



## Full wwPDB EM Validation Report ⓘ

Apr 22, 2025 – 05:37 pm BST

PDB ID : 9G6J / pdb\_00009g6j  
EMDB ID : EMD-51103  
Title : The structure of the *Candida albicans* ribosome with tRNA-fMet, mRNA, and compounds (GEN and MFQ) with strong density for the P-site tRNA  
Authors : Kolosova, O.; Zgadzay, Y.; Jenner, L.B.; Guskov, A.; Yusupov, M.  
Deposited on : 2024-07-18  
Resolution : 2.15 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

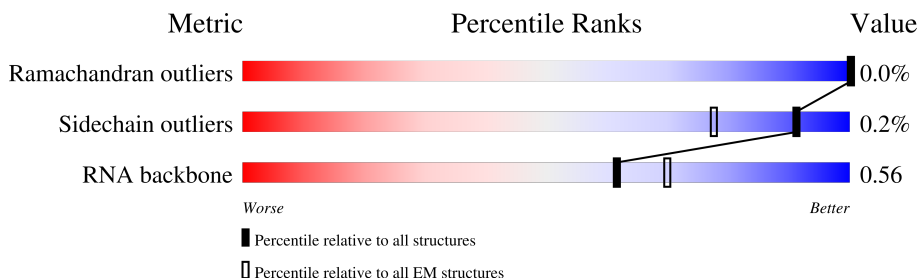
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.15 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	172	99% .
2	1	3359	76% 15% 9% .
3	2	160	99% ..
4	3	121	93% 7% .
5	4	158	85% 13% .
6	6	137	95% . .
7	7	155	40% 60%
8	8	142	85% 15%

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Mol	Chain	Length	Quality of chain
9	9	127	98%
10	A	1787	6%
11	B	261	80%
12	C	256	84%
13	D	249	86%
14	E	251	9%
15	F	262	6%
16	G	225	5%
17	H	236	13%
18	I	186	10%
19	J	206	11%
20	K	189	19%
21	L	118	19%
22	M	155	6%
23	N	143	42%
24	O	151	99%
25	P	132	95%
26	Q	142	13%
27	T	145	10%
28	R	142	98%
29	S	137	14%
30	U	145	97%
31	V	119	16%
32	W	87	99%
33	X	130	99%

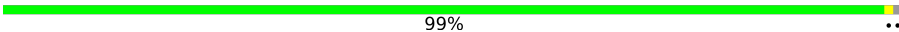

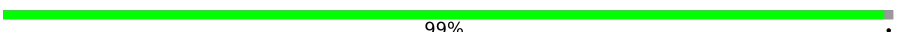
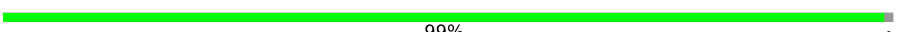








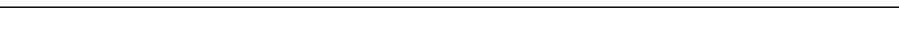

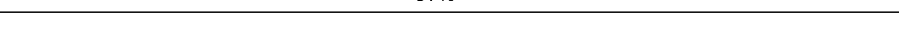
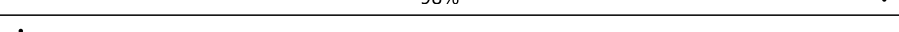
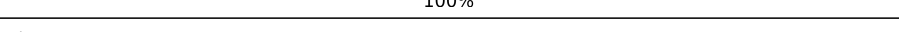
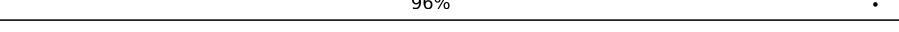
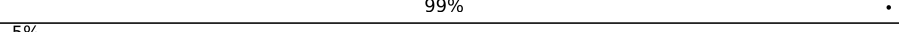
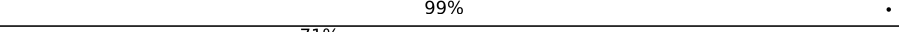


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Mol	Chain	Length	Quality of chain
34	Y	145	
35	Z	135	
36	a	105	
37	b	119	
38	c	82	
39	d	67	
40	e	56	
41	f	63	
42	g	193	
43	h	317	
44	j	254	
45	k	389	
46	l	363	
47	m	298	
48	n	176	
49	o	241	
50	p	262	
51	q	191	
52	r	220	
53	s	174	
54	t	202	
55	u	131	
56	v	204	
57	w	200	
58	x	185	

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Mol	Chain	Length	Quality of chain
59	y	186	 99% ..
60	z	190	 95% 5%
61	AA	136	 99% .
62	AB	149	 99% .
63	AC	63	 94% . 5%
64	AD	106	 91% 9%
65	AE	112	 7% 96% .
66	AF	131	 95% . 5%
67	AG	107	 99% .
68	AH	122	 91% . 8%
69	AI	120	 99% .
70	AJ	99	 98% .
71	AK	90	 96% .
72	AL	78	 8% 97% ..
73	AM	51	 98% .
74	AN	52	 100%
75	AO	25	 96% .
76	AP	106	 99% .
77	AQ	92	 5% 99% .
78	AT	77	 71% 69% 30% .
78	PT	77	 81% 18% .
79	MR	39	 28% 72%

## 2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 197424 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	171	Total	C	N	O	S	2	0
			1442	933	262	244	3		

- Molecule 2 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	3066	Total	C	N	O	P	0	0
			65536	29280	11774	21416	3066		

- Molecule 3 is a protein called Ribosomal 60S subunit protein L21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	159	Total	C	N	O	S	2	0
			1276	807	244	223	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	121	Total	C	N	O	P	0	0
			2579	1153	463	842	121		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	156	Total	C	N	O	P	0	0
			3313	1482	581	1094	156		

- Molecule 6 is a protein called Ribosomal 60S subunit protein L23B.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	131	Total	C	N	O	S	1	0
			986	621	186	171	8		

- Molecule 7 is a protein called Ribosomal 60S subunit protein L24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	62	Total	C	N	O	S	0	0
			516	328	102	85	1		

- Molecule 8 is a protein called Ribosomal 60S subunit protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	121	Total	C	N	O	S	0	0
			974	622	175	176	1		

- Molecule 9 is a protein called Ribosomal 60S subunit protein L26B.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	9	125	Total	C	N	O	0	0
			980	613	189	178		

- Molecule 10 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1692	Total	C	N	O	P	0	0
			36083	16130	6412	11849	1692		

- Molecule 11 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	208	Total	C	N	O	S	0	0
			1627	1041	284	297	5		

- Molecule 12 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	214	Total	C	N	O	S	0	0
			1724	1094	313	313	4		

- Molecule 13 is a protein called Ribosomal 40S subunit protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	216	Total	C	N	O	S	0	0
			1620	1033	287	295	5		

- Molecule 14 is a protein called Ribosomal 40S subunit protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	222	Total	C	N	O	S	0	0
			1701	1084	310	303	4		

- Molecule 15 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	260	Total	C	N	O	S	0	0
			2055	1306	386	358	5		

- Molecule 16 is a protein called Ribosomal 40S subunit protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	199	Total	C	N	O	S	0	0
			1572	983	294	291	4		

- Molecule 17 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	226	Total	C	N	O	S	0	0
			1820	1133	351	330	6		

- Molecule 18 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	182	Total	C	N	O	S	0	0
			1466	939	264	263			

- Molecule 19 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	203	Total	C	N	O	S	0	0
			1579	973	322	283	1		

- Molecule 20 is a protein called Ribosomal 40S subunit protein S9B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	178	Total	C	N	O	S	0	0
			1453	918	286	248	1		

- Molecule 21 is a protein called Ribosomal 40S subunit protein S10A.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	93	Total	C	N	O	S	0	0
			783	511	129	142	1		

- Molecule 22 is a protein called Ribosomal 40S subunit protein S11A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	141	Total	C	N	O	S	0	0
			1129	722	212	192	3		

- Molecule 23 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	71	Total	C	N	O	S	0	0
			539	341	95	99	4		

- Molecule 24 is a protein called Ribosomal 40S subunit protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	150	Total	C	N	O	S	0	0
			1187	757	219	210	1		

- Molecule 25 is a protein called Ribosomal 40S subunit protein S14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	127	Total	C	N	O	S	0	0
			942	579	186	174	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	119	IAS	ASP	conflict	UNP A0A1D8PDT3

- Molecule 26 is a protein called Ribosomal 40S subunit protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	115	Total	C	N	O	S	0	0
			906	578	164	158	6		

- Molecule 27 is a protein called Ribosomal 40S subunit protein S18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	142	Total	C	N	O	S	0	0
			1169	733	228	205	3		

- Molecule 28 is a protein called Ribosomal 40S subunit protein S16A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	141	Total	C	N	O	S	0	0
			1102	706	202	193	1		

- Molecule 29 is a protein called Ribosomal 40S subunit protein S17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	118	Total	C	N	O	S	0	0
			954	602	176	175	1		

- Molecule 30 is a protein called Ribosomal 40S subunit protein S19A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	141	Total	C	N	O	S	0	0
			1100	689	210	200	1		

- Molecule 31 is a protein called Ribosomal 40S subunit protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	100	Total	C	N	O	S	0	0
			790	499	146	143	2		

- Molecule 32 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	87	Total	C	N	O	S	0	0
			676	415	126	133	2		

- Molecule 33 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	X	129	Total	C	N	O	S	0	0
			1032	655	191	183	3		

- Molecule 34 is a protein called Ribosomal 40S subunit protein S23B.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Y	143	Total	C	N	O	S	0	0
			1110	701	219	188	2		

- Molecule 35 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Z	132	Total	C	N	O		0	0
			1072	670	216	186			

- Molecule 36 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	a	72	Total	C	N	O		0	0
			578	369	103	106			

- Molecule 37 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b	98	Total	C	N	O	S	0	0
			779	482	163	128	6		

- Molecule 38 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	81	Total	C	N	O	S	0	0
			614	383	110	114	7		

- Molecule 39 is a protein called Ribosomal 40S subunit protein S28B.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	62	Total	C	N	O	S	0	0
			487	299	98	88	2		

- Molecule 40 is a protein called Ribosomal 40S subunit protein S29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e	55	Total	C	N	O	S	0	0
			454	281	94	75	4		

- Molecule 41 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	58	Total	C	N	O	S	0	0
			461	289	93	77	2		

- Molecule 42 is a protein called Ubiquitin-ribosomal 40S subunit protein S31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g	70	Total	C	N	O	S	0	0
			565	358	111	90	6		

- Molecule 43 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	241	Total	C	N	O	S	0	0
			1854	1176	319	355	4		

- Molecule 44 is a protein called Ribosomal 60S subunit protein L2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	249	Total	C	N	O	S	1	0
			1894	1185	377	330	2		

- Molecule 45 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	386	Total	C	N	O	S	1	0
			3084	1955	584	538	7		

- Molecule 46 is a protein called Ribosomal 60S subunit protein L4B.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	361	Total	C	N	O	S	0	0
			2751	1729	529	490	3		

- Molecule 47 is a protein called Ribosomal 60S subunit protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	292	Total	C	N	O	S	0	0
			2394	1526	416	450	2		

- Molecule 48 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	n	155	Total	C	N	O	1	0
			1237	794	226	217		

- Molecule 49 is a protein called Ribosomal 60S subunit protein L7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	230	Total	C	N	O	S	1	0
			1860	1193	343	323	1		

- Molecule 50 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	p	231	Total	C	N	O	S	0	0
			1795	1150	319	323	3		

- Molecule 51 is a protein called Ribosomal 60S subunit protein L9B.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q	189	Total	C	N	O	S	0	0
			1510	953	275	278	4		

- Molecule 52 is a protein called Ribosomal 60S subunit protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r	218	Total	C	N	O	S	0	0
			1759	1110	336	305	8		

- Molecule 53 is a protein called Ribosomal 60S subunit protein L11B.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	172	Total	C	N	O	S	1	0
			1385	864	262	255	4		

- Molecule 54 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	t	195	Total	C	N	O	0	0
			1573	986	311	276		

- Molecule 55 is a protein called Ribosomal 60S subunit protein L14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	u	130	Total	C	N	O	S	0	0
			1029	660	193	175	1		

- Molecule 56 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	v	203	Total	C	N	O	S	0	0
			1713	1075	356	280	2		

- Molecule 57 is a protein called Ribosomal 60S subunit protein L16A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	w	199	Total	C	N	O	S	0	0
			1590	1025	294	269	2		

- Molecule 58 is a protein called Ribosomal 60S subunit protein L17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	x	172	Total	C	N	O		0	0
			1375	850	279	246			

- Molecule 59 is a protein called Ribosomal 60S subunit protein L18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	y	185	Total	C	N	O		3	0
			1478	930	302	246			

- Molecule 60 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	z	180	Total	C	N	O	S	1	0
			1471	910	313	245	3		

- Molecule 61 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AA	135	Total	C	N	O	S	0	0
			1087	705	197	183	2		

- Molecule 62 is a protein called Ribosomal 60S subunit protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AB	148	Total	C	N	O	S	0	0
			1170	741	231	197	1		

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AC	60	Total	C	N	O	S	1	0
			489	305	105	78	1		

- Molecule 64 is a protein called Ribosomal 60S subunit protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AD	96	Total	C	N	O	S	0	0
			729	469	121	137	2		

- Molecule 65 is a protein called Ribosomal 60S subunit protein L31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AE	108	Total	C	N	O	S	0	0
			881	558	166	155	2		

- Molecule 66 is a protein called Ribosomal 60S subunit protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AF	125	Total	C	N	O	S	1	0
			1015	649	197	168	1		

- Molecule 67 is a protein called Ribosomal 60S subunit protein L33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AG	106	Total	C	N	O	S	3	0
			867	558	166	142	1		

- Molecule 68 is a protein called Ribosomal 60S subunit protein L34B.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AH	112	Total	C	N	O	S	4	0
			913	567	188	154	4		

- Molecule 69 is a protein called Ribosomal 60S subunit protein L35A.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	AI	119	Total	C	N	O	1	0
			990	629	195	166		

- Molecule 70 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AJ	97	Total	C	N	O	S	1	0
			764	476	157	130	1		

- Molecule 71 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AK	86	Total	C	N	O	S	0	0
			677	413	148	110	6		

- Molecule 72 is a protein called Ribosomal 60S subunit protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	AL	77	Total	C	N	O	1	0
			623	398	116	109		

- Molecule 73 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	AM	50	Total	C	N	O	1	0
			446	280	100	66		

- Molecule 74 is a protein called Rpl40bp.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AN	52	Total	C	N	O	S	1	0
			427	265	89	67	6		

- Molecule 75 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AO	25	Total	C	N	O	S	0	0
			236	144	63	28	1		

- Molecule 76 is a protein called Ribosomal 60S subunit protein L42A.



Mol	Chain	Residues	Atoms					AltConf	Trace
76	AP	105	Total	C	N	O	S	2	0
			863	547	171	140	5		

- Molecule 77 is a protein called Ribosomal 60S subunit protein L43A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AQ	91	Total	C	N	O	S	0	0
			698	430	140	124	4		

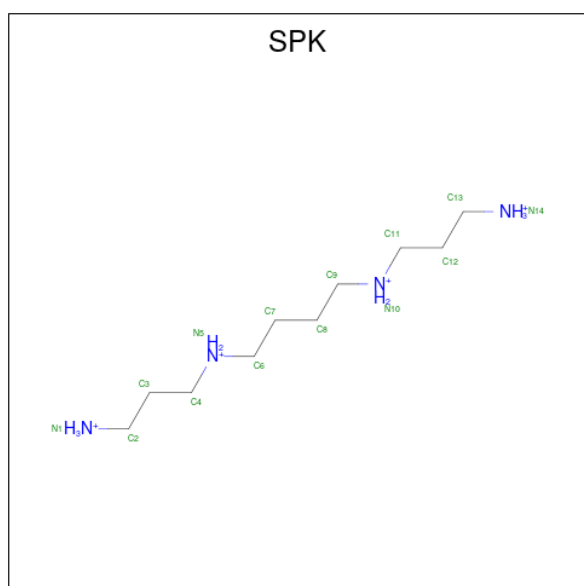
- Molecule 78 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	PT	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		
78	AT	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 79 is a RNA chain called mRNA.

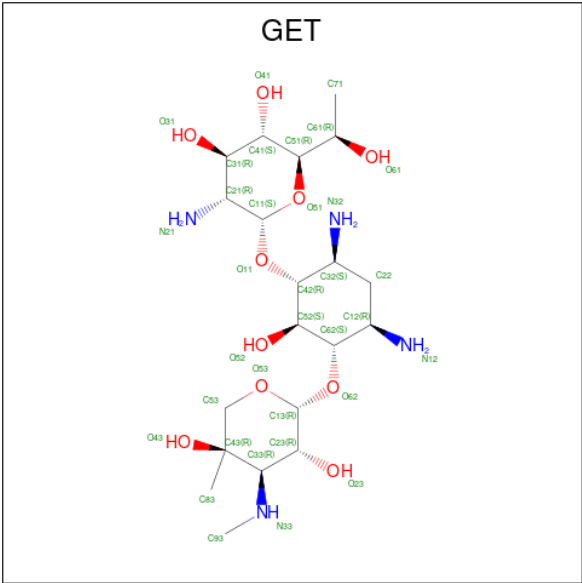
Mol	Chain	Residues	Atoms					AltConf	Trace
79	MR	11	Total	C	N	O	P	0	0
			229	103	36	79	11		

- Molecule 80 is SPERMINE (FULLY PROTONATED FORM) (CCD ID: SPK) (formula:  $C_{10}H_{30}N_4$ ).



Mol	Chain	Residues	Atoms			AltConf
80	1	1	Total	C	N	0
			14	10	4	

- Molecule 81 is GENETICIN (CCD ID: GET) (formula: C<sub>20</sub>H<sub>40</sub>N<sub>4</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	1	1	Total	C	N	O	0
			34	20	4	10	

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Mol	Chain	Residues	Atoms				AltConf
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	1	1	Total	C	N	O	0
			34	20	4	10	
81	A	1	Total	C	N	O	0
			34	20	4	10	
81	A	1	Total	C	N	O	0
			34	20	4	10	
81	A	1	Total	C	N	O	0
			34	20	4	10	
81	AT	1	Total	C	N	O	0
			34	20	4	10	

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	b	1	Total	Zn	0
			1	1	
82	e	1	Total	Zn	0
			1	1	
82	AH	1	Total	Zn	0
			1	1	
82	AK	1	Total	Zn	0
			1	1	
82	AN	1	Total	Zn	0
			1	1	
82	AP	1	Total	Zn	0
			1	1	
82	AQ	1	Total	Zn	0
			1	1	

- Molecule 83 is (11R,12S)- Mefloquine (CCD ID: YMZ) (formula: C<sub>17</sub>H<sub>16</sub>F<sub>6</sub>N<sub>2</sub>O) (labeled as "Ligand of Interest" by depositor).



### 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.

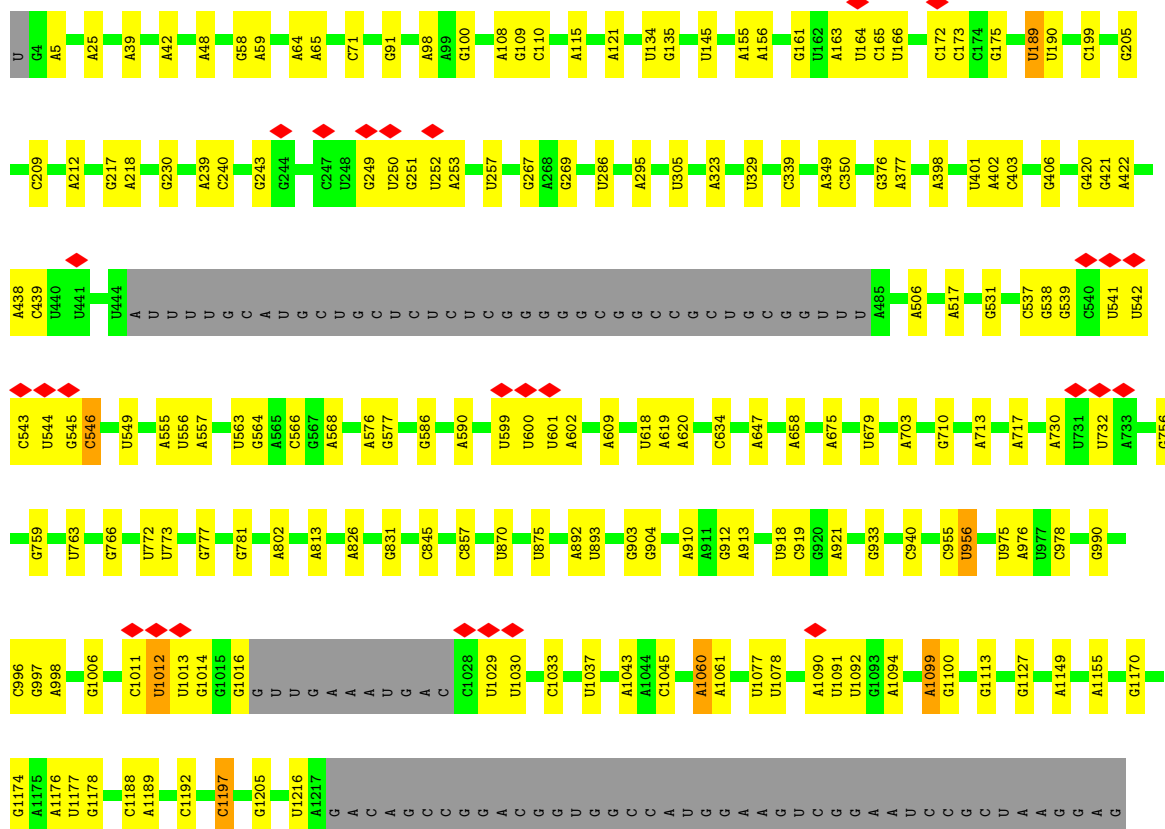
- Molecule 1: 60S ribosomal protein L20

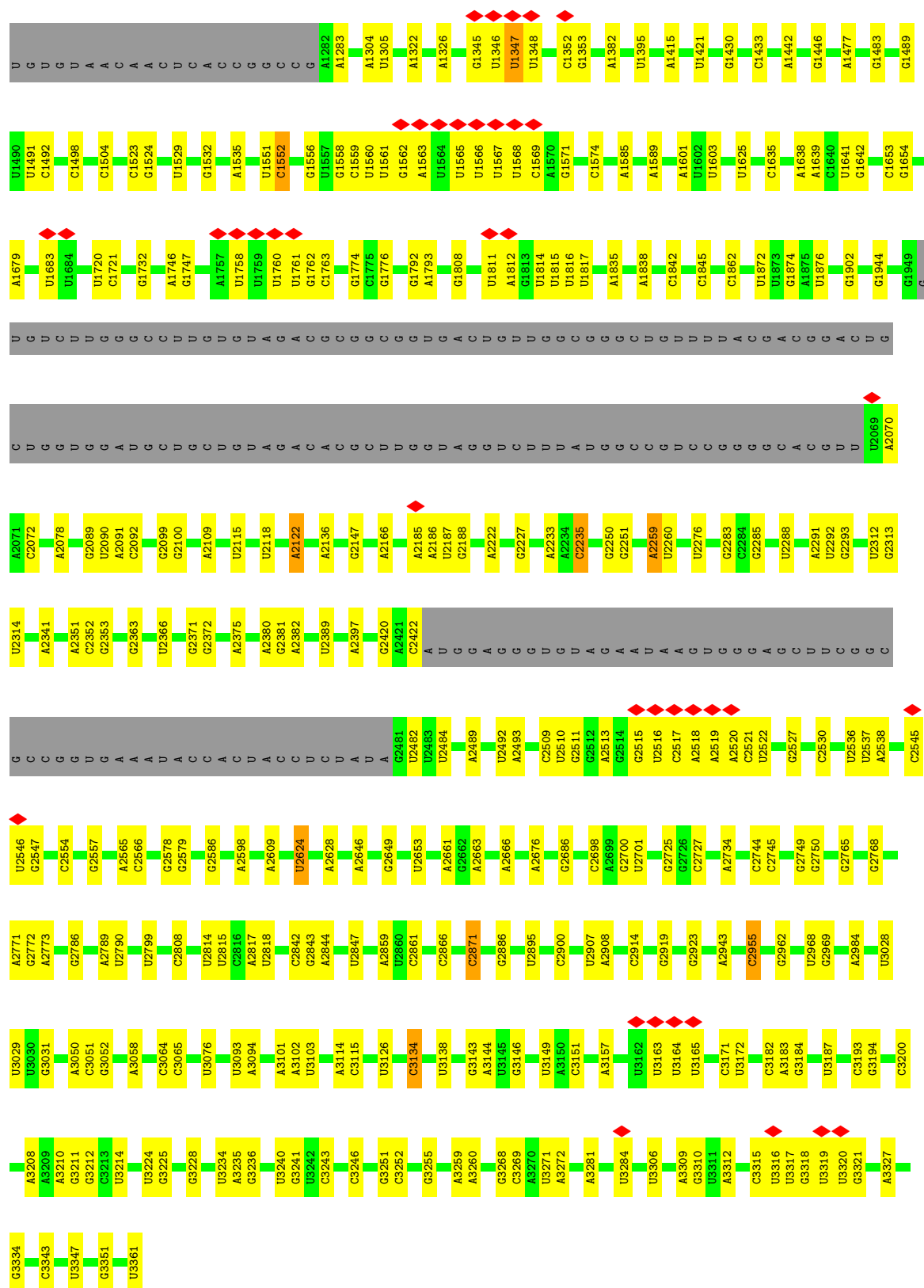
Chain 0:  99%



- Molecule 2: 25S rRNA

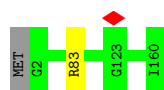
Chain 1:  76% 15% 9%



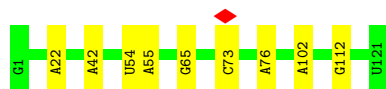


• Molecule 3: Ribosomal 60S subunit protein L21A

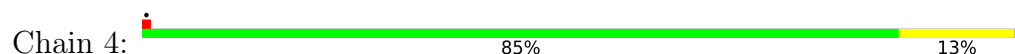
Chain 2: 99%



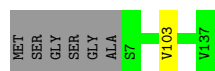
- Molecule 4: 5S rRNA



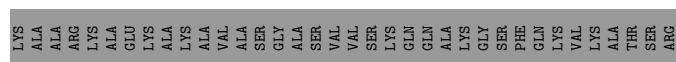
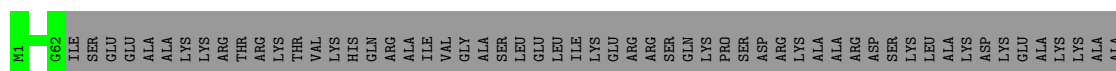
- Molecule 5: 5.8S rRNA



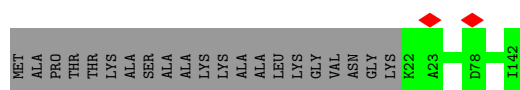
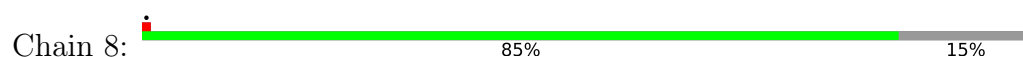
- Molecule 6: Ribosomal 60S subunit protein L23B



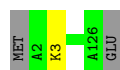
- Molecule 7: Ribosomal 60S subunit protein L24A



- Molecule 8: Ribosomal 60S subunit protein L25

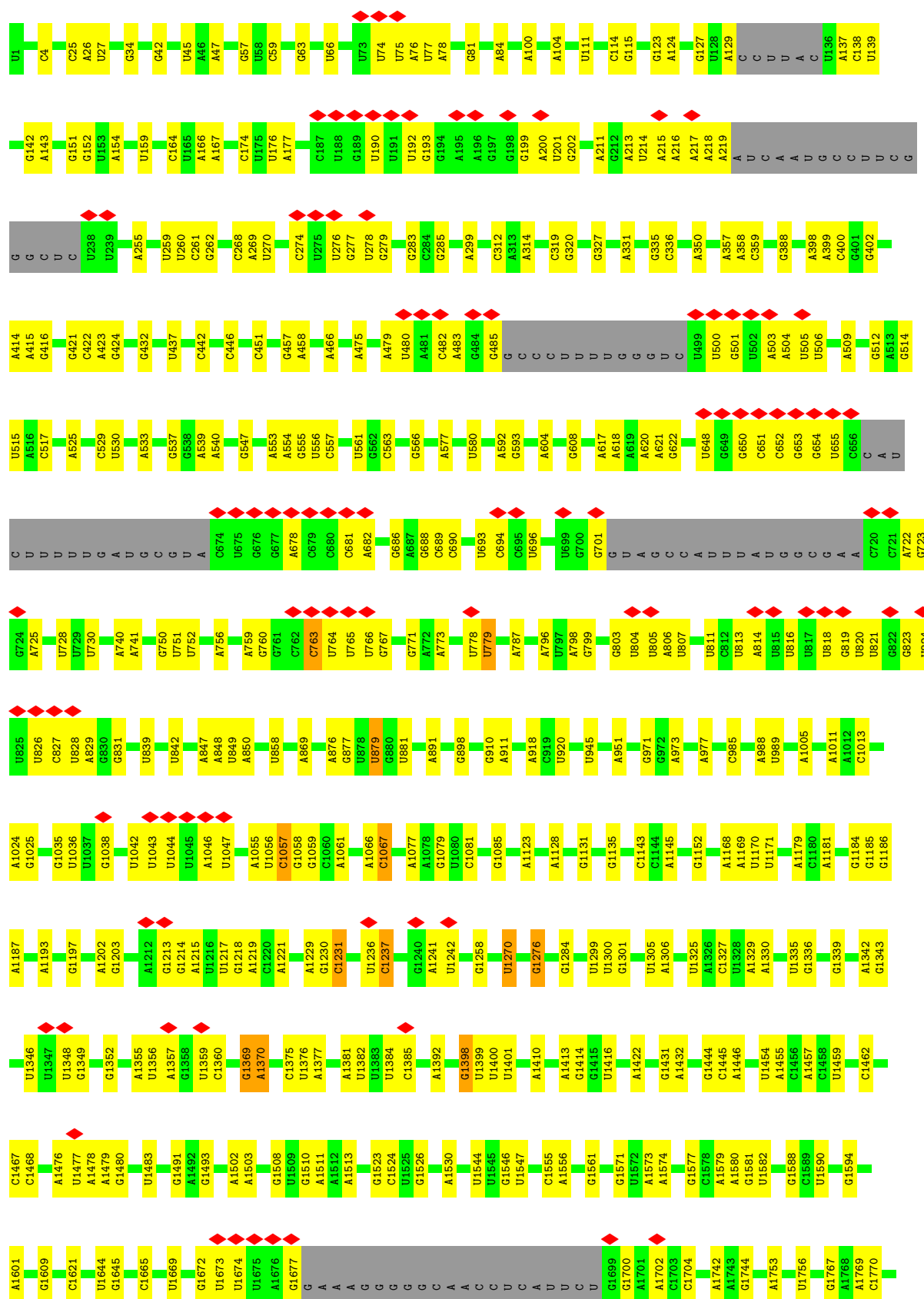


- Molecule 9: Ribosomal 60S subunit protein L26B



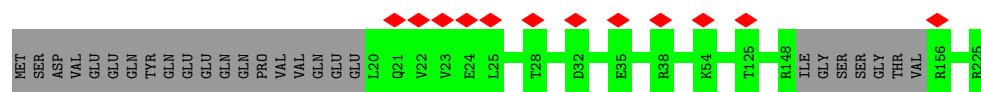
- Molecule 10: 18S rRNA

Chain A: 

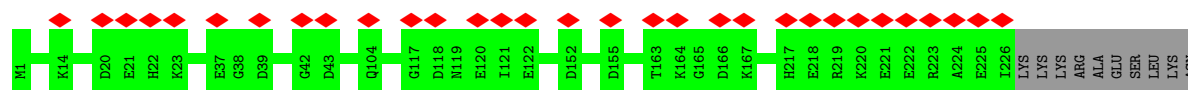




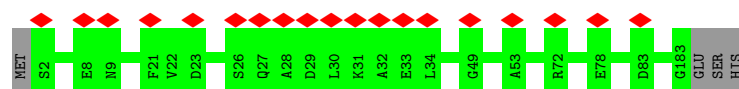




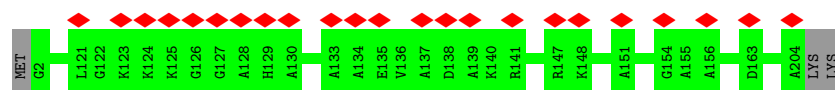
- Molecule 17: 40S ribosomal protein S6



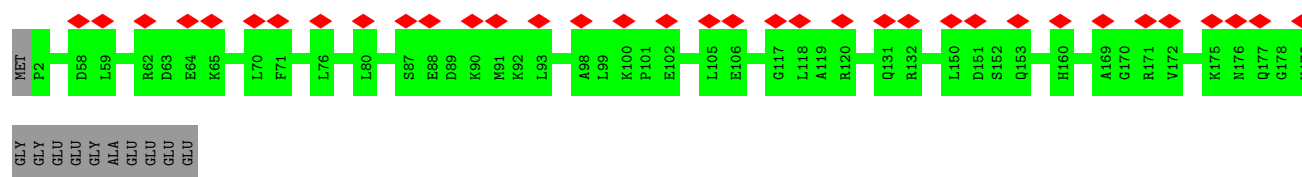
- Molecule 18: 40S ribosomal protein S7



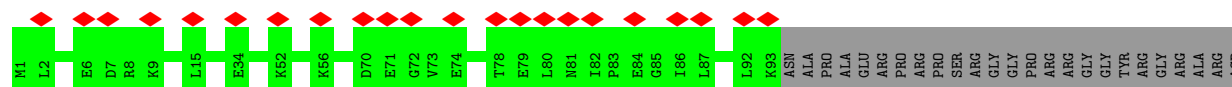
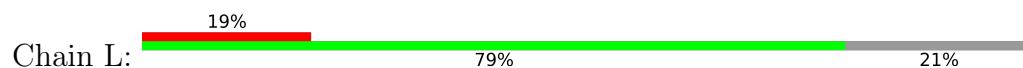
- Molecule 19: 40S ribosomal protein S8



- Molecule 20: Ribosomal 40S subunit protein S9B

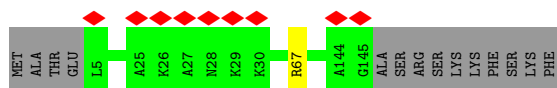


- Molecule 21: Ribosomal 40S subunit protein S10A

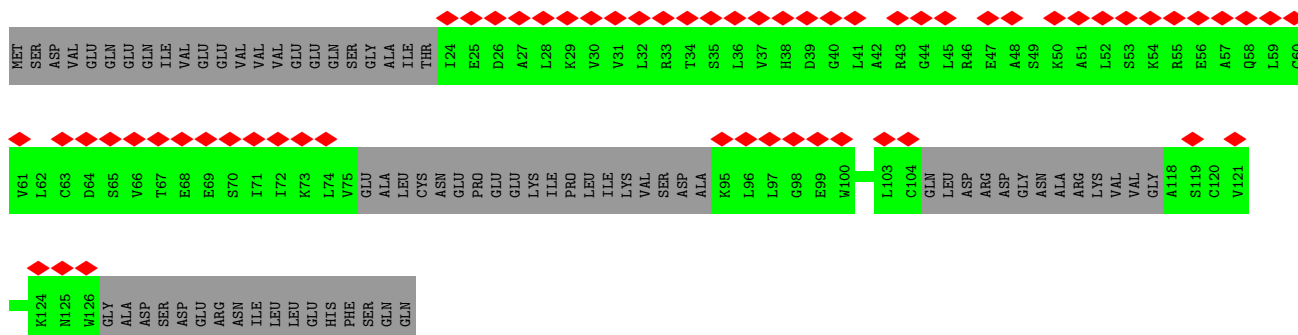
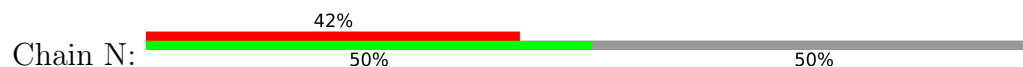


- Molecule 22: Ribosomal 40S subunit protein S11A





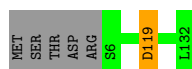
- Molecule 23: 40S ribosomal protein S12



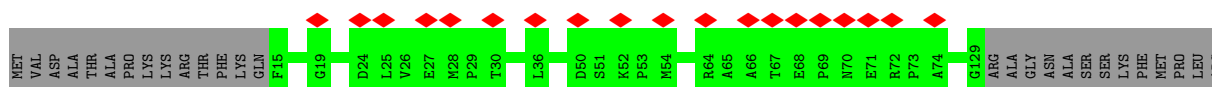
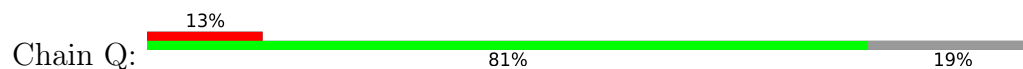
- Molecule 24: Ribosomal 40S subunit protein S13



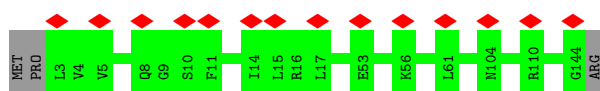
- Molecule 25: Ribosomal 40S subunit protein S14B



- Molecule 26: Ribosomal 40S subunit protein S15

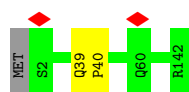


- Molecule 27: Ribosomal 40S subunit protein S18B




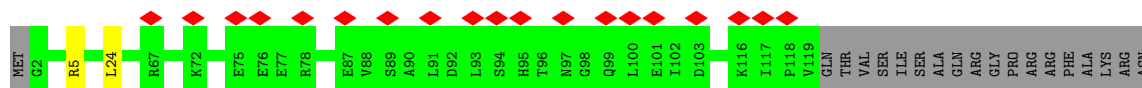
- Molecule 28: Ribosomal 40S subunit protein S16A

Chain R:  98%

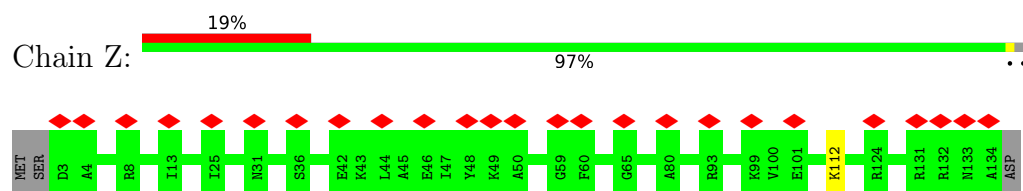


- Molecule 29: Ribosomal 40S subunit protein S17B

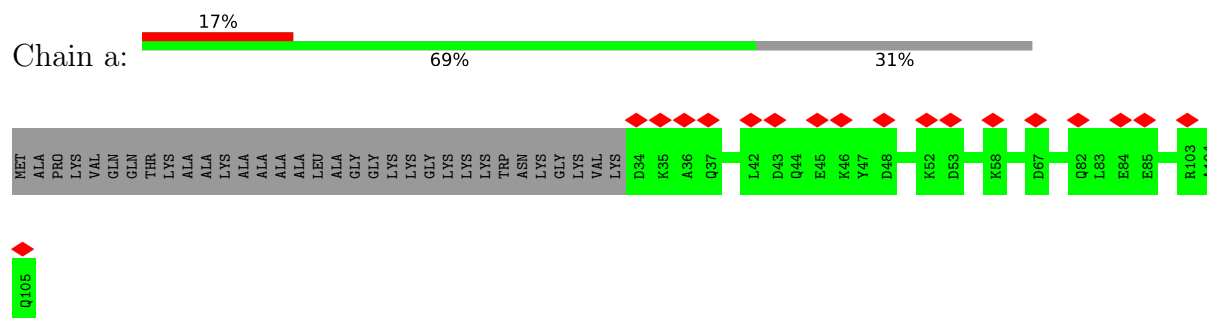
Chain S:  14% 85% 14%



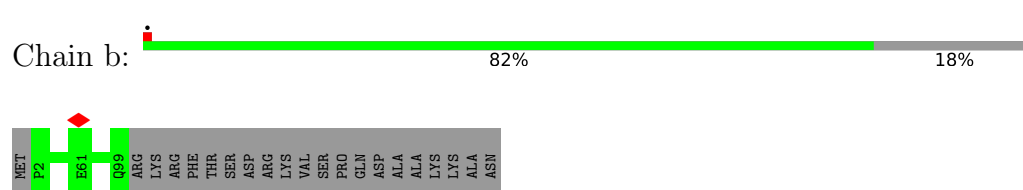
- Molecule 35: 40S ribosomal protein S24



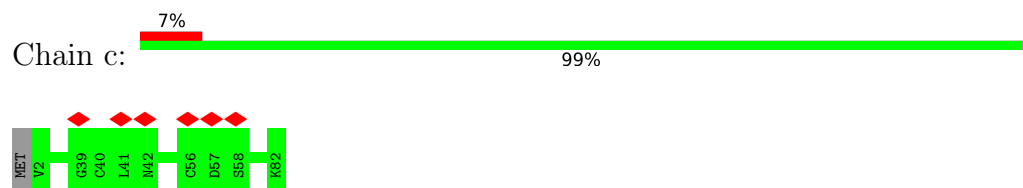
- Molecule 36: 40S ribosomal protein S25



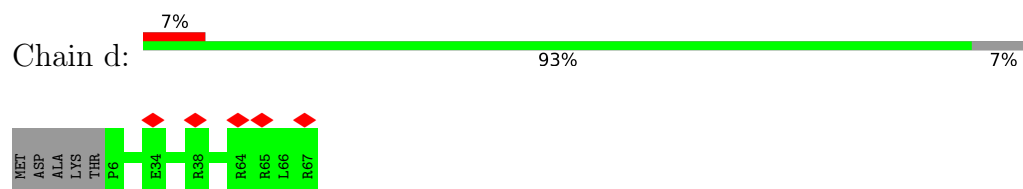
- Molecule 37: 40S ribosomal protein S26



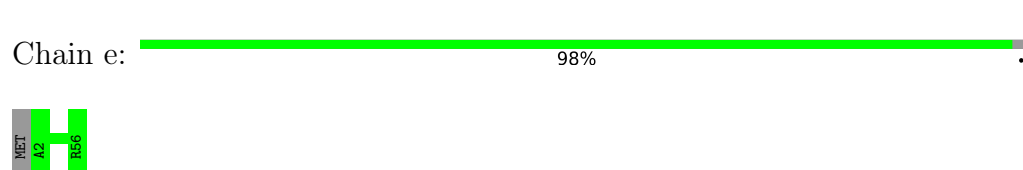
- Molecule 38: 40S ribosomal protein S27



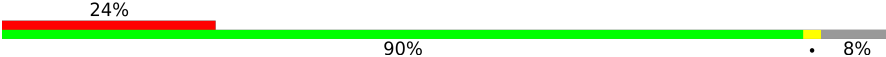
- Molecule 39: Ribosomal 40S subunit protein S28B

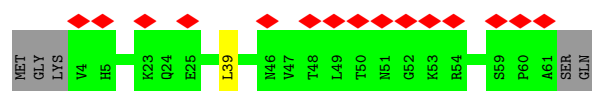


- Molecule 40: Ribosomal 40S subunit protein S29A



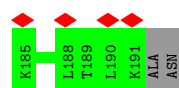
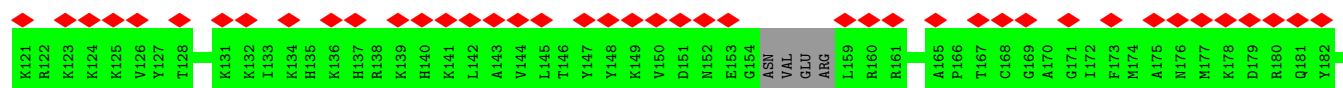
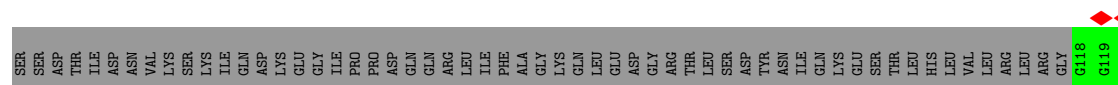
- Molecule 41: 40S ribosomal protein S30

Chain f: 




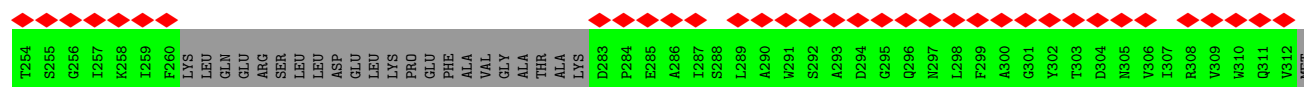
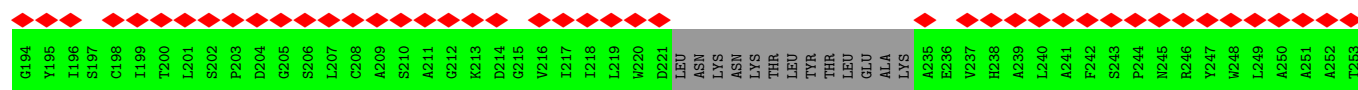
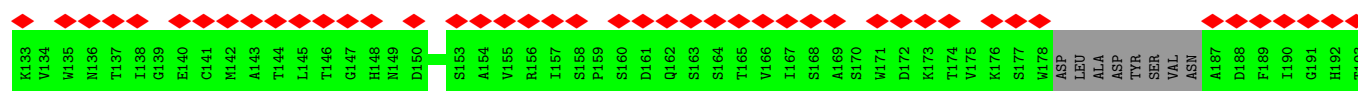
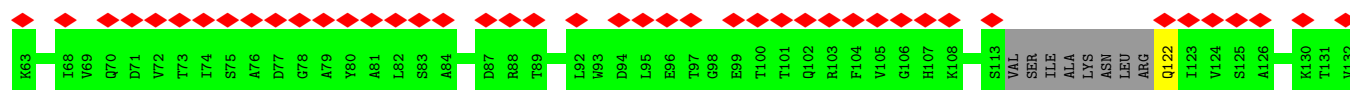
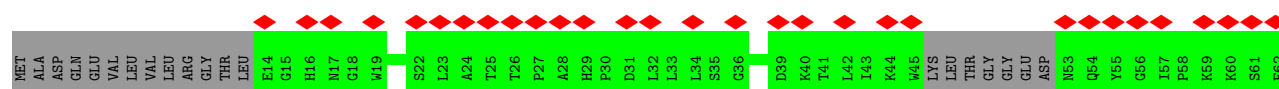
- Molecule 42: Ubiquitin-ribosomal 40S subunit protein S31 fusion protein

Chain g: 



- Molecule 43: Guanine nucleotide-binding protein subunit beta-like protein

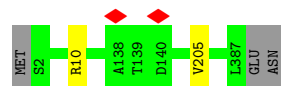
Chain h: 



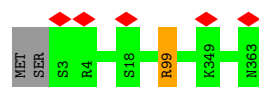
- Molecule 44: Ribosomal 60S subunit protein L2A

MET G2 K70 Q250 LYS THR ALA GLU

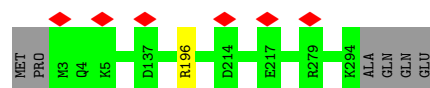
- Chain k:  99%

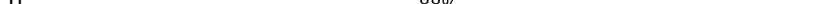


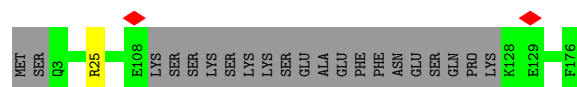
- Chain 1:  99%



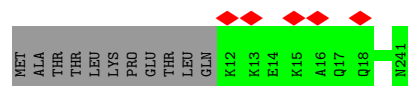
- Chain m: 



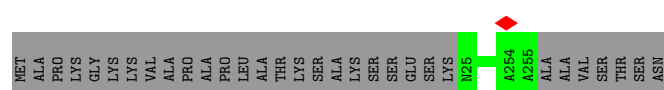
- Chain n:  88% 12%



- Chain 0:  95% 5%



- Chain p:  88% 12%



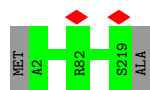
- Molecule 51: Ribosomal 60S subunit protein L9B

Chain q:  98% ..



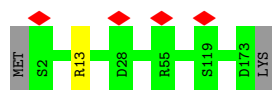
- Molecule 52: Ribosomal 60S subunit protein L10

Chain r:  99% .



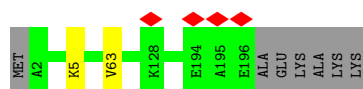
- Molecule 53: Ribosomal 60S subunit protein L11B

Chain s:  98% ..



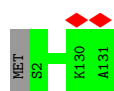
- Molecule 54: 60S ribosomal protein L13

Chain t:  96% ..



- Molecule 55: Ribosomal 60S subunit protein L14B

Chain u:  99% .



- Molecule 56: Ribosomal protein L15

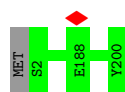
Chain v:  100%



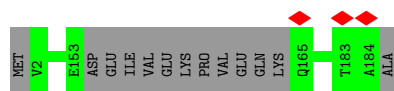
- Molecule 57: Ribosomal 60S subunit protein L16A

Chain w:  100%





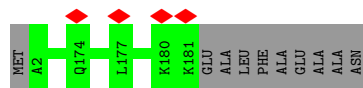
- Molecule 58: Ribosomal 60S subunit protein L17B



- Molecule 59: Ribosomal 60S subunit protein L18A



- Molecule 60: Ribosomal protein L19



- Molecule 61: 60S ribosomal protein L27



- Molecule 62: Ribosomal 60S subunit protein L28



- Molecule 63: 60S ribosomal protein L29



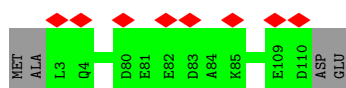
- Molecule 64: Ribosomal 60S subunit protein L30

Chain AD:  91% 9%



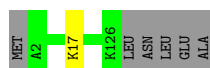
- Molecule 65: Ribosomal 60S subunit protein L31B

Chain AE:  7% 96%



- Molecule 66: Ribosomal 60S subunit protein L32

Chain AF:  95% 5%



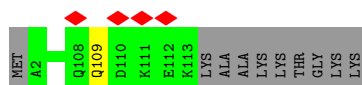
- Molecule 67: Ribosomal 60S subunit protein L33A

Chain AG:  99%



- Molecule 68: Ribosomal 60S subunit protein L34B

Chain AH:  91% 8%



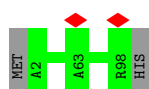
- Molecule 69: Ribosomal 60S subunit protein L35A

Chain AI:  99%



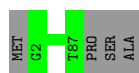
- Molecule 70: 60S ribosomal protein L36

Chain AJ:  98%



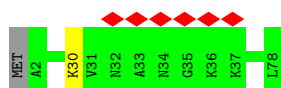
- Molecule 71: Ribosomal protein L37

Chain AK:  96% .



- Molecule 72: Ribosomal 60S subunit protein L38

Chain AL:  97% ..



- Molecule 73: 60S ribosomal protein L39

Chain AM:  98% .



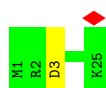
- Molecule 74: Rpl40bp

Chain AN:  100%



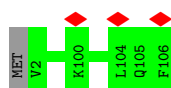
- Molecule 75: Small ribosomal subunit protein eS32

Chain AO:  96% .



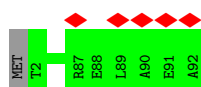
- Molecule 76: Ribosomal 60S subunit protein L42A

Chain AP:  99% .



- Molecule 77: Ribosomal 60S subunit protein L43A

Chain AQ:  99% .





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63238	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	29.7	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.999	Depositor
Minimum map value	-0.786	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.174	Depositor
Map size ( $\text{\AA}$ )	510.3, 510.3, 510.3	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.729, 0.729, 0.729	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: YMZ, SPK, GET, IAS, OMC, OMG, MLZ, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.39	0/1483	0.61	0/1997
2	1	0.82	0/73296	0.90	60/114257 (0.1%)
3	2	0.39	0/1305	0.57	0/1749
4	3	0.70	0/2884	0.78	0/4492
5	4	0.82	0/3702	0.86	0/5764
6	6	0.39	0/994	0.64	1/1339 (0.1%)
7	7	0.40	0/528	0.63	0/701
8	8	0.37	0/990	0.61	0/1337
9	9	0.37	0/990	0.61	0/1322
10	A	0.65	0/40362	0.90	49/62888 (0.1%)
11	B	0.34	0/1666	0.57	0/2273
12	C	0.34	0/1750	0.58	0/2354
13	D	0.36	0/1648	0.57	0/2237
14	E	0.32	0/1725	0.60	0/2316
15	F	0.32	0/2096	0.58	0/2822
16	G	0.32	0/1588	0.58	0/2139
17	H	0.31	0/1845	0.60	0/2464
18	I	0.33	0/1490	0.60	0/2004
19	J	0.33	0/1606	0.62	0/2150
20	K	0.32	0/1478	0.61	0/1978
21	L	0.31	0/801	0.61	0/1081
22	M	0.36	0/1154	0.60	0/1553
23	N	0.27	0/541	0.57	0/726
24	O	0.36	0/1210	0.57	0/1631
25	P	0.36	0/944	0.64	0/1265
26	Q	0.34	0/924	0.62	0/1243
27	T	0.32	0/1186	0.63	0/1590
28	R	0.32	0/1120	0.61	0/1500
29	S	0.32	0/966	0.60	1/1295 (0.1%)
30	U	0.33	0/1120	0.57	0/1508
31	V	0.31	0/800	0.58	0/1082
32	W	0.37	0/683	0.67	1/918 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	X	0.37	0/1049	0.60	0/1412
34	Y	0.33	0/1128	0.61	0/1505
35	Z	0.31	0/1086	0.62	0/1447
36	a	0.32	0/585	0.62	0/789
37	b	0.36	0/791	0.64	0/1060
38	c	0.32	0/624	0.53	0/843
39	d	0.34	0/489	0.72	0/654
40	e	0.34	0/466	0.59	0/620
41	f	0.36	0/469	0.66	1/626 (0.2%)
42	g	0.30	0/575	0.61	0/760
43	h	0.28	0/1898	0.58	0/2584
44	j	0.42	0/1931	0.65	0/2592
45	k	0.41	1/3156 (0.0%)	0.61	1/4246 (0.0%)
46	l	0.36	0/2799	0.59	0/3777
47	m	0.37	0/2447	0.59	0/3294
48	n	0.37	0/1258	0.57	0/1696
49	o	0.38	0/1896	0.60	0/2544
50	p	0.36	0/1825	0.57	0/2458
51	q	0.35	0/1528	0.58	0/2055
52	r	0.35	0/1795	0.58	0/2411
53	s	0.35	0/1404	0.63	0/1880
54	t	0.39	0/1600	0.62	0/2147
55	u	0.35	0/1044	0.60	0/1407
56	v	0.42	0/1753	0.64	0/2347
57	w	0.39	0/1620	0.57	0/2167
58	x	0.38	0/1398	0.61	0/1879
59	y	0.36	0/1511	0.65	0/2022
60	z	0.36	0/1492	0.63	0/1983
61	AA	0.37	0/1112	0.53	0/1488
62	AB	0.38	0/1199	0.61	0/1607
63	AC	0.36	0/502	0.54	0/666
64	AD	0.39	0/738	0.51	0/994
65	AE	0.35	0/894	0.60	0/1201
66	AF	0.41	0/1039	0.61	0/1390
67	AG	0.39	0/895	0.59	0/1201
68	AH	0.38	0/934	0.65	0/1242
69	AI	0.36	0/1004	0.64	0/1337
70	AJ	0.34	0/772	0.62	0/1023
71	AK	0.38	0/690	0.69	0/916
72	AL	0.38	0/632	0.57	0/842
73	AM	0.35	0/458	0.64	0/609
74	AN	0.34	0/436	0.62	0/577
75	AO	0.31	0/237	0.85	0/304

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	AP	0.37	0/861	0.57	0/1136
77	AQ	0.37	0/705	0.63	0/940
78	AT	0.36	0/1813	0.90	1/2825 (0.0%)
78	PT	0.51	0/1813	0.82	0/2825
79	MR	0.45	0/254	0.81	0/392
All	All	0.63	1/211480 (0.0%)	0.80	115/310695 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	P	0	1
28	R	0	1
46	l	0	1
48	n	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	k	205	VAL	CB-CG1	-5.51	1.41	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	451	C	C2-N1-C1'	8.64	128.30	118.80
2	1	406	G	O4'-C1'-N9	8.31	114.85	108.20
2	1	831	G	O4'-C1'-N9	7.96	114.56	108.20
2	1	3271	U	N3-C2-O2	-7.41	117.01	122.20
2	1	3126	U	C2-N1-C1'	7.19	126.33	117.70
10	A	451	C	N1-C2-O2	7.12	123.17	118.90
2	1	1491	U	C5-C6-N1	-7.04	119.18	122.70
10	A	681	C	N3-C2-O2	-6.77	117.16	121.90
10	A	1305	U	N3-C2-O2	-6.60	117.58	122.20
2	1	165	C	C2-N1-C1'	6.59	126.05	118.80
10	A	1375	C	C2-N1-C1'	6.48	125.92	118.80
2	1	2259	A	O4'-C1'-N9	6.42	113.33	108.20
2	1	3126	U	N3-C2-O2	-6.35	117.76	122.20
2	1	2698	C	N3-C2-O2	-6.25	117.53	121.90
10	A	1237	C	C2-N1-C1'	6.18	125.60	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	879	U	N3-C2-O2	-6.15	117.89	122.20
10	A	561	U	N3-C2-O2	-6.15	117.90	122.20
2	1	918	U	C2-N1-C1'	6.14	125.07	117.70
10	A	1067	C	C2-N1-C1'	6.11	125.52	118.80
10	A	1327	C	N1-C2-O2	6.08	122.55	118.90
2	1	1552	C	N3-C2-O2	-6.06	117.66	121.90
2	1	3243	C	C2-N1-C1'	6.05	125.45	118.80
10	A	4	C	N3-C2-O2	-5.99	117.71	121.90
10	A	451	C	N3-C2-O2	-5.99	117.71	121.90
10	A	849	U	N3-C2-O2	-5.96	118.03	122.20
2	1	2283	G	O4'-C1'-N9	5.95	112.96	108.20
2	1	1197	C	N1-C2-O2	5.94	122.46	118.90
10	A	1231	C	C2-N1-C1'	5.91	125.30	118.80
2	1	3243	C	N1-C2-O2	5.91	122.44	118.90
10	A	451	C	C6-N1-C2	-5.89	117.94	120.30
10	A	451	C	C6-N1-C1'	-5.88	113.75	120.80
2	1	956	U	C2-N1-C1'	5.84	124.71	117.70
2	1	3243	C	N3-C2-O2	-5.83	117.82	121.90
2	1	1197	C	N3-C2-O2	-5.82	117.83	121.90
2	1	1552	C	N1-C2-O2	5.82	122.39	118.90
10	A	1375	C	N1-C2-O2	5.80	122.38	118.90
10	A	1459	U	C2-N1-C1'	5.79	124.65	117.70
10	A	1276	G	N3-C4-C5	5.76	131.48	128.60
10	A	811	U	C5-C4-O4	5.75	129.35	125.90
2	1	3327	A	O4'-C1'-N9	5.73	112.78	108.20
2	1	2115	U	O4'-C1'-N1	5.73	112.78	108.20
10	A	608	G	C4-N9-C1'	5.71	133.93	126.50
2	1	766	G	O4'-C1'-N9	5.71	112.77	108.20
2	1	1491	U	C4-C5-C6	5.68	123.11	119.70
2	1	2818	U	N3-C2-O2	-5.66	118.24	122.20
2	1	2235	C	C2-N1-C1'	5.64	125.00	118.80
10	A	879	U	N1-C2-O2	5.62	126.73	122.80
10	A	1276	G	N3-C4-N9	-5.61	122.64	126.00
2	1	2235	C	N3-C2-O2	-5.59	117.99	121.90
6	6	103	VAL	C-N-CA	5.58	135.64	121.70
78	AT	20	G	O4'-C1'-N9	-5.57	103.74	108.20
2	1	2698	C	C6-N1-C2	-5.56	118.08	120.30
2	1	3126	U	C6-N1-C2	-5.55	117.67	121.00
2	1	3327	A	C2-N3-C4	-5.54	107.83	110.60
10	A	985	C	N3-C2-O2	-5.52	118.04	121.90
10	A	1398	G	OP2-P-O3'	5.50	117.30	105.20
2	1	100	G	O4'-C1'-N9	5.50	112.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2799	U	O4'-C1'-N1	5.49	112.59	108.20
10	A	847	A	O4'-C1'-N9	5.49	112.59	108.20
2	1	2624	U	N3-C2-O2	-5.48	118.36	122.20
2	1	115	A	O4'-C1'-N9	5.48	112.58	108.20
2	1	2955	C	N3-C2-O2	-5.43	118.10	121.90
2	1	2955	C	C2-N1-C1'	5.43	124.77	118.80
2	1	2122	A	O4'-C1'-N9	5.39	112.52	108.20
2	1	3134	C	C2-N1-C1'	5.39	124.73	118.80
2	1	3029	U	N3-C2-O2	-5.38	118.43	122.20
2	1	1492	C	C6-N1-C2	-5.37	118.15	120.30
2	1	2842	C	C6-N1-C1'	5.36	127.24	120.80
10	A	1370	A	O4'-C1'-N9	5.35	112.48	108.20
2	1	267	G	O4'-C1'-N9	-5.32	103.94	108.20
10	A	1398	G	P-O3'-C3'	5.32	126.08	119.70
10	A	1369	G	P-O3'-C3'	5.32	126.08	119.70
10	A	1237	C	N1-C2-O2	5.31	122.09	118.90
29	S	24	LEU	CA-CB-CG	5.29	127.48	115.30
10	A	1547	U	N3-C2-O2	-5.28	118.50	122.20
2	1	1489	G	O4'-C1'-N9	5.28	112.42	108.20
10	A	1547	U	C2-N1-C1'	5.27	124.02	117.70
2	1	100	G	C8-N9-C1'	-5.24	120.19	127.00
10	A	608	G	C8-N9-C1'	-5.24	120.19	127.00
10	A	4	C	N1-C2-O2	5.21	122.03	118.90
10	A	1276	G	N3-C2-N2	-5.21	116.26	119.90
32	W	79	LEU	CA-CB-CG	5.20	127.27	115.30
10	A	1057	C	C2-N1-C1'	5.20	124.52	118.80
2	1	1012	U	P-O3'-C3'	5.19	125.93	119.70
10	A	763	C	P-O3'-C3'	5.19	125.92	119.70
2	1	546	C	C2-N1-C1'	5.18	124.50	118.80
2	1	2842	C	C2-N1-C1'	-5.17	113.11	118.80
2	1	1099	A	OP2-P-O3'	5.17	116.57	105.20
2	1	2509	C	C2-N1-C1'	5.13	124.45	118.80
10	A	985	C	C2-N1-C1'	5.12	124.43	118.80
2	1	189	U	C2-N1-C1'	-5.11	111.57	117.70
2	1	165	C	C6-N1-C1'	-5.10	114.68	120.80
10	A	164	C	C6-N1-C2	-5.10	118.26	120.30
10	A	850	A	O4'-C1'-N9	5.10	112.28	108.20
10	A	1444	G	C4-N9-C1'	5.10	133.12	126.50
2	1	100	G	C4-N9-C1'	5.10	133.12	126.50
10	A	517	C	C2-N1-C1'	5.09	124.40	118.80
10	A	1237	C	N3-C2-O2	-5.09	118.34	121.90
10	A	779	U	C2-N1-C1'	5.08	123.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	756	G	O4'-C1'-N9	5.06	112.25	108.20
2	1	1642	G	O4'-C1'-N9	5.06	112.24	108.20
10	A	827	C	C2-N1-C1'	5.05	124.35	118.80
2	1	2871	C	N3-C2-O2	-5.04	118.37	121.90
45	k	10	ARG	CG-CD-NE	-5.03	101.23	111.80
2	1	2235	C	N1-C2-O2	5.03	121.92	118.90
2	1	1060	A	P-O3'-C3'	5.03	125.73	119.70
10	A	1416	U	N3-C2-O2	-5.03	118.68	122.20
2	1	2235	C	C6-N1-C2	-5.02	118.29	120.30
2	1	918	U	N1-C2-O2	5.02	126.31	122.80
10	A	1270	U	C2-N1-C1'	5.01	123.71	117.70
10	A	1410	A	O4'-C1'-N9	5.01	112.21	108.20
2	1	2955	C	C6-N1-C2	-5.01	118.30	120.30
10	A	1416	U	C2-N1-C1'	5.00	123.71	117.70
2	1	1347	U	P-O3'-C3'	5.00	125.70	119.70
41	f	39	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	P	119	IAS	Peptide
28	R	39	GLN	Peptide
46	l	99	ARG	Sidechain
48	n	25	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	171/172 (99%)	169 (99%)	2 (1%)	0	100	100
3	2	159/160 (99%)	156 (98%)	3 (2%)	0	100	100
6	6	129/137 (94%)	127 (98%)	2 (2%)	0	100	100
7	7	60/155 (39%)	59 (98%)	1 (2%)	0	100	100
8	8	119/142 (84%)	117 (98%)	2 (2%)	0	100	100
9	9	123/127 (97%)	120 (98%)	3 (2%)	0	100	100
11	B	206/261 (79%)	192 (93%)	14 (7%)	0	100	100
12	C	212/256 (83%)	203 (96%)	9 (4%)	0	100	100
13	D	214/249 (86%)	209 (98%)	5 (2%)	0	100	100
14	E	220/251 (88%)	211 (96%)	9 (4%)	0	100	100
15	F	258/262 (98%)	240 (93%)	18 (7%)	0	100	100
16	G	195/225 (87%)	187 (96%)	8 (4%)	0	100	100
17	H	224/236 (95%)	212 (95%)	12 (5%)	0	100	100
18	I	180/186 (97%)	170 (94%)	10 (6%)	0	100	100
19	J	201/206 (98%)	193 (96%)	8 (4%)	0	100	100
20	K	176/189 (93%)	163 (93%)	13 (7%)	0	100	100
21	L	91/118 (77%)	84 (92%)	7 (8%)	0	100	100
22	M	139/155 (90%)	132 (95%)	7 (5%)	0	100	100
23	N	65/143 (46%)	53 (82%)	12 (18%)	0	100	100
24	O	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
25	P	124/132 (94%)	122 (98%)	2 (2%)	0	100	100
26	Q	113/142 (80%)	103 (91%)	10 (9%)	0	100	100
27	T	140/145 (97%)	125 (89%)	15 (11%)	0	100	100
28	R	139/142 (98%)	132 (95%)	6 (4%)	1 (1%)	19	13
29	S	116/137 (85%)	111 (96%)	5 (4%)	0	100	100
30	U	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
31	V	98/119 (82%)	93 (95%)	5 (5%)	0	100	100
32	W	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
33	X	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
34	Y	141/145 (97%)	134 (95%)	7 (5%)	0	100	100
35	Z	130/135 (96%)	118 (91%)	12 (9%)	0	100	100
36	a	70/105 (67%)	62 (89%)	8 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	b	96/119 (81%)	92 (96%)	4 (4%)	0	100	100
38	c	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
39	d	60/67 (90%)	57 (95%)	3 (5%)	0	100	100
40	e	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
41	f	56/63 (89%)	53 (95%)	3 (5%)	0	100	100
42	g	66/193 (34%)	51 (77%)	15 (23%)	0	100	100
43	h	229/317 (72%)	198 (86%)	31 (14%)	0	100	100
44	j	248/254 (98%)	239 (96%)	9 (4%)	0	100	100
45	k	385/389 (99%)	376 (98%)	9 (2%)	0	100	100
46	l	359/363 (99%)	349 (97%)	10 (3%)	0	100	100
47	m	290/298 (97%)	278 (96%)	12 (4%)	0	100	100
48	n	152/176 (86%)	147 (97%)	5 (3%)	0	100	100
49	o	229/241 (95%)	224 (98%)	5 (2%)	0	100	100
50	p	229/262 (87%)	222 (97%)	7 (3%)	0	100	100
51	q	187/191 (98%)	181 (97%)	6 (3%)	0	100	100
52	r	216/220 (98%)	212 (98%)	4 (2%)	0	100	100
53	s	171/174 (98%)	170 (99%)	1 (1%)	0	100	100
54	t	193/202 (96%)	183 (95%)	8 (4%)	2 (1%)	13	8
55	u	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
56	v	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
57	w	197/200 (98%)	194 (98%)	3 (2%)	0	100	100
58	x	168/185 (91%)	162 (96%)	6 (4%)	0	100	100
59	y	186/186 (100%)	180 (97%)	6 (3%)	0	100	100
60	z	179/190 (94%)	177 (99%)	2 (1%)	0	100	100
61	AA	133/136 (98%)	133 (100%)	0	0	100	100
62	AB	146/149 (98%)	142 (97%)	4 (3%)	0	100	100
63	AC	59/63 (94%)	59 (100%)	0	0	100	100
64	AD	94/106 (89%)	93 (99%)	1 (1%)	0	100	100
65	AE	106/112 (95%)	102 (96%)	4 (4%)	0	100	100
66	AF	124/131 (95%)	124 (100%)	0	0	100	100
67	AG	107/107 (100%)	105 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	AH	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
69	AI	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
70	AJ	96/99 (97%)	95 (99%)	1 (1%)	0	100	100
71	AK	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
72	AL	76/78 (97%)	74 (97%)	2 (3%)	0	100	100
73	AM	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
74	AN	51/52 (98%)	51 (100%)	0	0	100	100
75	AO	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	0
76	AP	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
77	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
All	All	10641/11747 (91%)	10202 (96%)	435 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	R	40	PRO
54	t	5	LYS
54	t	63	VAL
75	AO	3	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	158/157 (101%)	158 (100%)	0	100	100
3	2	135/134 (101%)	134 (99%)	1 (1%)	81	86
6	6	101/103 (98%)	101 (100%)	0	100	100
7	7	56/127 (44%)	56 (100%)	0	100	100
8	8	108/121 (89%)	108 (100%)	0	100	100
9	9	110/112 (98%)	109 (99%)	1 (1%)	75	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	B	176/215 (82%)	176 (100%)	0	100	100
12	C	194/229 (85%)	194 (100%)	0	100	100
13	D	174/198 (88%)	173 (99%)	1 (1%)	84	89
14	E	173/196 (88%)	172 (99%)	1 (1%)	84	89
15	F	218/220 (99%)	218 (100%)	0	100	100
16	G	173/197 (88%)	173 (100%)	0	100	100
17	H	195/204 (96%)	195 (100%)	0	100	100
18	I	163/167 (98%)	163 (100%)	0	100	100
19	J	157/160 (98%)	157 (100%)	0	100	100
20	K	153/160 (96%)	153 (100%)	0	100	100
21	L	87/104 (84%)	87 (100%)	0	100	100
22	M	122/134 (91%)	121 (99%)	1 (1%)	79	84
23	N	60/123 (49%)	60 (100%)	0	100	100
24	O	129/130 (99%)	129 (100%)	0	100	100
25	P	96/101 (95%)	96 (100%)	0	100	100
26	Q	99/121 (82%)	99 (100%)	0	100	100
27	T	126/129 (98%)	126 (100%)	0	100	100
28	R	115/116 (99%)	115 (100%)	0	100	100
29	S	106/122 (87%)	105 (99%)	1 (1%)	75	81
30	U	113/117 (97%)	113 (100%)	0	100	100
31	V	90/105 (86%)	90 (100%)	0	100	100
32	W	71/71 (100%)	71 (100%)	0	100	100
33	X	112/113 (99%)	112 (100%)	0	100	100
34	Y	116/118 (98%)	116 (100%)	0	100	100
35	Z	109/112 (97%)	108 (99%)	1 (1%)	75	81
36	a	64/85 (75%)	64 (100%)	0	100	100
37	b	84/102 (82%)	84 (100%)	0	100	100
38	c	72/73 (99%)	72 (100%)	0	100	100
39	d	54/58 (93%)	54 (100%)	0	100	100
40	e	47/48 (98%)	47 (100%)	0	100	100
41	f	50/54 (93%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	g	60/175 (34%)	60 (100%)	0	100	100
43	h	199/263 (76%)	198 (100%)	1 (0%)	86	91
44	j	191/194 (98%)	189 (99%)	2 (1%)	73	78
45	k	326/328 (99%)	326 (100%)	0	100	100
46	l	290/292 (99%)	289 (100%)	1 (0%)	91	94
47	m	247/252 (98%)	246 (100%)	1 (0%)	89	92
48	n	135/154 (88%)	135 (100%)	0	100	100
49	o	195/204 (96%)	195 (100%)	0	100	100
50	p	193/216 (89%)	193 (100%)	0	100	100
51	q	168/170 (99%)	167 (99%)	1 (1%)	84	89
52	r	185/186 (100%)	185 (100%)	0	100	100
53	s	148/149 (99%)	147 (99%)	1 (1%)	81	86
54	t	163/168 (97%)	163 (100%)	0	100	100
55	u	108/109 (99%)	108 (100%)	0	100	100
56	v	177/178 (99%)	177 (100%)	0	100	100
57	w	166/167 (99%)	166 (100%)	0	100	100
58	x	142/154 (92%)	142 (100%)	0	100	100
59	y	156/154 (101%)	154 (99%)	2 (1%)	65	71
60	z	148/153 (97%)	148 (100%)	0	100	100
61	AA	117/118 (99%)	117 (100%)	0	100	100
62	AB	120/121 (99%)	120 (100%)	0	100	100
63	AC	48/49 (98%)	46 (96%)	2 (4%)	25	24
64	AD	81/90 (90%)	81 (100%)	0	100	100
65	AE	97/100 (97%)	97 (100%)	0	100	100
66	AF	111/115 (96%)	109 (98%)	2 (2%)	54	59
67	AG	94/92 (102%)	94 (100%)	0	100	100
68	AH	99/102 (97%)	98 (99%)	1 (1%)	73	78
69	AI	106/106 (100%)	106 (100%)	0	100	100
70	AJ	78/79 (99%)	78 (100%)	0	100	100
71	AK	70/73 (96%)	70 (100%)	0	100	100
72	AL	69/69 (100%)	67 (97%)	2 (3%)	37	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	AM	47/47 (100%)	47 (100%)	0	100	100
74	AN	48/47 (102%)	48 (100%)	0	100	100
75	AO	24/24 (100%)	24 (100%)	0	100	100
76	AP	90/89 (101%)	90 (100%)	0	100	100
77	AQ	72/73 (99%)	72 (100%)	0	100	100
All	All	9134/9896 (92%)	9111 (100%)	23 (0%)	91	94

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	83	ARG
9	9	3	LYS
13	D	136	ARG
14	E	77	ARG
22	M	67	ARG
29	S	5	ARG
35	Z	112	LYS
43	h	122	GLN
44	j	70[A]	LYS
44	j	70[B]	LYS
46	l	99	ARG
47	m	196	ARG
51	q	157	ASN
53	s	13	ARG
59	y	31[A]	LYS
59	y	31[B]	LYS
63	AC	14[A]	ARG
63	AC	14[B]	ARG
66	AF	17[A]	LYS
66	AF	17[B]	LYS
68	AH	109	GLN
72	AL	30[A]	LYS
72	AL	30[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
12	C	124	ASN
16	G	37	GLN

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Mol	Chain	Res	Type
16	G	63	GLN
16	G	224	ASN
19	J	111	GLN
19	J	129	HIS
27	T	74	GLN
27	T	89	GLN
36	a	98	GLN
41	f	17	GLN
42	g	181	GLN
46	l	111	ASN
54	t	66	ASN
76	AP	22	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1685/1787 (94%)	385 (22%)	26 (1%)
2	1	3060/3359 (91%)	466 (15%)	34 (1%)
4	3	120/121 (99%)	9 (7%)	0
5	4	155/158 (98%)	20 (12%)	1 (0%)
78	AT	76/77 (98%)	21 (27%)	1 (1%)
78	PT	75/77 (97%)	14 (18%)	0
79	MR	10/39 (25%)	0	0
All	All	5181/5618 (92%)	915 (17%)	62 (1%)

All (915) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	1	5	A
2	1	25	A
2	1	39	A
2	1	42	A
2	1	48	A
2	1	58	G
2	1	59	A
2	1	64	A
2	1	65	A
2	1	71	C
2	1	91	G
2	1	98	A
2	1	108	A

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Mol	Chain	Res	Type
2	1	109	G
2	1	110	C
2	1	121	A
2	1	134	U
2	1	135	G
2	1	145	U
2	1	155	A
2	1	156	A
2	1	161	G
2	1	163	A
2	1	164	U
2	1	166	U
2	1	173	C
2	1	175	G
2	1	189	U
2	1	190	U
2	1	199	C
2	1	205	G
2	1	209	C
2	1	212	A
2	1	217	G
2	1	218	A
2	1	230	G
2	1	239	A
2	1	240	C
2	1	243	G
2	1	249	G
2	1	250	U
2	1	251	G
2	1	252	U
2	1	253	A
2	1	257	U
2	1	269	G
2	1	286	U
2	1	295	A
2	1	305	U
2	1	323	A
2	1	329	U
2	1	339	C
2	1	349	A
2	1	350	C
2	1	376	G

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Mol	Chain	Res	Type
2	1	377	A
2	1	398	A
2	1	401	U
2	1	402	A
2	1	403	C
2	1	420	G
2	1	421	G
2	1	422	A
2	1	438	A
2	1	439	C
2	1	506	A
2	1	517	A
2	1	531	G
2	1	537	C
2	1	538	G
2	1	539	G
2	1	541	U
2	1	542	U
2	1	543	C
2	1	544	U
2	1	545	G
2	1	546	C
2	1	549	U
2	1	555	A
2	1	556	U
2	1	557	A
2	1	564	G
2	1	566	C
2	1	568	A
2	1	576	A
2	1	577	G
2	1	590	A
2	1	599	U
2	1	600	U
2	1	602	A
2	1	609	A
2	1	618	U
2	1	619	A
2	1	620	A
2	1	634	C
2	1	647	A
2	1	658	A

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Mol	Chain	Res	Type
2	1	675	A
2	1	679	U
2	1	703	A
2	1	710	G
2	1	713	A
2	1	717	A
2	1	730	A
2	1	732	U
2	1	759	G
2	1	763	U
2	1	772	U
2	1	773	U
2	1	777	G
2	1	781	G
2	1	802	A
2	1	813	A
2	1	826	A
2	1	845	C
2	1	857	C
2	1	870	U
2	1	875	U
2	1	892	A
2	1	893	U
2	1	903	G
2	1	904	G
2	1	910	A
2	1	912	G
2	1	913	A
2	1	919	C
2	1	921	A
2	1	933	G
2	1	940	C
2	1	955	C
2	1	956	U
2	1	975	U
2	1	976	A
2	1	978	C
2	1	990	G
2	1	996	C
2	1	997	G
2	1	998	A
2	1	1006	G

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Mol	Chain	Res	Type
2	1	1011	C
2	1	1012	U
2	1	1013	U
2	1	1014	G
2	1	1016	G
2	1	1029	U
2	1	1030	U
2	1	1033	C
2	1	1037	U
2	1	1043	A
2	1	1045	C
2	1	1060	A
2	1	1061	A
2	1	1077	U
2	1	1078	U
2	1	1090	A
2	1	1091	U
2	1	1092	U
2	1	1094	A
2	1	1099	A
2	1	1100	G
2	1	1113	G
2	1	1127	G
2	1	1149	A
2	1	1155	A
2	1	1170	G
2	1	1174	G
2	1	1176	A
2	1	1177	U
2	1	1178	G
2	1	1188	C
2	1	1189	A
2	1	1192	C
2	1	1197	C
2	1	1205	G
2	1	1216	U
2	1	1283	A
2	1	1304	A
2	1	1305	U
2	1	1322	A
2	1	1326	A
2	1	1345	G

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Mol	Chain	Res	Type
2	1	1346	U
2	1	1347	U
2	1	1348	U
2	1	1352	C
2	1	1353	G
2	1	1382	A
2	1	1395	U
2	1	1415	A
2	1	1421	U
2	1	1430	G
2	1	1433	C
2	1	1442	A
2	1	1446	G
2	1	1477	A
2	1	1483	G
2	1	1498	C
2	1	1504	C
2	1	1523	C
2	1	1524	G
2	1	1529	U
2	1	1532	G
2	1	1535	A
2	1	1551	U
2	1	1552	C
2	1	1556	G
2	1	1558	G
2	1	1560	U
2	1	1561	U
2	1	1562	G
2	1	1563	A
2	1	1565	U
2	1	1566	U
2	1	1567	U
2	1	1568	U
2	1	1569	C
2	1	1571	G
2	1	1574	C
2	1	1585	A
2	1	1589	A
2	1	1601	A
2	1	1603	U
2	1	1625	U

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Mol	Chain	Res	Type
2	1	1635	C
2	1	1638	A
2	1	1639	A
2	1	1641	U
2	1	1653	C
2	1	1654	G
2	1	1679	A
2	1	1683	U
2	1	1720	U
2	1	1721	C
2	1	1732	G
2	1	1746	A
2	1	1747	G
2	1	1758	U
2	1	1760	U
2	1	1761	U
2	1	1762	G
2	1	1763	C
2	1	1774	G
2	1	1776	G
2	1	1792	G
2	1	1793	A
2	1	1808	G
2	1	1811	U
2	1	1812	A
2	1	1814	U
2	1	1815	U
2	1	1816	U
2	1	1817	U
2	1	1835	A
2	1	1838	A
2	1	1842	C
2	1	1845	C
2	1	1862	C
2	1	1872	U
2	1	1874	G
2	1	1876	U
2	1	1902	G
2	1	1944	G
2	1	2070	A
2	1	2072	C
2	1	2078	A

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Mol	Chain	Res	Type
2	1	2089	G
2	1	2090	U
2	1	2091	A
2	1	2092	C
2	1	2099	G
2	1	2100	G
2	1	2109	A
2	1	2118	U
2	1	2122	A
2	1	2136	A
2	1	2147	G
2	1	2166	A
2	1	2185	A
2	1	2186	A
2	1	2187	U
2	1	2188	G
2	1	2222	A
2	1	2227	G
2	1	2233	A
2	1	2235	C
2	1	2250	G
2	1	2251	G
2	1	2259	A
2	1	2260	U
2	1	2276	U
2	1	2285	G
2	1	2288	U
2	1	2291	A
2	1	2292	U
2	1	2293	G
2	1	2312	U
2	1	2313	G
2	1	2314	U
2	1	2341	A
2	1	2351	A
2	1	2352	C
2	1	2353	G
2	1	2363	G
2	1	2366	U
2	1	2371	G
2	1	2372	G
2	1	2375	A

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Mol	Chain	Res	Type
2	1	2380	A
2	1	2381	G
2	1	2382	A
2	1	2389	U
2	1	2397	A
2	1	2420	G
2	1	2422	C
2	1	2482	U
2	1	2484	U
2	1	2489	A
2	1	2492	U
2	1	2493	A
2	1	2510	U
2	1	2511	G
2	1	2513	A
2	1	2515	G
2	1	2516	U
2	1	2517	C
2	1	2518	A
2	1	2519	A
2	1	2520	A
2	1	2521	C
2	1	2522	U
2	1	2527	G
2	1	2530	C
2	1	2536	U
2	1	2537	U
2	1	2538	A
2	1	2545	C
2	1	2546	U
2	1	2547	G
2	1	2554	C
2	1	2557	G
2	1	2565	A
2	1	2566	C
2	1	2578	G
2	1	2579	G
2	1	2586	G
2	1	2598	A
2	1	2609	A
2	1	2624	U
2	1	2628	A

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Mol	Chain	Res	Type
2	1	2646	A
2	1	2649	G
2	1	2653	U
2	1	2661	A
2	1	2663	A
2	1	2666	A
2	1	2676	A
2	1	2686	G
2	1	2700	G
2	1	2701	U
2	1	2725	G
2	1	2727	C
2	1	2734	A
2	1	2744	C
2	1	2745	C
2	1	2749	G
2	1	2750	G
2	1	2768	G
2	1	2771	A
2	1	2772	G
2	1	2773	A
2	1	2786	G
2	1	2789	A
2	1	2790	U
2	1	2814	U
2	1	2815	U
2	1	2817	A
2	1	2843	G
2	1	2844	A
2	1	2847	U
2	1	2859	A
2	1	2861	C
2	1	2866	C
2	1	2871	C
2	1	2886	G
2	1	2895	U
2	1	2900	C
2	1	2907	U
2	1	2908	A
2	1	2914	C
2	1	2919	G
2	1	2923	G

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Mol	Chain	Res	Type
2	1	2943	A
2	1	2955	C
2	1	2962	G
2	1	2968	U
2	1	2969	G
2	1	2984	A
2	1	3028	U
2	1	3031	G
2	1	3050	A
2	1	3051	C
2	1	3052	G
2	1	3058	A
2	1	3064	C
2	1	3065	C
2	1	3076	U
2	1	3094	A
2	1	3101	A
2	1	3102	A
2	1	3103	U
2	1	3114	A
2	1	3115	C
2	1	3134	C
2	1	3138	U
2	1	3143	G
2	1	3144	A
2	1	3146	G
2	1	3149	U
2	1	3151	C
2	1	3157	A
2	1	3163	U
2	1	3164	U
2	1	3165	U
2	1	3171	C
2	1	3172	U
2	1	3182	C
2	1	3183	A
2	1	3184	G
2	1	3187	U
2	1	3194	G
2	1	3200	C
2	1	3208	A
2	1	3210	A

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Mol	Chain	Res	Type
2	1	3211	G
2	1	3212	G
2	1	3214	U
2	1	3224	U
2	1	3225	G
2	1	3228	G
2	1	3235	A
2	1	3236	G
2	1	3241	G
2	1	3246	C
2	1	3251	G
2	1	3252	C
2	1	3255	G
2	1	3259	A
2	1	3260	A
2	1	3269	C
2	1	3272	A
2	1	3281	A
2	1	3284	U
2	1	3306	U
2	1	3309	A
2	1	3310	G
2	1	3312	A
2	1	3316	U
2	1	3318	G
2	1	3319	U
2	1	3320	U
2	1	3321	G
2	1	3334	G
2	1	3343	C
2	1	3347	U
2	1	3351	G
2	1	3361	U
4	3	22	A
4	3	42	A
4	3	54	U
4	3	55	A
4	3	65	G
4	3	73	C
4	3	76	A
4	3	102	A
4	3	112	G

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Mol	Chain	Res	Type
5	4	34	U
5	4	35	C
5	4	53	A
5	4	59	A
5	4	62	C
5	4	63	G
5	4	81	A
5	4	84	C
5	4	86	U
5	4	87	G
5	4	95	G
5	4	102	U
5	4	104	A
5	4	105	A
5	4	106	C
5	4	111	A
5	4	113	U
5	4	125	U
5	4	126	A
5	4	152	G
10	A	25	C
10	A	26	A
10	A	27	U
10	A	34	G
10	A	42	G
10	A	45	U
10	A	47	A
10	A	57	G
10	A	59	C
10	A	63	G
10	A	66	U
10	A	74	U
10	A	75	U
10	A	76	A
10	A	77	U
10	A	78	A
10	A	81	G
10	A	84	A
10	A	100	A
10	A	104	A
10	A	111	U
10	A	114	C

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Mol	Chain	Res	Type
10	A	115	G
10	A	123	G
10	A	124	A
10	A	127	G
10	A	129	A
10	A	138	C
10	A	139	U
10	A	142	G
10	A	143	A
10	A	151	G
10	A	152	G
10	A	154	A
10	A	159	U
10	A	166	A
10	A	167	A
10	A	174	C
10	A	176	U
10	A	177	A
10	A	190	U
10	A	192	U
10	A	193	G
10	A	199	G
10	A	200	A
10	A	201	U
10	A	202	G
10	A	211	A
10	A	213	A
10	A	215	A
10	A	216	A
10	A	217	A
10	A	218	A
10	A	219	A
10	A	255	A
10	A	259	U
10	A	260	U
10	A	261	C
10	A	262	G
10	A	268	C
10	A	269	A
10	A	270	U
10	A	274	C
10	A	276	U

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Mol	Chain	Res	Type
10	A	277	G
10	A	278	U
10	A	279	G
10	A	283	G
10	A	285	G
10	A	299	A
10	A	312	C
10	A	314	A
10	A	319	C
10	A	320	G
10	A	327	G
10	A	331	A
10	A	335	G
10	A	336	C
10	A	350	A
10	A	357	A
10	A	358	A
10	A	359	C
10	A	388	G
10	A	398	A
10	A	399	A
10	A	400	C
10	A	402	G
10	A	414	A
10	A	416	G
10	A	421	G
10	A	422	C
10	A	423	A
10	A	424	G
10	A	432	G
10	A	437	U
10	A	442	C
10	A	446	C
10	A	457	G
10	A	458	A
10	A	466	A
10	A	475	A
10	A	479	A
10	A	480	U
10	A	482	C
10	A	483	A
10	A	485	G

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Mol	Chain	Res	Type
10	A	500	U
10	A	501	G
10	A	503	A
10	A	505	U
10	A	506	U
10	A	509	A
10	A	512	G
10	A	515	U
10	A	525	A
10	A	530	U
10	A	533	A
10	A	537	G
10	A	539	A
10	A	540	A
10	A	547	G
10	A	553	A
10	A	554	A
10	A	555	G
10	A	556	U
10	A	557	C
10	A	563	C
10	A	566	G
10	A	577	A
10	A	580	U
10	A	592	A
10	A	593	G
10	A	604	A
10	A	617	A
10	A	618	A
10	A	620	A
10	A	621	A
10	A	622	G
10	A	648	U
10	A	650	G
10	A	651	C
10	A	652	C
10	A	653	G
10	A	654	G
10	A	655	U
10	A	678	A
10	A	682	A
10	A	686	G

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Mol	Chain	Res	Type
10	A	688	G
10	A	689	C
10	A	690	C
10	A	693	U
10	A	694	C
10	A	696	U
10	A	701	G
10	A	722	A
10	A	723	G
10	A	725	A
10	A	728	U
10	A	730	U
10	A	740	A
10	A	741	A
10	A	750	G
10	A	751	U
10	A	752	U
10	A	756	A
10	A	759	A
10	A	760	G
10	A	763	C
10	A	764	U
10	A	765	U
10	A	766	U
10	A	767	G
10	A	771	G
10	A	773	A
10	A	778	U
10	A	779	U
10	A	787	A
10	A	796	A
10	A	798	A
10	A	799	G
10	A	803	G
10	A	804	U
10	A	805	U
10	A	806	A
10	A	807	U
10	A	813	U
10	A	814	A
10	A	816	U
10	A	818	U

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Mol	Chain	Res	Type
10	A	819	G
10	A	820	U
10	A	821	U
10	A	823	G
10	A	824	U
10	A	826	U
10	A	828	U
10	A	829	A
10	A	831	G
10	A	839	U
10	A	842	U
10	A	848	A
10	A	858	U
10	A	869	A
10	A	877	G
10	A	879	U
10	A	881	U
10	A	891	A
10	A	898	G
10	A	910	G
10	A	911	A
10	A	918	A
10	A	920	U
10	A	945	U
10	A	951	A
10	A	971	G
10	A	973	A
10	A	977	A
10	A	988	A
10	A	989	U
10	A	1005	A
10	A	1011	A
10	A	1013	C
10	A	1024	A
10	A	1025	G
10	A	1035	G
10	A	1036	U
10	A	1038	G
10	A	1042	U
10	A	1043	U
10	A	1044	U
10	A	1046	A

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Mol	Chain	Res	Type
10	A	1047	U
10	A	1055	A
10	A	1056	U
10	A	1057	C
10	A	1058	G
10	A	1059	G
10	A	1061	A
10	A	1066	A
10	A	1067	C
10	A	1077	A
10	A	1079	G
10	A	1081	C
10	A	1085	G
10	A	1123	A
10	A	1128	A
10	A	1131	G
10	A	1135	G
10	A	1143	C
10	A	1145	A
10	A	1152	G
10	A	1168	A
10	A	1169	A
10	A	1170	U
10	A	1171	U
10	A	1179	A
10	A	1181	A
10	A	1184	G
10	A	1185	G
10	A	1186	G
10	A	1187	A
10	A	1193	A
10	A	1197	G
10	A	1202	A
10	A	1203	G
10	A	1213	G
10	A	1214	G
10	A	1215	A
10	A	1217	U
10	A	1218	G
10	A	1219	A
10	A	1221	A
10	A	1229	A

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Mol	Chain	Res	Type
10	A	1230	G
10	A	1231	C
10	A	1236	U
10	A	1237	C
10	A	1241	A
10	A	1242	U
10	A	1258	G
10	A	1270	U
10	A	1276	G
10	A	1284	G
10	A	1299	U
10	A	1300	U
10	A	1301	G
10	A	1306	A
10	A	1325	U
10	A	1329	A
10	A	1330	A
10	A	1336	G
10	A	1339	G
10	A	1342	A
10	A	1343	G
10	A	1346	U
10	A	1348	U
10	A	1349	G
10	A	1352	G
10	A	1355	A
10	A	1356	U
10	A	1357	A
10	A	1359	U
10	A	1360	C
10	A	1369	G
10	A	1370	A
10	A	1376	U
10	A	1377	A
10	A	1381	A
10	A	1382	U
10	A	1384	U
10	A	1385	C
10	A	1392	A
10	A	1398	G
10	A	1399	U
10	A	1400	U

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Mol	Chain	Res	Type
10	A	1401	U
10	A	1413	A
10	A	1414	G
10	A	1422	A
10	A	1431	G
10	A	1432	A
10	A	1445	C
10	A	1446	A
10	A	1454	U
10	A	1455	A
10	A	1457	A
10	A	1462	C
10	A	1468	C
10	A	1476	A
10	A	1477	U
10	A	1478	A
10	A	1479	A
10	A	1480	G
10	A	1483	U
10	A	1491	G
10	A	1493	G
10	A	1502	A
10	A	1503	A
10	A	1508	G
10	A	1510	G
10	A	1511	A
10	A	1513	A
10	A	1523	G
10	A	1524	C
10	A	1526	G
10	A	1530	A
10	A	1544	U
10	A	1546	G
10	A	1556	A
10	A	1561	G
10	A	1571	G
10	A	1574	A
10	A	1577	G
10	A	1580	A
10	A	1582	U
10	A	1588	G
10	A	1590	U

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Mol	Chain	Res	Type
10	A	1594	G
10	A	1601	A
10	A	1609	G
10	A	1621	C
10	A	1644	U
10	A	1645	G
10	A	1665	C
10	A	1669	U
10	A	1672	G
10	A	1673	U
10	A	1674	U
10	A	1677	G
10	A	1700	G
10	A	1702	A
10	A	1704	C
10	A	1742	A
10	A	1744	G
10	A	1753	A
10	A	1756	U
10	A	1767	G
10	A	1769	A
10	A	1770	C
10	A	1779	G
10	A	1780	G
10	A	1781	A
10	A	1782	U
10	A	1783	C
78	PT	3	C
78	PT	4	G
78	PT	5	G
78	PT	9	G
78	PT	17	C
78	PT	20	G
78	PT	21	U
78	PT	22	A
78	PT	48	U
78	PT	49	C
78	PT	50	G
78	PT	53	G
78	PT	75	C
78	PT	77	A
78	AT	3	C

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Mol	Chain	Res	Type
78	AT	5	G
78	AT	6	G
78	AT	9	G
78	AT	10	G
78	AT	14	A
78	AT	16	C
78	AT	18(A)	U
78	AT	22	A
78	AT	24	C
78	AT	43	G
78	AT	48	U
78	AT	49	C
78	AT	50	G
78	AT	53	G
78	AT	55	U
78	AT	62	C
78	AT	63	C
78	AT	75	C
78	AT	76	C
78	AT	77	A

All (62) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	172	C
2	1	538	G
2	1	563	U
2	1	586	G
2	1	601	U
2	1	892	A
2	1	912	G
2	1	1012	U
2	1	1029	U
2	1	1060	A
2	1	1099	A
2	1	1346	U
2	1	1347	U
2	1	1430	G
2	1	1559	C
2	1	1567	U
2	1	1762	G
2	1	1815	U

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Mol	Chain	Res	Type
2	1	2090	U
2	1	2515	G
2	1	2519	A
2	1	2557	G
2	1	2789	A
2	1	2790	U
2	1	3028	U
2	1	3093	U
2	1	3163	U
2	1	3193	C
2	1	3234	U
2	1	3240	U
2	1	3268	G
2	1	3309	A
2	1	3315	C
2	1	3317	U
5	4	85	G
10	A	25	C
10	A	137	A
10	A	151	G
10	A	176	U
10	A	214	U
10	A	259	U
10	A	415	A
10	A	504	A
10	A	505	U
10	A	514	G
10	A	529	C
10	A	553	A
10	A	740	A
10	A	763	C
10	A	820	U
10	A	876	A
10	A	1168	A
10	A	1335	U
10	A	1369	G
10	A	1398	G
10	A	1467	C
10	A	1479	A
10	A	1555	C
10	A	1573	A
10	A	1579	A

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Mol	Chain	Res	Type
10	A	1581	G
78	AT	2	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	MLZ	6	110	6	8,9,10	0.77	0	4,9,11	0.56	0
76	MLZ	AP	55	76	8,9,10	0.71	0	4,9,11	0.64	0
2	OMG	1	2765	2	18,26,27	2.34	8 (44%)	19,38,41	1.53	4 (21%)
25	IAS	P	119	25	6,7,8	1.19	0	5,8,10	1.44	1 (20%)
76	MLZ	AP	40	76	8,9,10	0.80	0	4,9,11	0.62	0
2	OMC	1	2808	2	19,22,23	2.84	8 (42%)	26,31,34	1.13	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MLZ	6	110	6	-	2/7/8/10	-
76	MLZ	AP	55	76	-	1/7/8/10	-
2	OMG	1	2765	2	-	0/5/27/28	0/3/3/3
25	IAS	P	119	25	-	2/5/6/8	-
76	MLZ	AP	40	76	-	3/7/8/10	-
2	OMC	1	2808	2	-	2/9/27/28	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2808	OMC	C2-N3	5.76	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2808	OMC	C6-C5	5.61	1.48	1.35
2	1	2765	OMG	C2-N3	4.96	1.45	1.33
2	1	2808	OMC	C2-N1	4.57	1.49	1.40
2	1	2808	OMC	C4-N4	4.56	1.44	1.33
2	1	2765	OMG	C4-N3	4.40	1.48	1.37
2	1	2808	OMC	C4-N3	4.34	1.43	1.34
2	1	2765	OMG	C2-N2	3.77	1.43	1.34
2	1	2808	OMC	O2-C2	-3.37	1.17	1.23
2	1	2765	OMG	C6-N1	3.17	1.42	1.37
2	1	2765	OMG	C5-C4	-3.04	1.35	1.43
2	1	2765	OMG	O6-C6	-2.97	1.17	1.23
2	1	2808	OMC	C6-N1	2.93	1.45	1.38
2	1	2765	OMG	C5-C6	2.57	1.52	1.47
2	1	2808	OMC	C5-C4	2.33	1.48	1.42
2	1	2765	OMG	C2-N1	2.07	1.42	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2765	OMG	C5-C6-N1	3.68	120.45	113.95
2	1	2808	OMC	O2-C2-N3	-3.18	117.15	122.33
2	1	2765	OMG	C2-N1-C6	-2.85	119.84	125.10
2	1	2765	OMG	C8-N7-C5	2.51	107.78	102.99
25	P	119	IAS	CA-CB-CG	-2.43	98.55	113.74
2	1	2808	OMC	C6-C5-C4	2.36	121.31	117.50
2	1	2765	OMG	O6-C6-C5	-2.32	119.83	124.37

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	2808	OMC	O4'-C1'-N1-C2
2	1	2808	OMC	O4'-C1'-N1-C6
25	P	119	IAS	C-CA-CB-CG
76	AP	40	MLZ	CG-CD-CE-NZ
6	6	110	MLZ	CE-CD-CG-CB
25	P	119	IAS	N-CA-CB-CG
76	AP	55	MLZ	CA-CB-CG-CD
76	AP	40	MLZ	CE-CD-CG-CB
6	6	110	MLZ	CD-CE-NZ-CM
76	AP	40	MLZ	CD-CE-NZ-CM

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 7 are monoatomic - leaving 18 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	$\# Z  > 2$
81	GET	1	3412	-	33,36,36	0.53	0	43,55,55	0.63	0
81	GET	1	3410	-	33,36,36	0.42	0	43,55,55	0.71	1 (2%)
81	GET	A	1801	-	33,36,36	0.46	0	43,55,55	0.84	3 (6%)
81	GET	1	3413	-	33,36,36	0.44	0	43,55,55	0.98	2 (4%)
81	GET	1	3406	-	33,36,36	0.49	0	43,55,55	0.92	1 (2%)
83	YMZ	AQ	301	-	28,28,28	1.20	1 (3%)	41,43,43	1.47	5 (12%)
81	GET	1	3409	-	33,36,36	0.50	0	43,55,55	0.78	1 (2%)
81	GET	1	3411	-	33,36,36	0.46	0	43,55,55	0.77	2 (4%)
81	GET	AT	101	-	33,36,36	0.49	0	43,55,55	0.64	1 (2%)
80	SPK	1	3401	-	13,13,13	0.39	0	12,12,12	0.90	0
81	GET	1	3405	-	33,36,36	0.43	0	43,55,55	0.80	1 (2%)
81	GET	1	3407	-	33,36,36	0.45	0	43,55,55	0.77	2 (4%)
81	GET	1	3408	-	33,36,36	0.42	0	43,55,55	0.69	1 (2%)
81	GET	A	1803	-	33,36,36	0.47	0	43,55,55	0.81	2 (4%)
81	GET	1	3403	-	33,36,36	0.56	0	43,55,55	0.92	2 (4%)
81	GET	1	3402	-	33,36,36	0.44	0	43,55,55	0.63	1 (2%)
81	GET	1	3404	-	33,36,36	0.55	0	43,55,55	0.88	2 (4%)
81	GET	A	1802	-	33,36,36	0.44	0	43,55,55	0.87	2 (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
81	GET	1	3412	-	-	1/13/74/74	0/3/3/3
81	GET	1	3410	-	-	1/13/74/74	0/3/3/3
81	GET	A	1801	-	-	1/13/74/74	1/3/3/3
81	GET	1	3413	-	-	3/13/74/74	0/3/3/3
81	GET	1	3406	-	-	1/13/74/74	0/3/3/3
83	YMZ	AQ	301	-	-	7/20/28/28	0/3/3/3
81	GET	1	3409	-	-	3/13/74/74	1/3/3/3
81	GET	1	3411	-	-	1/13/74/74	0/3/3/3
81	GET	AT	101	-	-	2/13/74/74	1/3/3/3
80	SPK	1	3401	-	-	6/11/11/11	-
81	GET	1	3405	-	-	1/13/74/74	0/3/3/3
81	GET	1	3407	-	-	1/13/74/74	0/3/3/3
81	GET	1	3408	-	-	1/13/74/74	0/3/3/3
81	GET	A	1803	-	-	7/13/74/74	0/3/3/3
81	GET	1	3403	-	-	7/13/74/74	1/3/3/3
81	GET	1	3402	-	-	1/13/74/74	0/3/3/3
81	GET	1	3404	-	-	3/13/74/74	1/3/3/3
81	GET	A	1802	-	-	1/13/74/74	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	AQ	301	YMZ	CAW-CAX	5.17	1.60	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	AQ	301	YMZ	CAK-CAR-NAP	4.54	128.32	125.50
81	1	3405	GET	O11-C11-C21	4.33	115.67	108.22
81	1	3406	GET	O11-C11-C21	4.02	115.14	108.22
81	A	1802	GET	O11-C11-C21	3.63	114.47	108.22
81	1	3413	GET	O11-C11-C21	3.60	114.41	108.22
81	1	3404	GET	O62-C62-C12	-3.28	101.36	109.18
83	AQ	301	YMZ	CAK-CAS-CAW	-3.25	117.66	120.30
81	1	3413	GET	O11-C42-C32	-3.19	101.56	109.18
83	AQ	301	YMZ	CAS-CAK-CAR	-3.19	117.11	118.87
81	1	3410	GET	O11-C11-C21	3.19	113.70	108.22

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	A	1803	GET	O11-C42-C32	-3.05	101.89	109.18
81	1	3408	GET	O11-C11-C21	2.97	113.33	108.22
81	1	3403	GET	O62-C62-C52	-2.96	99.41	107.28
81	1	3402	GET	O11-C11-C21	2.95	113.30	108.22
83	AQ	301	YMZ	CAK-CAR-CAY	-2.88	116.46	120.10
81	AT	101	GET	O62-C62-C12	-2.79	102.52	109.18
81	1	3404	GET	O11-C11-C21	2.70	112.86	108.22
81	1	3407	GET	O62-C62-C12	-2.68	102.78	109.18
81	A	1802	GET	O62-C62-C12	-2.66	102.83	109.18
81	1	3409	GET	O11-C11-C21	2.65	112.78	108.22
83	AQ	301	YMZ	CAR-NAP-CAV	-2.58	114.47	116.89
81	1	3407	GET	O11-C11-C21	2.53	112.58	108.22
81	A	1803	GET	O11-C11-C21	2.35	112.26	108.22
81	1	3411	GET	O62-C62-C12	-2.34	103.59	109.18
81	A	1801	GET	O11-C42-C32	-2.20	103.93	109.18
81	A	1801	GET	O11-C11-C21	2.19	111.99	108.22
81	1	3403	GET	O11-C11-C21	2.18	111.97	108.22
81	A	1801	GET	O62-C62-C12	-2.08	104.22	109.18
81	1	3411	GET	O11-C11-C21	2.03	111.72	108.22

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	1	3402	GET	C23-C33-N33-C93
81	1	3403	GET	C21-C11-O11-C42
81	1	3403	GET	C41-C51-C61-O61
81	1	3403	GET	C41-C51-C61-C71
81	1	3403	GET	O51-C51-C61-C71
81	1	3404	GET	C23-C33-N33-C93
81	1	3405	GET	C23-C33-N33-C93
81	1	3406	GET	C23-C33-N33-C93
81	1	3407	GET	C23-C33-N33-C93
81	1	3408	GET	C23-C33-N33-C93
81	1	3410	GET	C23-C33-N33-C93
81	1	3411	GET	C23-C33-N33-C93
81	1	3412	GET	C23-C33-N33-C93
81	1	3413	GET	C23-C33-N33-C93
81	A	1801	GET	C23-C33-N33-C93
81	A	1802	GET	C23-C33-N33-C93
81	A	1803	GET	C41-C51-C61-O61
81	A	1803	GET	C41-C51-C61-C71

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Mol	Chain	Res	Type	Atoms
81	A	1803	GET	O51-C51-C61-O61
81	A	1803	GET	O51-C51-C61-C71
81	A	1803	GET	C23-C33-N33-C93
81	AT	101	GET	C23-C33-N33-C93
80	1	3401	SPK	N5-C6-C7-C8
80	1	3401	SPK	C3-C4-N5-C6
80	1	3401	SPK	C7-C6-N5-C4
81	1	3409	GET	O51-C11-O11-C42
81	1	3413	GET	C52-C42-O11-C11
81	AT	101	GET	O51-C11-O11-C42
81	A	1803	GET	C52-C42-O11-C11
83	AQ	301	YMZ	CAK-CAS-CAW-OAA
83	AQ	301	YMZ	CAU-CAS-CAW-OAA
83	AQ	301	YMZ	CAS-CAW-CAX-NAQ
81	1	3403	GET	O51-C11-O11-C42
81	1	3404	GET	O53-C13-O62-C62
81	1	3413	GET	C32-C42-O11-C11
81	A	1803	GET	C32-C42-O11-C11
80	1	3401	SPK	C6-C7-C8-C9
83	AQ	301	YMZ	CAV-CAT-CAZ-FAE
81	1	3409	GET	C52-C42-O11-C11
81	1	3404	GET	C23-C13-O62-C62
83	AQ	301	YMZ	CAS-CAW-CAX-CAO
83	AQ	301	YMZ	OAA-CAW-CAX-CAO
80	1	3401	SPK	C12-C11-N10-C9
81	1	3403	GET	O51-C51-C61-O61
81	1	3403	GET	C52-C62-O62-C13
81	1	3409	GET	C23-C33-N33-C93
80	1	3401	SPK	C8-C9-N10-C11
83	AQ	301	YMZ	CAI-CAT-CAZ-FAE

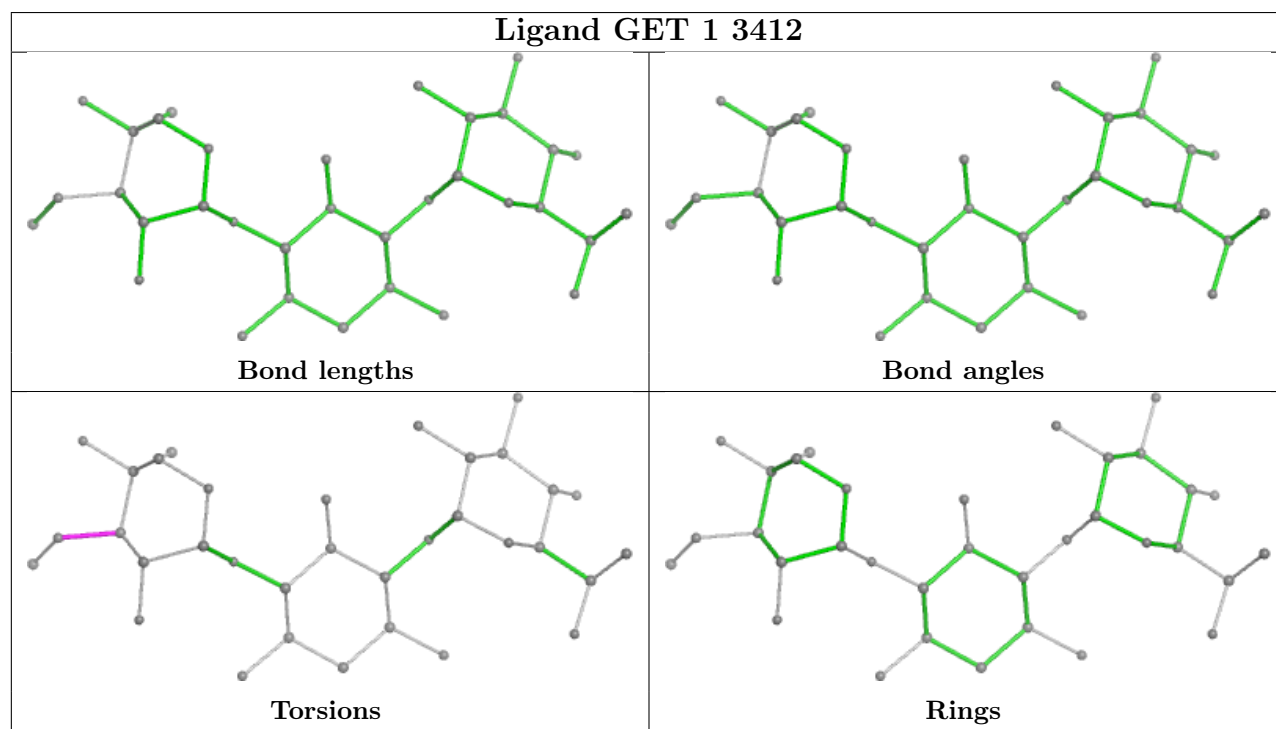
All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	1	3403	GET	C11-C21-C31-C41-C51-O51
81	1	3409	GET	C13-C23-C33-C43-C53-O53
81	1	3404	GET	C13-C23-C33-C43-C53-O53
81	A	1801	GET	C13-C23-C33-C43-C53-O53
81	AT	101	GET	C11-C21-C31-C41-C51-O51

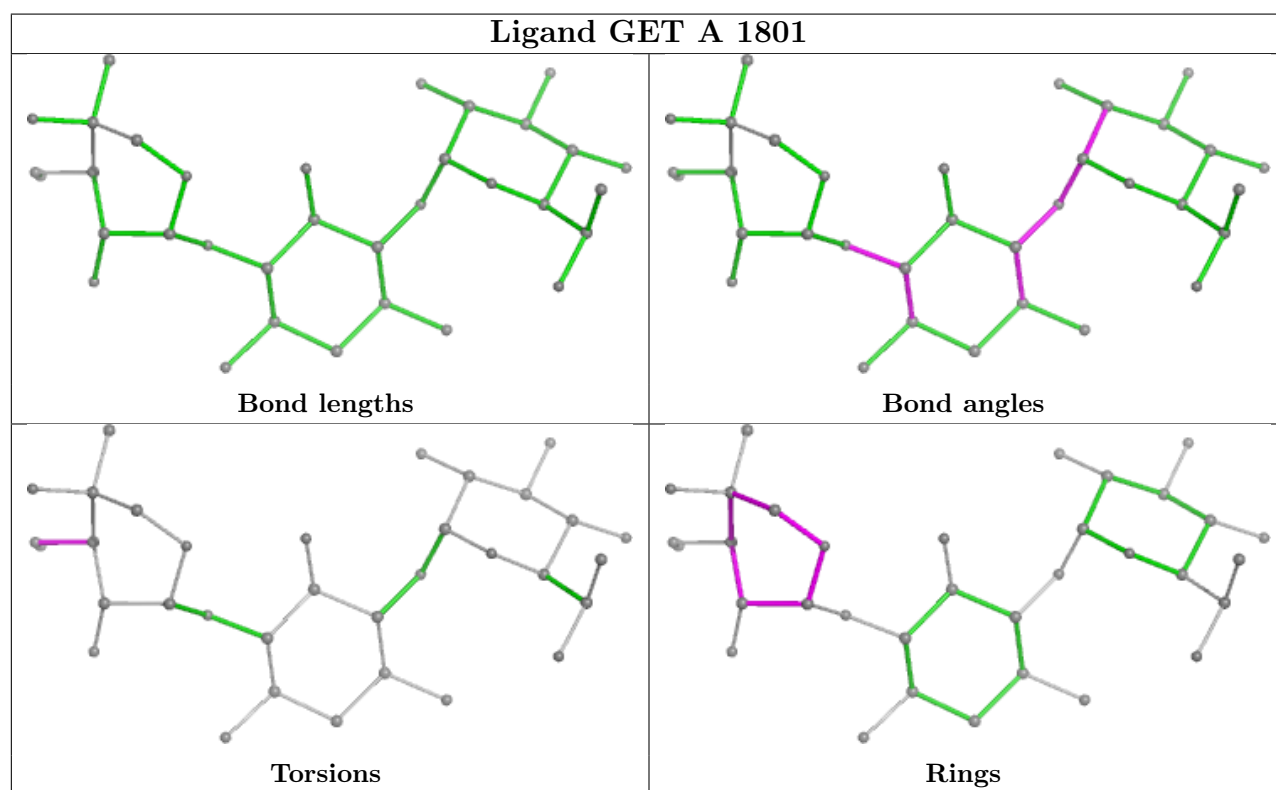
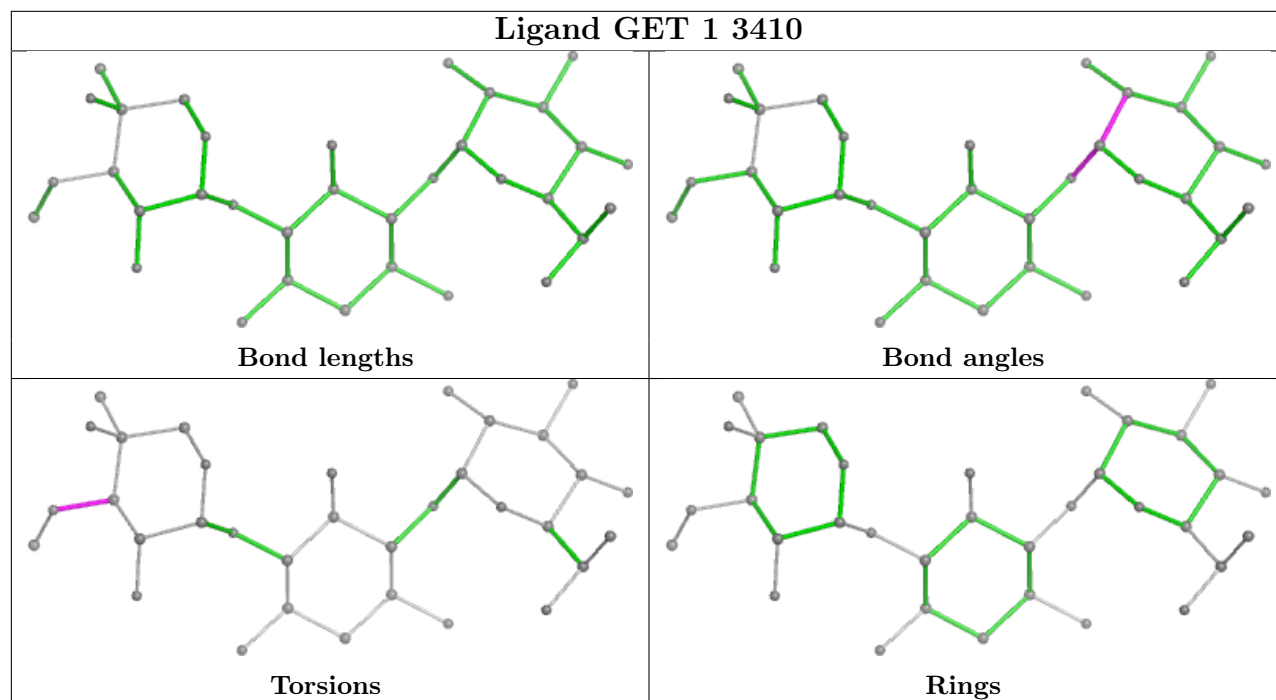
No monomer is involved in short contacts.

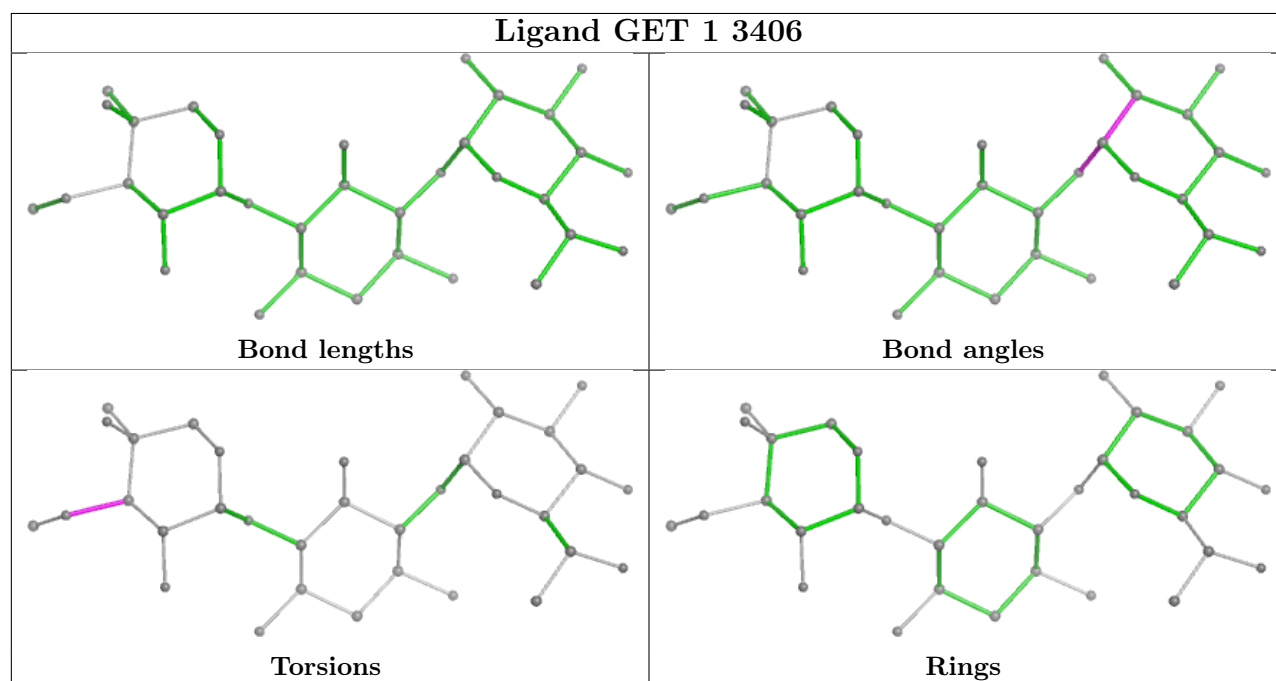
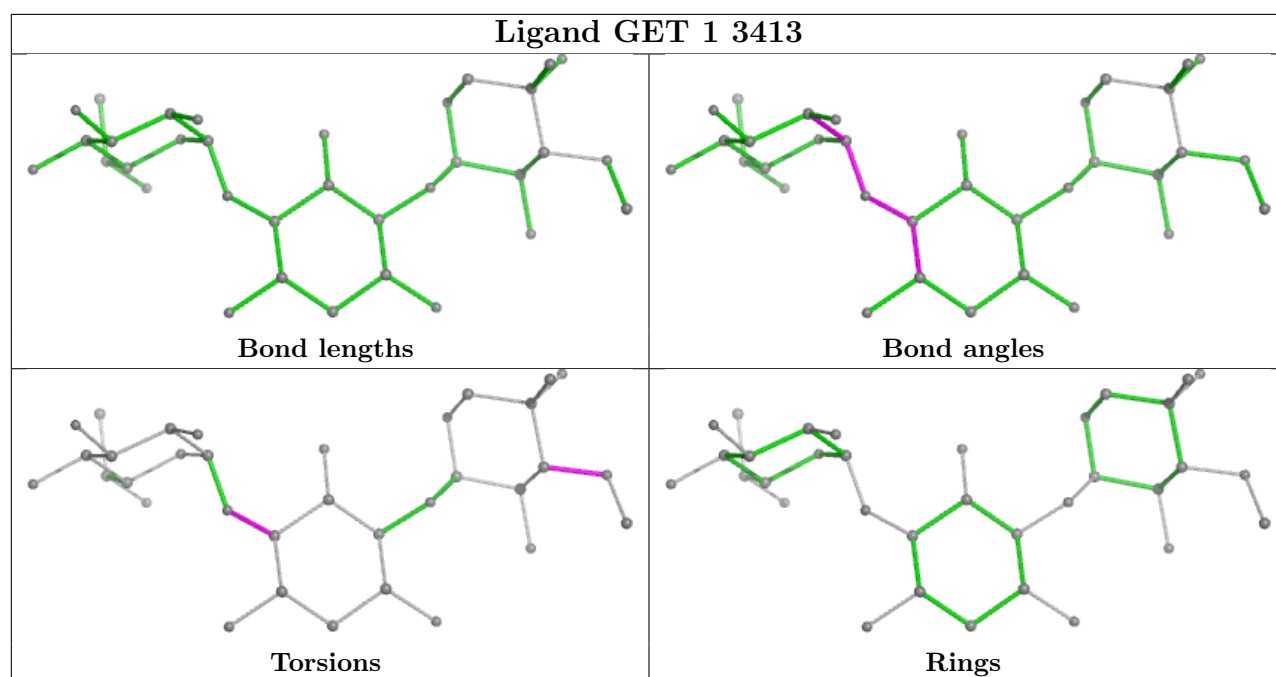
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

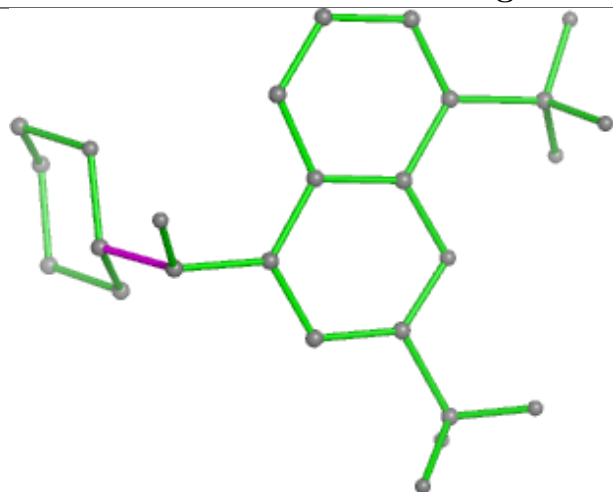




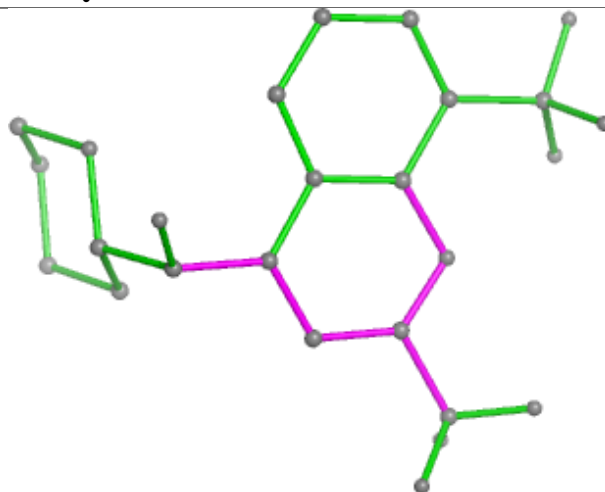




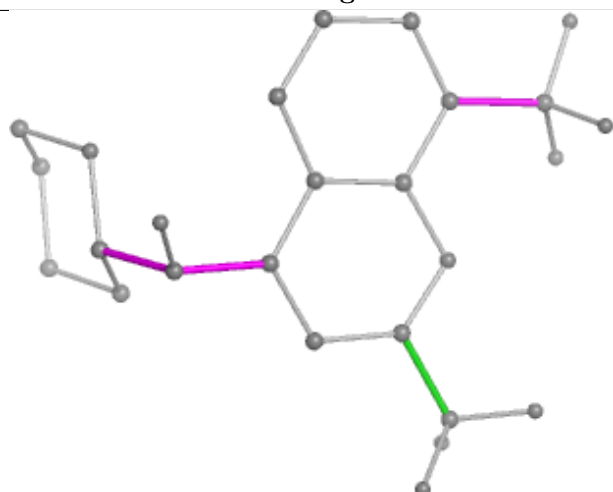
## Ligand YMZ AQ 301



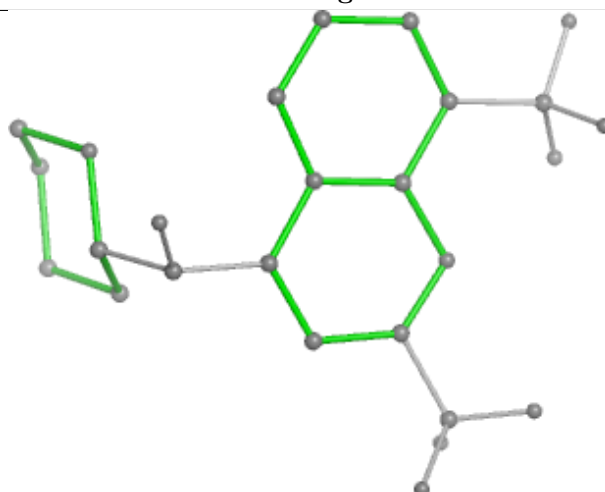
Bond lengths



Bond angles

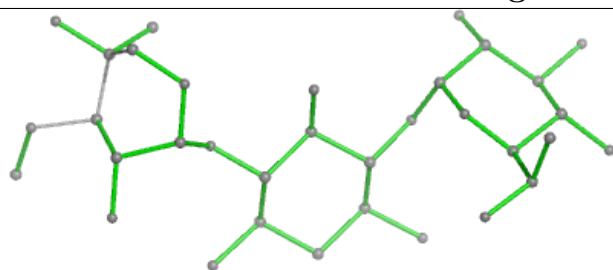


Torsions

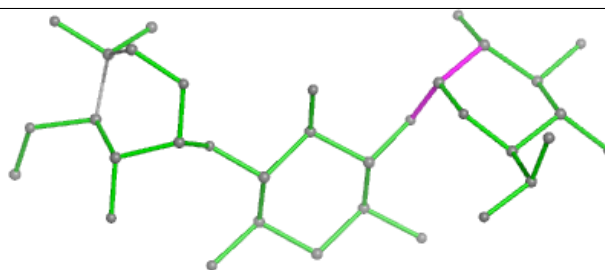


Rings

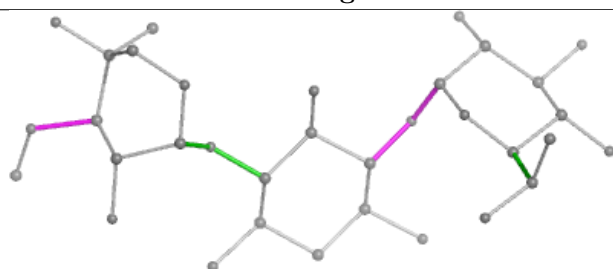
## Ligand GET 1 3409



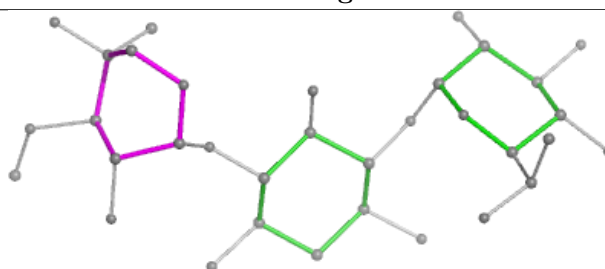
Bond lengths



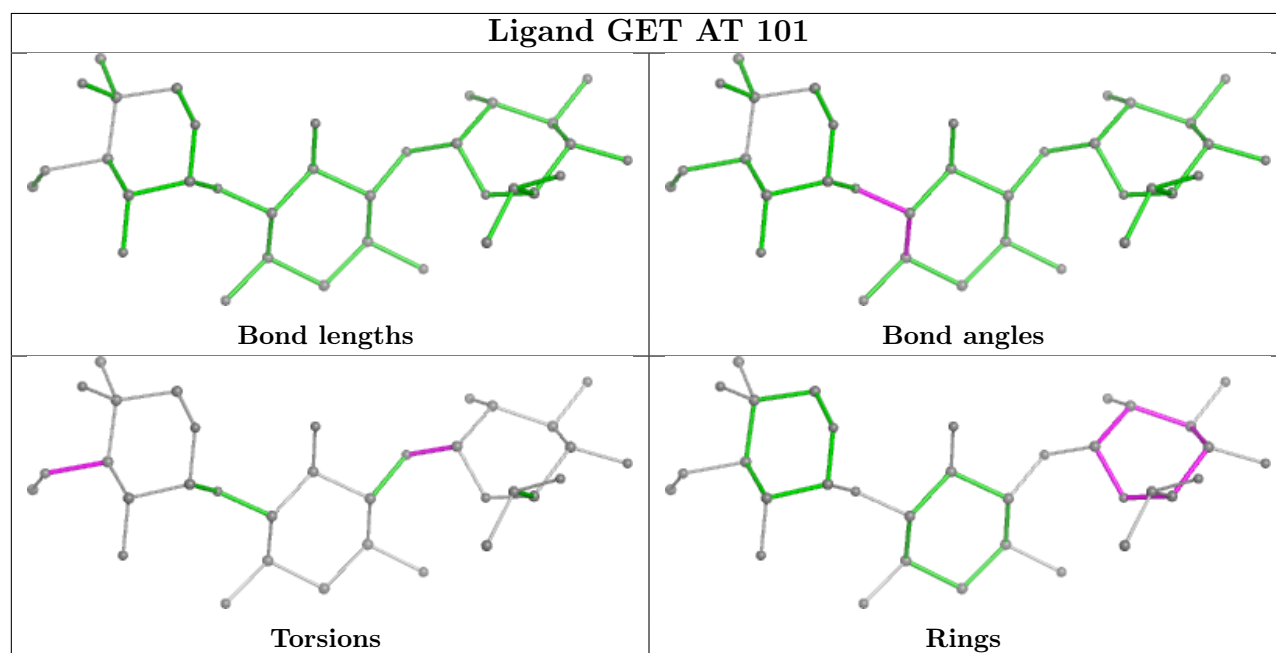
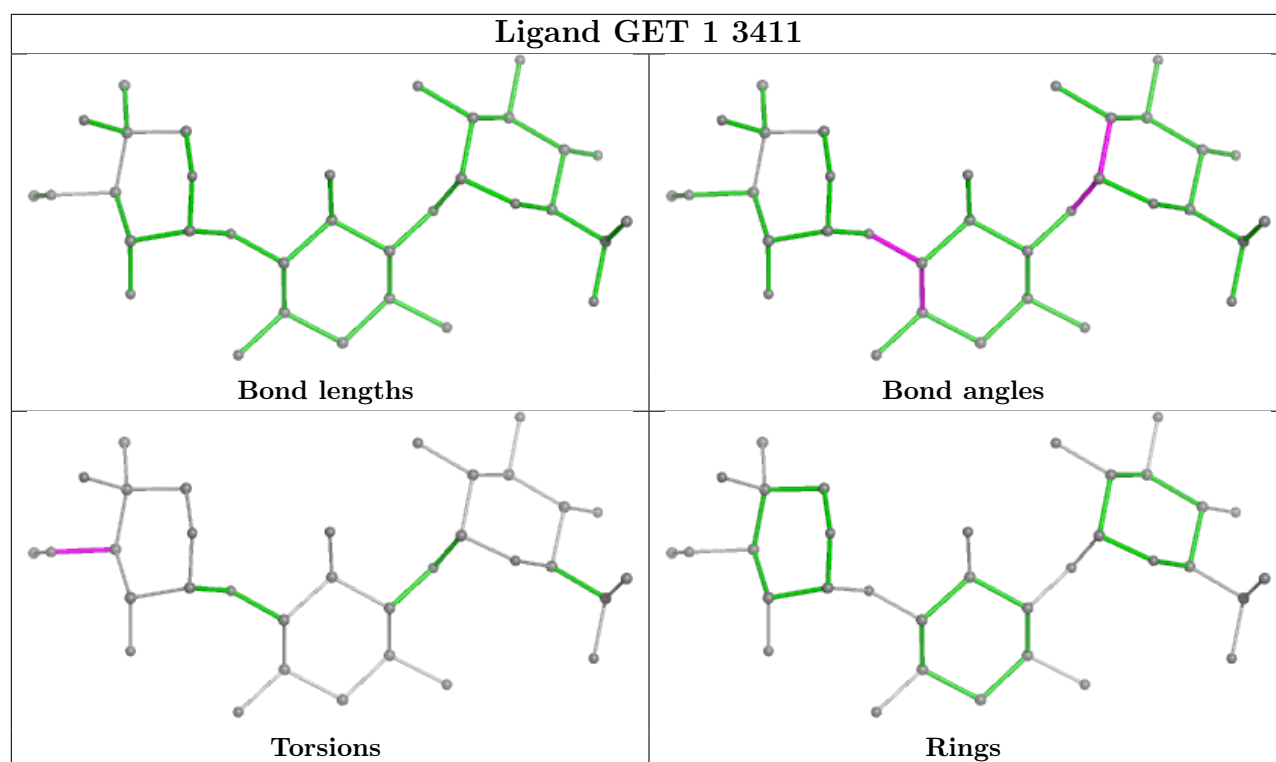
Bond angles

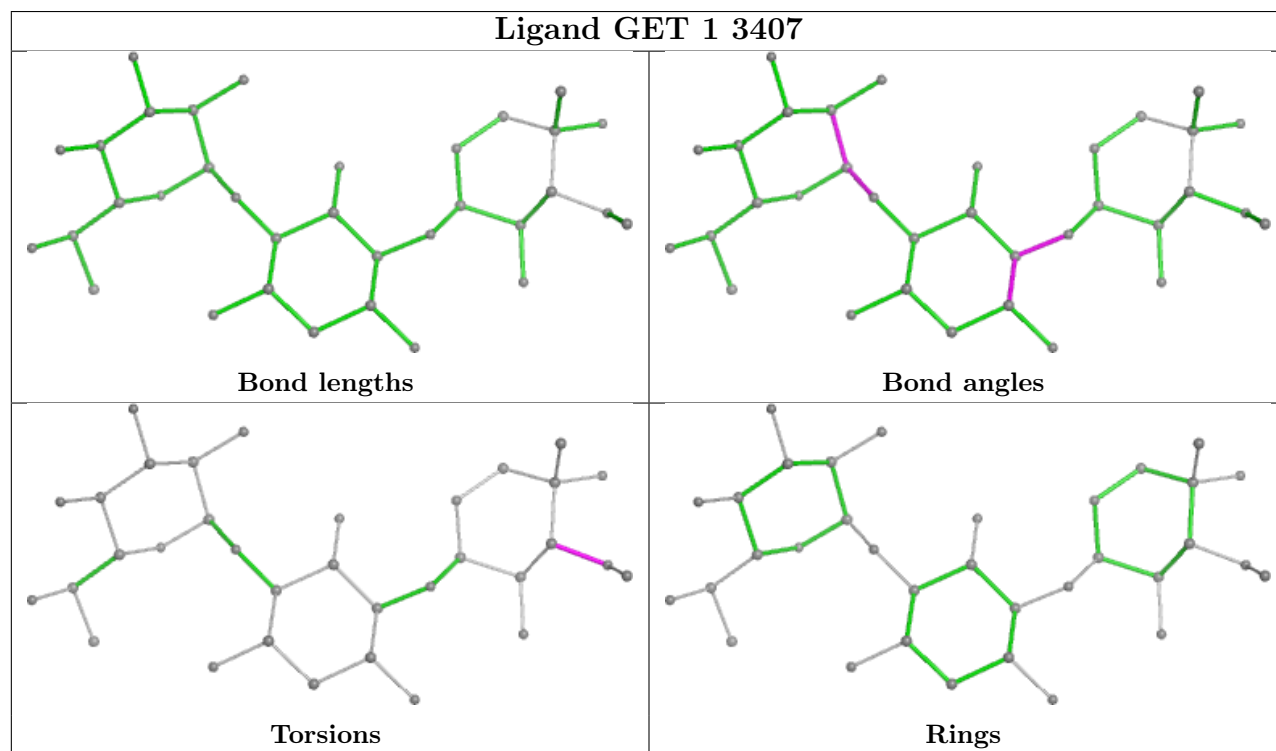
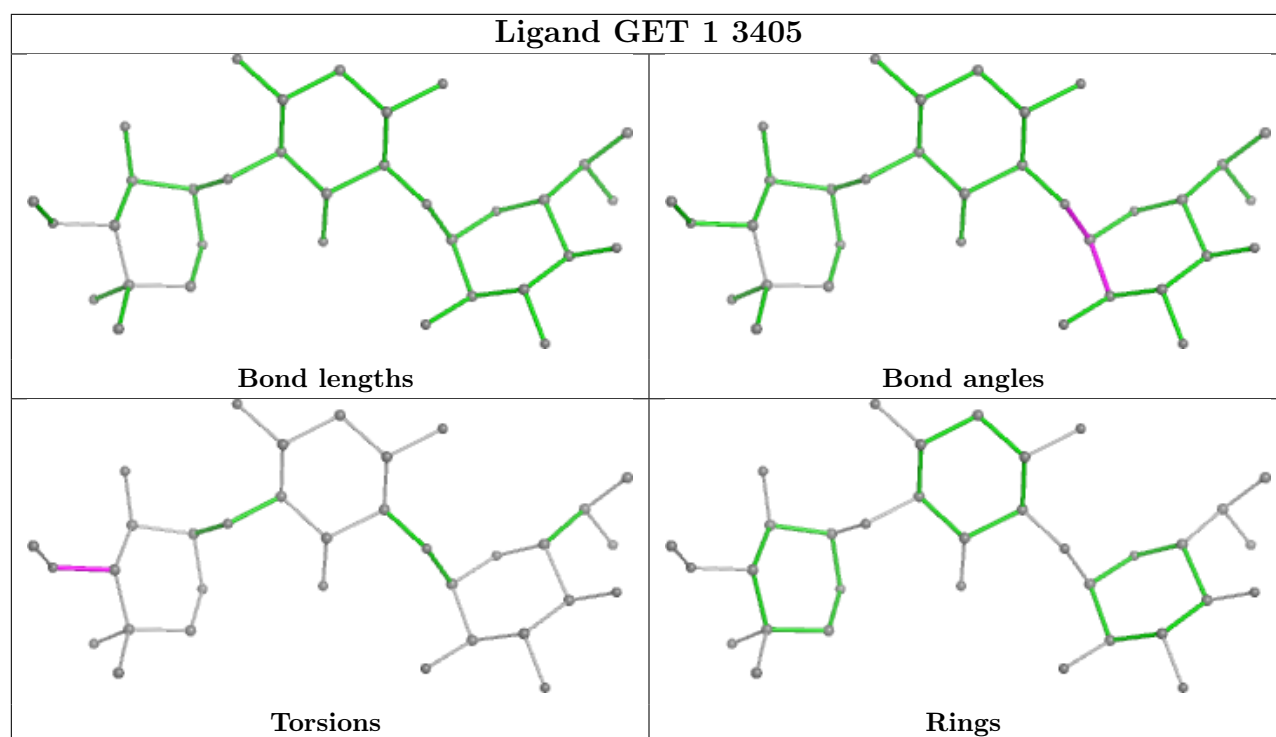


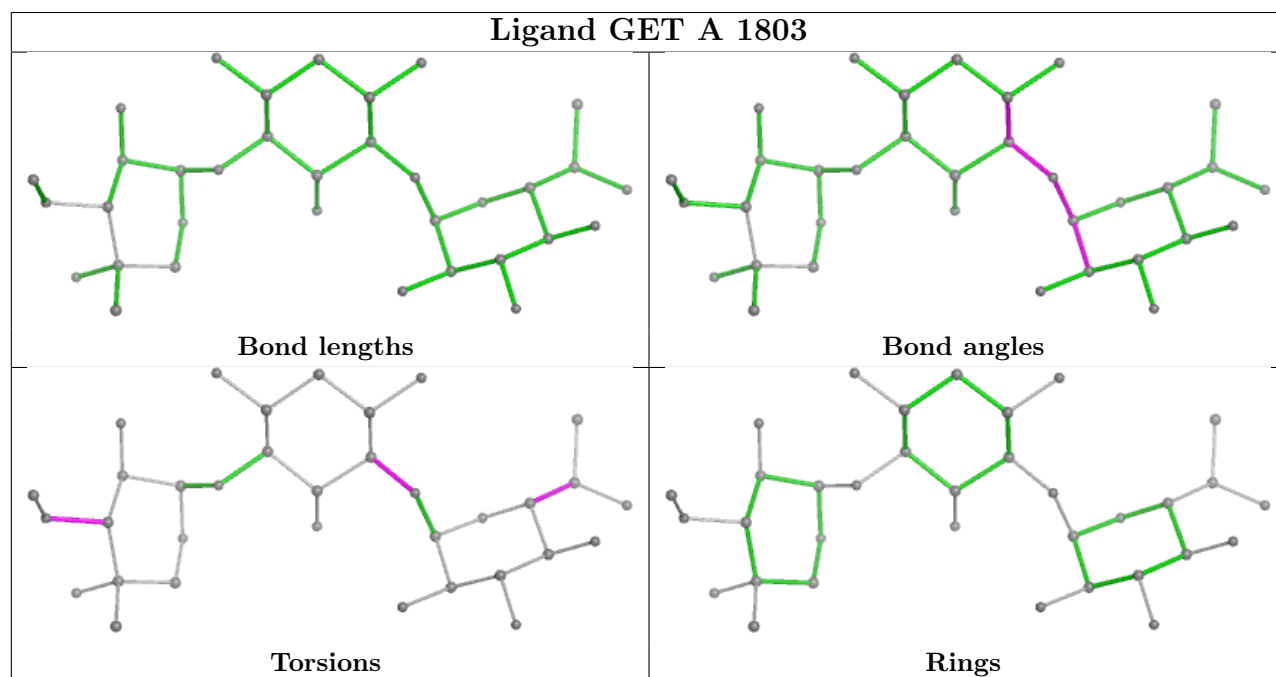
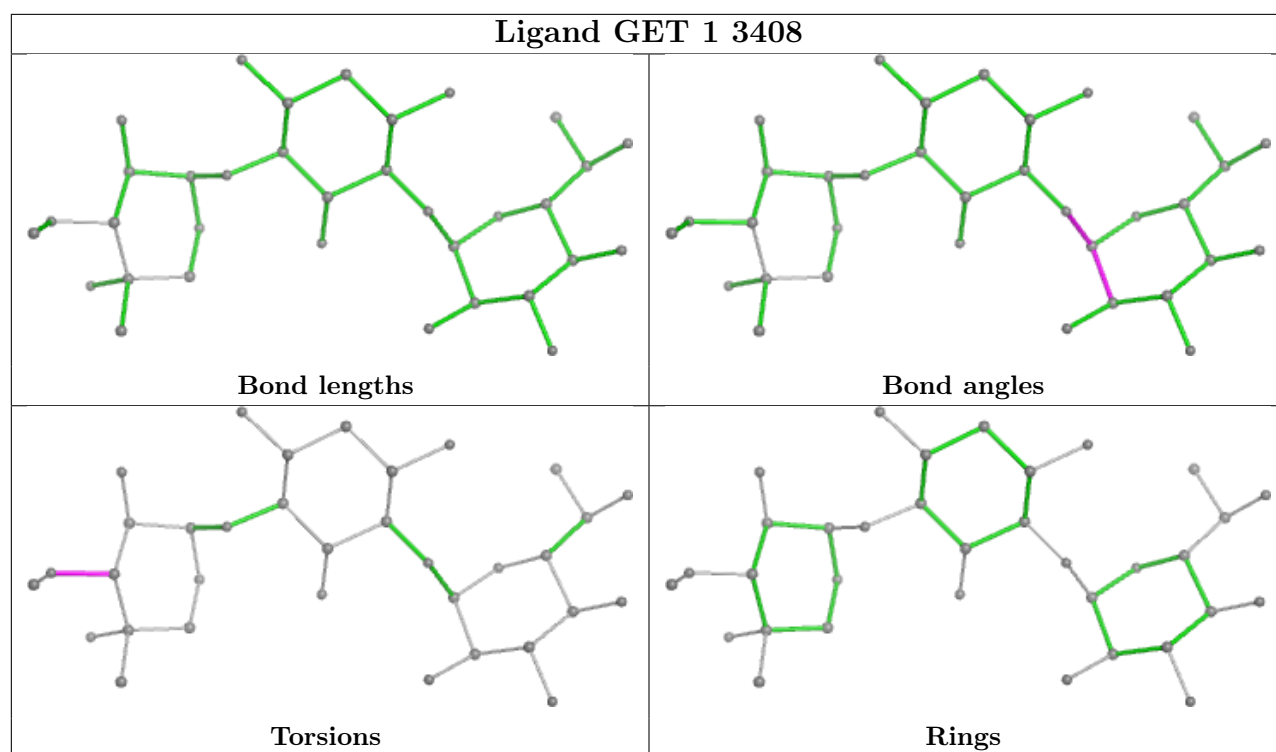
Torsions

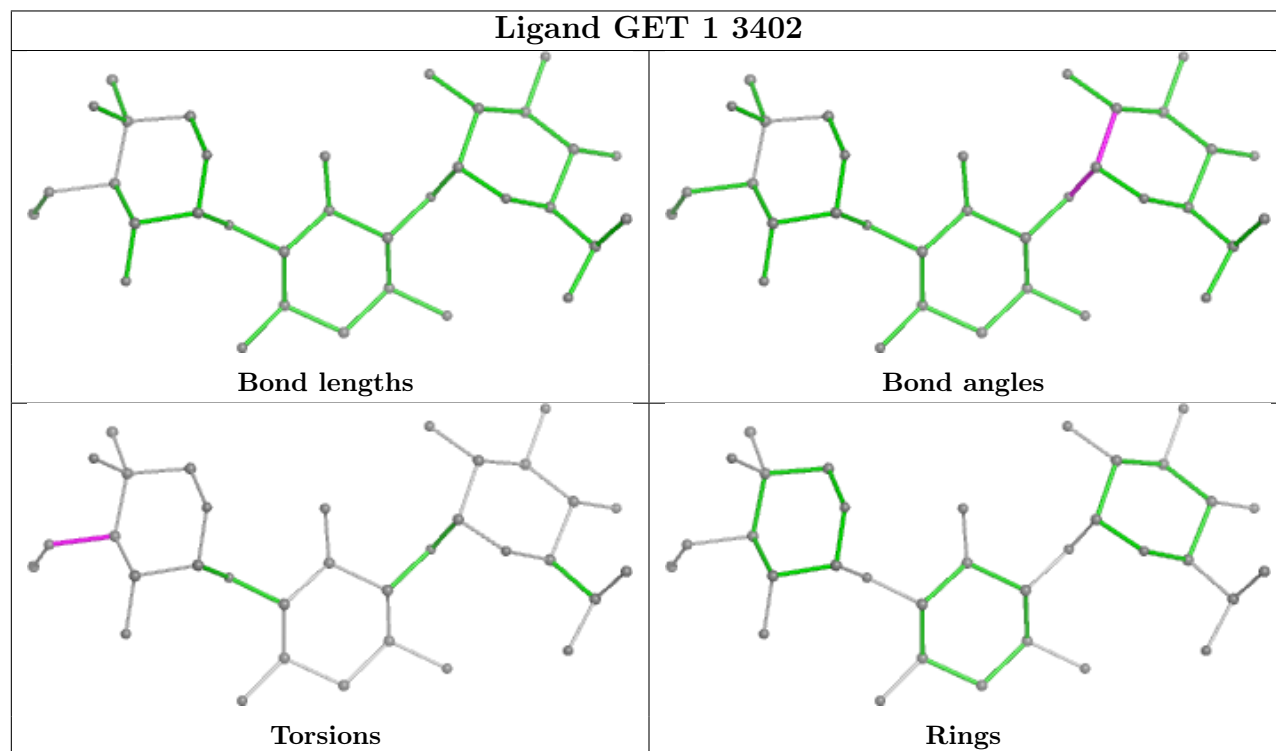
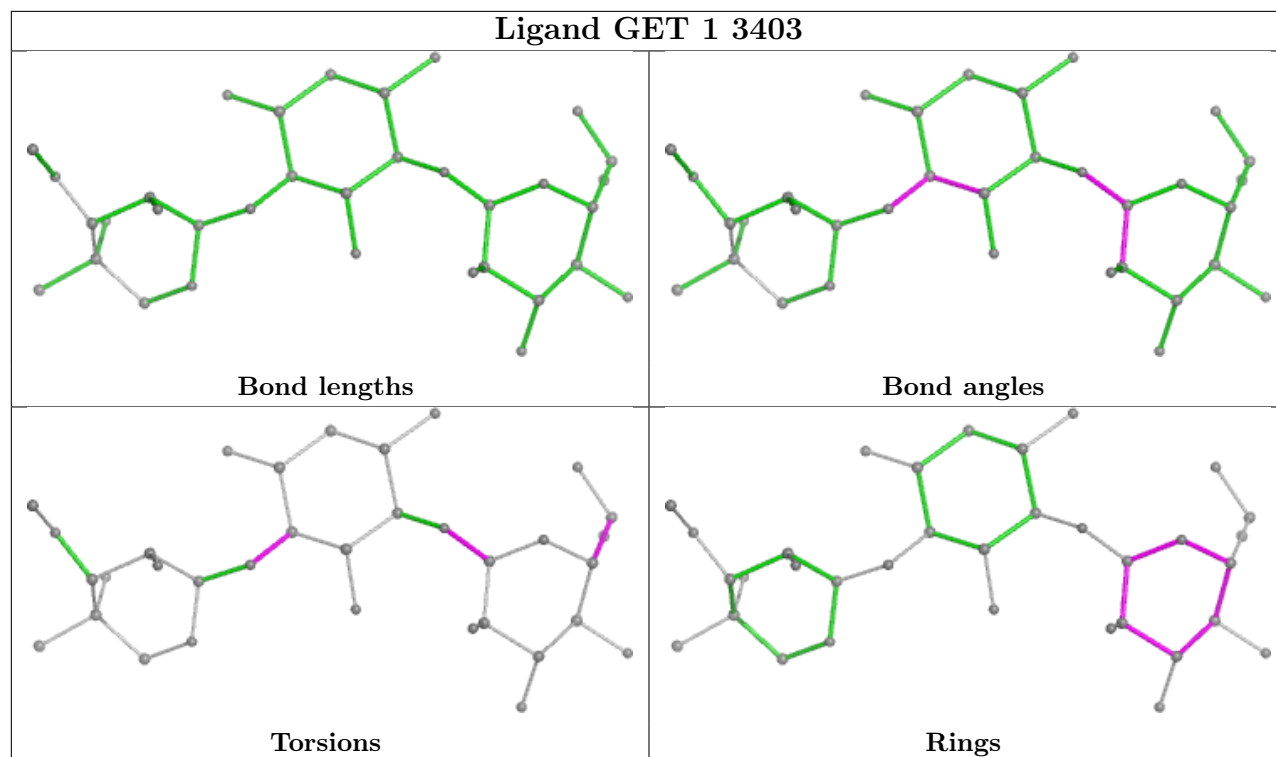


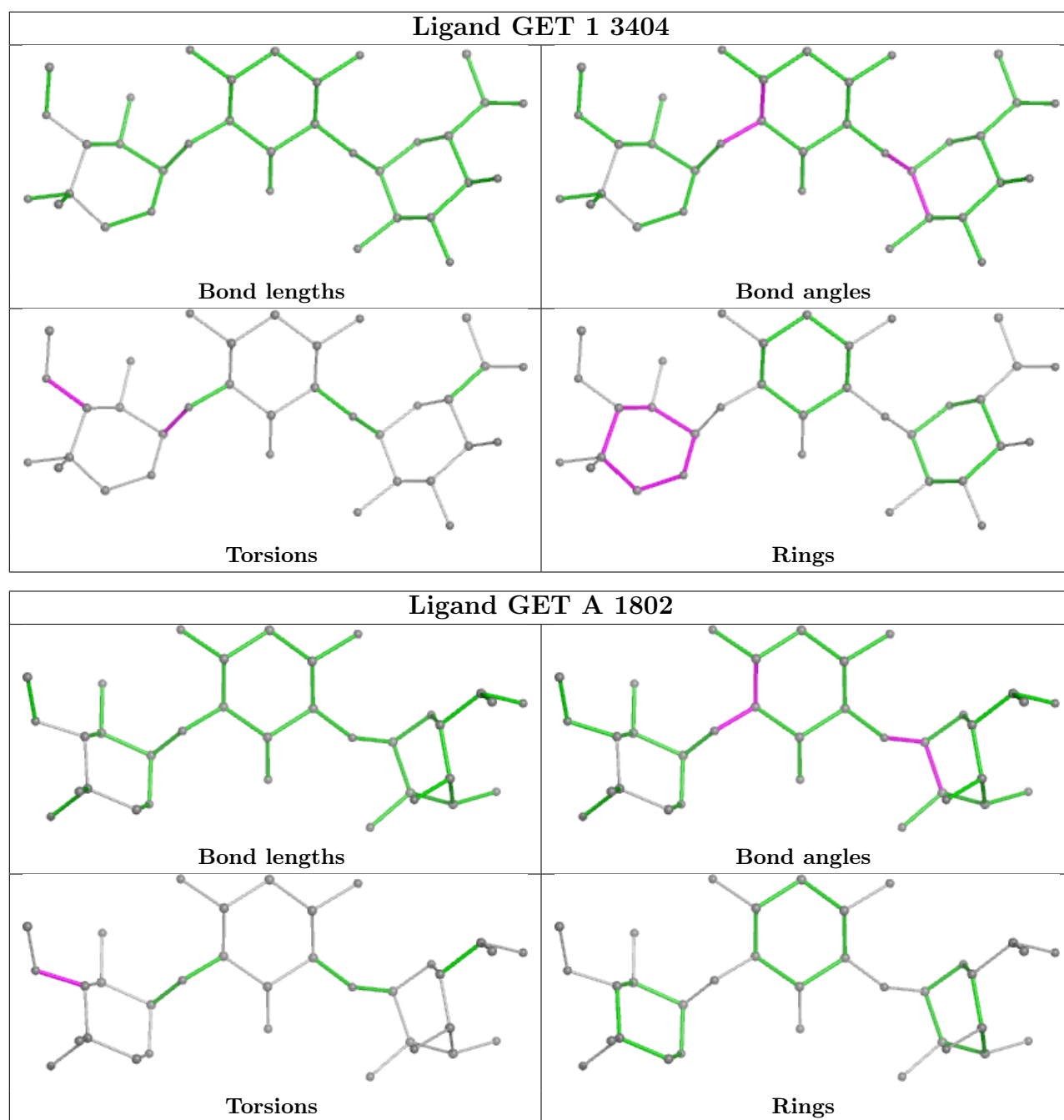
Rings











## 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.



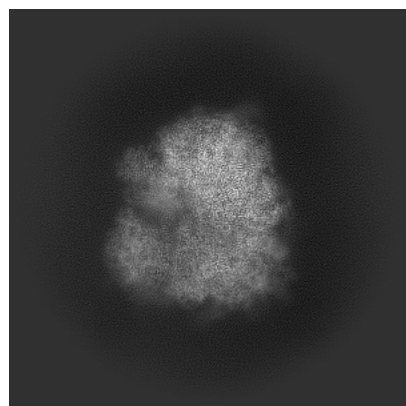
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51103. These allow visual inspection of the internal detail of the map and identification of artifacts.

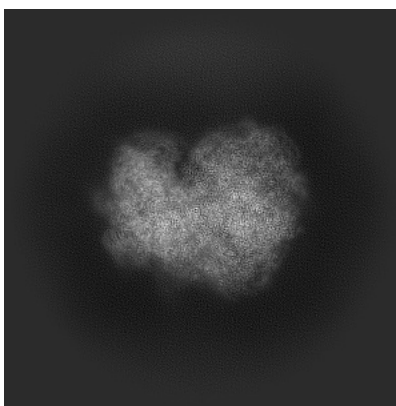
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

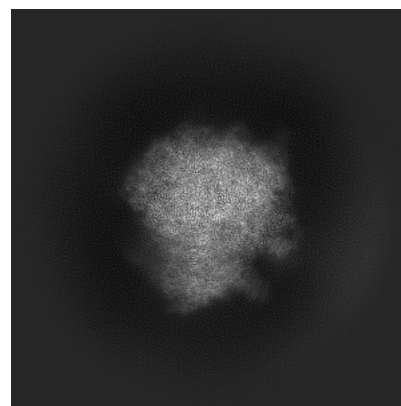
#### 6.1.1 Primary map



X

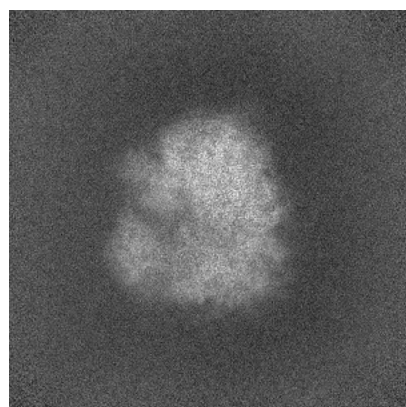


Y

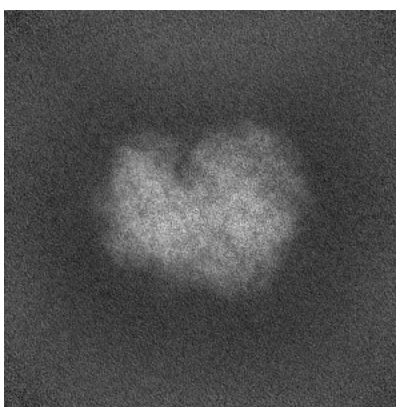


Z

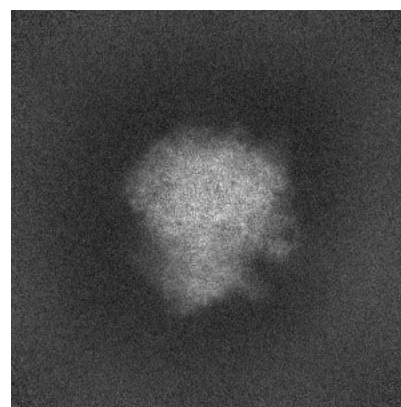
#### 6.1.2 Raw map



X



Y

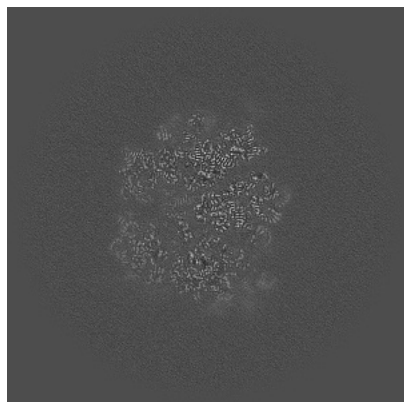


Z

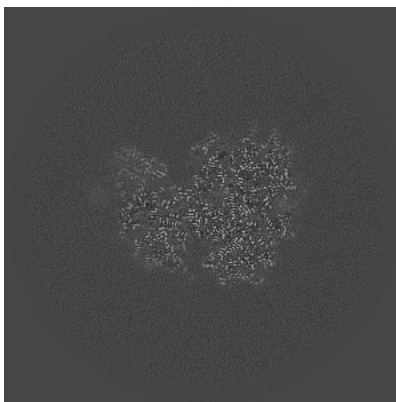
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

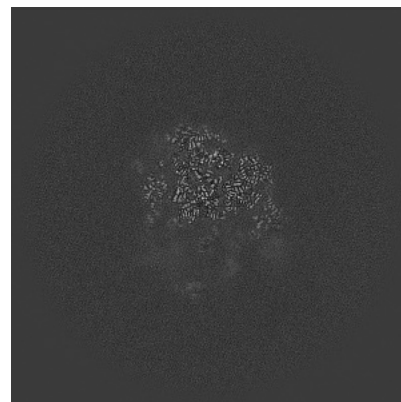
### 6.2.1 Primary map



X Index: 350

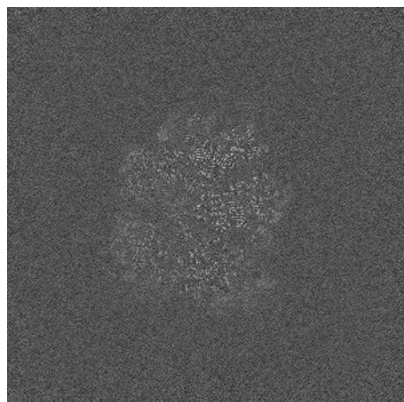


Y Index: 350

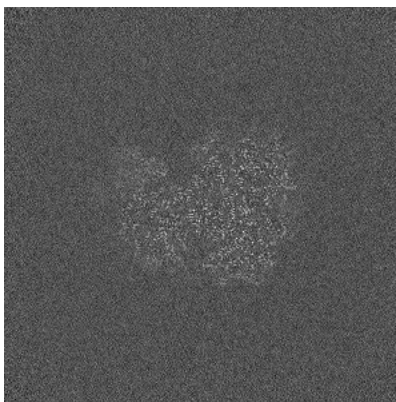


Z Index: 350

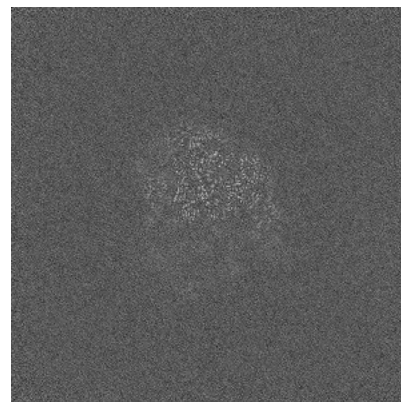
### 6.2.2 Raw map



X Index: 350



Y Index: 350

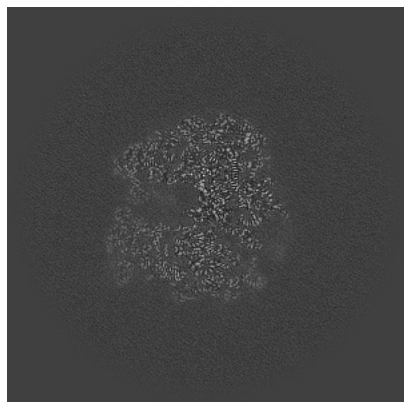


Z Index: 350

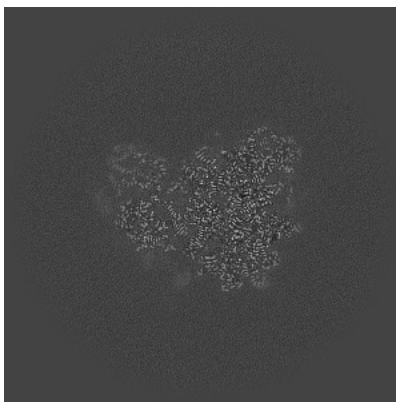
The images above show central slices of the map in three orthogonal directions.

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

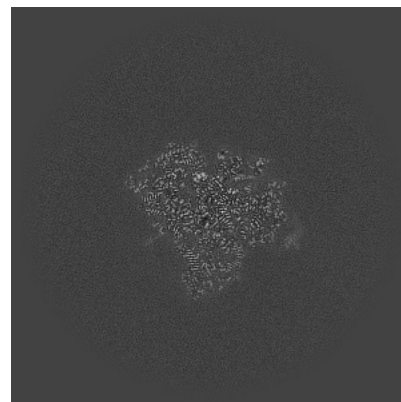
### 6.3.1 Primary map



X Index: 324

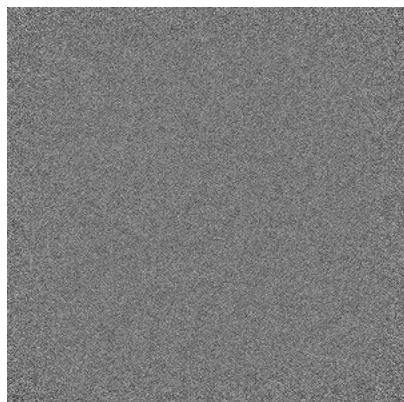


Y Index: 363

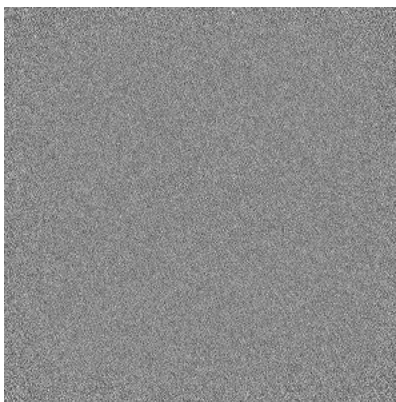


Z Index: 423

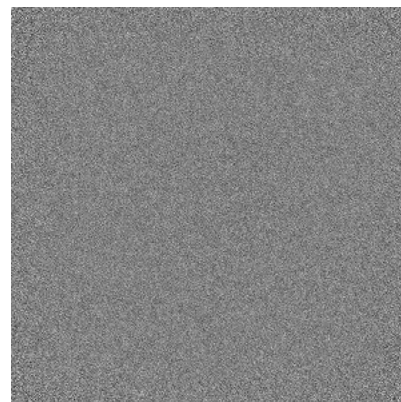
### 6.3.2 Raw map



X Index: 0



Y Index: 0



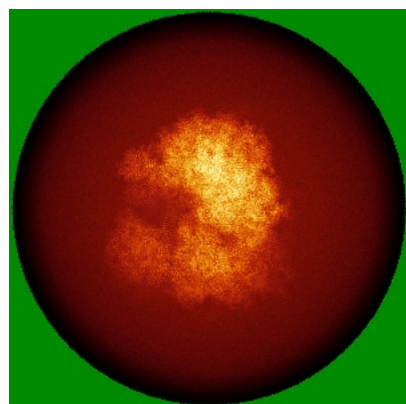
Z Index: 0

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

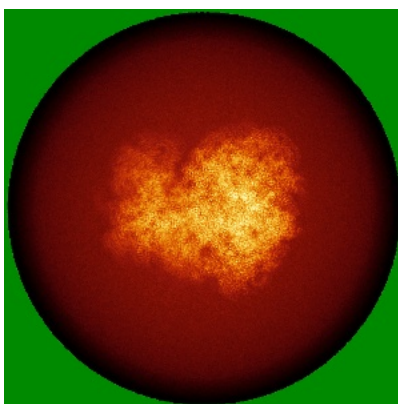


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

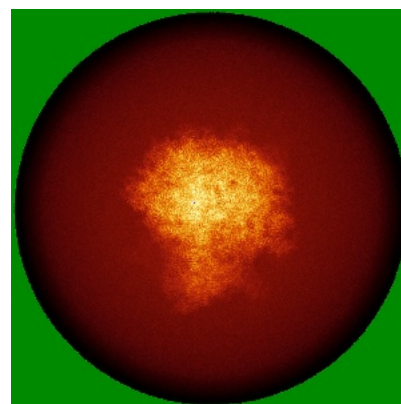
### 6.4.1 Primary map



X

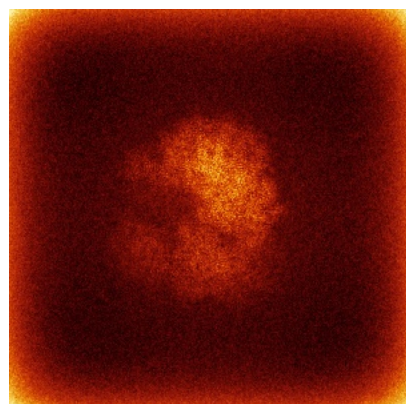


Y

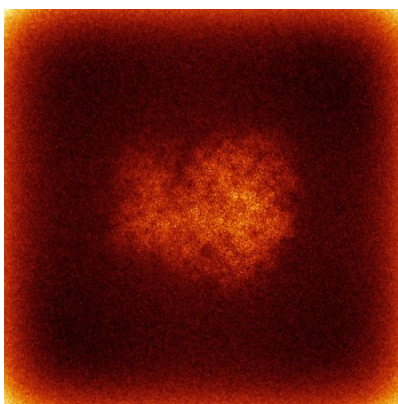


Z

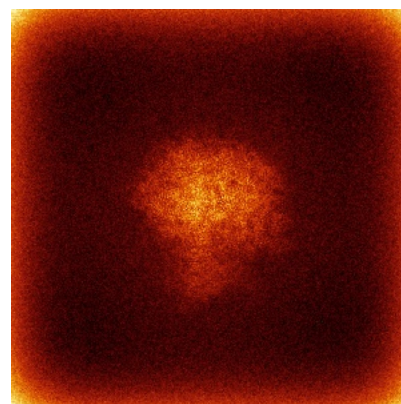
### 6.4.2 Raw map



X



Y

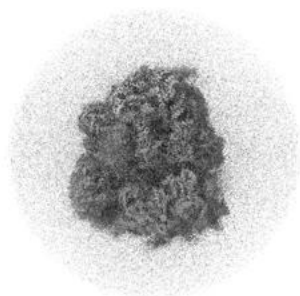


Z

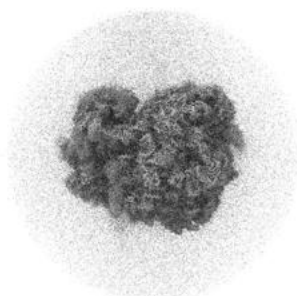
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

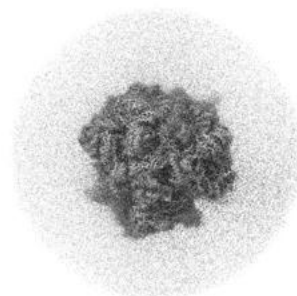
### 6.5.1 Primary map



X



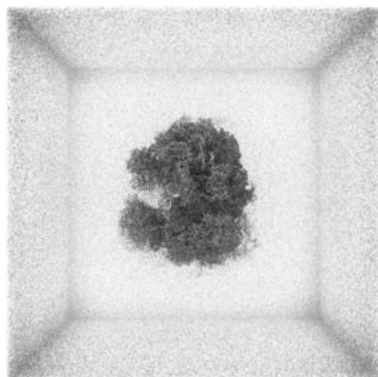
Y



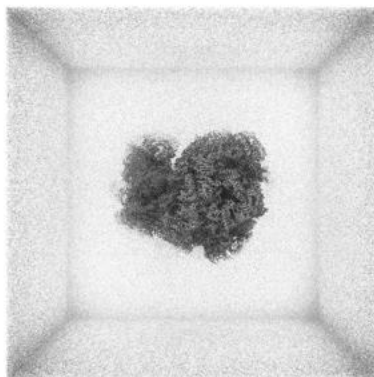
Z

The images above show the 3D surface view of the map at the recommended contour level 0.174. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

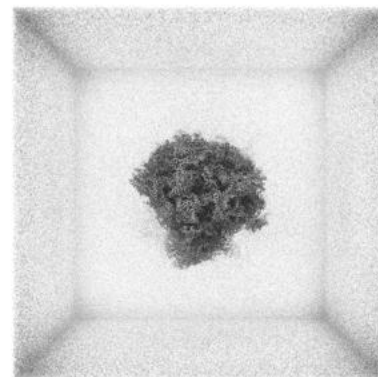
### 6.5.2 Raw map



X



Y



Z

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.

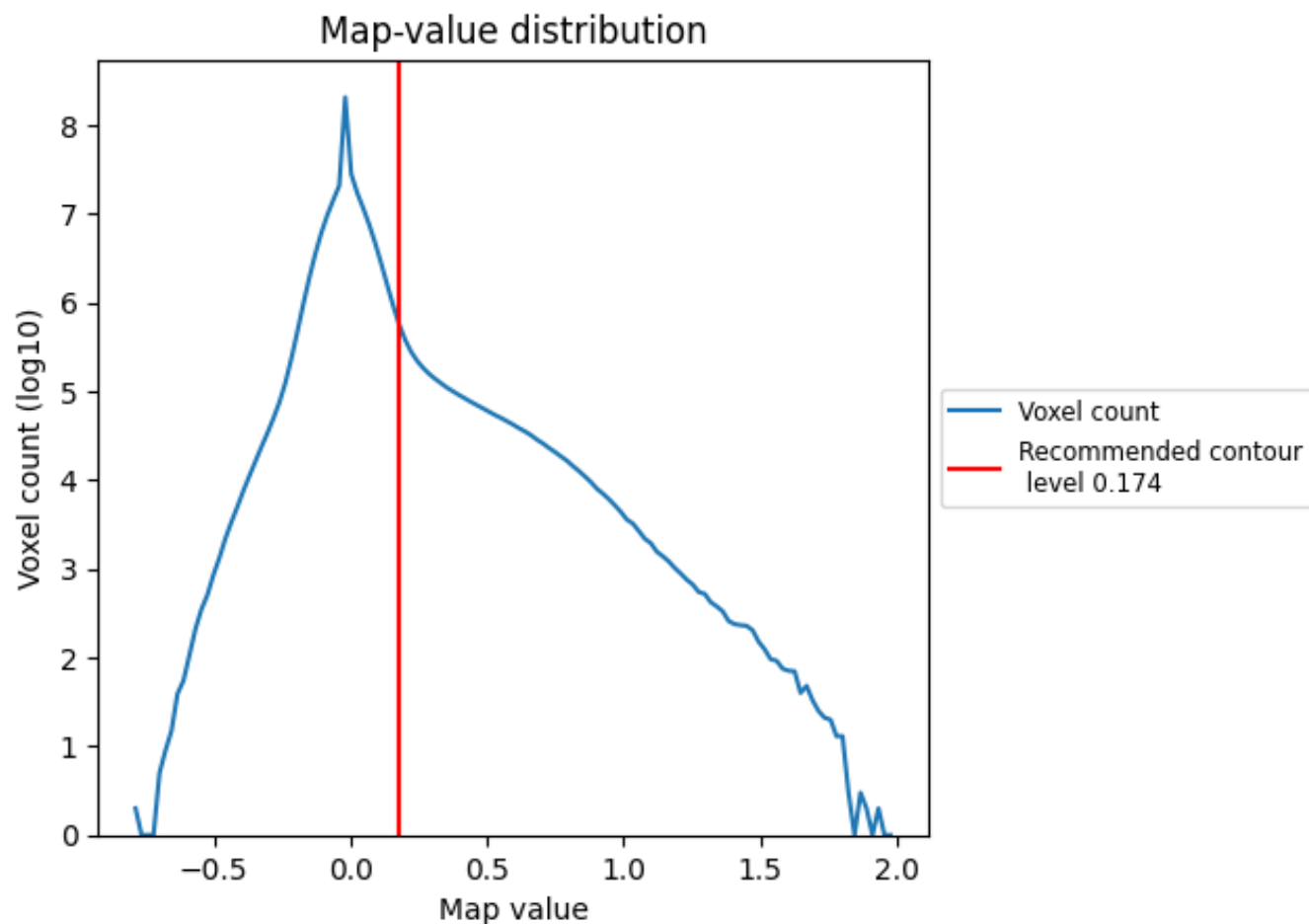
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

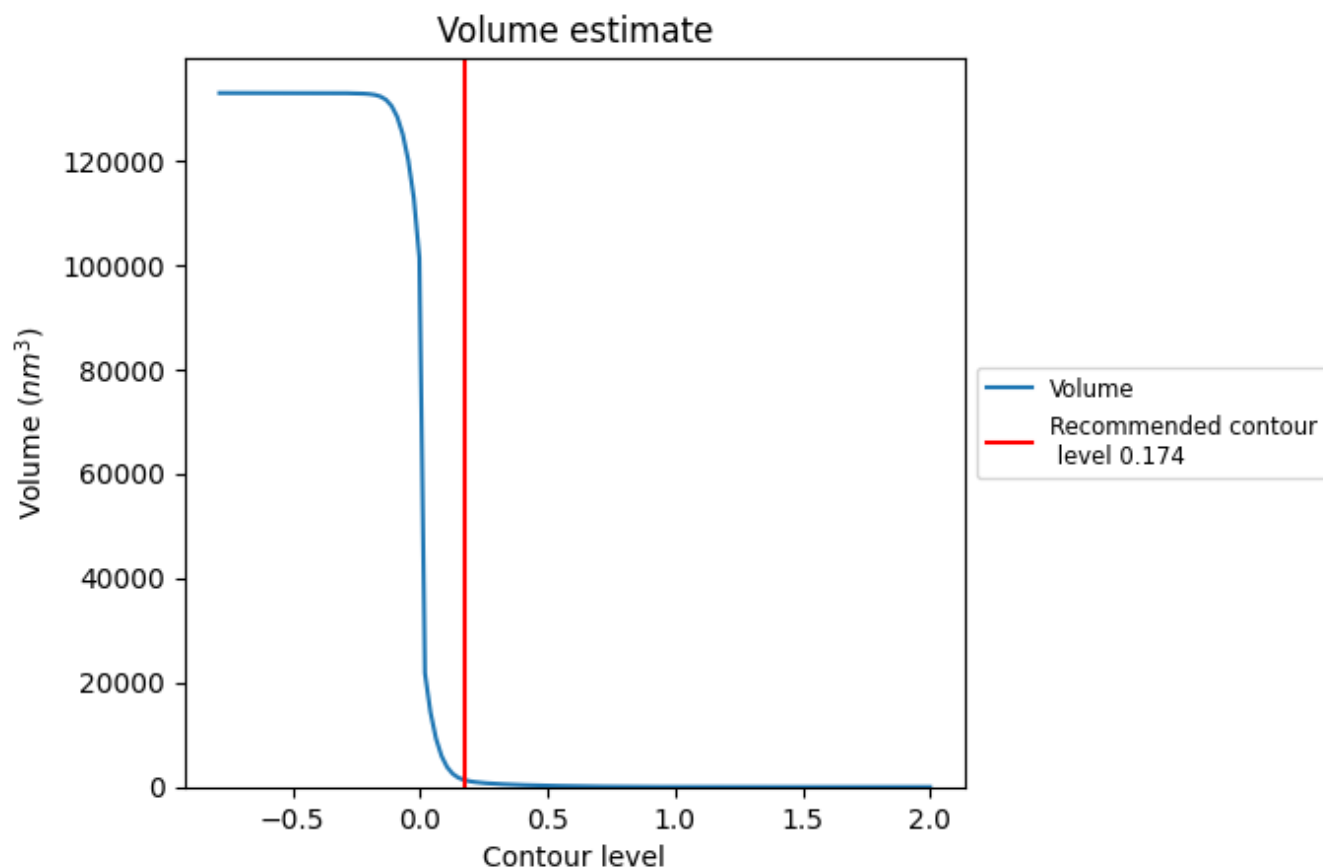
This section contains the results of statistical analysis of the map.

### 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.

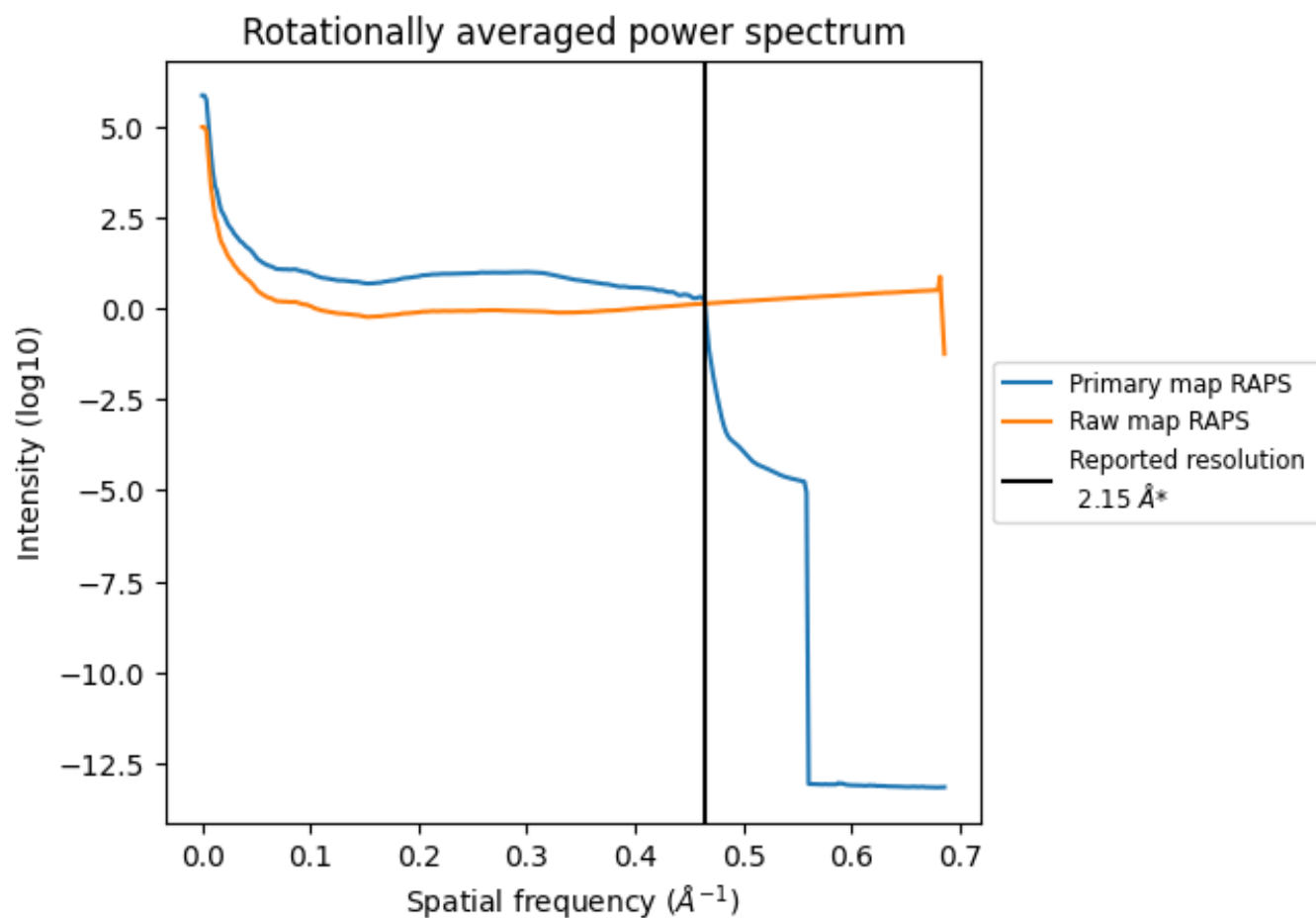
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1328  $\text{nm}^3$ ; this corresponds to an approximate mass of 1200 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 ⓘ



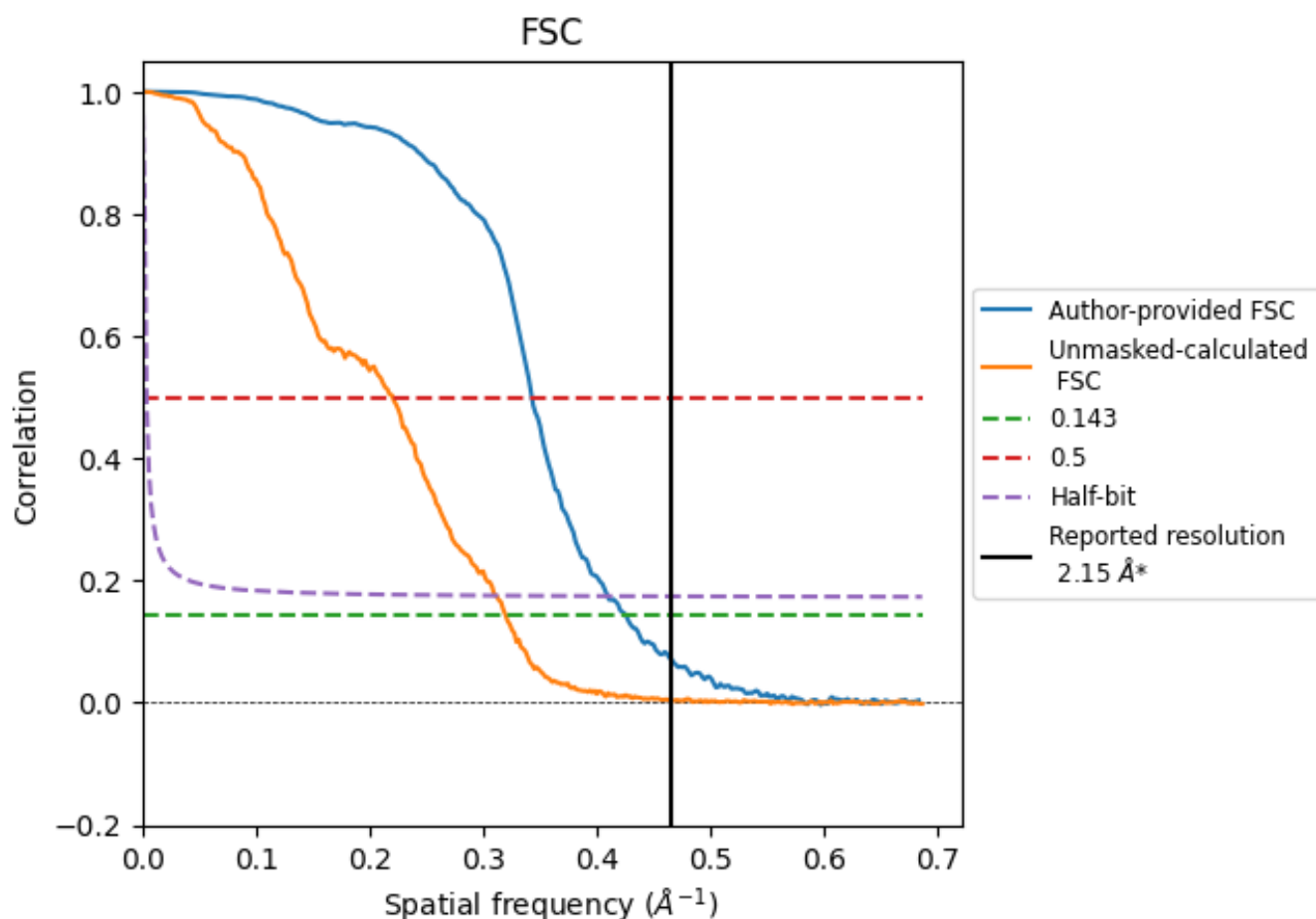
\*Reported resolution corresponds to spatial frequency of 0.465  $\text{\AA}^{-1}$



## 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 0.465  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

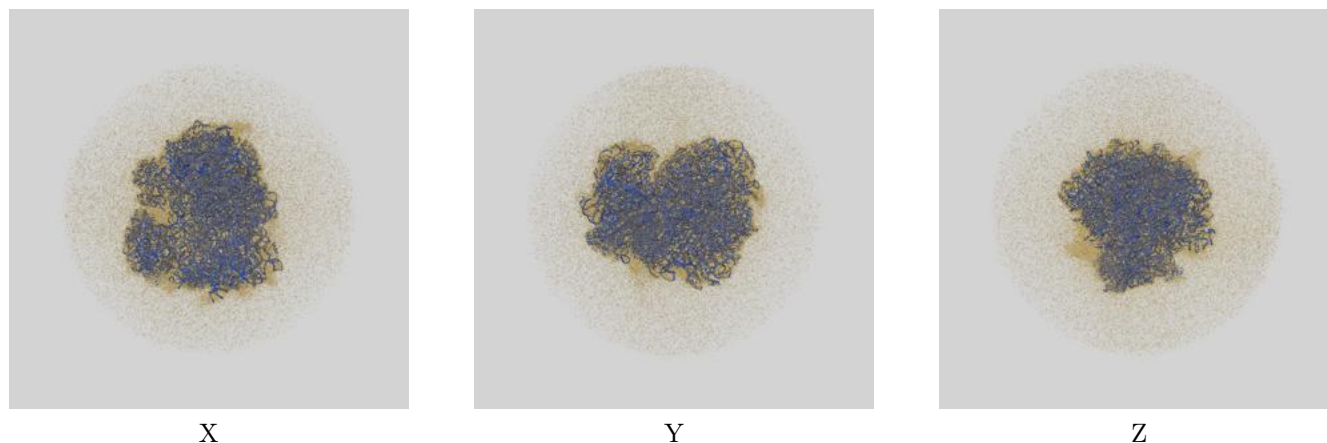
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.35	2.92	2.44
Unmasked-calculated*	3.13	4.54	3.21

\*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 3.13 differs from the reported value 2.15 by more than 10 %

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

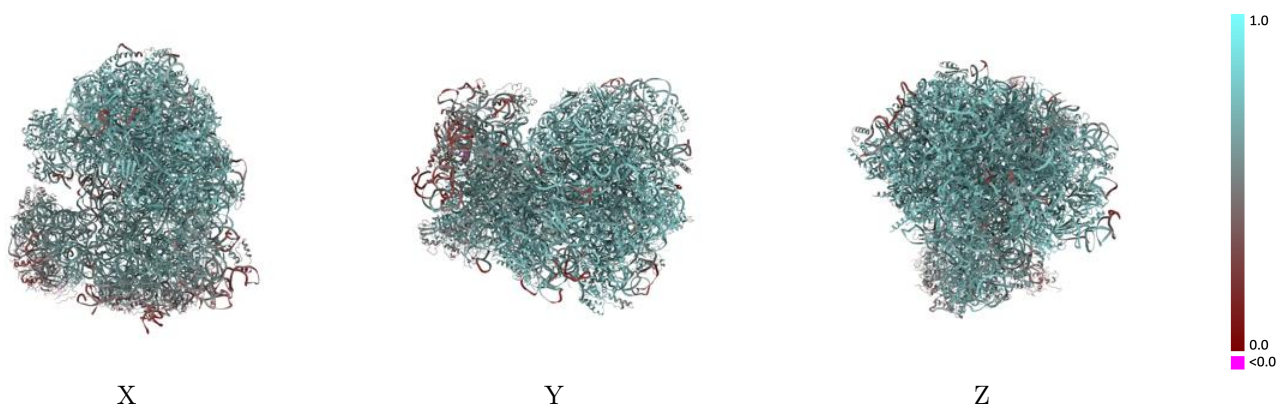
This section contains information regarding the fit between EMDB map EMD-51103 and PDB model 9G6J. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



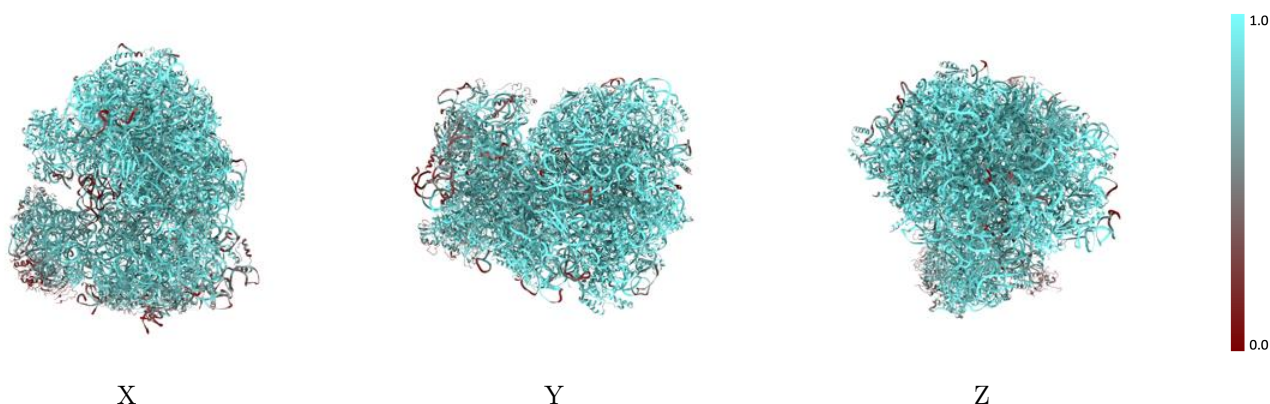
The images above show the 3D surface view of the map at the recommended contour level 0.174 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



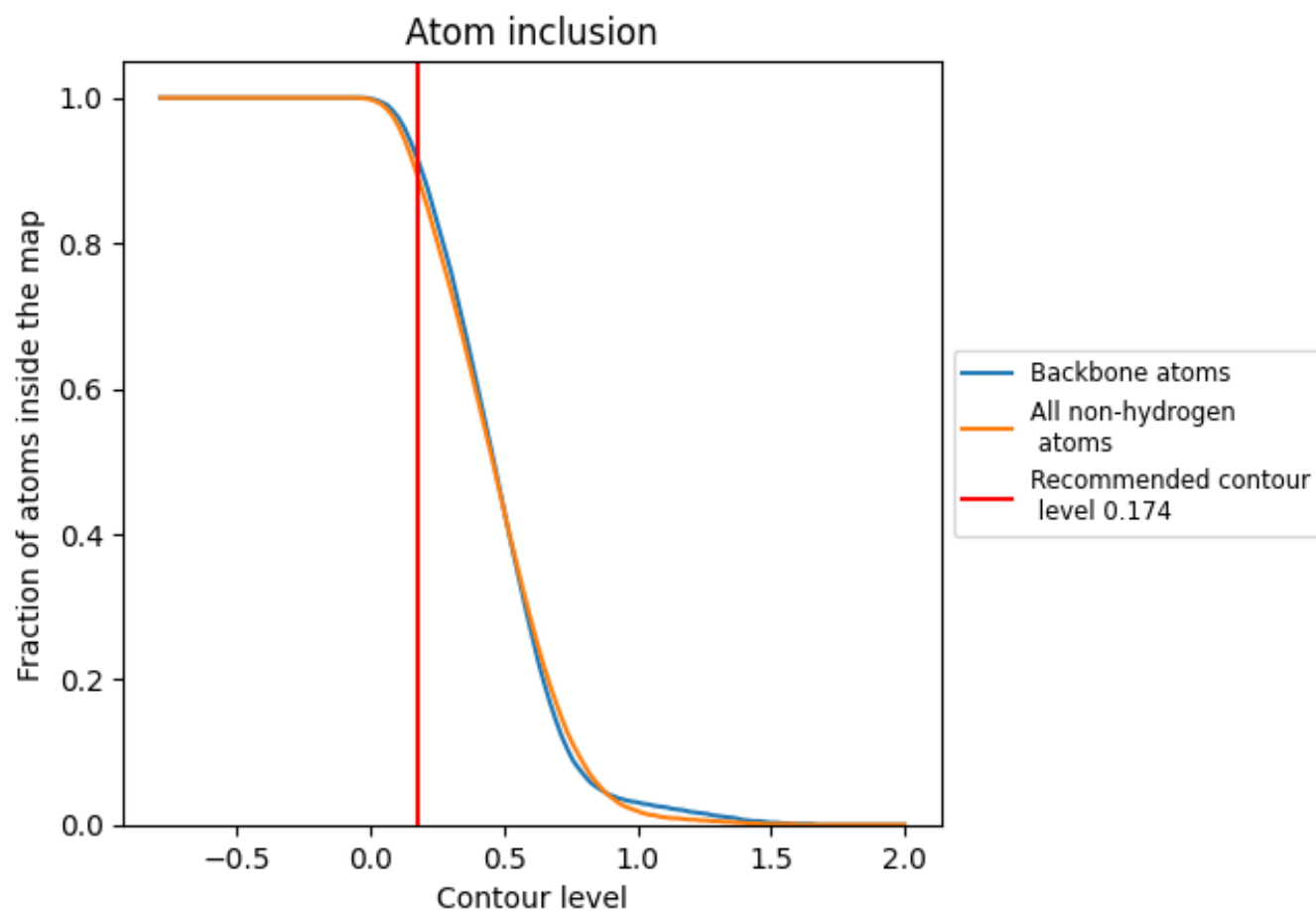
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.174).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.174) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.6390
0	 0.9620	 0.6990
1	 0.9580	 0.6800
2	 0.9310	 0.6870
3	 0.9860	 0.6790
4	 0.9750	 0.6880
6	 0.9680	 0.7110
7	 0.9560	 0.7010
8	 0.9570	 0.6950
9	 0.9450	 0.6940
A	 0.8870	 0.5980
AA	 0.9270	 0.6730
AB	 0.9780	 0.7240
AC	 0.9190	 0.6710
AD	 0.9360	 0.6800
AE	 0.9040	 0.6790
AF	 0.9610	 0.7080
AG	 0.9770	 0.7170
AH	 0.9280	 0.6880
AI	 0.9400	 0.6750
AJ	 0.9140	 0.6570
AK	 0.9860	 0.7250
AL	 0.8020	 0.6000
AM	 0.9620	 0.6940
AN	 0.9210	 0.6730
AO	 0.7440	 0.6170
AP	 0.9150	 0.6830
AQ	 0.8930	 0.6780
AT	 0.2820	 0.4020
B	 0.8530	 0.6000
C	 0.9060	 0.6490
D	 0.9310	 0.6590
E	 0.7600	 0.5540
F	 0.7410	 0.4980
G	 0.8000	 0.5790











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Chain	Atom inclusion	Q-score
H	 0.7030	 0.5070
I	 0.7310	 0.5470
J	 0.8130	 0.5820
K	 0.6390	 0.4360
L	 0.6160	 0.4630
M	 0.8750	 0.6210
MR	 0.8080	 0.5800
N	 0.2060	 0.3150
O	 0.9300	 0.6550
P	 0.9510	 0.6710
PT	 0.8480	 0.5940
Q	 0.6670	 0.5060
R	 0.8150	 0.5850
S	 0.7050	 0.5240
T	 0.7210	 0.5210
U	 0.7790	 0.5500
V	 0.6990	 0.5040
W	 0.8740	 0.6260
X	 0.9630	 0.6990
Y	 0.8980	 0.6320
Z	 0.6050	 0.4280
a	 0.5830	 0.4750
b	 0.9330	 0.6720
c	 0.8620	 0.6260
d	 0.7520	 0.5520
e	 0.9250	 0.6320
f	 0.5950	 0.4550
g	 0.3290	 0.3560
h	 0.2570	 0.3990
j	 0.9780	 0.7280
k	 0.9680	 0.7140
l	 0.9450	 0.6960
m	 0.8840	 0.6410
n	 0.9080	 0.6450
o	 0.9450	 0.6970
p	 0.9320	 0.6730
q	 0.9170	 0.6610
r	 0.9270	 0.6700
s	 0.8280	 0.5810
t	 0.9280	 0.6860
u	 0.9490	 0.6810
v	 0.9930	 0.7330

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Chain	Atom inclusion	Q-score
w	 0.9600	 0.7090
x	 0.9560	 0.7060
y	 0.9770	 0.7140
z	 0.9130	 0.6680