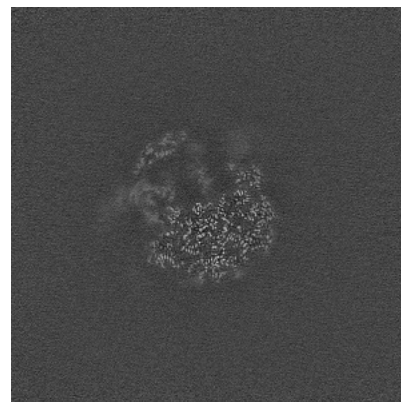
6.2.2 Raw map



X Index: 340



Y Index: 340

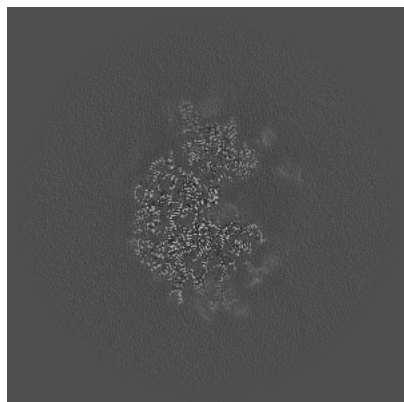


Z Index: 340

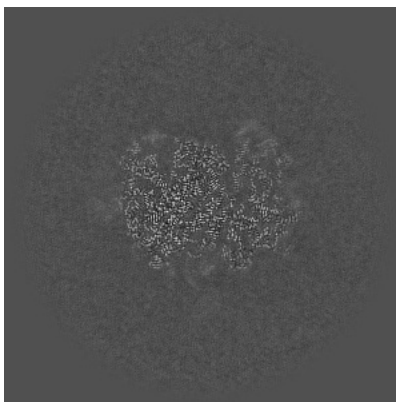
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

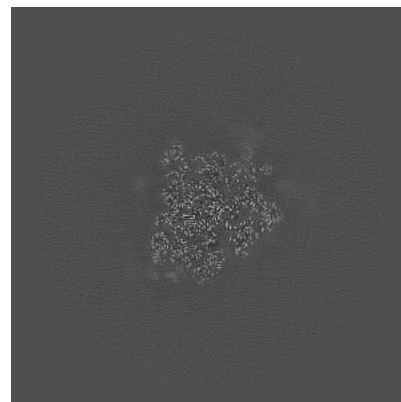
6.3.1 Primary map



X Index: 335

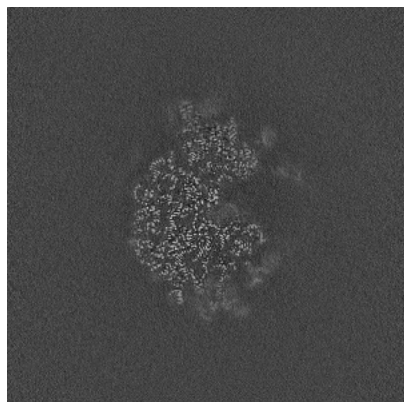


Y Index: 331

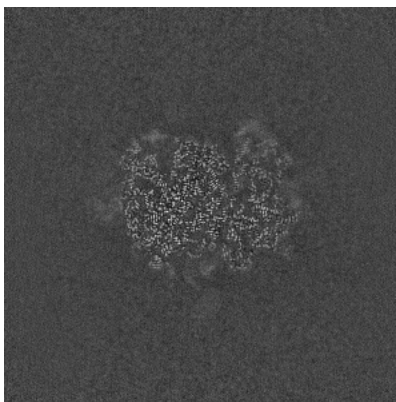


Z Index: 298

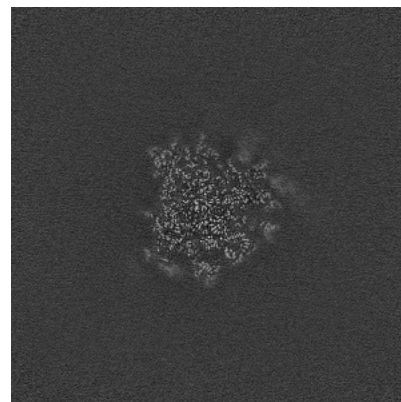
6.3.2 Raw map



X Index: 335



Y Index: 331

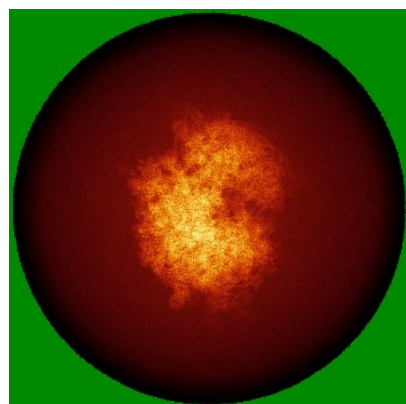


Z Index: 281

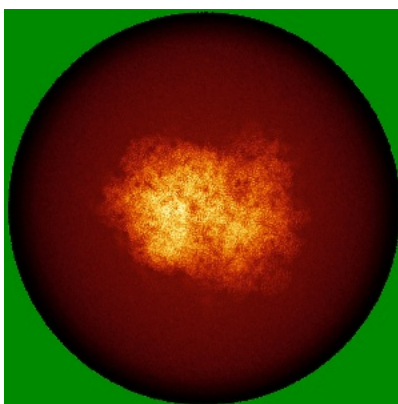
The images above show the largest variance slices of the map in three orthogonal directions.

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

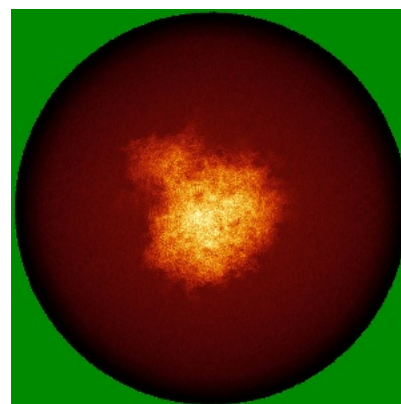
6.4.1 Primary map



X

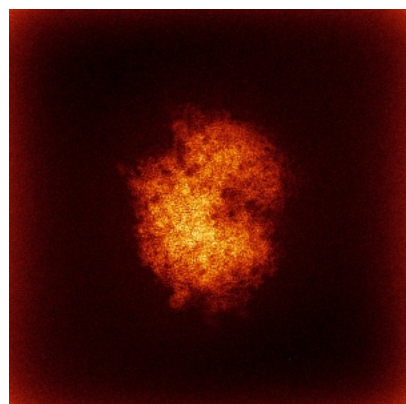


Y

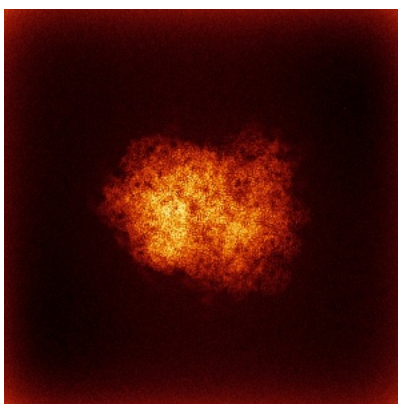


Z

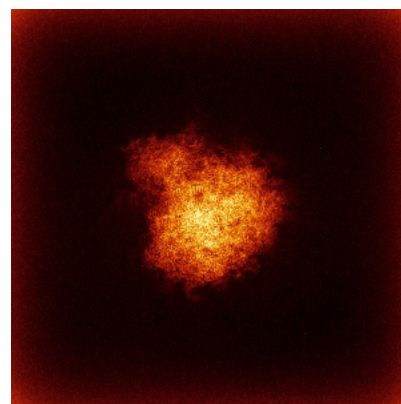
6.4.2 Raw map



X



Y

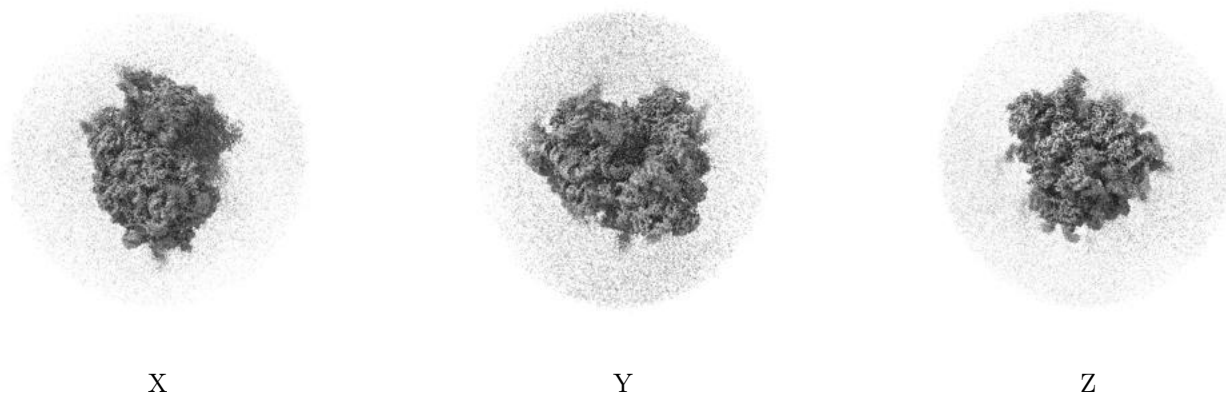


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

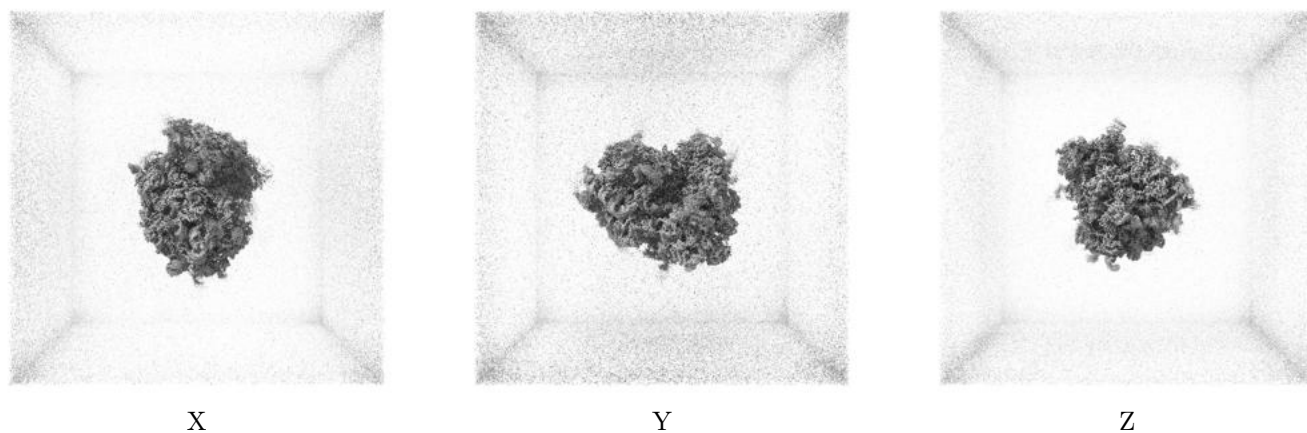
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

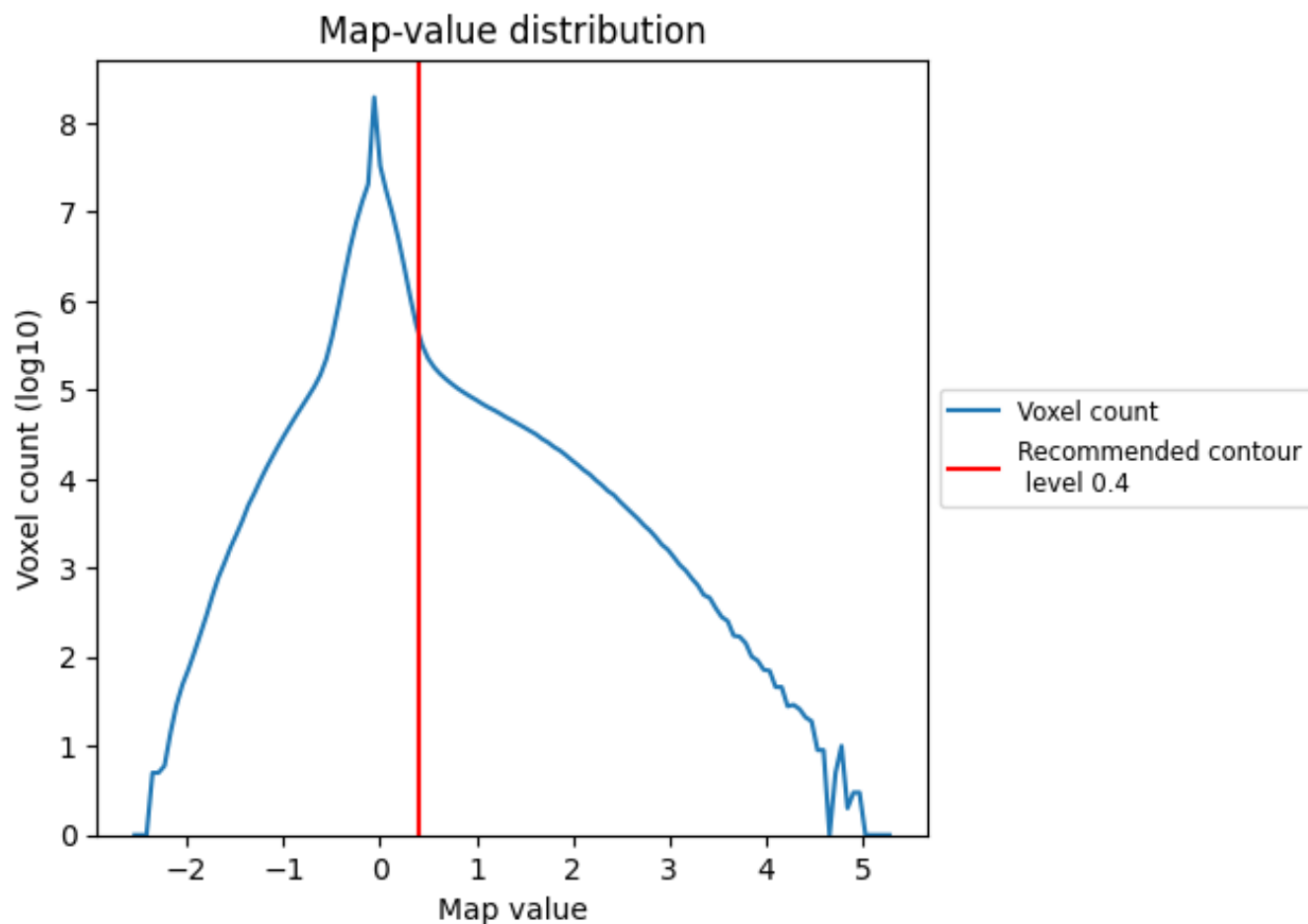
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

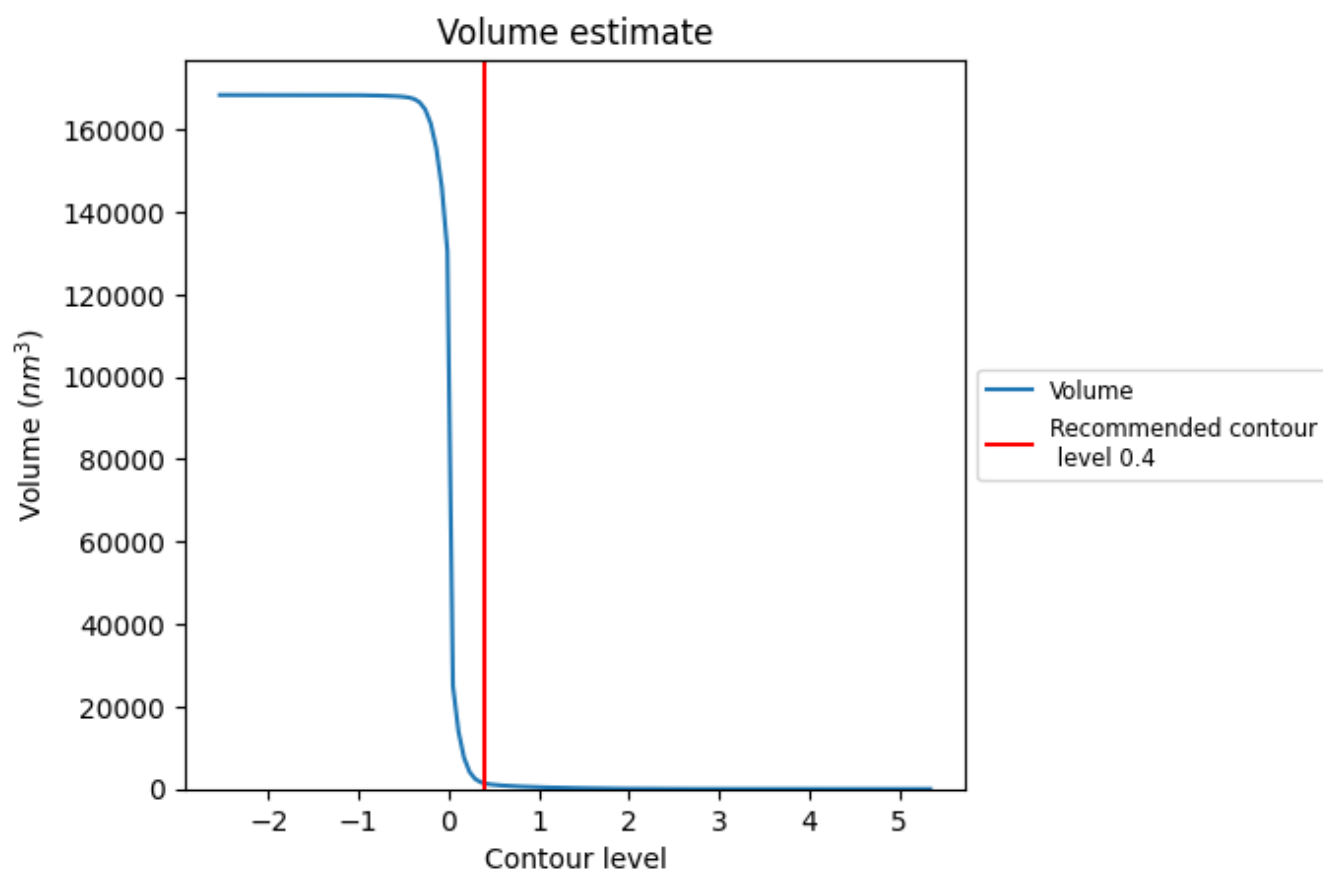
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

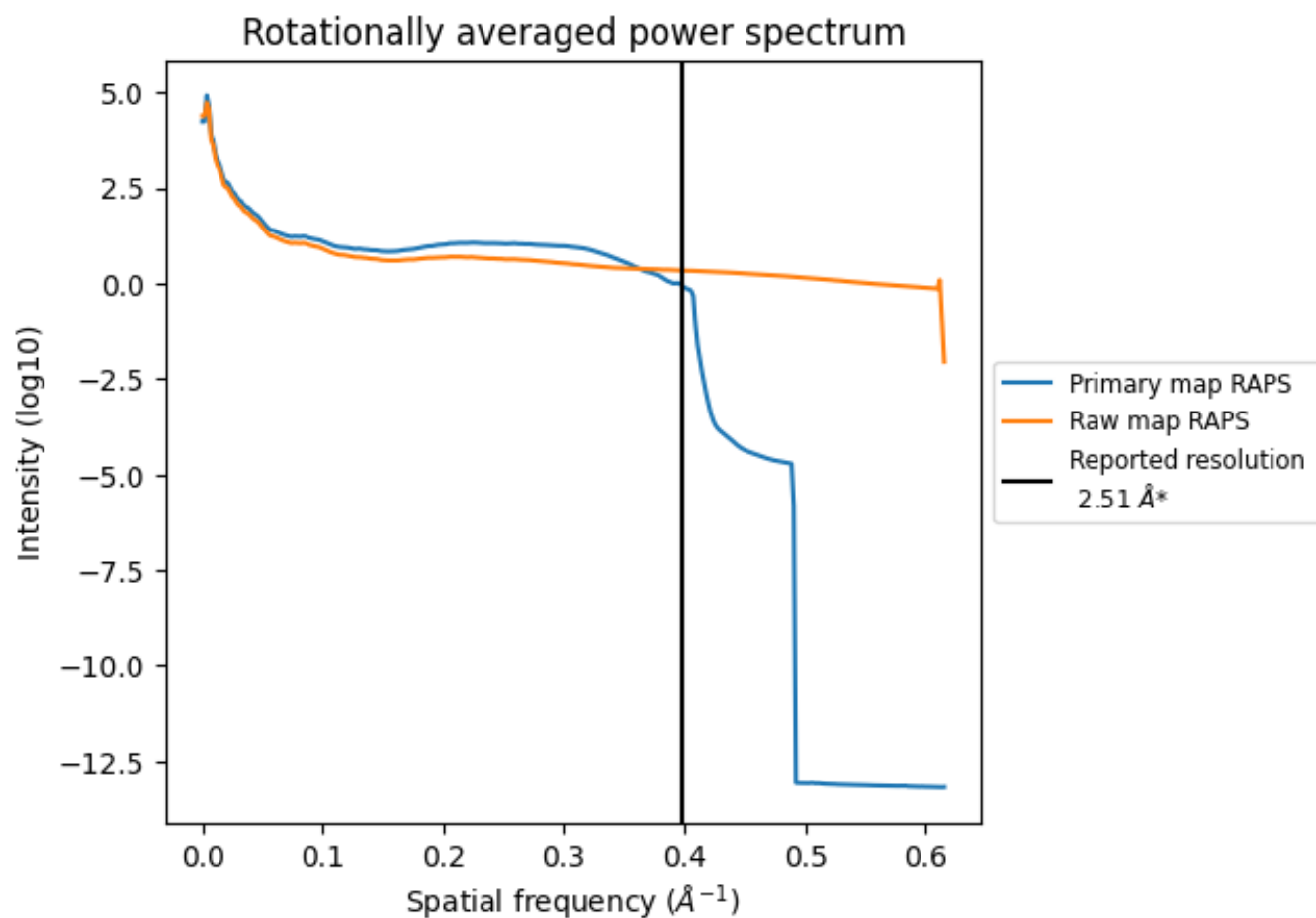
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1362 nm³; this corresponds to an approximate mass of 1231 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 ⓘ

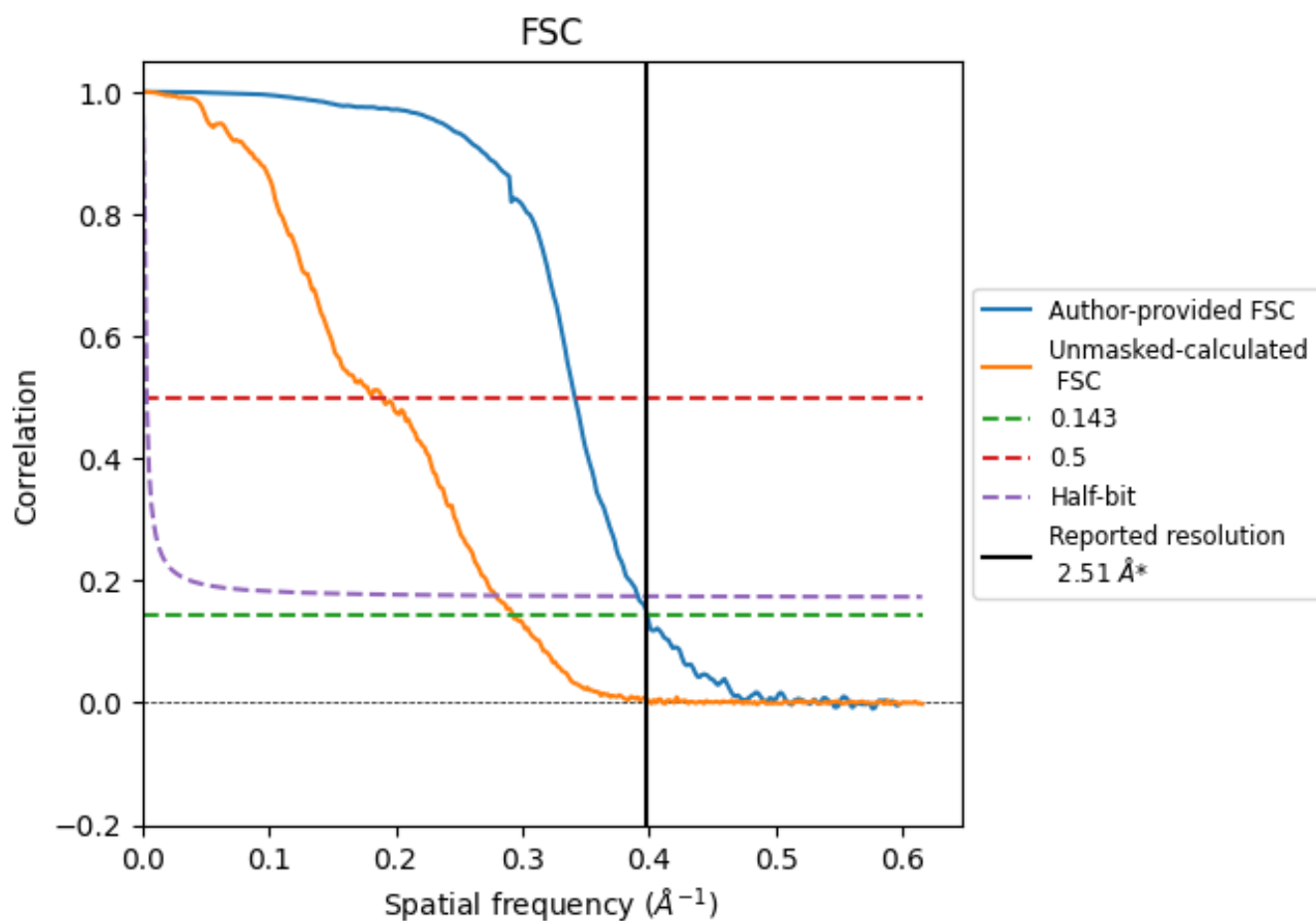


*Reported resolution corresponds to spatial frequency of 0.398 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.398 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

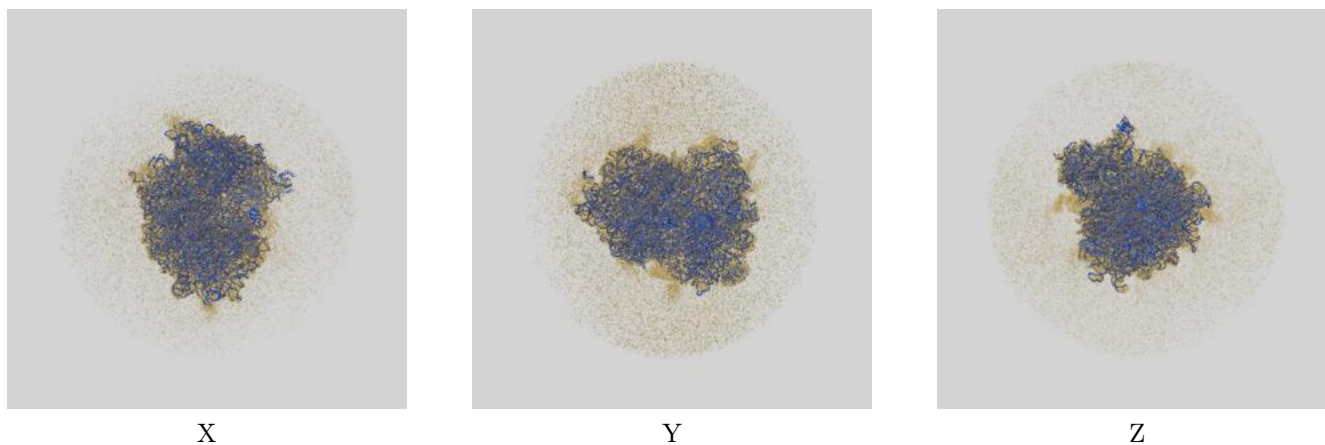
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.51	-	-
Author-provided FSC curve	2.51	2.93	2.56
Unmasked-calculated*	3.42	5.28	3.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 2.51 by more than 10 %

9 Map-model fit [i](#)

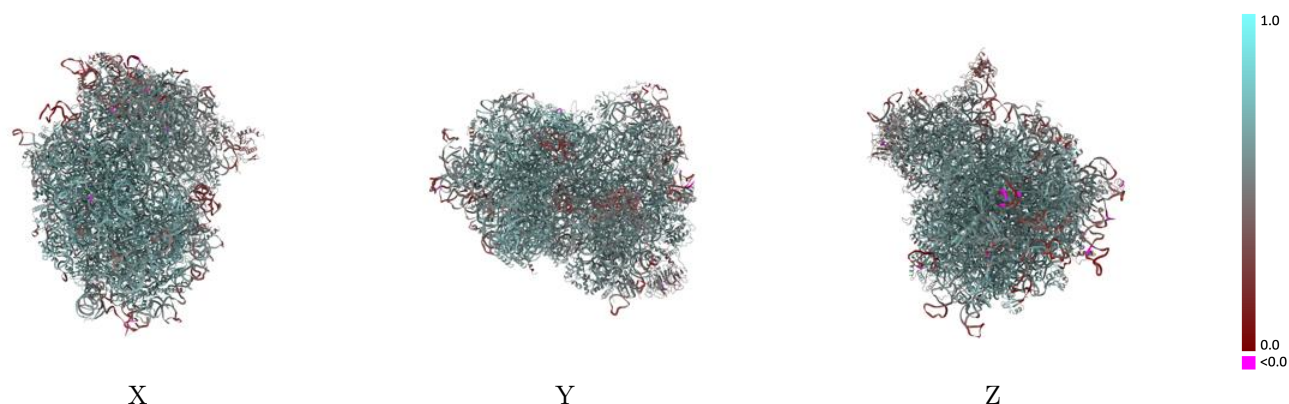
This section contains information regarding the fit between EMDB map EMD-65434 and PDB model 9VXN. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



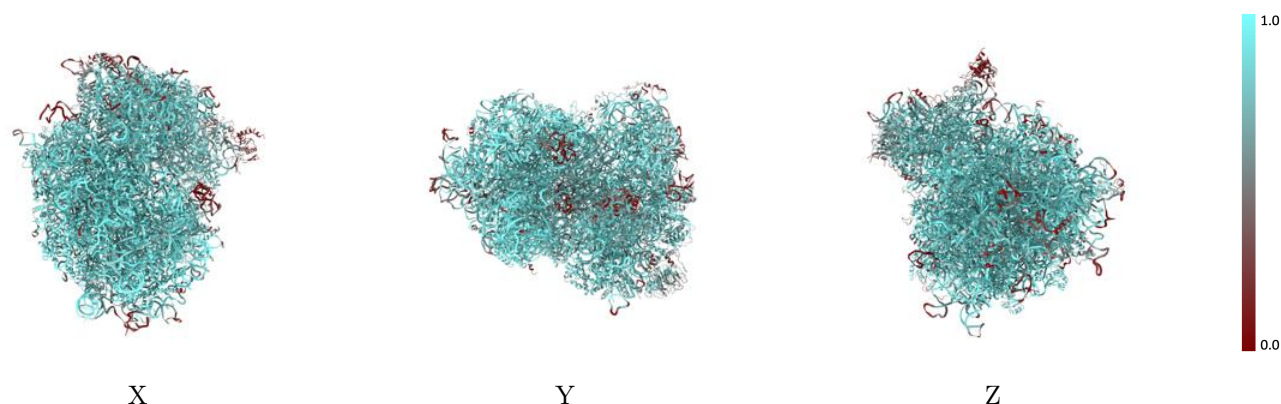
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



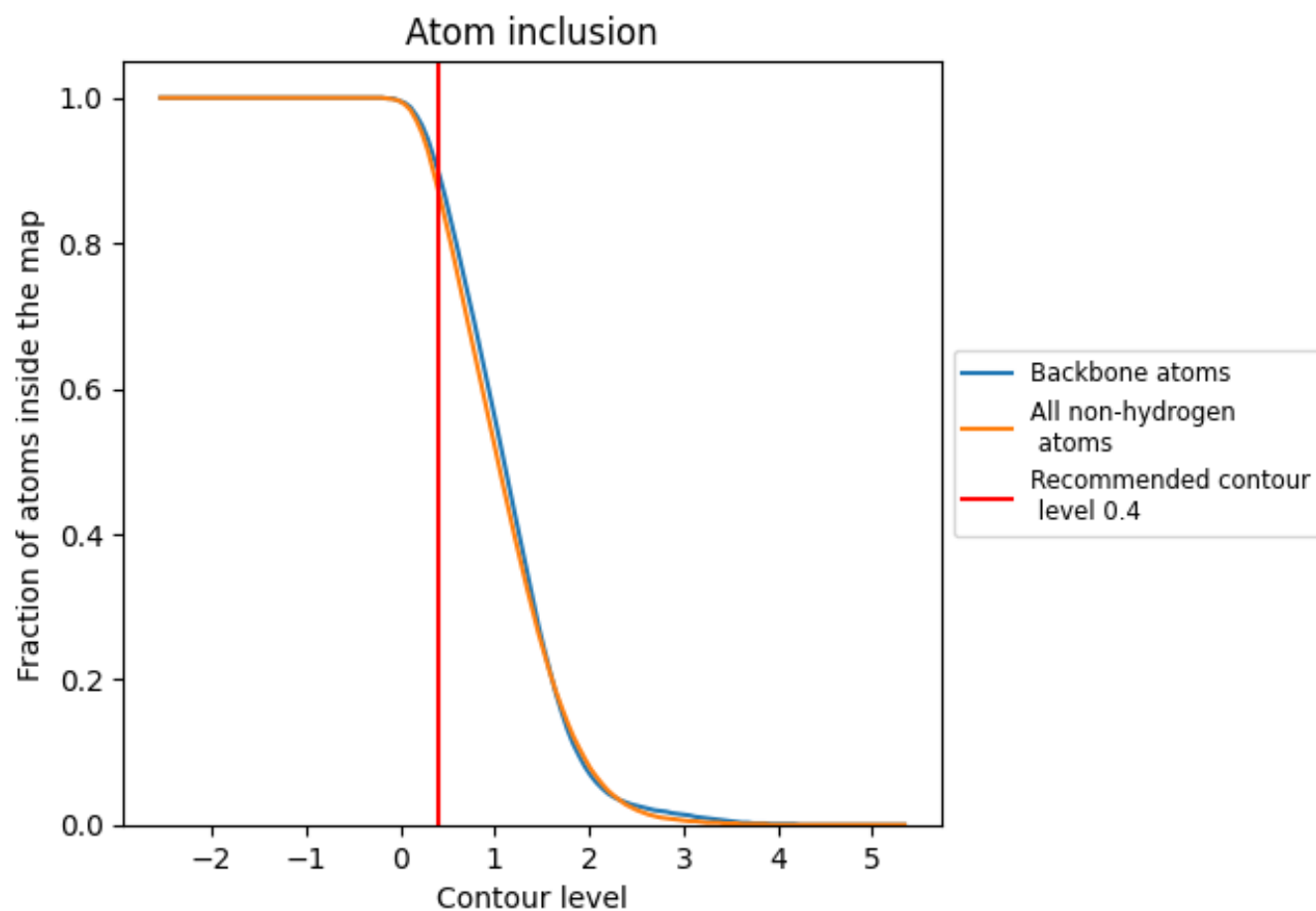
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5850
L5	 0.8990	 0.5870
L7	 0.9790	 0.6320
L8	 0.9360	 0.6160
LA	 0.9710	 0.6640
LB	 0.9380	 0.6450
LC	 0.9390	 0.6430
LD	 0.9170	 0.6140
LE	 0.8430	 0.5860
LF	 0.9490	 0.6540
LG	 0.8280	 0.5790
LH	 0.9230	 0.6310
LI	 0.8970	 0.6200
LJ	 0.8640	 0.5920
LL	 0.8850	 0.6140
LM	 0.9290	 0.6210
LN	 0.9810	 0.6670
LO	 0.9420	 0.6450
LP	 0.9650	 0.6600
LQ	 0.9590	 0.6610
LR	 0.8560	 0.6070
LS	 0.9620	 0.6540
LT	 0.9230	 0.6350
LU	 0.8050	 0.5500
LV	 0.9400	 0.6540
LW	 0.7070	 0.5320
LX	 0.9100	 0.6320
LY	 0.9400	 0.6430
LZ	 0.9010	 0.6100
La	 0.9720	 0.6620
Lb	 0.8860	 0.6090
Lc	 0.8850	 0.6170
Ld	 0.9220	 0.6280
Le	 0.9660	 0.6650
Lf	 0.9760	 0.6670



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Chain	Atom inclusion	Q-score
Lg	 0.9400	 0.6450
Lh	 0.9040	 0.6230
Li	 0.9170	 0.6220
Lj	 0.9750	 0.6640
Lk	 0.8340	 0.5830
Ll	 0.9600	 0.6450
Lm	 0.9460	 0.6420
Ln	 0.9140	 0.6380
Lo	 0.9420	 0.6520
Lp	 0.9580	 0.6610
Lr	 0.9620	 0.6480
S2	 0.8760	 0.5520
SA	 0.8220	 0.5750
SB	 0.8790	 0.6090
SC	 0.8720	 0.6000
SD	 0.7020	 0.5240
SE	 0.8340	 0.5850
SF	 0.7850	 0.5480
SG	 0.7090	 0.5230
SH	 0.6850	 0.5110
SI	 0.7970	 0.5530
SJ	 0.8470	 0.5970
SK	 0.6620	 0.5050
SL	 0.8090	 0.5950
SM	 0.1610	 0.3230
SN	 0.8750	 0.6090
SO	 0.8610	 0.5850
SP	 0.8210	 0.5630
SQ	 0.7840	 0.5450
SR	 0.7190	 0.5370
SS	 0.8330	 0.5760
ST	 0.7860	 0.5460
SU	 0.5980	 0.4630
SV	 0.8570	 0.5890
SW	 0.9210	 0.6190
SX	 0.8950	 0.6270
SY	 0.7440	 0.5240
SZ	 0.7340	 0.5370
Sa	 0.8610	 0.5990
Sb	 0.8170	 0.5780
Sc	 0.7200	 0.5290
Sd	 0.8560	 0.5820

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Chain	Atom inclusion	Q-score
Se	 0.6890	 0.5260
Sf	 0.2290	 0.3610
Sg	 0.6030	 0.4460
u	 0.6300	 0.4910
v	 0.7750	 0.4950
w	 0.9200	 0.5980