wwPDB EM Validation Summary Report (i)

Nov 8, 2022 – 09:52 AM EST

PDB ID	:	6MTE
EMDB ID	:	EMD-9242
Title	:	Rabbit 80S ribosome with eEF2 and SERBP1 (rotated state)
Authors	:	Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.
Deposited on	:	2018-10-19
Resolution	:	3.40 Å(reported)
Based on initial model	:	5LZV

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

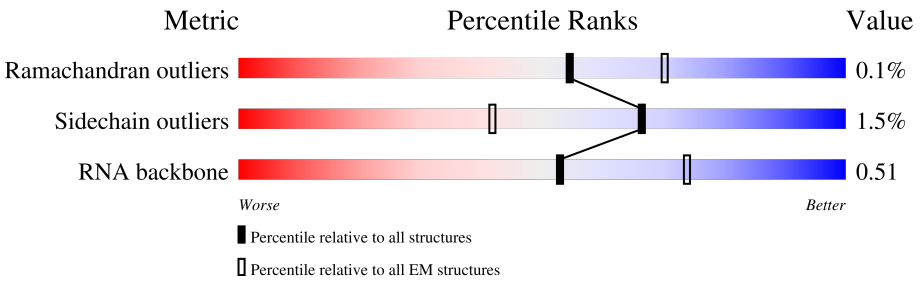
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5	3597	70% 26%
2	7	120	82% 18%
3	8	151	75% 21%
4	A	248	99%
5	B	394	98%
6	C	362	98%
7	D	293	99%
8	E	291	72% 26%

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Mol	Chain	Length	Quality of chain
9	F	225	99%
10	G	319	71% 27%
11	H	190	99%
12	I	214	94%
13	J	170	99%
14	L	210	98%
15	M	138	99%
16	N	203	97%
17	O	199	98%
18	P	153	98%
19	Q	187	99%
20	R	180	99%
21	S	176	98%
22	T	159	97%
23	U	99	99%
24	V	131	98%
25	W	157	13% 64% 36%
26	X	118	98%
27	Y	134	99%
28	Z	135	100%
29	a	147	99%
30	b	245	42% 58%
31	c	98	99%
32	d	107	98%
33	e	128	98%

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Mol	Chain	Length	Quality of chain
34	f	109	99%
35	g	114	97%
36	h	122	99%
37	i	102	96%
38	j	86	98%
39	k	69	100%
40	l	50	98%
41	m	52	98%
42	n	25	96%
43	o	103	97%
44	p	91	100%
45	r	124	98%
46	s	196	99%
47	t	153	29% 97%
48	v	848	6% 97%
49	w	55	20% 100%
50	9	1698	70% 26%
51	AA	217	99%
52	BB	213	7% 96%
53	CC	221	99%
54	DD	228	6% 98%
55	EE	262	97%
56	FF	204	11% 87% 9%
57	GG	237	12% 96%
58	HH	194	6% 94% 5%

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Mol	Chain	Length	Quality of chain
59	II	206	12% 97%
60	JJ	185	98%
61	KK	96	98%
62	LL	158	6% 89% 9%
63	MM	117	32% 97%
64	NN	149	99%
65	OO	136	7% 99%
66	PP	125	12% 94% 6%
67	QQ	142	6% 98%
68	RR	132	8% 97%
69	SS	144	15% 97%
70	TT	141	7% 98%
71	UU	100	9% 99%
72	VV	83	98%
73	WW	129	98%
74	XX	141	96%
75	YY	124	98%
76	ZZ	75	19% 100%
77	aa	101	99%
78	bb	83	6% 100%
79	cc	62	23% 95% 5%
80	dd	55	96%
81	ee	55	13% 95% 5%
82	ff	68	26% 99%
83	gg	313	11% 98%

2 Entry composition (i)

There are 86 unique types of molecules in this entry. The entry contains 220739 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	3597	77254	34469	14127	25061	3597	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	7	120	2558	1141	456	842	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	8	151	3209	1433	564	1062	150	0	0

- Molecule 4 is a protein called uL2.

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

- Molecule 5 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	394	3172	2020	597	542	13	0	0

- Molecule 6 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	362	2884	1813	577	480	14	0	0

- Molecule 7 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	293	2391	1512	438	427	14	0	0

- Molecule 8 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	216	1729	1115	329	282	3	0	0

- Molecule 9 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	225	1875	1205	358	303	9	0	0

- Molecule 10 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	233	1879	1199	361	315	4	0	0

- Molecule 11 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	190	1516	954	284	272	6	0	0

- Molecule 12 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	205	1664	1056	321	274	13	0	0

- Molecule 13 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	170	1362	861	254	241	6	0	0

- Molecule 14 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	L	210	1702	1065	354	279	4	0	0

- Molecule 15 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	M	138	1137	727	221	182	7	0	0

- Molecule 16 is a protein called eL15.

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

- Molecule 17 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	O	199	1630	1051	319	255	5	0	0

- Molecule 18 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	P	153	1242	777	241	215	9	0	0

- Molecule 19 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Q	187	1515	946	315	250	4	0	0

- Molecule 20 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	R	180	1508	933	328	238	9	0	0

- Molecule 21 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	S	176	1462	930	285	236	11	0	0

- Molecule 22 is a protein called eL21.

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

- Molecule 23 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	U	99	809	519	141	147	2	0	0

- Molecule 24 is a protein called uL14.

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

- Molecule 25 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	W	100	816	512	164	136	4	0	0

- Molecule 26 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	X	118	967	618	181	167	1	0	0

- Molecule 27 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Y	134	1115	700	226	186	3	0	0

- Molecule 28 is a protein called eL27.

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

- Molecule 29 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	147	1162	734	239	185	4	0	0

- Molecule 30 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	104	848	527	189	129	3	0	0

- Molecule 31 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	98	761	481	134	140	6	0	0

- Molecule 32 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	d	107	888	560	171	155	2	0	0

- Molecule 33 is a protein called eL32.

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

- Molecule 34 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	f	109	876	555	174	143	4	0	0

- Molecule 35 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	114	906	566	187	147	6	0	0

- Molecule 36 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	h	122	1013	640	204	168	1	0	0

- Molecule 37 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	i	102	830	520	176	129	5	0	0

- Molecule 38 is a protein called eL37.

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

- Molecule 39 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	k	69	569	366	103	99	1	0	0

- Molecule 40 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	l	50	447	286	96	64	1	0	0

- Molecule 41 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	m	52	430	267	90	67	6	0	0

- Molecule 42 is a protein called eL41.

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

- Molecule 43 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	103	842	528	172	136	6	0	0

- Molecule 44 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	91	708	445	136	120	7	0	0

- Molecule 45 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	r	124	994	616	205	167	6	0	0

- Molecule 46 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	s	196	1507	959	263	276	9	0	0

- Molecule 47 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	t	153	1160	722	218	217	3	0	0

- Molecule 48 is a protein called eEF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	v	848	6628	4211	1138	1235	44	0	0

- Molecule 49 is a protein called SERBP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	w	55	440	263	87	90	0	0

- Molecule 50 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	9	1698	36291	16217	6509	11868	1697	0	0

- Molecule 51 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	AA	217	1710	1086	300	316	8	0	0

- Molecule 52 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	BB	213	1729	1098	309	308	14	0	0

- Molecule 53 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	CC	221	1716	1111	295	301	9	0	0

- Molecule 54 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	DD	228	1768	1126	318	316	8	0	0

- Molecule 55 is a protein called eS4.

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

- Molecule 56 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	FF	185	1471	921	277	266	7	0	0

- Molecule 57 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	GG	237	1923	1200	387	329	7	0	0

- Molecule 58 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	HH	185	1488	952	271	264	1	0	0

- Molecule 59 is a protein called eS8.

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

- Molecule 60 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	JJ	185	1525	969	306	248	2	0	0

- Molecule 61 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	KK	96	810	530	143	131	6	0	0

- Molecule 62 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	LL	143	1175	749	222	198	6	0	0

- Molecule 63 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	MM	117	908	570	161	169	8	0	0

- Molecule 64 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	NN	149	1202	770	228	203	1	0	0

- Molecule 65 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	OO	136	1016	621	199	190	6	0	0

- Molecule 66 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	PP	125	1025	652	192	174	7	0	0

- Molecule 67 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	QQ	142	1128	717	213	195	3	0	0

- Molecule 68 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	RR	132	1068	670	199	195	4	0	0

- Molecule 69 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	SS	144	1190	746	241	202	1	0	0

- Molecule 70 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	TT	141	1097	688	211	195	3	0	0

- Molecule 71 is a protein called uS10.

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

- Molecule 72 is a protein called eS21.

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

- Molecule 73 is a protein called uS8.

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

- Molecule 74 is a protein called uS12.

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

- Molecule 75 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	YY	124	1011	640	198	168	5	0	0

- Molecule 76 is a protein called eS25.

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

- Molecule 77 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	aa	101	814	507	170	132	5	0	0

- Molecule 78 is a protein called eS27.

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

- Molecule 79 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	cc	62	488	297	97	92	2	0	0

- Molecule 80 is a protein called uS14.

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

- Molecule 81 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	ee	55	443	274	97	71	1	0	0

- Molecule 82 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	ff	68	555	351	103	94	7	0	0

- Molecule 83 is a protein called RACK1.

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

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

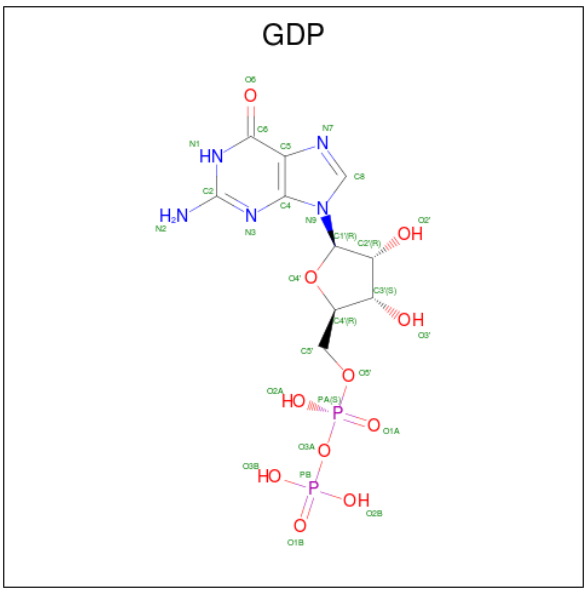
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
84	5	200	200	200	0
			Total	Mg	
84	7	7	7	7	0
			Total	Mg	
84	8	6	6	6	0
			Total	Mg	
84	A	1	1	1	0
			Total	Mg	
84	P	1	1	1	0
			Total	Mg	
84	V	1	1	1	0
			Total	Mg	
84	a	1	1	1	0
			Total	Mg	
84	j	1	1	1	0
			Total	Mg	
84	v	1	1	1	0
			Total	Mg	
84	9	78	78	78	0
			Total	Mg	
84	TT	1	1	1	0

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
85	g	1	1	1	0
			Total	Zn	
85	j	1	1	1	0
			Total	Zn	
85	m	1	1	1	0
			Total	Zn	
85	o	1	1	1	0
			Total	Zn	
85	p	1	1	1	0
			Total	Zn	
85	KK	1	1	1	0
			Total	Zn	
85	aa	1	1	1	0
			Total	Zn	
85	ff	1	1	1	0

- Molecule 86 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:

$C_{10}H_{15}N_5O_{11}P_2$).



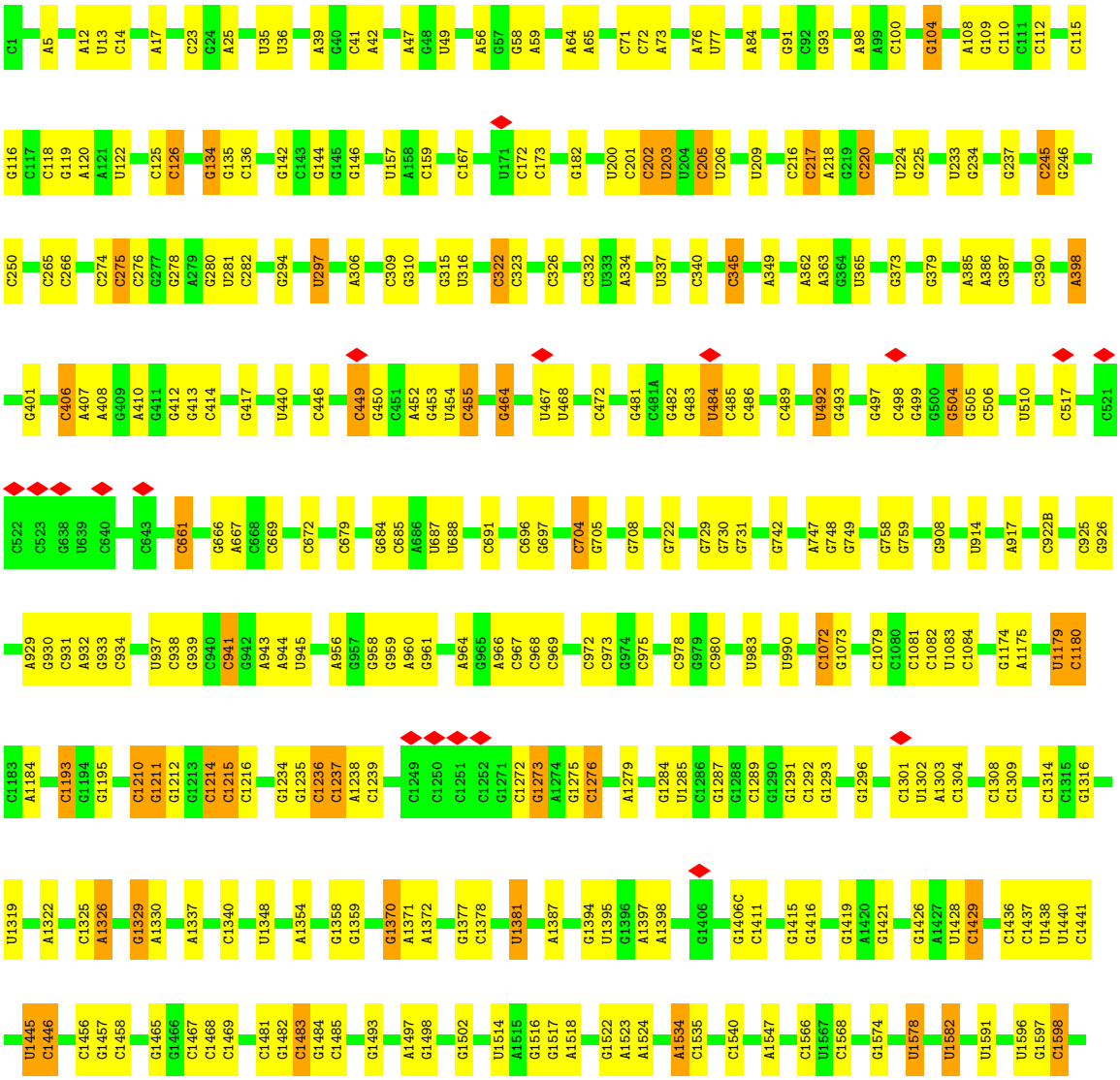
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
86	v	1	28	10	5	11	2	0

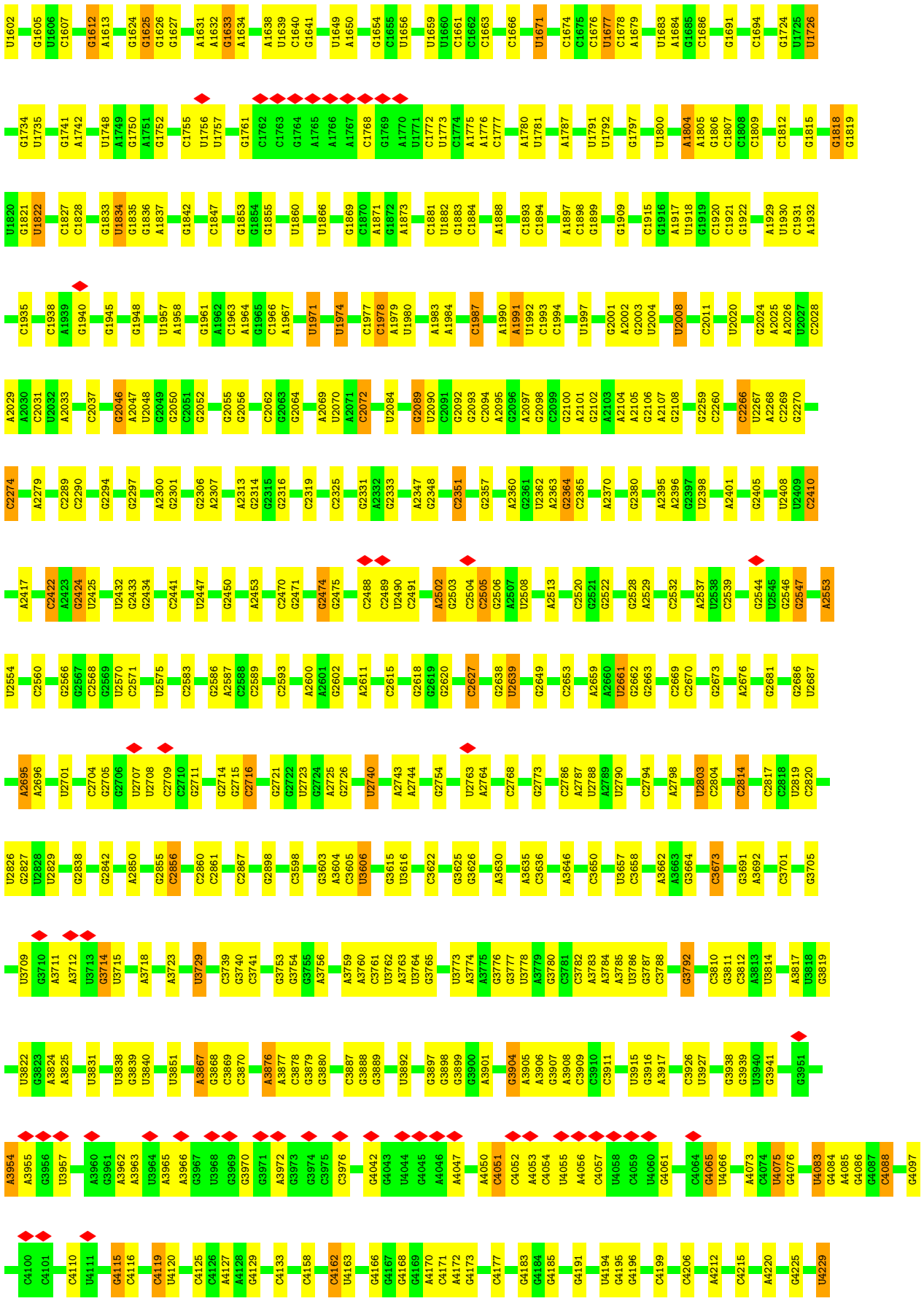
3 Residue-property plots (i)

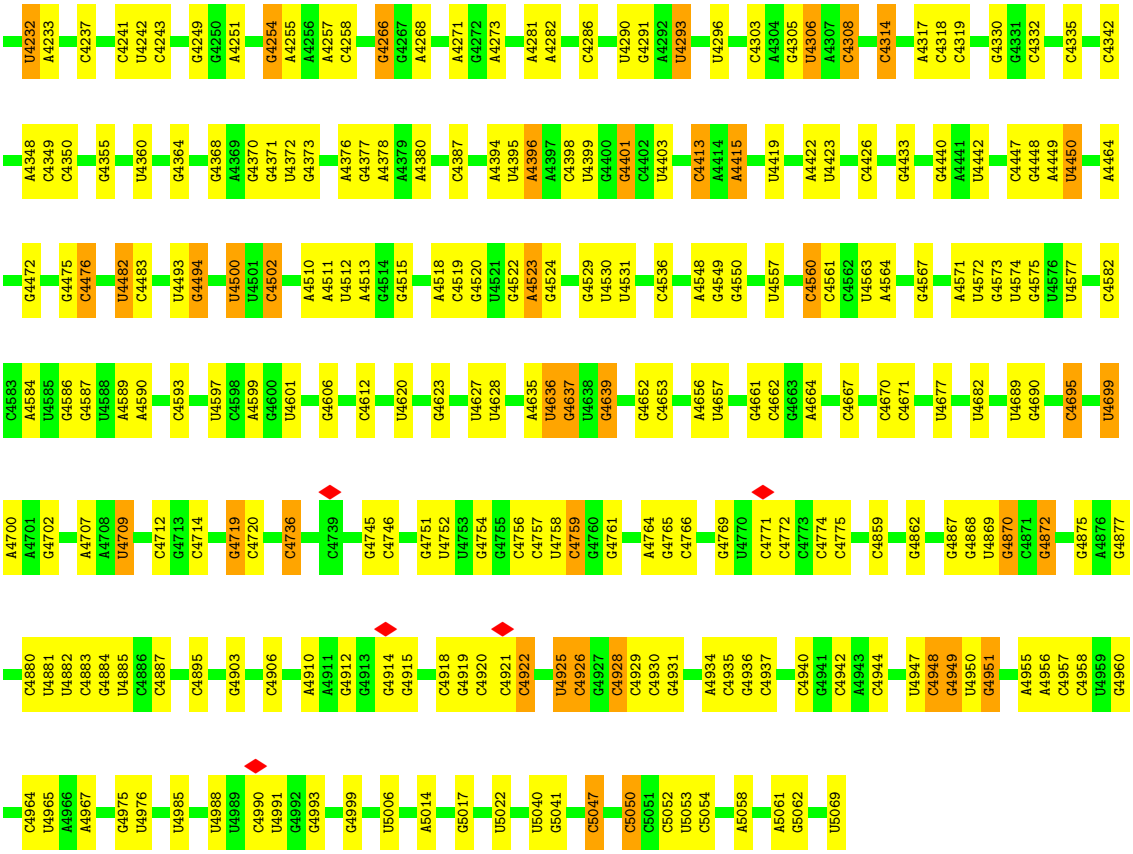
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 28S rRNA

Chain 5:

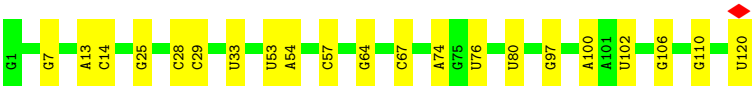



U1602 G1605 U1606 C1607 G1612 A1613 G1624 G1625 G1626 G1627 A1631 A1632 G1633 A1634 A1638 U1639 C1640 G1641 U1649 A1650 G1654 C1655 U1656 U1659 U1660 C1661 C1662 C1663 C1666 U1671 C1674 C1675 C1676 U1677 C1678 A1679 U1683 A1684 G1685 C1686 G1691 C1694 G1724 U1725 U1726
G1734 U1735 G1741 A1742 U1748 A1749 G1750 A1751 G1752 C1755 U1756 U1757 G1761 C1762 C1763 G1764 A1765 A1766 A1767 C1768 G1769 A1770 U1771 C1772 U1773 C1774 A1775 A1776 C1777 A1780 U1781 A1787 U1791 U1792 G1797 U1800 A1804 A1805 G1806 C1807 C1808 C1809 C1812 G1815 G1818 G1819
U1820 G1821 U1822 C1827 C1828 G1833 U1834 G1835 G1836 A1837 G1842 C1847 G1853 G1854 G1855 U1860 U1866 G1869 C1870 A1871 G1872 A1873 C1881 U1882 G1883 C1884 A1888 C1893 C1894 A1897 C1898 G1899 G1909 C1915 G1916 A1917 U1918 G1919 C1920 C1921 G1922 A1929 U1930 C1931 A1932
C1935 C1938 A1939 G1940 G1945 G1948 U1957 A1958 G1961 A1962 C1963 A1964 G1965 C1966 A1967 U1971 U1974 C1977 C1978 A1979 U1980 A1983 A1984 C1987 A1990 A1991 U1992 C1993 C1994 U1997 G2001 A2002 G2003 U2004 U2008 C2011 U2020 G2024 A2025 A2026 U2027 C2028
A2029 A2030 C2031 U2032 A2033 C2037 G2046 A2047 U2048 G2049 G2050 C2051 G2052 G2055 G2056 C2062 G2063 G2064 A2069 U2070 A2071 C2072 U2084 G2089 U2090 C2091 G2092 G2093 C2094 A2095 G2096 A2097 G2098 C2099 G2100 A2101 G2102 A2103 A2104 A2105 G2106 A2107 G2108 G2259 C2260 C2266 U2267 A2268 C2269 G2270
C2274 A2279 C2289 C2290 G2294 G2297 A2300 G2301 G2306 A2307 A2313 G2314 G2315 G2316 C2319 C2325 G2331 A2332 G2333 A2347 G2348 C2351 G2357 A2360 G2361 U2362 A2363 G2364 C2365 A2370 G2380 A2395 A2396 G2397 U2398 A2401 G2405 U2408 U2409 C2410
A2417 C2422 A2423 G2424 U2425 U2432 G2433 G2434 C2441 U2447 G2450 A2453 C2470 G2471 G2474 G2475 C2488 C2489 U2490 C2491 A2502 G2503 C2504 C2505 G2506 A2507 U2508 A2513 C2520 G2521 G2522 G2528 A2529 C2532 A2537 U2538 C2539 G2544 U2545 G2546 G2547 A2553
U2554 C2560 G2566 G2567 C2568 G2569 U2570 C2571 U2575 C2583 G2586 A2587 C2588 C2589 C2593 A2600 A2601 G2602 A2611 C2615 G2618 G2619 G2620 C2627 G2638 U2639 G2649 C2653 A2659 A2660 U2661 G2662 G2663 C2669 C2670 G2673 A2676 G2681 G2686 U2687
A2695 A2696 U2701 C2704 G2705 G2706 U2707 U2708 C2709 C2710 G2711 G2714 G2715 C2716 G2721 G2722 U2723 G2724 A2725 G2726 U2740 A2743 A2744 G2754 U2763 A2764 C2768 G2773 C2786 A2787 U2788 A2789 U2790 C2794 A2798 U2803 C2804 C2814 C2817 C2818 U2819 C2820
U2826 G2827 U2828 U2829 G2838 G2842 A2850 G2855 C2856 C2860 C2861 C2867 G2898 C3598 G3603 A3604 C3605 U3606 G3615 U3616 C3622 G3625 G3626 A3630 A3635 C3636 A3646 C3650 U3657 C3658 A3662 A3663 G3664 C3673 G3691 A3692 C3701 G3705
U3709 G3710 A3711 A3712 U3713 G3714 U3715 A3718 A3723 U3729 C3739 G3740 C3741 G3753 G3754 G3755 A3756 A3759 A3760 C3761 U3762 A3763 U3764 G3765 U3773 A3774 A3775 G3776 G3777 U3778 A3779 G3780 C3781 C3782 A3783 A3784 A3785 U3786 G3787 C3788 G3792 C3810 G3811 C3812 A3813 U3814 A3817 U3818 G3819
U3822 G3823 A3824 A3825 U3831 U3838 G3839 U3840 U3851 A3867 G3868 C3869 C3870 A3876 A3877 C3878 G3879 G3880 C3887 G3888 G3889 U3892 G3897 G3898 G3899 G3900 A3901 G3904 A3905 A3906 G3907 A3908 C3909 C3910 C3911 U3915 G3916 A3917 C3926 U3927 G3938 G3939 U3940 G3941 G3951
A3954 A3955 G3956 U3957 A3960 G3961 A3962 A3963 U3964 A3965 A3966 G3967 U3968 G3969 G3970 G3971 A3972 G3973 G3974 C3975 C3976 G4042 G4043 G4044 U4045 G4046 A4047 A4050 C4051 C4052 A4053 C4054 U4055 A4056 C4057 U4058 C4059 U4060 G4061 C4064 G4065 U4066 A4073 C4074 U4075 G4076 U4083 G4084 A4085 G4086 G4087 C4088 G4097
C4100 C4101 C4110 U4111 G4115 C4116 C4119 U4120 C4125 C4126 A4127 A4128 G4129 C4133 C4158 C4162 U4163 G4166 G4167 G4168 G4169 A4170 C4171 A4172 G4173 C4177 G4183 G4184 G4185 G4191 U4194 G4195 G4196 C4199 C4206 A4212 C4215 A4220 G4225 U4229



- Molecule 2: 5S rRNA

Chain 7:

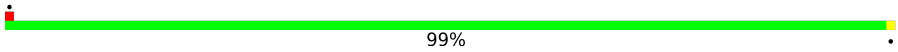


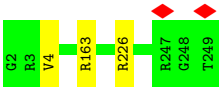
- Molecule 3: 5.8S rRNA

Chain 8:

- Molecule 4: uL2

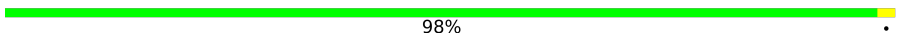
Chain A:





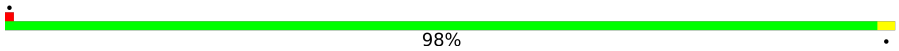
- Molecule 5: uL3

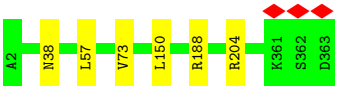
Chain B:



- Molecule 6: uL4

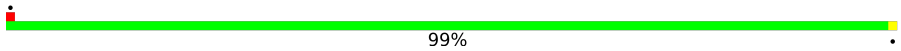
Chain C:

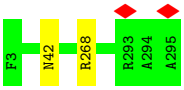




- Molecule 7: uL18

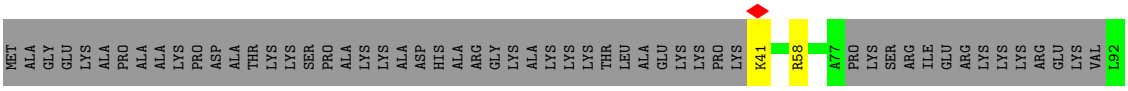
Chain D:





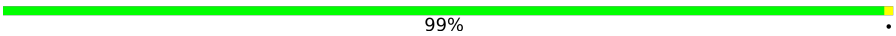
- Molecule 8: eL6

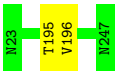
Chain E:



- Molecule 9: uL30

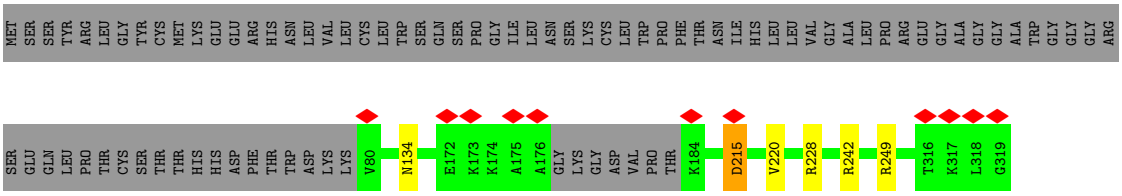
Chain F:





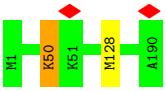
- Molecule 10: eL8

Chain G:



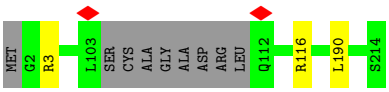
- Molecule 11: uL6

Chain H: 99%



• Molecule 12: uL16

Chain I: 94%

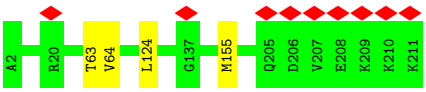


• Molecule 13: uL5

Chain J: 99%

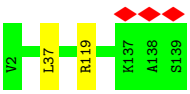
• Molecule 14: eL13

Chain L: 98%



• Molecule 15: eL14

Chain M: 99%



• Molecule 16: eL15

Chain N: 97%

• Molecule 17: uL13

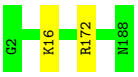
Chain O: 98%

• Molecule 18: uL22

Chain P: 98%

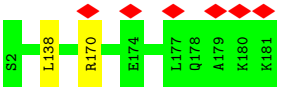
• Molecule 19: eL18

Chain Q: 99%



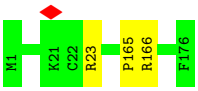
• Molecule 20: eL19

Chain R: 99%



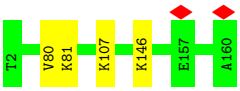
• Molecule 21: eL20

Chain S: 98%



• Molecule 22: eL21

Chain T: 97%

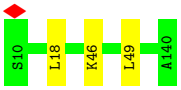


• Molecule 23: eL22

Chain U: 99%

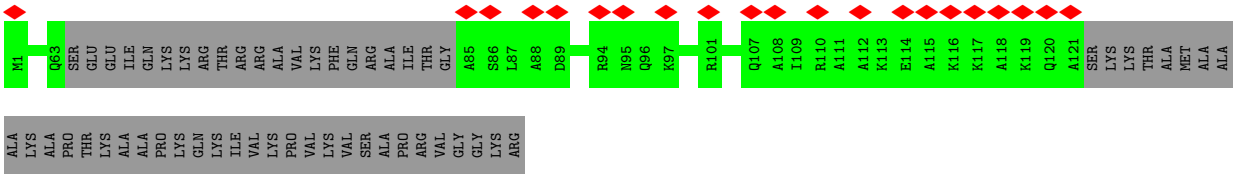
• Molecule 24: uL14

Chain V: 98%

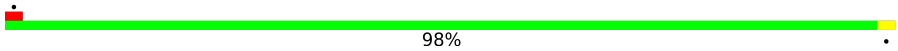


• Molecule 25: eL24

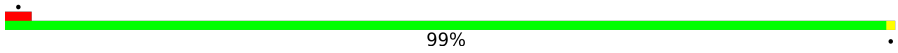
Chain W:

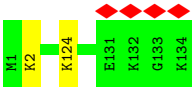


- Molecule 26: uL23

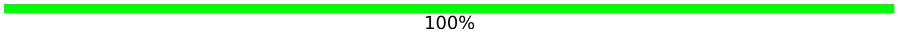
Chain X: 

- Molecule 27: uL24

Chain Y: 

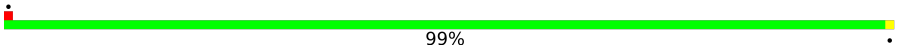


- Molecule 28: eL27

Chain Z: 

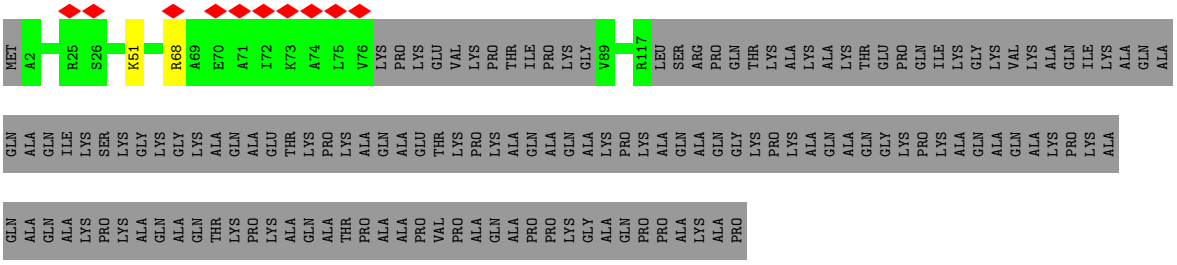
There are no outlier residues recorded for this chain.

- Molecule 29: uL15

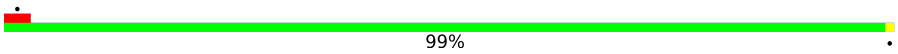
Chain a: 

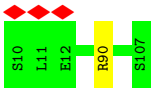
- Molecule 30: eL29

Chain b:

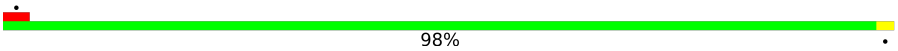


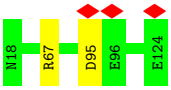
- Molecule 31: eL30

Chain c: 

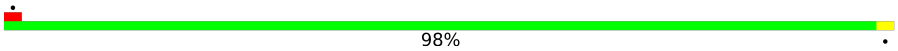


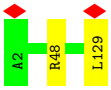
- Molecule 32: eL31

Chain d: 

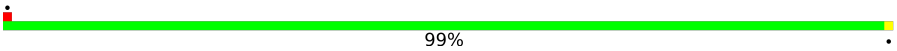


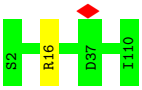
- Molecule 33: eL32

Chain e: 

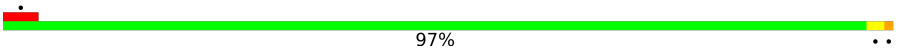


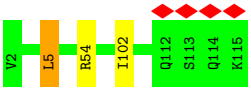
- Molecule 34: eL33

Chain f: 

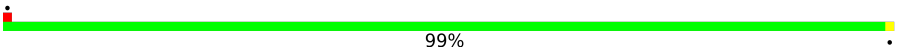


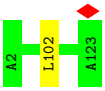
- Molecule 35: eL34

Chain g: 

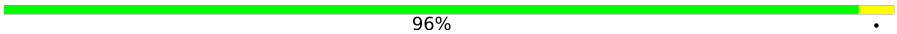


- Molecule 36: uL29

Chain h: 



- Molecule 37: eL36

Chain i: 

- Molecule 38: eL37

Chain j: 98%

- Molecule 39: eL38

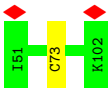
Chain k: 100%

- Molecule 40: eL39

Chain l: 98%

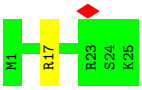
- Molecule 41: eL40

Chain m: 98%



- Molecule 42: eL41

Chain n: 96%



- Molecule 43: eL42

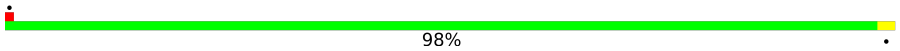
Chain o: 97%

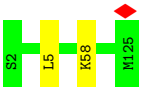
- Molecule 44: eL43

Chain p: 100%

- Molecule 45: eL28

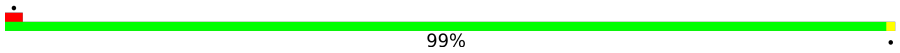
Chain r:

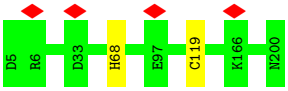




- Molecule 46: uL10

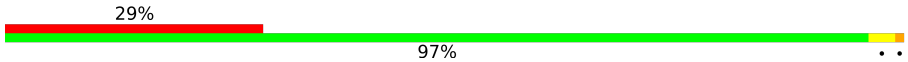
Chain s:

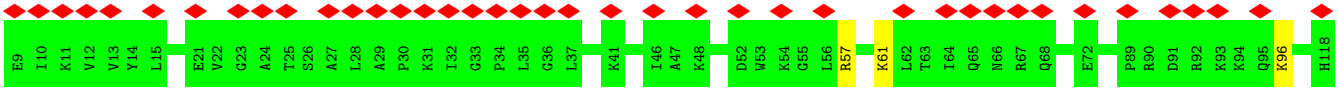


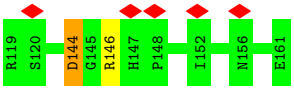


- Molecule 47: uL11

Chain t:

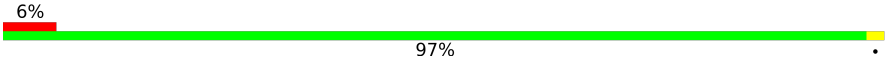


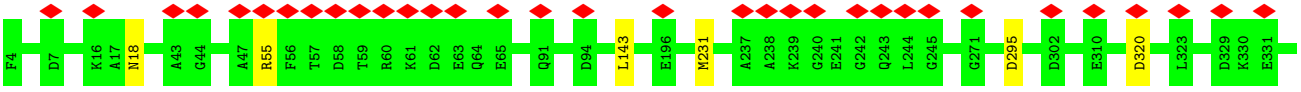


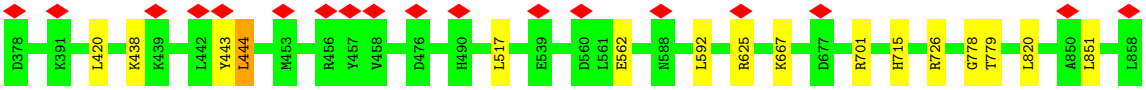


- Molecule 48: eEF2

Chain v:

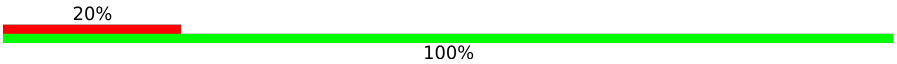


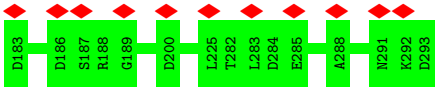




- Molecule 49: SERBP1

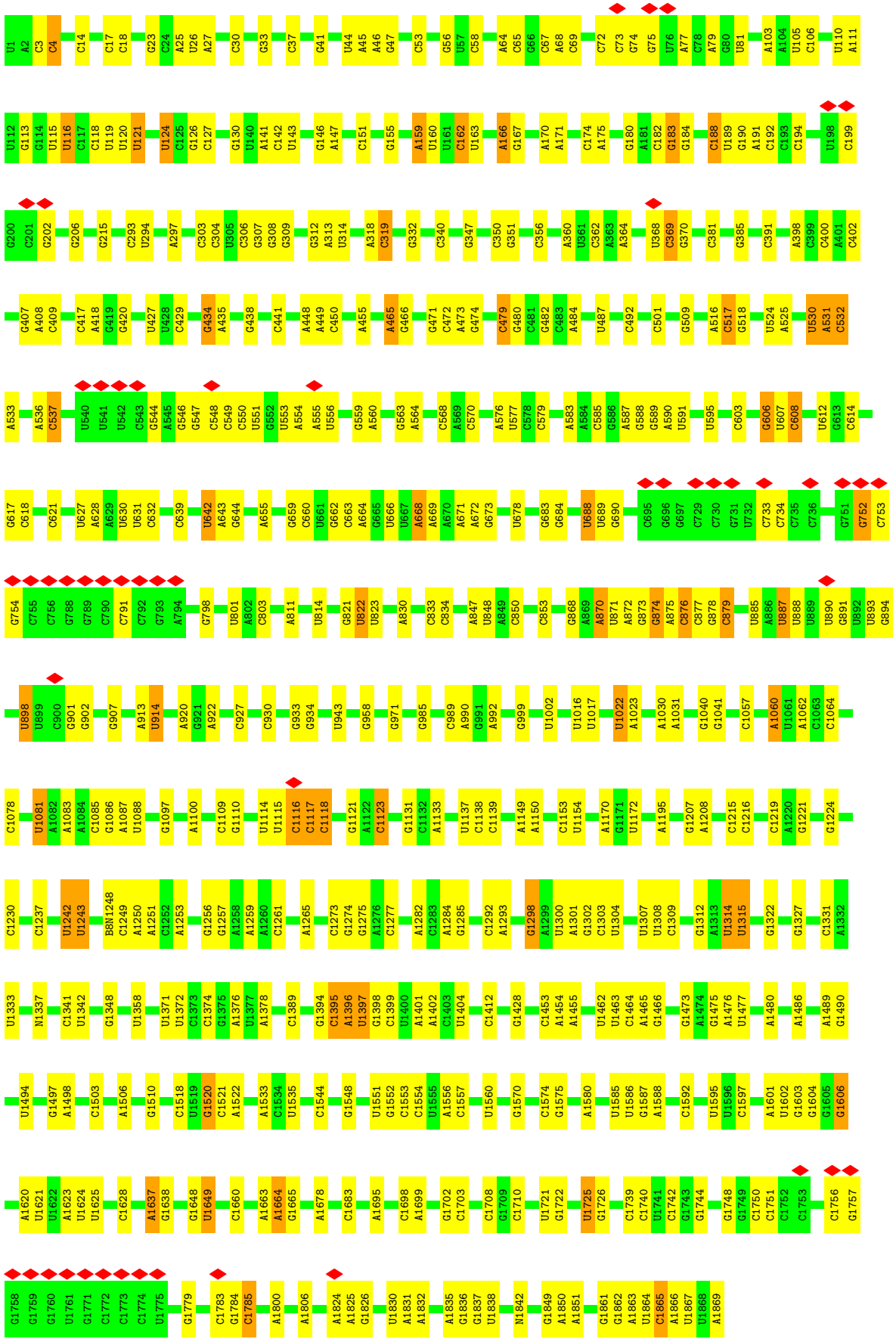
Chain w:





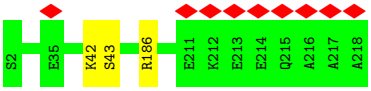
- Molecule 50: 18S rRNA

Chain 9:


U1 A2 C3 C4 C14 C17 C18 G23 C24 A25 U26 A27 C30 G33 C37 G41 U44 A45 A46 G47 C53 G56 U57 C58 A64 C65 G66 C67 A68 C69 C72 C73 G74 G75 U76 A77 C78 A79 G80 U81 A103 A104 U105 C106 U110 A111
U112 G113 G114 U115 U116 C117 C118 U119 U120 U121 U124 C125 G126 C127 G130 U140 A141 C142 U143 G146 A147 C151 G155 A159 U160 U161 C162 U163 A166 G167 A170 A171 C174 A175 G180 A181 C182 G183 G184 C188 U189 G190 A191 C192 C193 C194 U198 C199
G200 C201 G202 G206 G215 C293 U294 A297 C303 C304 U305 C306 G307 G308 G309 G312 A313 U314 A318 C319 G332 C340 G347 C350 G351 C356 A360 U361 C362 A363 A364 U368 C369 G370 C381 G385 C391 A398 C399 C400 A401 C402
G407 A408 C409 C417 A418 G419 G420 U427 U428 C429 G434 A435 G438 C441 A448 A449 C450 A455 A465 G466 G471 C472 A473 G474 C479 G480 C481 G482 C483 A484 U487 C492 C501 G509 A516 C517 G518 U524 A525 U530 A531 C532
A533 A536 C537 U540 U541 U542 C543 G544 A545 G546 G547 C548 C549 C550 U551 G552 U553 A554 A555 U556 G559 A560 G563 A564 C568 A569 C570 A576 U577 C578 C579 A583 A584 C585 G586 A587 G588 G589 A590 U591 U595 C603 G606 U607 C608 U612 G613 C614
G617 C618 C621 U627 A628 A629 U630 U631 C632 C639 U642 A643 G644 A655 G659 C660 U661 G662 C663 A664 G665 U666 U667 A668 A669 A670 A671 A672 G673 U678 G683 G684 U688 U689 G690 C695 G696 G697 C729 C730 G731 U732 C733 C734 C735 C736 G751 G752 C753
G754 C755 C756 G788 G789 C790 C791 C792 G793 A794 G798 U801 A802 C803 A811 U814 G821 U822 U823 A830 C833 C834 A847 U848 A849 C850 C853 G868 A869 A870 U871 A872 G873 G874 A875 C876 C877 G878 C879 U885 A886 U887 U888 U889 U890 G891 U892 U893 G894
U898 U899 C900 G901 G902 G907 A913 U914 A920 G921 A922 C927 C930 G933 G934 U943 G958 G971 G985 C989 A990 G991 A992 G999 U1002 U1016 U1017 U1022 A1023 A1030 A1031 G1040 G1041 C1057 A1060 U1061 A1062 C1063 C1064
C1078 U1081 A1082 A1083 A1084 C1085 G1086 A1087 U1088 G1097 A1100 C1109 G1110 U1114 U1115 C1116 C1117 C1118 G1121 A1122 C1123 G1131 C1132 A1133 U1137 C1138 C1139 A1149 A1150 C1153 U1154 A1170 G1171 U1172 A1195 G1207 A1208 C1215 C1216 C1219 A1220 G1221 G1224
C1230 C1237 U1242 U1243 B8N1248 C1249 A1250 A1251 C1252 A1253 G1256 G1257 A1258 A1259 A1260 C1261 A1265 C1273 G1274 G1275 A1276 C1277 A1282 C1283 A1284 G1285 C1292 A1293 G1298 A1299 U1300 A1301 G1302 C1303 U1304 U1307 U1308 C1309 G1312 A1313 U1314 U1315 G1322 G1327 C1331 A1332
U1333 N1337 C1341 U1342 G1348 U1358 U1371 U1372 C1373 C1374 G1375 A1376 U1377 A1378 C1389 G1394 C1395 A1396 U1397 G1398 C1399 U1400 A1401 A1402 C1403 U1404 C1412 G1428 C1453 A1454 A1455 U1462 U1463 C1464 A1465 G1466 G1473 A1474 G1475 A1476 U1477 A1480 A1486 A1489 G1490
U1494 G1497 A1498 C1503 A1506 G1510 C1518 U1519 G1520 C1521 A1522 A1533 C1534 U1535 C1544 G1548 U1551 G1552 C1553 C1554 U1555 A1556 C1557 U1560 G1570 C1574 G1575 A1580 U1585 U1586 G1587 A1588 C1592 U1595 U1596 C1597 A1601 U1602 G1603 G1604 G1605 G1606
A1620 U1621 U1622 A1623 U1624 U1625 C1628 A1637 G1638 G1648 U1649 C1660 A1663 A1664 G1665 A1678 C1683 A1695 C1698 A1699 G1702 C1703 C1708 G1709 C1710 U1721 G1722 U1725 G1726 C1739 C1740 U1741 C1742 G1743 G1744 G1748 G1749 C1750 C1751 C1752 C1753 C1756 G1757
G1758 G1759 G1760 U1761 G1771 C1772 C1773 C1774 U1775 G1779 C1783 G1784 C1785 A1800 A1806 A1824 A1825 G1826 U1830 A1831 A1832 A1835 G1836 G1837 U1838 N1842 G1849 A1850 A1851 G1861 G1862 A1863 U1864 C1865 A1866 U1867 U1868 A1869

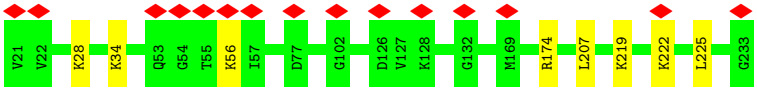
- Molecule 51: uS2

Chain AA: 99%



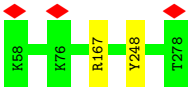
- Molecule 52: eS1

Chain BB: 7% 96%



- Molecule 53: uS5

Chain CC: 99%

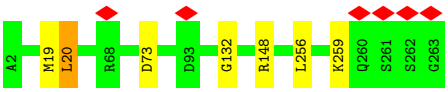


- Molecule 54: uS3

Chain DD: 6% 98%

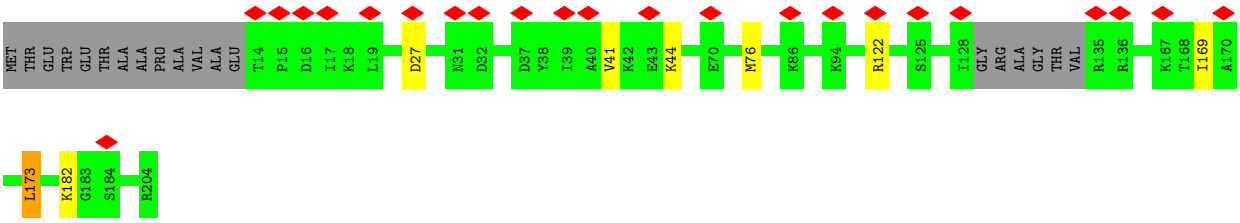
- Molecule 55: eS4

Chain EE: 97%



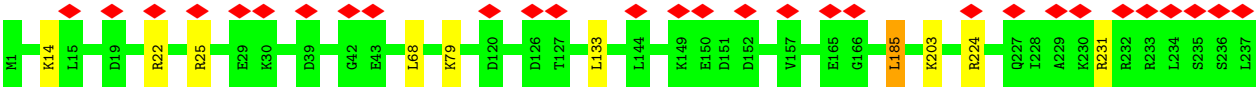
- Molecule 56: uS7

Chain FF: 11% 87% 9%



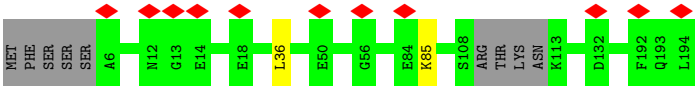
- Molecule 57: eS6

Chain GG: 12% 96%



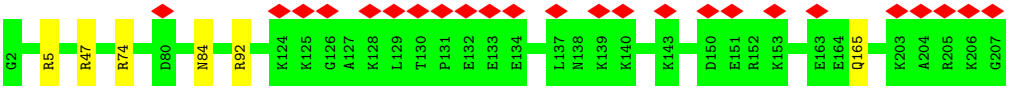
- Molecule 58: eS7

Chain HH: 6% 94% 5%



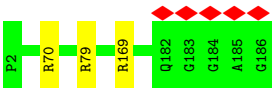
- Molecule 59: eS8

Chain II: 12% 97%



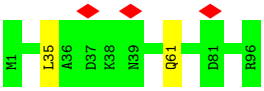
- Molecule 60: uS4

Chain JJ: 98%



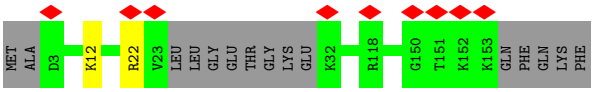
- Molecule 61: eS10

Chain KK: 98%



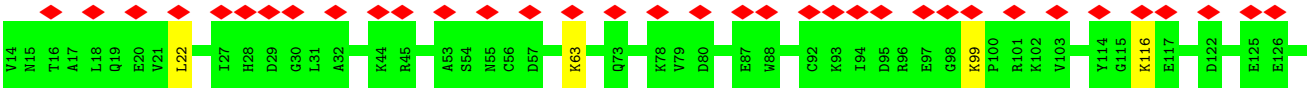
- Molecule 62: uS17

Chain LL: 6% 89% 9%



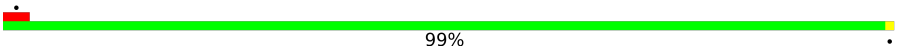
- Molecule 63: eS12

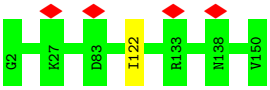
Chain MM: 32% 97%



- Molecule 64: uS15

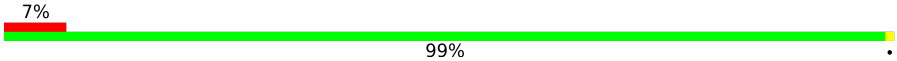
Chain NN:

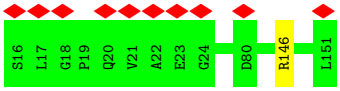




- Molecule 65: uS11

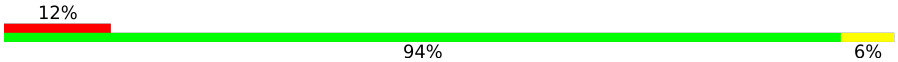
Chain OO:

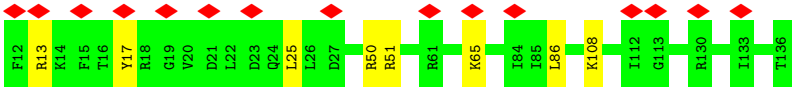




- Molecule 66: uS19

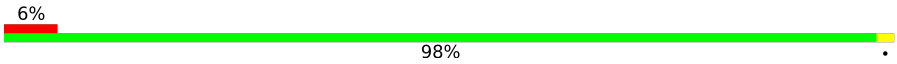
Chain PP:

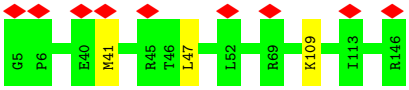




- Molecule 67: uS9

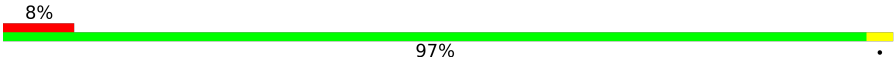
Chain QQ:

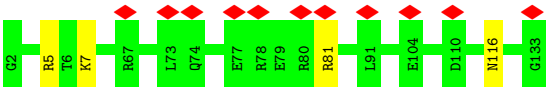




- Molecule 68: eS17

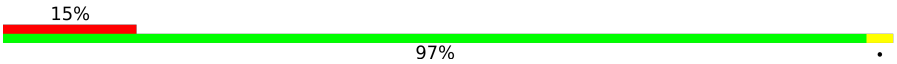
Chain RR:

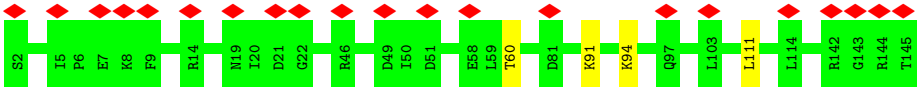




- Molecule 69: uS13

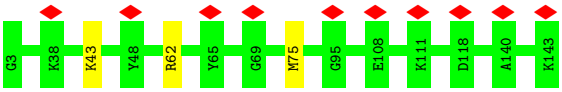
Chain SS:





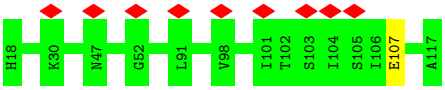
- Molecule 70: eS19

Chain TT: 7% 98%



- Molecule 71: uS10

Chain UU: 9% 99%

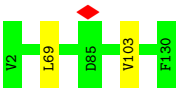


- Molecule 72: eS21

Chain VV: 98%

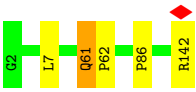
- Molecule 73: uS8

Chain WW: 98%



- Molecule 74: uS12

Chain XX: 96%

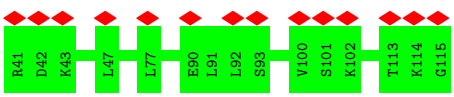


- Molecule 75: eS24

Chain YY: 98%

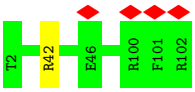
- Molecule 76: eS25

Chain ZZ: 19% 100%



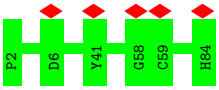
- Molecule 77: eS26

Chain aa: 99%



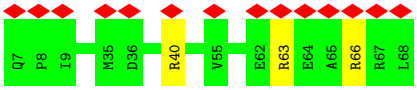
• Molecule 78: eS27

Chain bb: 6% 100%



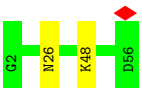
• Molecule 79: eS28

Chain cc: 23% 95% 5%



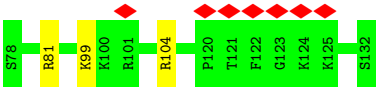
• Molecule 80: uS14

Chain dd: 96%



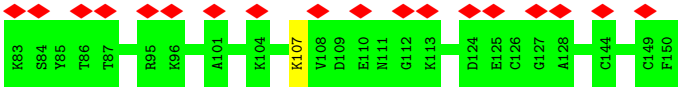
• Molecule 81: eS30

Chain ee: 13% 95% 5%



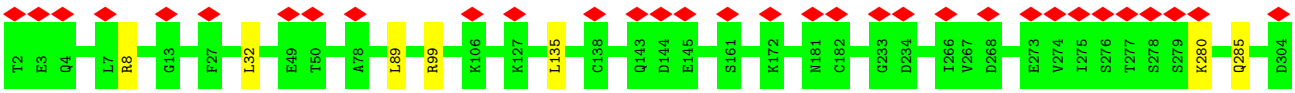
• Molecule 82: eS31

Chain ff: 26% 99%



• Molecule 83: RACK1

Chain gg: 11% 98%



R308
I314

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	133480	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.679	Depositor
Minimum map value	-0.386	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DDE, ZN, MHG, BGH, B9B, B8N, P4U, A2M, E3C, OMG, B8K, 5MU, B8H, E7G, OMU, GDP, I4U, B8Q, MG, UR3, OMC, M7A, B9H, 4AC, 1MA, E6G, P7G, 5MC, B8T, 6MZ, MLZ, MA6, 2MG, PSU, 7MG, B8W

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	5	0.80	0/83819	1.15	616/130590 (0.5%)
2	7	0.79	0/2858	1.09	13/4455 (0.3%)
3	8	0.77	0/3559	1.16	39/5543 (0.7%)
4	A	0.51	0/1936	0.62	0/2596
5	B	0.49	0/3240	0.66	2/4339 (0.0%)
6	C	0.47	0/2927	0.62	2/3932 (0.1%)
7	D	0.42	0/2437	0.55	0/3264
8	E	0.39	0/1762	0.64	0/2362
9	F	0.48	0/1911	0.62	0/2549
10	G	0.41	0/1910	0.61	0/2569
11	H	0.50	1/1535 (0.1%)	0.63	0/2063
12	I	0.48	0/1702	0.60	1/2272 (0.0%)
13	J	0.38	0/1385	0.66	1/1852 (0.1%)
14	L	0.42	0/1733	0.63	2/2316 (0.1%)
15	M	0.45	0/1158	0.58	1/1547 (0.1%)
16	N	0.50	0/1746	0.62	0/2338
17	O	0.51	0/1662	0.65	0/2222
18	P	0.49	0/1268	0.61	0/1700
19	Q	0.47	0/1539	0.62	0/2054
20	R	0.41	0/1524	0.65	1/2013 (0.0%)
21	S	0.53	0/1501	0.61	0/2012
22	T	0.47	0/1326	0.57	0/1770
23	U	0.37	0/823	0.64	0/1104
24	V	0.49	0/993	0.63	1/1332 (0.1%)
25	W	0.46	0/829	0.60	0/1099
26	X	0.43	0/984	0.64	1/1323 (0.1%)
27	Y	0.45	0/1132	0.60	0/1504
28	Z	0.46	0/1130	0.59	0/1507
29	a	0.49	0/1191	0.63	0/1590
30	b	0.34	0/861	0.56	0/1138

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	c	0.42	0/771	0.60	0/1034
32	d	0.43	0/903	0.61	0/1216
33	e	0.46	0/1071	0.58	1/1429 (0.1%)
34	f	0.51	0/895	0.68	0/1198
35	g	0.46	0/916	0.63	0/1220
36	h	0.41	0/1021	0.58	0/1348
37	i	0.39	0/841	0.59	1/1112 (0.1%)
38	j	0.46	0/720	0.65	0/952
39	k	0.40	0/575	0.58	0/761
40	l	0.40	0/459	0.61	1/608 (0.2%)
41	m	0.49	0/425	0.68	0/561
42	n	0.33	0/240	0.64	0/305
43	o	0.44	0/855	0.58	1/1128 (0.1%)
44	p	0.46	0/718	0.60	0/953
45	r	0.45	0/1010	0.62	1/1354 (0.1%)
46	s	0.33	0/1530	0.59	0/2064
47	t	0.31	0/1174	0.72	1/1582 (0.1%)
48	v	0.40	0/6736	0.69	8/9094 (0.1%)
49	w	0.33	0/447	0.58	0/592
50	9	0.64	0/39723	1.15	274/61870 (0.4%)
51	AA	0.40	0/1747	0.63	0/2374
52	BB	0.37	0/1756	0.72	4/2350 (0.2%)
53	CC	0.47	0/1753	0.64	0/2369
54	DD	0.38	0/1796	0.65	0/2417
55	EE	0.38	0/2118	0.69	5/2849 (0.2%)
56	FF	0.35	0/1492	0.68	2/2005 (0.1%)
57	GG	0.32	0/1946	0.68	3/2590 (0.1%)
58	HH	0.36	0/1510	0.67	1/2022 (0.0%)
59	II	0.36	0/1715	0.65	0/2287
60	JJ	0.39	0/1550	0.63	0/2069
61	KK	0.39	0/834	0.66	1/1125 (0.1%)
62	LL	0.44	0/1195	0.59	0/1597
63	MM	0.32	0/918	0.64	1/1233 (0.1%)
64	NN	0.36	0/1226	0.58	0/1649
65	OO	0.33	0/1029	0.63	0/1380
66	PP	0.34	0/1045	0.66	2/1396 (0.1%)
67	QQ	0.32	0/1146	0.66	1/1534 (0.1%)
68	RR	0.32	0/1082	0.62	0/1452
69	SS	0.32	0/1208	0.67	0/1618
70	TT	0.30	0/1115	0.59	0/1493
71	UU	0.32	0/805	0.61	0/1081
72	VV	0.41	0/643	0.61	0/860
73	WW	0.48	0/1051	0.69	1/1406 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	XX	0.46	0/1116	0.64	1/1490 (0.1%)
75	YY	0.33	0/1028	0.56	0/1366
76	ZZ	0.31	0/604	0.69	0/810
77	aa	0.37	0/828	0.56	0/1109
78	bb	0.33	0/665	0.59	0/891
79	cc	0.32	0/490	0.61	0/656
80	dd	0.40	0/470	0.60	0/623
81	ee	0.36	0/447	0.54	0/587
82	ff	0.32	0/567	0.60	0/753
83	gg	0.32	0/2493	0.64	2/3394 (0.1%)
All	All	0.63	1/232799 (0.0%)	0.97	992/340171 (0.3%)

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
6	C	0	1
8	E	0	2
9	F	0	1
10	G	0	1
11	H	0	1
16	N	0	3
21	S	0	1
22	T	0	1
32	d	0	1
35	g	0	1
46	s	0	1
47	t	0	1
48	v	0	4
51	AA	0	2
54	DD	0	1
55	EE	0	1
56	FF	0	1
59	II	0	1
66	PP	0	1
69	SS	0	1
71	UU	0	1
72	VV	0	1
74	XX	0	1
83	gg	0	1
All	All	0	31

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	128	MET	C-N	-5.34	1.21	1.34

The worst 5 of 992 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	9	1116	C	N1-C2-O2	12.69	126.52	118.90
50	9	1116	C	C2-N1-C1'	11.86	131.84	118.80
1	5	4056	A	OP1-P-O3'	-11.48	79.94	105.20
50	9	501	C	N1-C2-O2	11.03	125.52	118.90
1	5	1429	C	N1-C2-O2	10.96	125.47	118.90

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	73	VAL	Peptide
8	E	178	VAL	Peptide
8	E	179	THR	Peptide
9	F	195	THR	Peptide
10	G	215	ASP	Peptide

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	
4	A	246/248 (99%)	221 (90%)	25 (10%)	0	100	100
5	B	392/394 (100%)	365 (93%)	27 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	359/362 (99%)	339 (94%)	20 (6%)	0	100	100
7	D	291/293 (99%)	279 (96%)	12 (4%)	0	100	100
8	E	208/291 (72%)	198 (95%)	10 (5%)	0	100	100
9	F	223/225 (99%)	212 (95%)	10 (4%)	1 (0%)	34	67
10	G	229/319 (72%)	219 (96%)	10 (4%)	0	100	100
11	H	188/190 (99%)	171 (91%)	17 (9%)	0	100	100
12	I	201/214 (94%)	191 (95%)	10 (5%)	0	100	100
13	J	168/170 (99%)	160 (95%)	8 (5%)	0	100	100
14	L	208/210 (99%)	198 (95%)	8 (4%)	2 (1%)	15	46
15	M	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
16	N	201/203 (99%)	190 (94%)	11 (6%)	0	100	100
17	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
18	P	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
19	Q	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
20	R	178/180 (99%)	173 (97%)	5 (3%)	0	100	100
21	S	174/176 (99%)	164 (94%)	9 (5%)	1 (1%)	25	57
22	T	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	57
23	U	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
24	V	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
25	W	96/157 (61%)	89 (93%)	7 (7%)	0	100	100
26	X	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
27	Y	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
28	Z	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
29	a	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
30	b	100/245 (41%)	95 (95%)	5 (5%)	0	100	100
31	c	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
32	d	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
33	e	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
34	f	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
35	g	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
36	h	120/122 (98%)	119 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	i	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
38	j	84/86 (98%)	77 (92%)	7 (8%)	0	100	100
39	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
40	l	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
41	m	49/52 (94%)	46 (94%)	2 (4%)	1 (2%)	7	30
42	n	23/25 (92%)	23 (100%)	0	0	100	100
43	o	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
44	p	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
45	r	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
46	s	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
47	t	151/153 (99%)	128 (85%)	22 (15%)	1 (1%)	22	55
48	v	843/848 (99%)	774 (92%)	68 (8%)	1 (0%)	51	82
49	w	51/55 (93%)	46 (90%)	5 (10%)	0	100	100
51	AA	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
52	BB	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
53	CC	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
54	DD	226/228 (99%)	216 (96%)	10 (4%)	0	100	100
55	EE	260/262 (99%)	244 (94%)	16 (6%)	0	100	100
56	FF	181/204 (89%)	162 (90%)	19 (10%)	0	100	100
57	GG	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
58	HH	181/194 (93%)	173 (96%)	8 (4%)	0	100	100
59	II	204/206 (99%)	185 (91%)	19 (9%)	0	100	100
60	JJ	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
61	KK	94/96 (98%)	86 (92%)	8 (8%)	0	100	100
62	LL	139/158 (88%)	131 (94%)	8 (6%)	0	100	100
63	MM	115/117 (98%)	101 (88%)	14 (12%)	0	100	100
64	NN	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
65	OO	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
66	PP	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
67	QQ	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
68	RR	130/132 (98%)	121 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	SS	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
70	TT	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
71	UU	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
72	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
73	WW	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
74	XX	139/141 (99%)	132 (95%)	4 (3%)	3 (2%)	6	29
75	YY	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
76	ZZ	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
77	aa	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
78	bb	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
79	cc	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
80	dd	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
81	ee	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
82	ff	66/68 (97%)	55 (83%)	11 (17%)	0	100	100
83	gg	311/313 (99%)	282 (91%)	29 (9%)	0	100	100
All	All	12409/13005 (95%)	11674 (94%)	724 (6%)	11 (0%)	54	82

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	L	64	VAL
41	m	73	CYS
74	XX	62	PRO
14	L	63	THR
21	S	166	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	190/190 (100%)	187 (98%)	3 (2%)	62	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	342/342 (100%)	338 (99%)	4 (1%)	71	85
6	C	301/301 (100%)	297 (99%)	4 (1%)	69	84
7	D	247/247 (100%)	245 (99%)	2 (1%)	81	91
8	E	190/251 (76%)	186 (98%)	4 (2%)	53	76
9	F	196/196 (100%)	196 (100%)	0	100	100
10	G	200/272 (74%)	194 (97%)	6 (3%)	41	68
11	H	169/169 (100%)	168 (99%)	1 (1%)	86	94
12	I	175/181 (97%)	173 (99%)	2 (1%)	73	86
13	J	143/143 (100%)	143 (100%)	0	100	100
14	L	175/175 (100%)	175 (100%)	0	100	100
15	M	117/117 (100%)	116 (99%)	1 (1%)	78	90
16	N	171/171 (100%)	168 (98%)	3 (2%)	59	79
17	O	171/171 (100%)	167 (98%)	4 (2%)	50	74
18	P	134/134 (100%)	131 (98%)	3 (2%)	52	75
19	Q	164/164 (100%)	162 (99%)	2 (1%)	71	85
20	R	159/159 (100%)	158 (99%)	1 (1%)	86	94
21	S	157/157 (100%)	156 (99%)	1 (1%)	86	94
22	T	139/139 (100%)	137 (99%)	2 (1%)	67	83
23	U	89/89 (100%)	88 (99%)	1 (1%)	73	86
24	V	101/101 (100%)	99 (98%)	2 (2%)	55	77
25	W	82/126 (65%)	82 (100%)	0	100	100
26	X	106/106 (100%)	105 (99%)	1 (1%)	78	90
27	Y	124/124 (100%)	122 (98%)	2 (2%)	62	81
28	Z	117/117 (100%)	117 (100%)	0	100	100
29	a	119/119 (100%)	118 (99%)	1 (1%)	81	91
30	b	84/184 (46%)	82 (98%)	2 (2%)	49	74
31	c	84/84 (100%)	83 (99%)	1 (1%)	71	85
32	d	98/98 (100%)	97 (99%)	1 (1%)	76	88
33	e	114/114 (100%)	113 (99%)	1 (1%)	78	90
34	f	88/88 (100%)	87 (99%)	1 (1%)	73	86
35	g	98/98 (100%)	95 (97%)	3 (3%)	40	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	h	109/109 (100%)	108 (99%)	1 (1%)	78	90
37	i	86/86 (100%)	83 (96%)	3 (4%)	36	65
38	j	73/73 (100%)	71 (97%)	2 (3%)	44	70
39	k	64/64 (100%)	64 (100%)	0	100	100
40	l	47/47 (100%)	47 (100%)	0	100	100
41	m	47/47 (100%)	47 (100%)	0	100	100
42	n	24/24 (100%)	23 (96%)	1 (4%)	30	59
43	o	91/91 (100%)	89 (98%)	2 (2%)	52	75
44	p	74/74 (100%)	74 (100%)	0	100	100
45	r	108/108 (100%)	107 (99%)	1 (1%)	78	90
46	s	164/164 (100%)	163 (99%)	1 (1%)	86	94
47	t	126/126 (100%)	123 (98%)	3 (2%)	49	74
48	v	722/722 (100%)	712 (99%)	10 (1%)	67	83
49	w	46/46 (100%)	46 (100%)	0	100	100
51	AA	180/181 (99%)	179 (99%)	1 (1%)	86	94
52	BB	194/194 (100%)	190 (98%)	4 (2%)	53	76
53	CC	187/187 (100%)	185 (99%)	2 (1%)	73	86
54	DD	190/190 (100%)	186 (98%)	4 (2%)	53	76
55	EE	224/224 (100%)	221 (99%)	3 (1%)	69	84
56	FF	158/170 (93%)	152 (96%)	6 (4%)	33	61
57	GG	207/207 (100%)	199 (96%)	8 (4%)	32	61
58	HH	165/174 (95%)	164 (99%)	1 (1%)	86	94
59	II	178/178 (100%)	173 (97%)	5 (3%)	43	70
60	JJ	161/161 (100%)	158 (98%)	3 (2%)	57	78
61	KK	87/87 (100%)	86 (99%)	1 (1%)	73	86
62	LL	130/142 (92%)	128 (98%)	2 (2%)	65	82
63	MM	99/99 (100%)	96 (97%)	3 (3%)	41	68
64	NN	130/130 (100%)	129 (99%)	1 (1%)	81	91
65	OO	106/106 (100%)	105 (99%)	1 (1%)	78	90
66	PP	111/111 (100%)	106 (96%)	5 (4%)	27	58
67	QQ	117/117 (100%)	115 (98%)	2 (2%)	60	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	RR	119/119 (100%)	115 (97%)	4 (3%)	37	65
69	SS	125/125 (100%)	122 (98%)	3 (2%)	49	74
70	TT	111/111 (100%)	108 (97%)	3 (3%)	44	70
71	UU	92/92 (100%)	92 (100%)	0	100	100
72	VV	67/67 (100%)	66 (98%)	1 (2%)	65	82
73	WW	112/112 (100%)	111 (99%)	1 (1%)	78	90
74	XX	113/113 (100%)	112 (99%)	1 (1%)	78	90
75	YY	107/107 (100%)	105 (98%)	2 (2%)	57	78
76	ZZ	66/66 (100%)	66 (100%)	0	100	100
77	aa	88/88 (100%)	87 (99%)	1 (1%)	73	86
78	bb	75/75 (100%)	75 (100%)	0	100	100
79	cc	55/55 (100%)	52 (94%)	3 (6%)	21	51
80	dd	48/48 (100%)	46 (96%)	2 (4%)	30	59
81	ee	46/46 (100%)	43 (94%)	3 (6%)	17	46
82	ff	61/61 (100%)	60 (98%)	1 (2%)	62	81
83	gg	272/272 (100%)	268 (98%)	4 (2%)	65	82
All	All	10806/11123 (97%)	10642 (98%)	164 (2%)	66	82

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	II	84	ASN
70	TT	62	ARG
60	JJ	169	ARG
66	PP	51	ARG
77	aa	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
7	D	42	ASN
15	M	48	GLN
22	T	69	GLN
55	EE	36	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3520/3597 (97%)	818 (23%)	59 (1%)
2	7	119/120 (99%)	14 (11%)	0
3	8	149/151 (98%)	25 (16%)	1 (0%)
50	9	1670/1698 (98%)	388 (23%)	18 (1%)
All	All	5458/5566 (98%)	1245 (22%)	78 (1%)

5 of 1245 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	5	A
1	5	12	A
1	5	13	U
1	5	17	A
1	5	25	A

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	4936	G
50	9	1137	U
3	8	124	U
50	9	553	U
50	9	1520	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	P7G	5	3880	1	24,28,29	3.87	10 (41%)	27,41,44	1.58	3 (11%)
50	4AC	9	1842	50	21,24,25	3.13	10 (47%)	29,34,37	1.16	4 (13%)
1	I4U	5	4194	1	21,24,25	4.95	16 (76%)	27,34,37	1.18	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
50	A2M	9	1678	50	18,25,26	4.83	9 (50%)	18,36,39	2.59	3 (16%)
1	A2M	5	1326	1	18,25,26	4.64	9 (50%)	18,36,39	2.61	3 (16%)
1	B8H	5	1860	1	19,22,23	6.79	6 (31%)	22,32,35	2.26	5 (22%)
1	B8W	5	4185	1	18,26,27	5.21	8 (44%)	21,38,41	6.11	12 (57%)
1	UR3	5	4597	1	19,22,23	2.53	6 (31%)	26,32,35	1.20	3 (11%)
50	M7A	9	1806	50	20,25,26	2.04	3 (15%)	28,37,40	3.73	8 (28%)
48	DDE	v	715	48	14,20,21	1.02	0	14,28,30	1.24	3 (21%)
1	OMG	5	2424	1	18,26,27	2.51	8 (44%)	19,38,41	1.55	4 (21%)
1	PSU	5	1582	1	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
1	6MZ	5	4220	1	18,25,26	2.17	4 (22%)	16,36,39	1.81	3 (18%)
1	MHG	5	4371	1	29,32,33	4.01	11 (37%)	34,46,49	2.28	11 (32%)
1	A2M	5	3825	1	18,25,26	4.71	8 (44%)	18,36,39	2.70	3 (16%)
1	OMG	5	3792	1	18,26,27	2.51	8 (44%)	19,38,41	1.60	4 (21%)
1	5MU	5	4083	1	19,22,23	4.67	7 (36%)	28,32,35	3.47	9 (32%)
1	OMG	5	4370	1	18,26,27	2.43	8 (44%)	19,38,41	1.56	4 (21%)
1	PSU	5	4403	1	18,21,22	1.02	1 (5%)	22,30,33	1.83	4 (18%)
50	E3C	9	568	50	18,23,24	3.37	6 (33%)	21,33,36	2.22	5 (23%)
1	PSU	5	4636	1	18,21,22	1.05	2 (11%)	22,30,33	1.97	4 (18%)
50	A2M	9	27	50,84	18,25,26	4.68	9 (50%)	18,36,39	2.69	4 (22%)
50	5MU	9	814	50	19,22,23	4.87	7 (36%)	28,32,35	3.58	12 (42%)
1	PSU	5	4450	84,1	18,21,22	1.07	3 (16%)	22,30,33	1.96	4 (18%)
1	5MC	5	3782	1	18,22,23	3.56	7 (38%)	26,32,35	1.06	1 (3%)
50	5MC	9	1374	50	18,22,23	3.69	7 (38%)	26,32,35	1.34	3 (11%)
1	1MA	5	4415	1	16,25,26	3.91	4 (25%)	18,37,40	1.78	3 (16%)
1	A2M	5	2401	84,1	18,25,26	4.68	10 (55%)	18,36,39	2.73	4 (22%)
1	B8W	5	4472	1	18,26,27	5.33	8 (44%)	21,38,41	5.88	10 (47%)
1	OMG	5	1316	1	18,26,27	2.46	8 (44%)	19,38,41	1.69	4 (21%)
1	BGH	5	3899	84,1	25,29,30	4.24	16 (64%)	31,43,46	2.57	13 (41%)
1	OMG	5	373	1	18,26,27	2.46	8 (44%)	19,38,41	1.68	5 (26%)
50	B8N	9	1248	50,84	24,29,30	2.79	6 (25%)	29,42,45	1.74	5 (17%)
3	OMU	8	14	3,1	19,22,23	2.84	7 (36%)	26,31,34	1.85	7 (26%)
1	OMC	5	2422	84,1	19,22,23	2.86	7 (36%)	26,31,34	0.98	1 (3%)
1	PSU	5	1683	1	18,21,22	1.11	2 (11%)	22,30,33	1.82	4 (18%)
50	B8Q	9	1219	50	17,22,23	2.92	4 (23%)	22,32,35	2.32	7 (31%)
1	PSU	5	3729	1	18,21,22	1.07	1 (5%)	22,30,33	1.72	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMG	5	4637	1	18,26,27	2.41	8 (44%)	19,38,41	1.49	4 (21%)
50	PSU	9	119	50	18,21,22	0.93	1 (5%)	22,30,33	1.59	4 (18%)
1	A2M	5	1524	1	18,25,26	4.72	10 (55%)	18,36,39	2.75	3 (16%)
1	PSU	5	1677	1	18,21,22	1.12	2 (11%)	22,30,33	1.90	4 (18%)
50	OMG	9	509	50,84	18,26,27	2.46	8 (44%)	19,38,41	1.46	4 (21%)
1	2MG	5	1517	1	18,26,27	2.52	7 (38%)	16,38,41	1.53	4 (25%)
6	MLZ	C	333	6	8,9,10	0.84	0	4,9,11	0.70	0
1	OMU	5	4620	1	19,22,23	2.70	7 (36%)	26,31,34	1.84	5 (19%)
1	B8Q	5	1456	1	17,22,23	2.73	5 (29%)	22,32,35	2.03	4 (18%)
1	OMU	5	4306	1	19,22,23	2.79	8 (42%)	26,31,34	1.75	5 (19%)
50	6MZ	9	1832	50,84	18,25,26	2.23	3 (16%)	16,36,39	1.52	1 (6%)
50	PSU	9	823	50	18,21,22	1.08	1 (5%)	22,30,33	1.81	4 (18%)
1	OMG	5	2364	1	18,26,27	2.47	8 (44%)	19,38,41	1.66	4 (21%)
1	A2M	5	3785	1	18,25,26	4.58	10 (55%)	18,36,39	2.57	3 (16%)
1	B8T	5	4483	1	19,22,23	3.00	8 (42%)	26,31,34	1.05	2 (7%)
50	A2M	9	668	50,84	18,25,26	4.67	8 (44%)	18,36,39	2.70	5 (27%)
1	B8W	5	4529	84,1	18,26,27	5.30	8 (44%)	21,38,41	6.42	10 (47%)
50	OMC	9	1710	50	19,22,23	2.94	7 (36%)	26,31,34	0.93	1 (3%)
1	PSU	5	4442	1	18,21,22	1.06	2 (11%)	22,30,33	1.84	5 (22%)
1	B8W	5	2380	1	18,26,27	5.22	8 (44%)	21,38,41	6.07	7 (33%)
1	PSU	5	4500	1	18,21,22	1.05	3 (16%)	22,30,33	1.91	4 (18%)
1	P7G	5	1909	1	24,28,29	4.12	10 (41%)	27,41,44	1.47	3 (11%)
1	OMC	5	2804	1	19,22,23	2.85	7 (36%)	26,31,34	0.81	0
1	E7G	5	1797	1	24,27,28	3.64	11 (45%)	30,40,43	2.21	10 (33%)
1	E6G	5	4355	1	20,27,28	5.75	9 (45%)	22,39,42	2.14	7 (31%)
1	OMC	5	3701	84,1	19,22,23	2.80	7 (36%)	26,31,34	0.76	0
1	1MA	5	1322	84,1	16,25,26	3.77	4 (25%)	18,37,40	1.76	3 (16%)
50	MA6	9	1851	50	19,26,27	0.98	1 (5%)	18,38,41	2.69	2 (11%)
1	2MG	5	4872	1	18,26,27	2.63	7 (38%)	16,38,41	1.76	4 (25%)
50	OMU	9	116	50	19,22,23	2.88	7 (36%)	26,31,34	1.75	5 (19%)
1	PSU	5	4628	1	18,21,22	1.13	3 (16%)	22,30,33	2.06	5 (22%)
1	A2M	5	398	1	18,25,26	4.82	8 (44%)	18,36,39	2.56	3 (16%)
1	7MG	5	2522	1	22,26,27	3.45	10 (45%)	29,39,42	1.97	8 (27%)
1	B8T	5	4671	1	19,22,23	2.99	8 (42%)	26,31,34	0.96	1 (3%)
1	OMG	5	4623	1	18,26,27	2.46	8 (44%)	19,38,41	1.64	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMG	5	2773	1	18,26,27	2.50	8 (44%)	19,38,41	1.53	4 (21%)
1	7MG	5	4550	1	22,26,27	3.48	10 (45%)	29,39,42	1.95	10 (34%)
1	OMC	5	3909	1	19,22,23	2.84	7 (36%)	26,31,34	1.26	3 (11%)
1	PSU	5	4531	1	18,21,22	1.09	2 (11%)	22,30,33	1.91	5 (22%)
50	MA6	9	1850	50	19,26,27	1.01	1 (5%)	18,38,41	2.81	3 (16%)
1	OMC	5	2861	1	19,22,23	2.83	7 (36%)	26,31,34	0.89	1 (3%)
50	OMC	9	517	50	19,22,23	2.84	7 (36%)	26,31,34	0.65	0
1	A2M	5	2363	84,1	18,25,26	4.80	10 (55%)	18,36,39	2.67	3 (16%)
1	PSU	5	3764	1	18,21,22	1.03	1 (5%)	22,30,33	1.68	4 (18%)
1	UR3	5	4530	1	19,22,23	2.67	6 (31%)	26,32,35	1.43	4 (15%)
1	OMG	5	2050	1	18,26,27	2.44	8 (44%)	19,38,41	1.48	4 (21%)
1	I4U	5	1659	1	21,24,25	4.95	16 (76%)	27,34,37	1.45	2 (7%)
1	7MG	5	1605	1	22,26,27	3.44	10 (45%)	29,39,42	2.05	9 (31%)
1	5MC	5	4335	1	18,22,23	3.61	7 (38%)	26,32,35	1.21	3 (11%)
50	UR3	9	1830	50	19,22,23	2.71	6 (31%)	26,32,35	1.57	4 (15%)
1	OMC	5	2365	1	19,22,23	2.83	7 (36%)	26,31,34	0.69	0
50	OMU	9	121	50	19,22,23	2.95	8 (42%)	26,31,34	1.76	5 (19%)
1	OMG	5	1883	1	18,26,27	2.50	8 (44%)	19,38,41	1.70	4 (21%)
1	A2M	5	4571	1	18,25,26	4.76	8 (44%)	18,36,39	2.68	4 (22%)
1	B9B	5	237	1	21,28,29	6.35	8 (38%)	23,40,43	2.37	7 (30%)
1	A2M	5	4523	84,1	18,25,26	4.82	10 (55%)	18,36,39	2.61	3 (16%)
1	UR3	5	1866	1	19,22,23	2.52	6 (31%)	26,32,35	1.37	4 (15%)
50	PSU	9	1243	50,84	18,21,22	1.07	1 (5%)	22,30,33	1.82	4 (18%)
1	A2M	5	3867	1	18,25,26	4.70	9 (50%)	18,36,39	2.62	4 (22%)
1	B8K	5	4690	1	24,28,29	4.95	16 (66%)	30,42,45	2.71	11 (36%)
1	5MC	5	4447	1	18,22,23	3.66	7 (38%)	26,32,35	1.08	1 (3%)
1	OMG	5	1522	1	18,26,27	2.44	8 (44%)	19,38,41	1.58	4 (21%)
1	OMG	5	4870	1	18,26,27	2.44	8 (44%)	19,38,41	1.53	4 (21%)
50	PSU	9	612	50	18,21,22	0.98	1 (5%)	22,30,33	1.73	4 (18%)
50	4AC	9	1337	50	21,24,25	3.19	9 (42%)	29,34,37	1.23	3 (10%)
1	OMC	5	3869	1	19,22,23	2.79	7 (36%)	26,31,34	0.83	1 (3%)
1	OMG	5	4494	1	18,26,27	2.46	8 (44%)	19,38,41	1.55	4 (21%)
50	OMG	9	644	50	18,26,27	2.47	8 (44%)	19,38,41	1.52	4 (21%)
1	B8K	5	3897	1	24,28,29	4.82	17 (70%)	30,42,45	2.49	12 (40%)
1	A2M	5	3723	1	18,25,26	4.86	9 (50%)	18,36,39	2.59	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
41	MLZ	m	72	41	8,9,10	0.77	0	4,9,11	0.78	0
50	A2M	9	166	50	18,25,26	4.79	9 (50%)	18,36,39	2.78	4 (22%)
1	E7G	5	2297	1	24,27,28	3.45	11 (45%)	30,40,43	2.12	9 (30%)
1	A2M	5	1534	84,1	18,25,26	4.66	9 (50%)	18,36,39	2.80	4 (22%)
50	A2M	9	1031	50	18,25,26	4.74	8 (44%)	18,36,39	2.78	4 (22%)
1	B9B	5	1574	1	21,28,29	6.30	9 (42%)	23,40,43	1.91	6 (26%)
1	B8H	5	4296	1	19,22,23	6.83	6 (31%)	22,32,35	2.48	5 (22%)
1	A2M	5	1871	84,1	18,25,26	4.70	9 (50%)	18,36,39	2.76	3 (16%)
1	OMC	5	3887	1	19,22,23	2.86	7 (36%)	26,31,34	0.94	1 (3%)
50	OMC	9	174	50	19,22,23	2.95	7 (36%)	26,31,34	0.81	0
1	PSU	5	2508	1	18,21,22	1.00	1 (5%)	22,30,33	1.66	4 (18%)
1	2MG	5	729	1	18,26,27	2.41	7 (38%)	16,38,41	1.43	4 (25%)
50	A2M	9	159	50	18,25,26	4.83	8 (44%)	18,36,39	2.76	4 (22%)
1	B8W	5	4129	1	18,26,27	5.30	8 (44%)	21,38,41	6.40	10 (47%)
1	M7A	5	4564	1	20,25,26	2.06	4 (20%)	28,37,40	3.76	7 (25%)
50	OMC	9	1703	50	19,22,23	2.94	7 (36%)	26,31,34	0.83	1 (3%)
50	A2M	9	484	50	18,25,26	4.71	9 (50%)	18,36,39	2.72	3 (16%)
50	PSU	9	1081	50	18,21,22	1.06	1 (5%)	22,30,33	1.77	5 (22%)
1	PSU	5	3715	1	18,21,22	1.02	1 (5%)	22,30,33	1.69	4 (18%)
1	OMG	5	1625	84,1	18,26,27	2.45	8 (44%)	19,38,41	1.48	4 (21%)
1	B8H	5	3762	1	19,22,23	6.81	6 (31%)	22,32,35	2.48	5 (22%)
50	PSU	9	822	50	18,21,22	1.03	2 (11%)	22,30,33	1.92	5 (22%)
1	PSU	5	4293	1	18,21,22	1.08	2 (11%)	22,30,33	1.75	3 (13%)
1	OMC	5	4536	1	19,22,23	2.81	7 (36%)	26,31,34	1.04	2 (7%)
50	OMG	9	683	50	18,26,27	2.46	8 (44%)	19,38,41	1.55	5 (26%)
1	OMG	5	4196	1	18,26,27	2.41	8 (44%)	19,38,41	1.49	4 (21%)
1	A2M	5	3718	1	18,25,26	4.79	10 (55%)	18,36,39	2.47	3 (16%)
1	B9B	5	2754	84,1	21,28,29	6.35	9 (42%)	23,40,43	2.05	6 (26%)
1	B9H	5	2786	1	20,25,26	2.98	3 (15%)	22,35,38	1.62	2 (9%)
1	P4U	5	1348	84,1	21,24,25	3.38	8 (38%)	27,33,36	1.26	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
1	P7G	5	3880	1	-	2/10/40/41	0/3/3/3
50	4AC	9	1842	50	-	0/11/29/30	0/2/2/2
1	I4U	5	4194	1	-	4/9/29/30	0/2/2/2
50	A2M	9	1678	50	-	0/5/27/28	0/3/3/3
1	A2M	5	1326	1	-	0/5/27/28	0/3/3/3
1	B8H	5	1860	1	-	2/7/25/26	0/2/2/2
1	B8W	5	4185	1	-	4/5/27/28	0/3/3/3
1	UR3	5	4597	1	-	0/7/25/26	0/2/2/2
50	M7A	9	1806	50	-	0/7/37/38	0/3/3/3
48	DDE	v	715	48	-	15/20/21/23	0/1/1/1
1	OMG	5	2424	1	-	2/5/27/28	0/3/3/3
1	PSU	5	1582	1	-	2/7/25/26	0/2/2/2
1	6MZ	5	4220	1	-	0/5/27/28	0/3/3/3
1	MHG	5	4371	1	-	6/16/46/47	0/3/3/3
1	A2M	5	3825	1	-	0/5/27/28	0/3/3/3
1	OMG	5	3792	1	-	2/5/27/28	0/3/3/3
1	5MU	5	4083	1	-	6/7/25/26	0/2/2/2
1	OMG	5	4370	1	-	0/5/27/28	0/3/3/3
1	PSU	5	4403	1	-	2/7/25/26	0/2/2/2
50	E3C	9	568	50	-	4/9/44/45	0/2/2/2
1	PSU	5	4636	1	-	4/7/25/26	0/2/2/2
50	A2M	9	27	50,84	-	0/5/27/28	0/3/3/3
50	5MU	9	814	50	-	0/7/25/26	0/2/2/2
1	PSU	5	4450	84,1	-	4/7/25/26	0/2/2/2
1	5MC	5	3782	1	-	0/7/25/26	0/2/2/2
50	5MC	9	1374	50	-	0/7/25/26	0/2/2/2
1	1MA	5	4415	1	-	2/3/25/26	0/3/3/3
1	A2M	5	2401	84,1	-	2/5/27/28	0/3/3/3
1	B8W	5	4472	1	-	2/5/27/28	0/3/3/3
1	OMG	5	1316	1	-	0/5/27/28	0/3/3/3
1	BGH	5	3899	84,1	-	2/13/43/44	0/3/3/3
1	OMG	5	373	1	-	1/5/27/28	0/3/3/3
50	B8N	9	1248	50,84	-	3/16/34/35	0/2/2/2
3	OMU	8	14	3,1	-	1/9/27/28	0/2/2/2
1	OMC	5	2422	84,1	-	1/9/27/28	0/2/2/2
1	PSU	5	1683	1	-	0/7/25/26	0/2/2/2
50	B8Q	9	1219	50	-	0/7/42/43	0/2/2/2
1	PSU	5	3729	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	5	4637	1	-	3/5/27/28	0/3/3/3
50	PSU	9	119	50	-	2/7/25/26	0/2/2/2
1	A2M	5	1524	1	-	0/5/27/28	0/3/3/3
1	PSU	5	1677	1	-	2/7/25/26	0/2/2/2
50	OMG	9	509	50,84	-	0/5/27/28	0/3/3/3
1	2MG	5	1517	1	-	0/5/27/28	0/3/3/3
6	MLZ	C	333	6	-	2/7/8/10	-
1	OMU	5	4620	1	-	0/9/27/28	0/2/2/2
1	B8Q	5	1456	1	-	2/7/42/43	0/2/2/2
1	OMU	5	4306	1	-	0/9/27/28	0/2/2/2
50	6MZ	9	1832	50,84	-	2/5/27/28	0/3/3/3
50	PSU	9	823	50	-	0/7/25/26	0/2/2/2
1	OMG	5	2364	1	-	2/5/27/28	0/3/3/3
1	A2M	5	3785	1	-	2/5/27/28	0/3/3/3
1	B8T	5	4483	1	-	2/7/27/28	0/2/2/2
50	A2M	9	668	50,84	-	4/5/27/28	0/3/3/3
1	B8W	5	4529	84,1	-	2/5/27/28	0/3/3/3
50	OMC	9	1710	50	-	0/9/27/28	0/2/2/2
1	PSU	5	4442	1	-	0/7/25/26	0/2/2/2
1	B8W	5	2380	1	-	5/5/27/28	0/3/3/3
1	PSU	5	4500	1	-	3/7/25/26	0/2/2/2
1	P7G	5	1909	1	-	4/10/40/41	0/3/3/3
1	OMC	5	2804	1	-	0/9/27/28	0/2/2/2
1	E7G	5	1797	1	-	3/9/39/40	0/3/3/3
1	E6G	5	4355	1	-	5/6/28/29	0/3/3/3
1	OMC	5	3701	84,1	-	4/9/27/28	0/2/2/2
1	1MA	5	1322	84,1	-	0/3/25/26	0/3/3/3
50	MA6	9	1851	50	-	3/7/29/30	0/3/3/3
1	2MG	5	4872	1	-	2/5/27/28	0/3/3/3
50	OMU	9	116	50	-	3/9/27/28	0/2/2/2
1	PSU	5	4628	1	-	0/7/25/26	0/2/2/2
1	A2M	5	398	1	-	2/5/27/28	0/3/3/3
1	7MG	5	2522	1	-	0/7/37/38	0/3/3/3
1	B8T	5	4671	1	-	0/7/27/28	0/2/2/2
1	OMG	5	4623	1	-	0/5/27/28	0/3/3/3
1	OMG	5	2773	1	-	0/5/27/28	0/3/3/3
1	7MG	5	4550	1	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	5	3909	1	-	1/9/27/28	0/2/2/2
1	PSU	5	4531	1	-	0/7/25/26	0/2/2/2
50	MA6	9	1850	50	-	1/7/29/30	0/3/3/3
1	OMC	5	2861	1	-	0/9/27/28	0/2/2/2
50	OMC	9	517	50	-	2/9/27/28	0/2/2/2
1	A2M	5	2363	84,1	-	0/5/27/28	0/3/3/3
1	PSU	5	3764	1	-	2/7/25/26	0/2/2/2
1	UR3	5	4530	1	-	1/7/25/26	0/2/2/2
1	OMG	5	2050	1	-	0/5/27/28	0/3/3/3
1	I4U	5	1659	1	-	2/9/29/30	0/2/2/2
1	7MG	5	1605	1	-	0/7/37/38	0/3/3/3
1	5MC	5	4335	1	-	0/7/25/26	0/2/2/2
50	UR3	9	1830	50	-	4/7/25/26	0/2/2/2
1	OMC	5	2365	1	-	0/9/27/28	0/2/2/2
50	OMU	9	121	50	-	2/9/27/28	0/2/2/2
1	OMG	5	1883	1	-	0/5/27/28	0/3/3/3
1	A2M	5	4571	1	-	0/5/27/28	0/3/3/3
1	B9B	5	237	1	-	4/7/29/30	0/3/3/3
1	A2M	5	4523	84,1	-	2/5/27/28	0/3/3/3
1	UR3	5	1866	1	-	0/7/25/26	0/2/2/2
50	PSU	9	1243	50,84	-	2/7/25/26	0/2/2/2
1	A2M	5	3867	1	-	4/5/27/28	0/3/3/3
1	B8K	5	4690	1	-	0/11/41/42	0/3/3/3
1	5MC	5	4447	1	-	4/7/25/26	0/2/2/2
1	OMG	5	1522	1	-	0/5/27/28	0/3/3/3
1	OMG	5	4870	1	-	4/5/27/28	0/3/3/3
50	PSU	9	612	50	-	0/7/25/26	0/2/2/2
50	4AC	9	1337	50	-	0/11/29/30	0/2/2/2
1	OMC	5	3869	1	-	0/9/27/28	0/2/2/2
1	OMG	5	4494	1	-	2/5/27/28	0/3/3/3
50	OMG	9	644	50	-	1/5/27/28	0/3/3/3
1	B8K	5	3897	1	-	3/11/41/42	0/3/3/3
1	A2M	5	3723	1	-	0/5/27/28	0/3/3/3
41	MLZ	m	72	41	-	3/7/8/10	-
50	A2M	9	166	50	-	2/5/27/28	0/3/3/3
1	E7G	5	2297	1	-	1/9/39/40	0/3/3/3
1	A2M	5	1534	84,1	-	2/5/27/28	0/3/3/3
50	A2M	9	1031	50	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B9B	5	1574	1	-	4/7/29/30	0/3/3/3
1	B8H	5	4296	1	-	1/7/25/26	0/2/2/2
1	A2M	5	1871	84,1	-	0/5/27/28	0/3/3/3
1	OMC	5	3887	1	-	1/9/27/28	0/2/2/2
50	OMC	9	174	50	-	0/9/27/28	0/2/2/2
1	PSU	5	2508	1	-	0/7/25/26	0/2/2/2
1	2MG	5	729	1	-	2/5/27/28	0/3/3/3
50	A2M	9	159	50	-	3/5/27/28	0/3/3/3
1	B8W	5	4129	1	-	2/5/27/28	0/3/3/3
1	M7A	5	4564	1	-	0/7/37/38	0/3/3/3
50	OMC	9	1703	50	-	2/9/27/28	0/2/2/2
50	A2M	9	484	50	-	0/5/27/28	0/3/3/3
50	PSU	9	1081	50	-	3/7/25/26	0/2/2/2
1	PSU	5	3715	1	-	0/7/25/26	0/2/2/2
1	OMG	5	1625	84,1	-	3/5/27/28	0/3/3/3
1	B8H	5	3762	1	-	0/7/25/26	0/2/2/2
50	PSU	9	822	50	-	2/7/25/26	0/2/2/2
1	PSU	5	4293	1	-	0/7/25/26	0/2/2/2
1	OMC	5	4536	1	-	0/9/27/28	0/2/2/2
50	OMG	9	683	50	-	2/5/27/28	0/3/3/3
1	OMG	5	4196	1	-	0/5/27/28	0/3/3/3
1	A2M	5	3718	1	-	0/5/27/28	0/3/3/3
1	B9B	5	2754	84,1	-	1/7/29/30	0/3/3/3
1	B9H	5	2786	1	-	3/12/47/48	0/2/2/2
1	P4U	5	1348	84,1	-	4/10/29/30	0/2/2/2

The worst 5 of 938 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2754	B9B	C2'-C1'	-17.99	1.26	1.53
1	5	1574	B9B	C2'-C1'	-17.90	1.26	1.53
1	5	237	B9B	C2'-C1'	-17.83	1.26	1.53
1	5	237	B9B	O4'-C1'	17.18	1.65	1.41
1	5	1574	B9B	O4'-C1'	16.86	1.64	1.41

The worst 5 of 595 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4529	B8W	N2-C2-N3	17.10	145.65	117.79
1	5	4129	B8W	N2-C2-N3	16.96	145.43	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4185	B8W	N2-C2-N3	16.75	145.08	117.79
1	5	2380	B8W	N2-C2-N3	16.70	145.01	117.79
1	5	4472	B8W	N2-C2-N3	15.95	143.78	117.79

There are no chirality outliers.

5 of 216 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	5	237	B9B	C5-C6-O6-C61
1	5	237	B9B	N1-C6-O6-C61
1	5	237	B9B	C3'-C4'-C5'-O5'
1	5	237	B9B	O4'-C4'-C5'-O5'
1	5	1348	P4U	N3-C4-O4-C41

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 307 ligands modelled in this entry, 306 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	GDP	v	900	-	24,30,30	0.96	1 (4%)	30,47,47	1.33	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	GDP	v	900	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	v	900	GDP	C6-N1	-2.63	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	v	900	GDP	PA-O3A-PB	-3.89	119.47	132.83
86	v	900	GDP	C5-C6-N1	2.53	118.42	113.95
86	v	900	GDP	C8-N7-C5	2.32	107.41	102.99
86	v	900	GDP	O6-C6-C5	-2.10	120.27	124.37

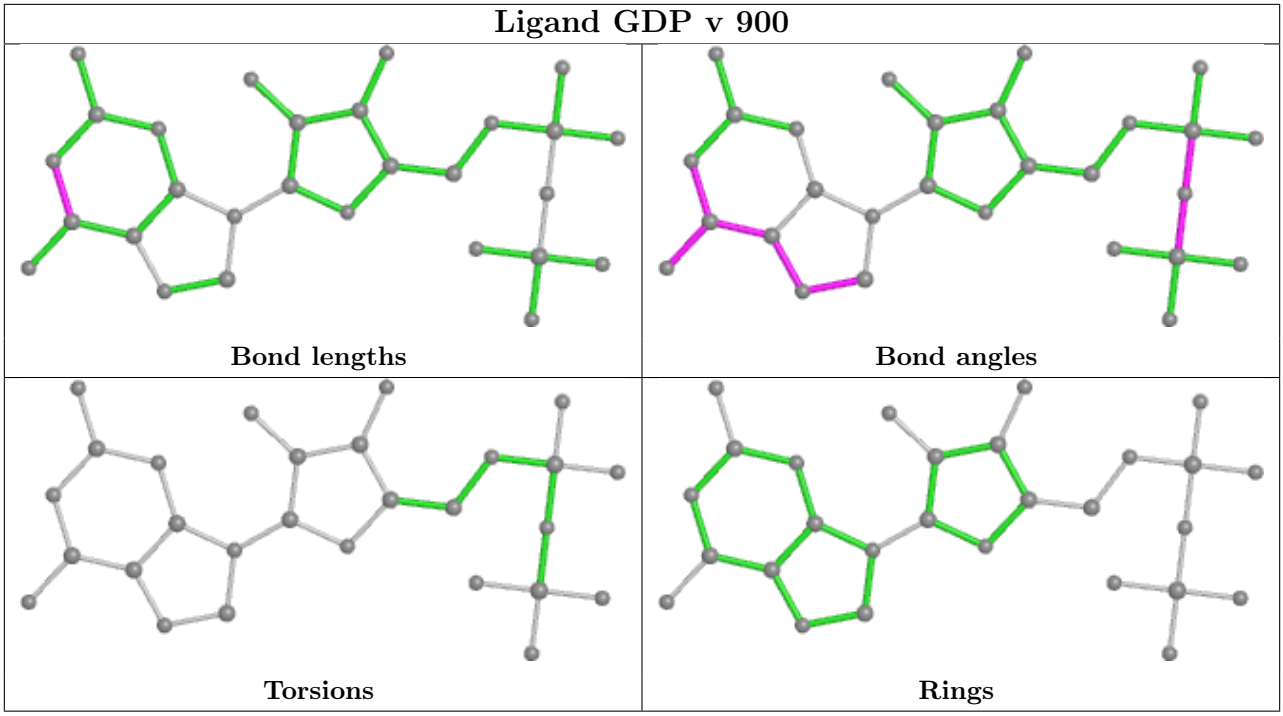
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	49
50	9	18
49	w	1
48	v	1
3	8	1

The worst 5 of 70 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	225:LEU	C	282:THR	N	57.95
1	5	2113:G	O3'	2258:C	P	39.61
1	5	1252:C	O3'	1271:G	P	35.94
1	5	1405:C	O3'	1406:G	P	22.80
1	5	1406(C):G	O3'	1411:C	P	20.78

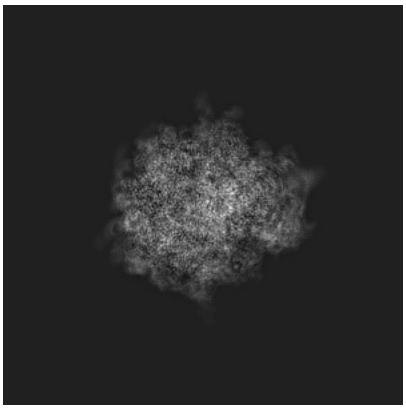
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9242. These allow visual inspection of the internal detail of the map and identification of artifacts.

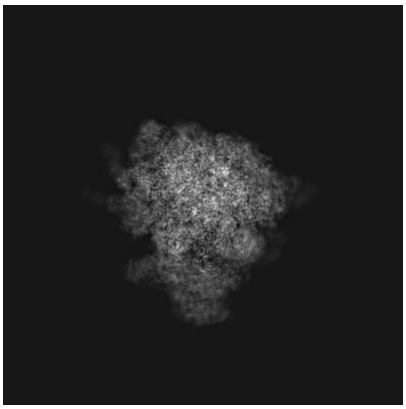
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

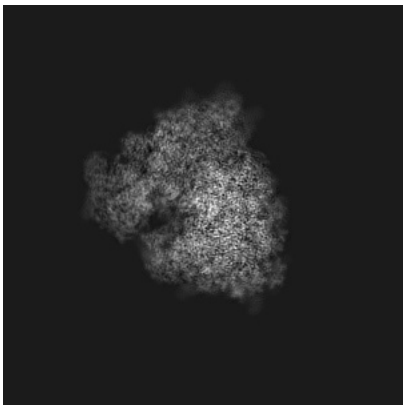
6.1.1 Primary map



X

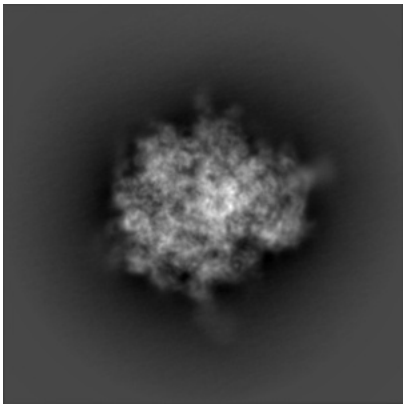


Y

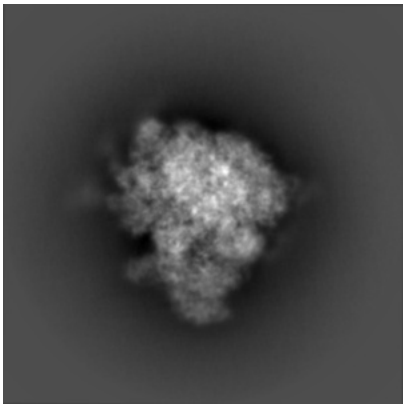


Z

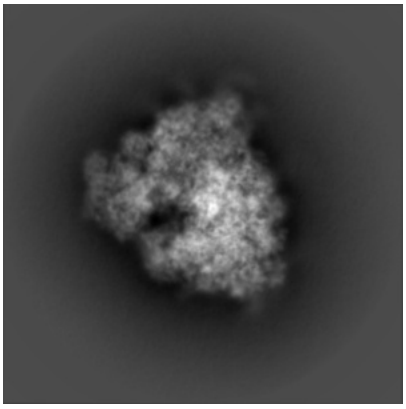
6.1.2 Raw map



X



Y

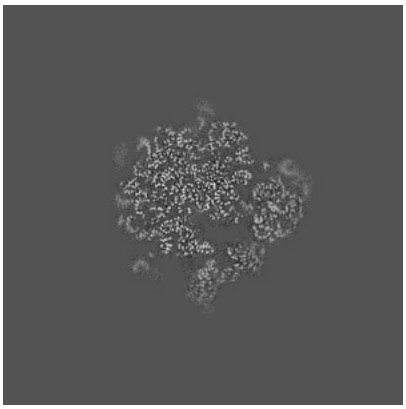


Z

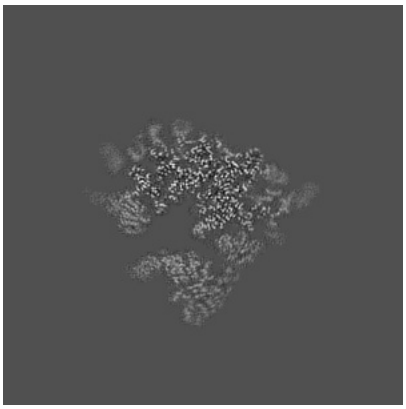
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

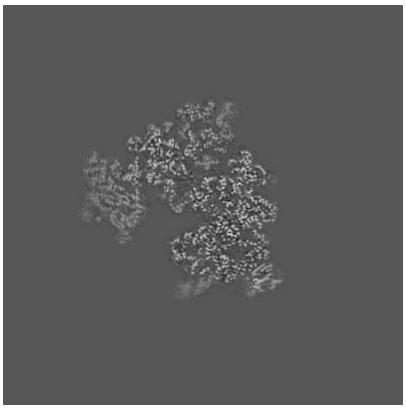
6.2.1 Primary map



X Index: 200

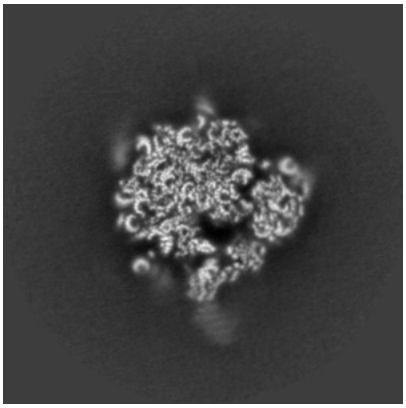


Y Index: 200

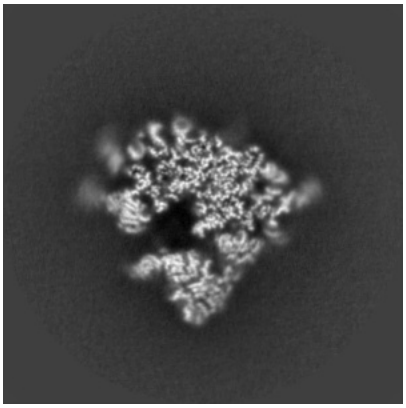


Z Index: 200

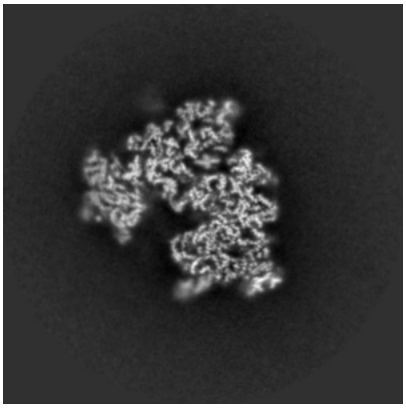
6.2.2 Raw map



X Index: 200



Y Index: 200

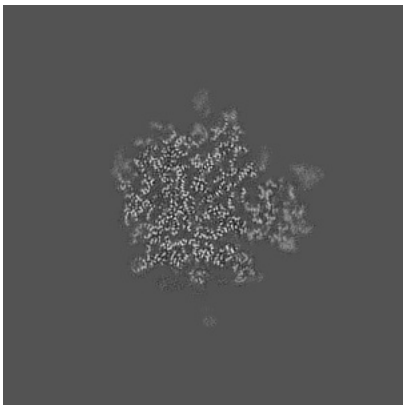


Z Index: 200

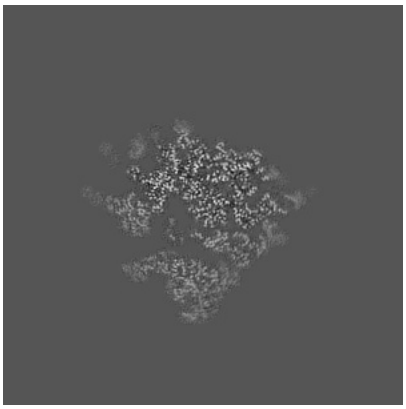
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

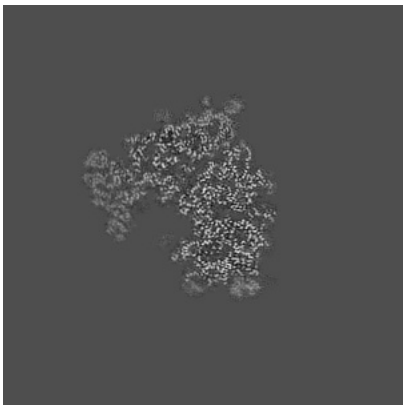
6.3.1 Primary map



X Index: 213

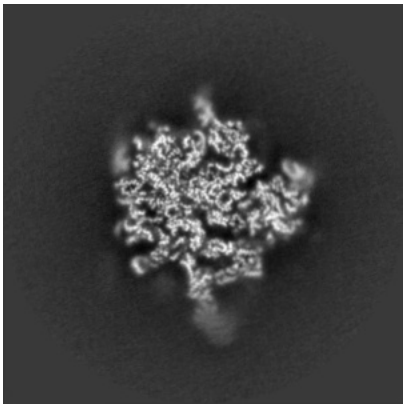


Y Index: 206

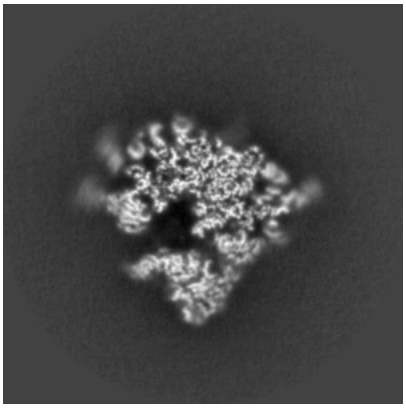


Z Index: 210

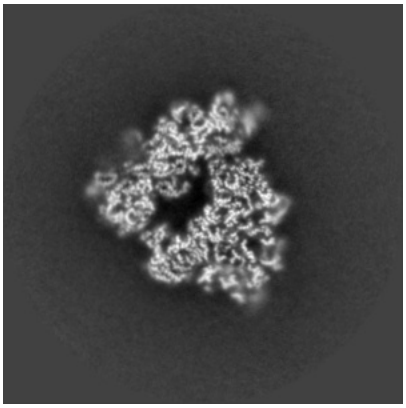
6.3.2 Raw map



X Index: 206



Y Index: 201

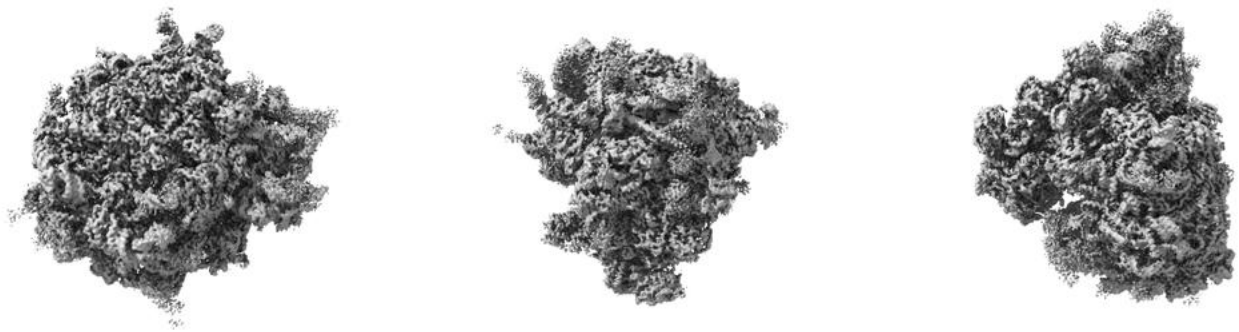


Z Index: 176

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

6.4 Orthogonal surface views (i)

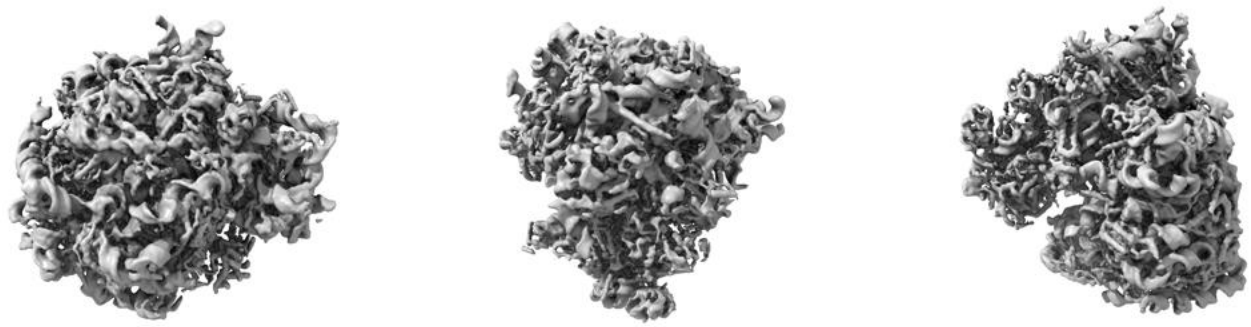
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

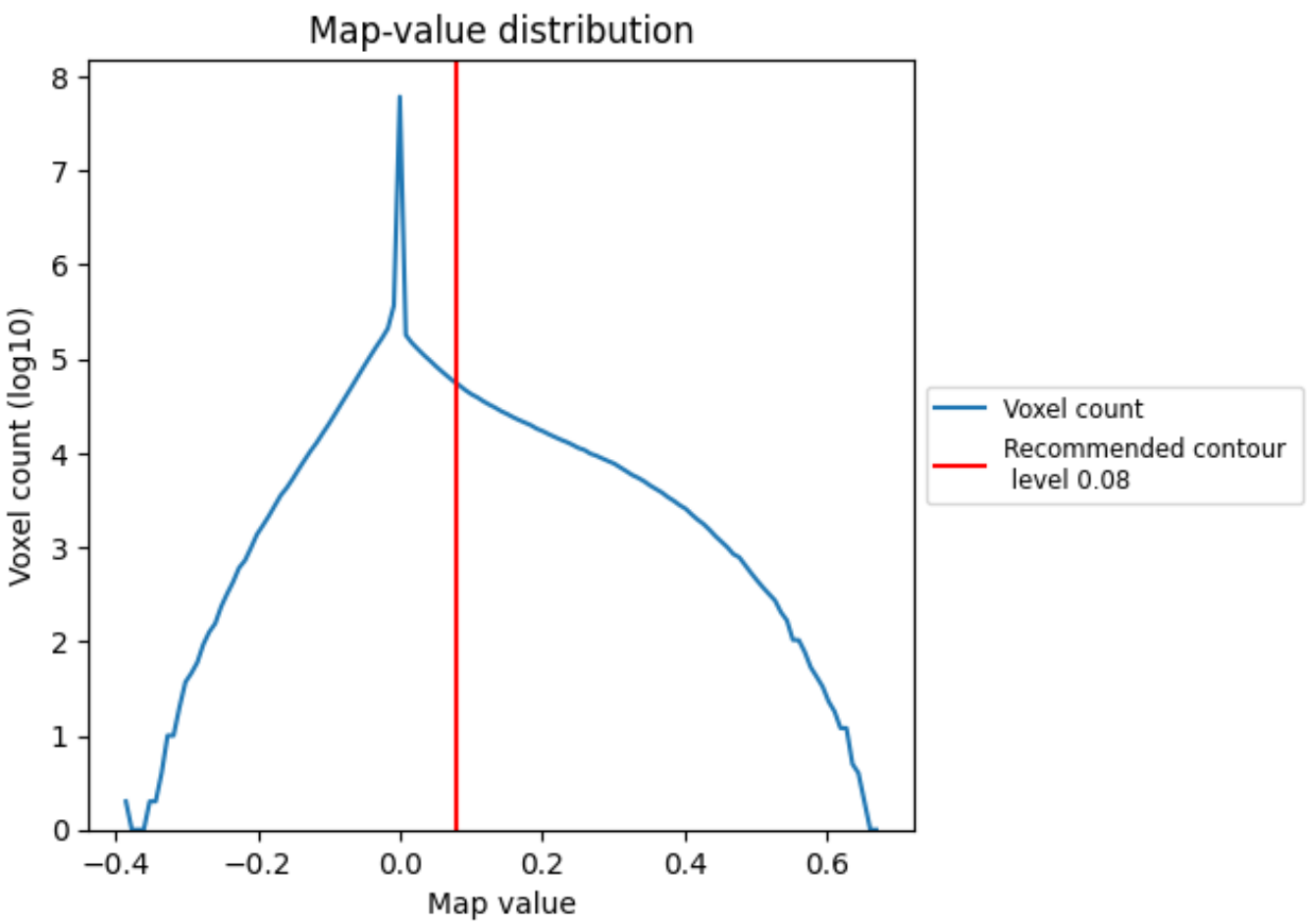
6.5 Mask visualisation (i)

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

7 Map analysis (i)

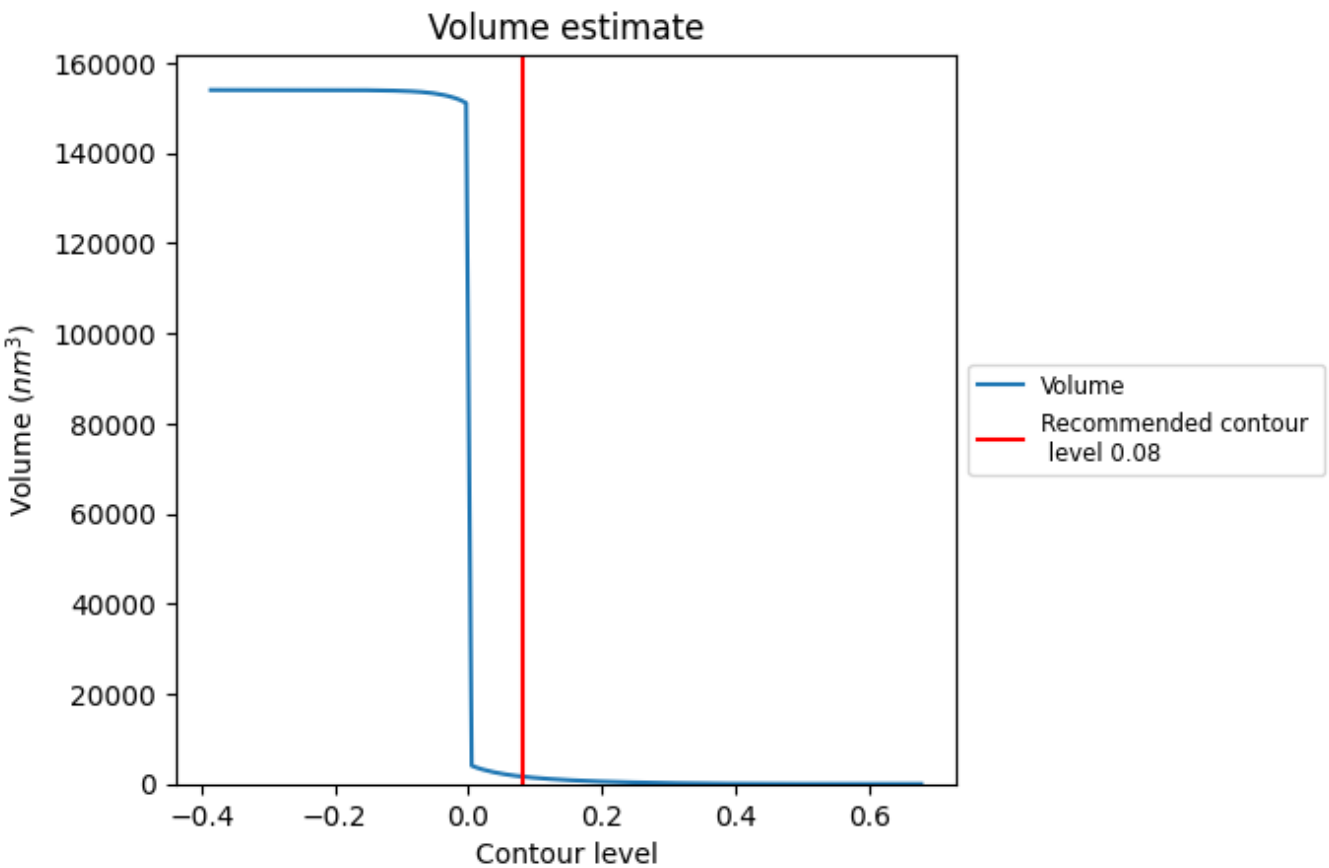
This section contains the results of statistical analysis of the map.

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.

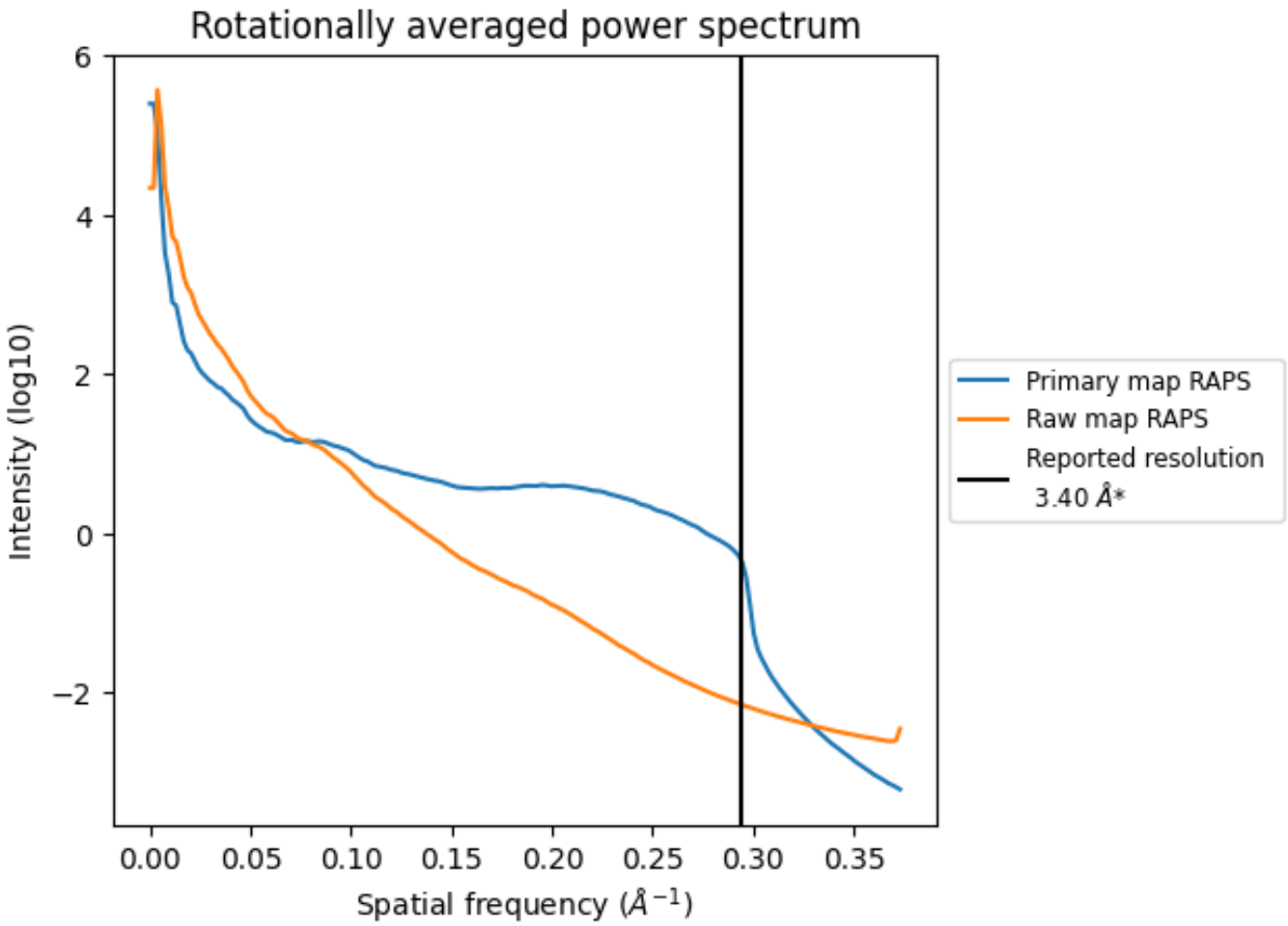
7.2 Volume estimate (i)



The volume at the recommended contour level is 1651 nm^3; this corresponds to an approximate mass of 1492 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 (i)

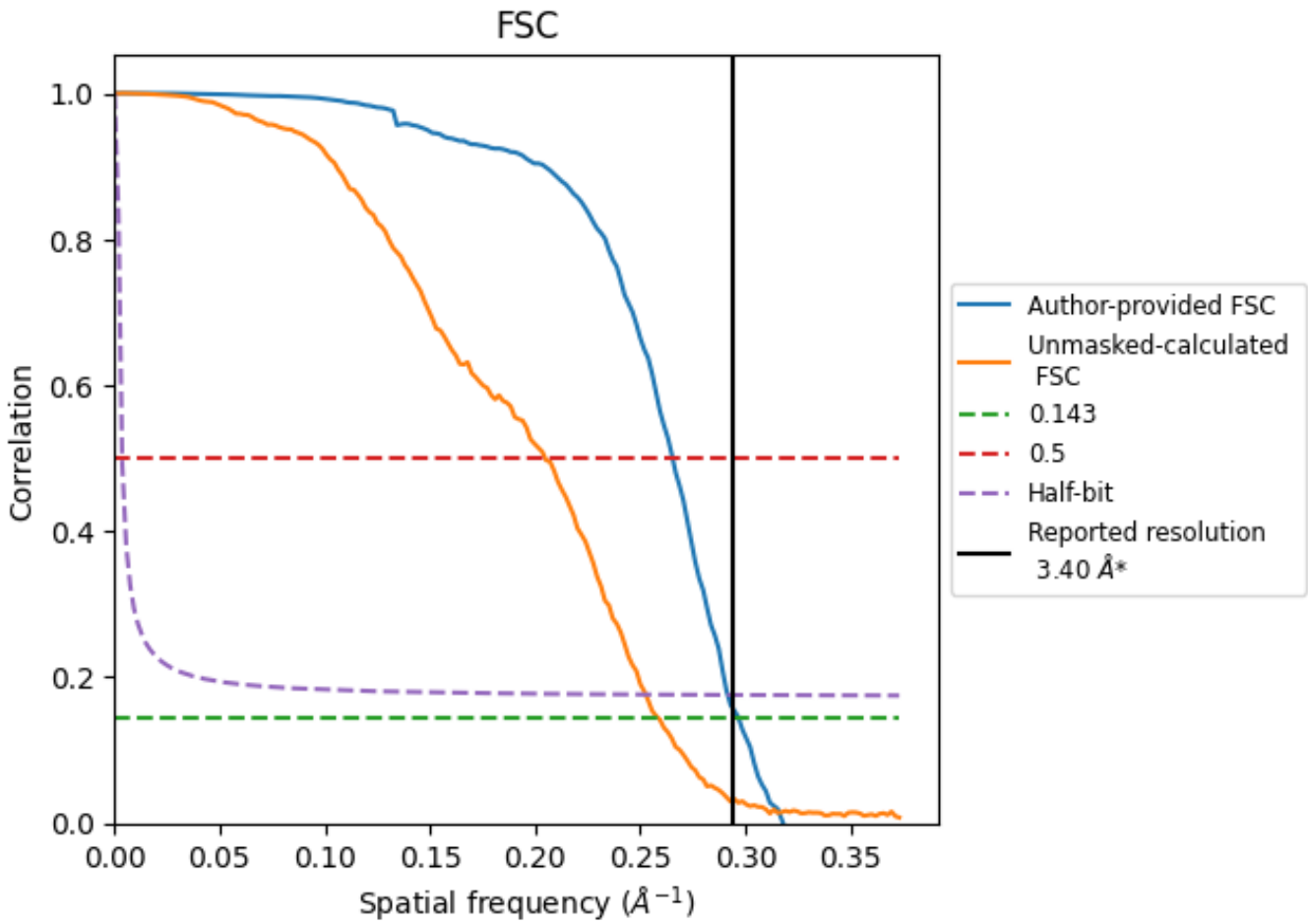


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

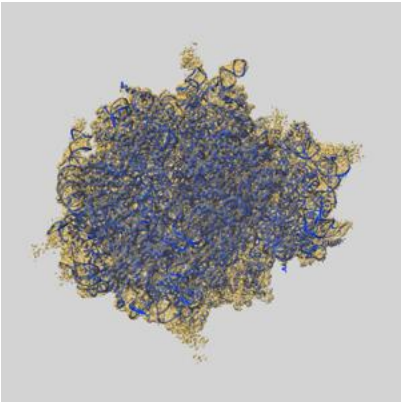
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	3.77	3.43
Unmasked-calculated*	3.86	4.89	3.96

*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 3.86 differs from the reported value 3.4 by more than 10 %

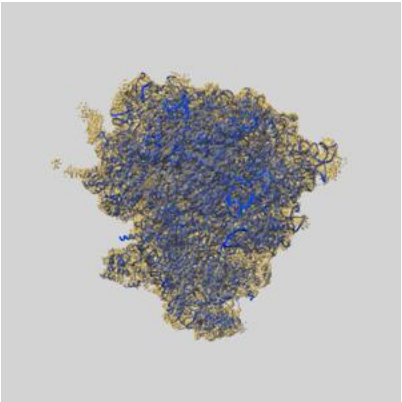
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9242 and PDB model 6MTE. Per-residue inclusion information can be found in section 3 on page 20.

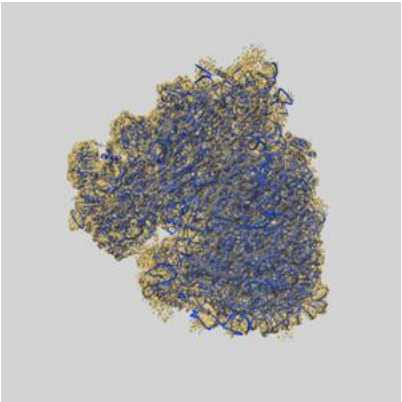
9.1 Map-model overlay (i)



X



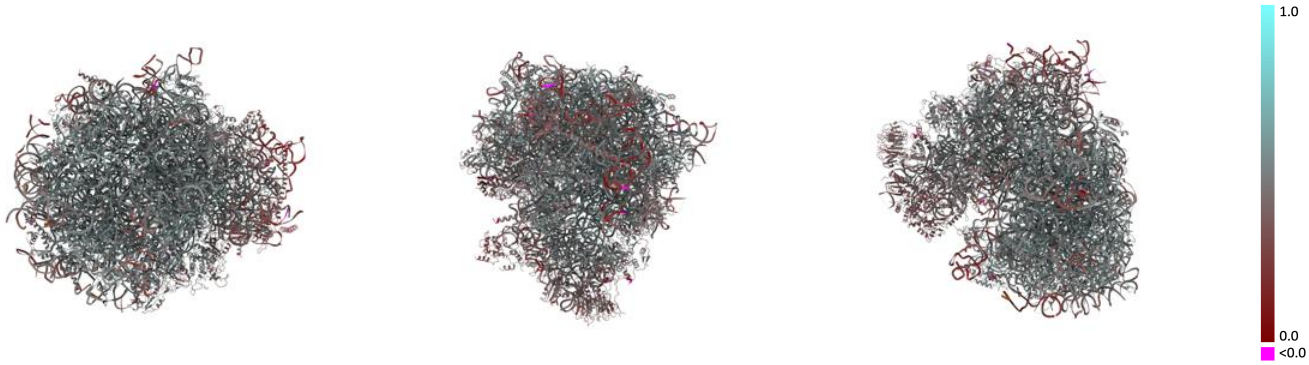
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

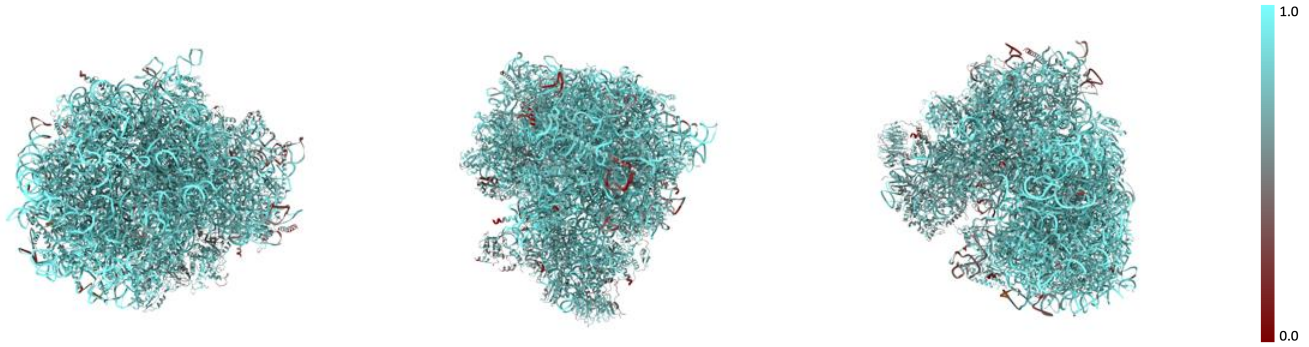
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

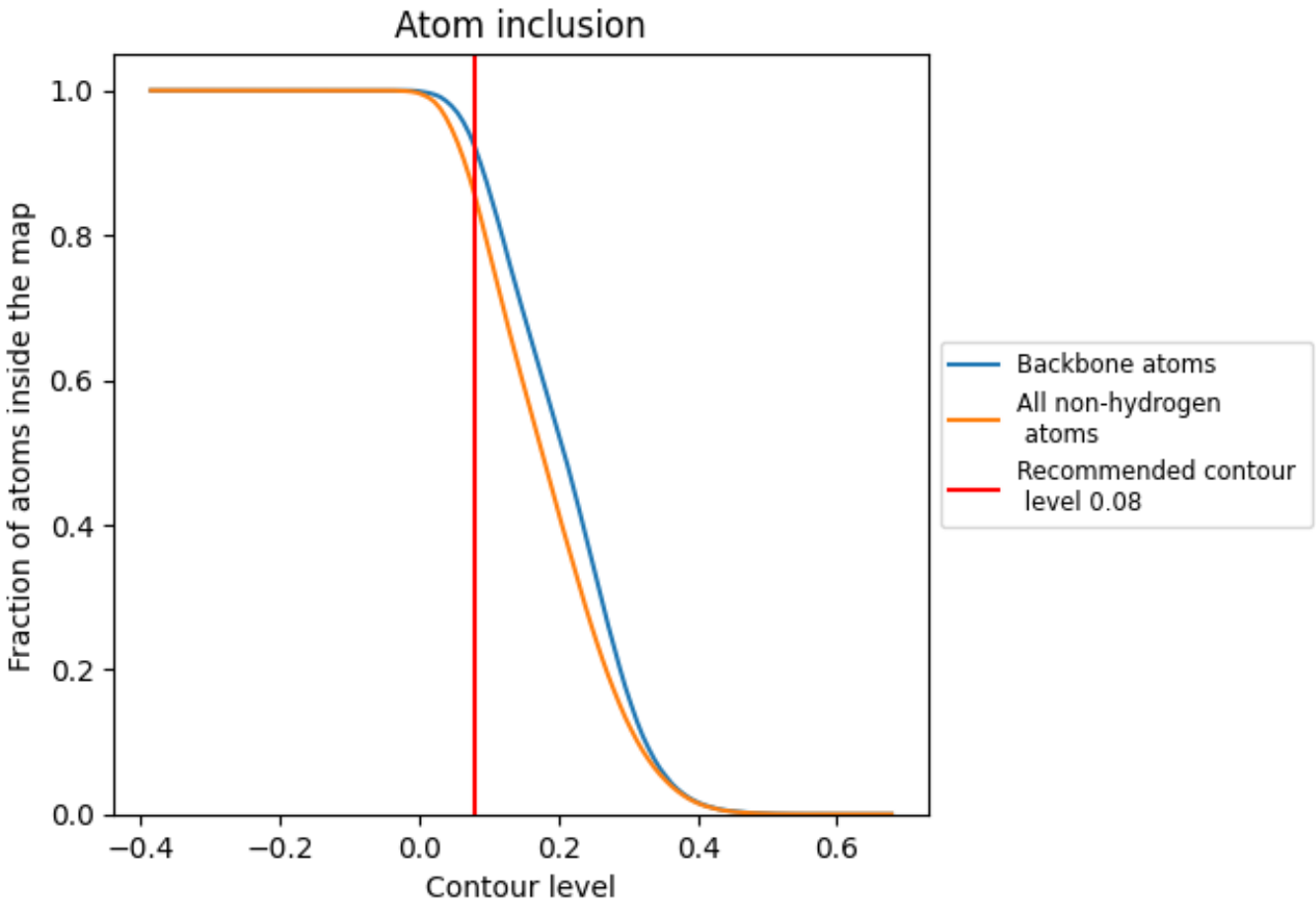
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8539	0.4760
5	0.9157	0.4870
7	0.9626	0.5120
8	0.9260	0.4850
9	0.8930	0.4420
A	0.8584	0.5490
AA	0.7837	0.4740
B	0.8837	0.5420
BB	0.7010	0.4310
C	0.8661	0.5310
CC	0.8254	0.5120
D	0.8465	0.5020
DD	0.7130	0.4450
E	0.8541	0.5080
EE	0.7990	0.4840
F	0.8583	0.5320
FF	0.6034	0.3480
G	0.7973	0.4890
GG	0.6663	0.3620
H	0.8512	0.5290
HH	0.7242	0.4390
I	0.8525	0.5330
II	0.7240	0.4290
J	0.8259	0.4880
JJ	0.8102	0.4880
KK	0.7509	0.4370
L	0.8286	0.5080
LL	0.7737	0.4820
M	0.8608	0.5280
MM	0.5280	0.2930
N	0.8914	0.5470
NN	0.7693	0.4710
O	0.8738	0.5320
OO	0.7356	0.4470
P	0.8558	0.5340

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Chain	Atom inclusion	Q-score
PP	0.6707	0.3650
Q	0.8593	0.5360
QQ	0.6822	0.3980
R	0.8140	0.5060
RR	0.6744	0.4170
S	0.8835	0.5440
SS	0.6524	0.3520
T	0.8361	0.5270
TT	0.6807	0.3710
U	0.8015	0.4710
UU	0.7158	0.4240
V	0.8539	0.5480
VV	0.8135	0.4980
W	0.6743	0.4520
WW	0.8446	0.5270
X	0.8245	0.5210
XX	0.8394	0.5340
Y	0.8442	0.5140
YY	0.7625	0.4410
Z	0.8462	0.5110
ZZ	0.5712	0.3140
a	0.8813	0.5420
aa	0.7647	0.4840
b	0.7374	0.4590
bb	0.7340	0.4710
c	0.8091	0.4910
cc	0.5723	0.3790
d	0.8320	0.5150
dd	0.8231	0.4670
e	0.8545	0.5450
ee	0.7441	0.4750
f	0.8907	0.5500
ff	0.5896	0.3200
g	0.8276	0.5230
gg	0.6550	0.3720
h	0.8325	0.5160
i	0.8178	0.4960
j	0.9036	0.5430
k	0.8025	0.4920
l	0.8431	0.5220
m	0.8657	0.5360
n	0.7569	0.5070

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Chain	Atom inclusion	Q-score
o	0.8397	0.5420
p	0.8041	0.5270
r	0.8777	0.5310
s	0.7502	0.4490
t	0.5360	0.3330
v	0.7431	0.4550
w	0.6215	0.4480