wwPDB EM Validation Summary Report (i)

Dec 16, 2024 – 10:13 PM EST

PDB ID	:	6MTD
EMDB ID	:	EMD-9240
Title	:	Rabbit 80S ribosome with eEF2 and SERBP1 (unrotated state with 40S head swivel)
Authors	:	Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.
Deposited on	:	2018-10-19
Resolution	:	3.30 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:

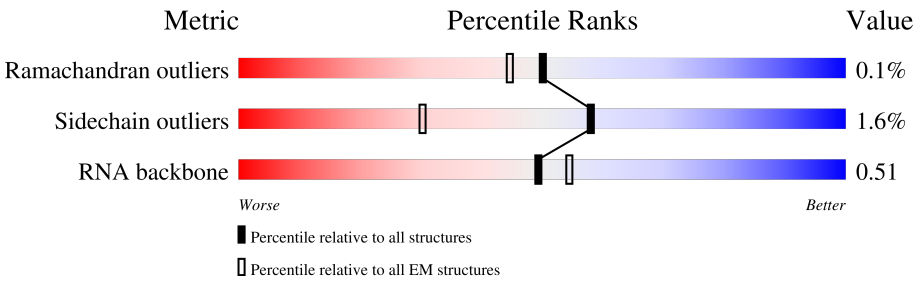
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	83% 15%
3	8	151	75% 21%
4	A	248	98%
5	B	394	98%
6	C	362	99%
7	D	293	99%
8	E	291	73% 26%

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Mol	Chain	Length	Quality of chain
9	F	225	100%
10	G	319	6%, 71%, 27%
11	H	190	97%
12	I	214	94%
13	J	170	99%
14	L	210	97%
15	M	138	99%
16	N	203	97%
17	O	199	99%
18	P	153	99%
19	Q	187	99%
20	R	180	6%, 99%
21	S	176	98%
22	T	159	100%
23	U	99	97%
24	V	131	98%
25	W	157	18%, 67%, 32%
26	X	118	100%
27	Y	134	99%
28	Z	135	97%
29	a	147	99%
30	b	245	42%, 58%
31	c	98	96%
32	d	107	99%
33	e	128	99%

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Mol	Chain	Length	Quality of chain
34	f	109	98%
35	g	114	5%, 98%
36	h	122	99%
37	i	102	98%
38	j	86	99%
39	k	69	100%
40	l	50	96%
41	m	52	96%
42	n	25	100%
43	o	103	98%
44	p	91	100%
45	r	124	97%
46	s	196	12%, 99%
47	t	153	52%, 95%, 5%
48	u	206	96%, 95%, 5%
49	v	839	30%, 96%
50	w	26	65%, 92%, 8%
51	9	1698	5%, 70%, 26%
52	AA	217	5%, 98%
53	BB	213	99%
54	CC	221	100%
55	DD	228	7%, 96%
56	EE	262	98%
57	FF	204	86%, 9%
58	GG	237	11%, 99%

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Mol	Chain	Length	Quality of chain
59	HH	194	9% 94% 5%
60	II	206	7% 100%
61	JJ	185	98%
62	KK	96	5% 98%
63	LL	158	6% 89% 9%
64	MM	117	40% 96%
65	NN	149	99%
66	OO	136	7% 99%
67	PP	120	9% 95% 5%
68	QQ	142	6% 97%
69	RR	132	8% 98%
70	SS	144	7% 97%
71	TT	141	99%
72	UU	100	6% 99%
73	VV	83	98%
74	WW	129	99%
75	XX	141	97%
76	YY	124	6% 99%
77	ZZ	75	9% 97%
78	aa	101	99%
79	bb	83	6% 96%
80	cc	62	8% 98%
81	dd	55	100%
82	ee	55	15% 96%
83	ff	68	35% 99%

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Mol	Chain	Length	Quality of chain
84	gg	313	9% 99%

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 222072 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	106	860	538	174	144	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 eL11.

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 uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	u	206	1654	1058	297	291	8	0	0

- Molecule 49 is a protein called eEF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	v	839	6544	4162	1122	1216	44	0	0

- Molecule 50 is a protein called SERBP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	w	26	216	129	43	44	0	0

- Molecule 51 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	9	1698	36263	16190	6509	11867	1697	0	0

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	PP	120	997	635	187	168	7	0	0

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
85	5	198	198	198	0
85	7	7	7	7	0
85	8	6	6	6	0
85	A	1	1	1	0
85	B	1	1	1	0
85	P	1	1	1	0
85	V	1	1	1	0
85	a	1	1	1	0
85	g	1	1	1	0
85	j	1	1	1	0
85	v	1	1	1	0
85	9	74	74	74	0
85	SS	2	2	2	0
85	TT	1	1	1	0
85	dd	1	1	1	0

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
86	g	1	1	1	0
86	j	1	1	1	0

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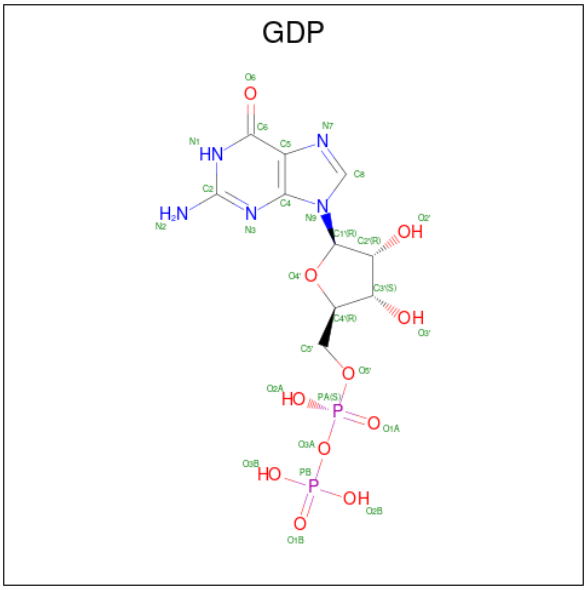
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
86	m	1	1	1	0
86	o	1	1	1	0
86	p	1	1	1	0
86	aa	1	1	1	0
86	dd	1	1	1	0
86	ff	1	1	1	0

- Molecule 87 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



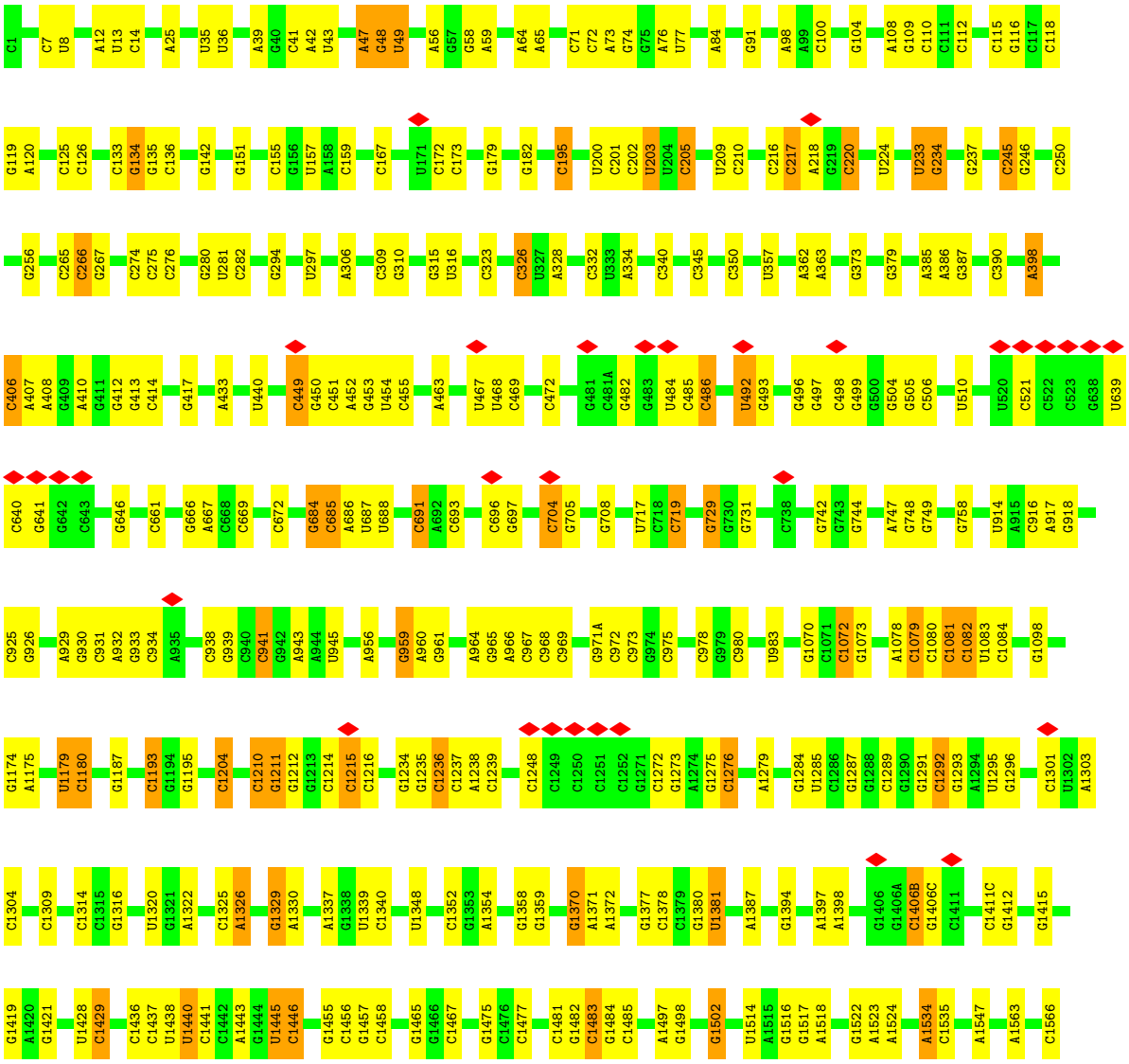
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
87	v	1	28	10	5	11	2	0

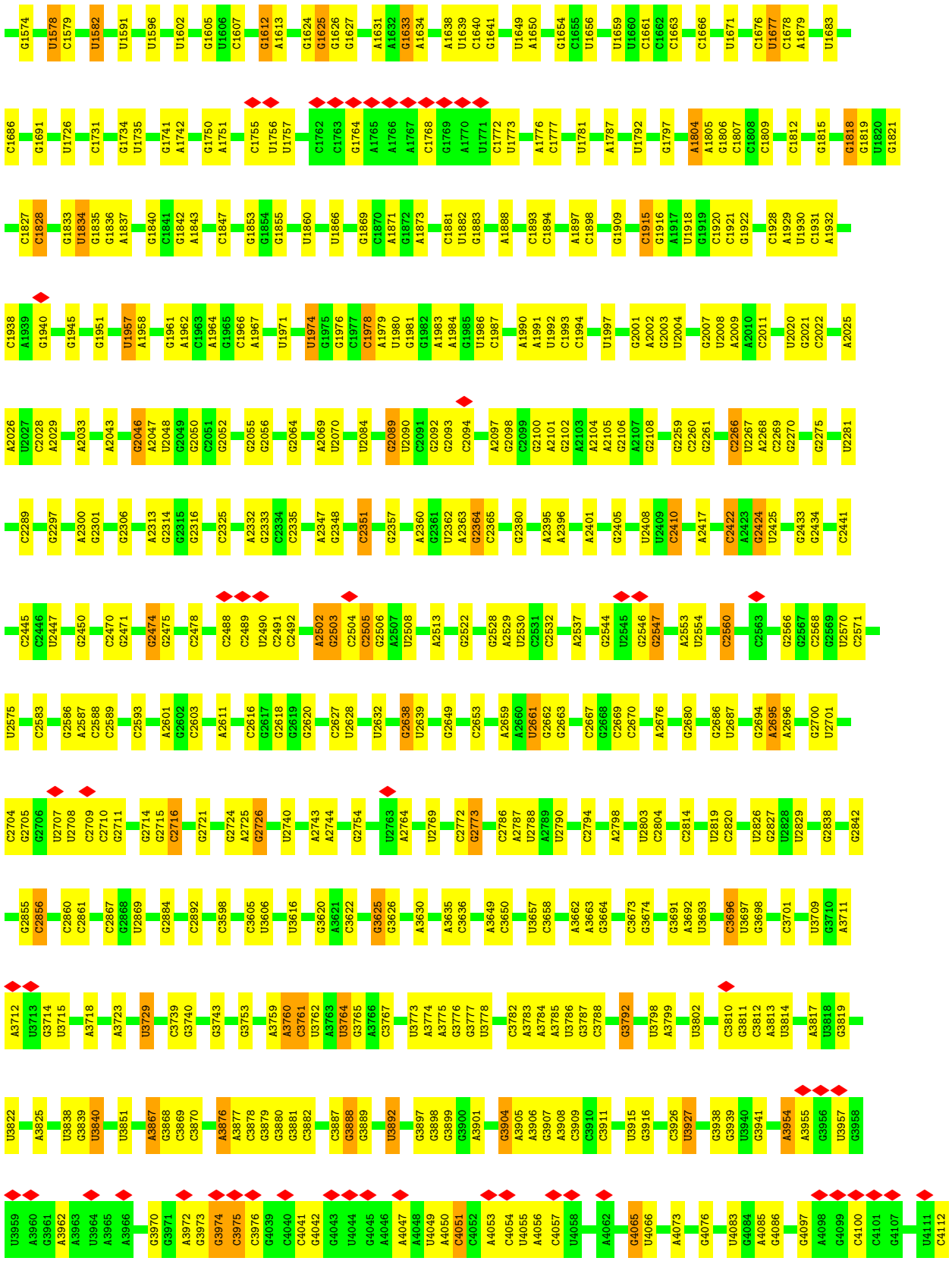
3 Residue-property plots (i)

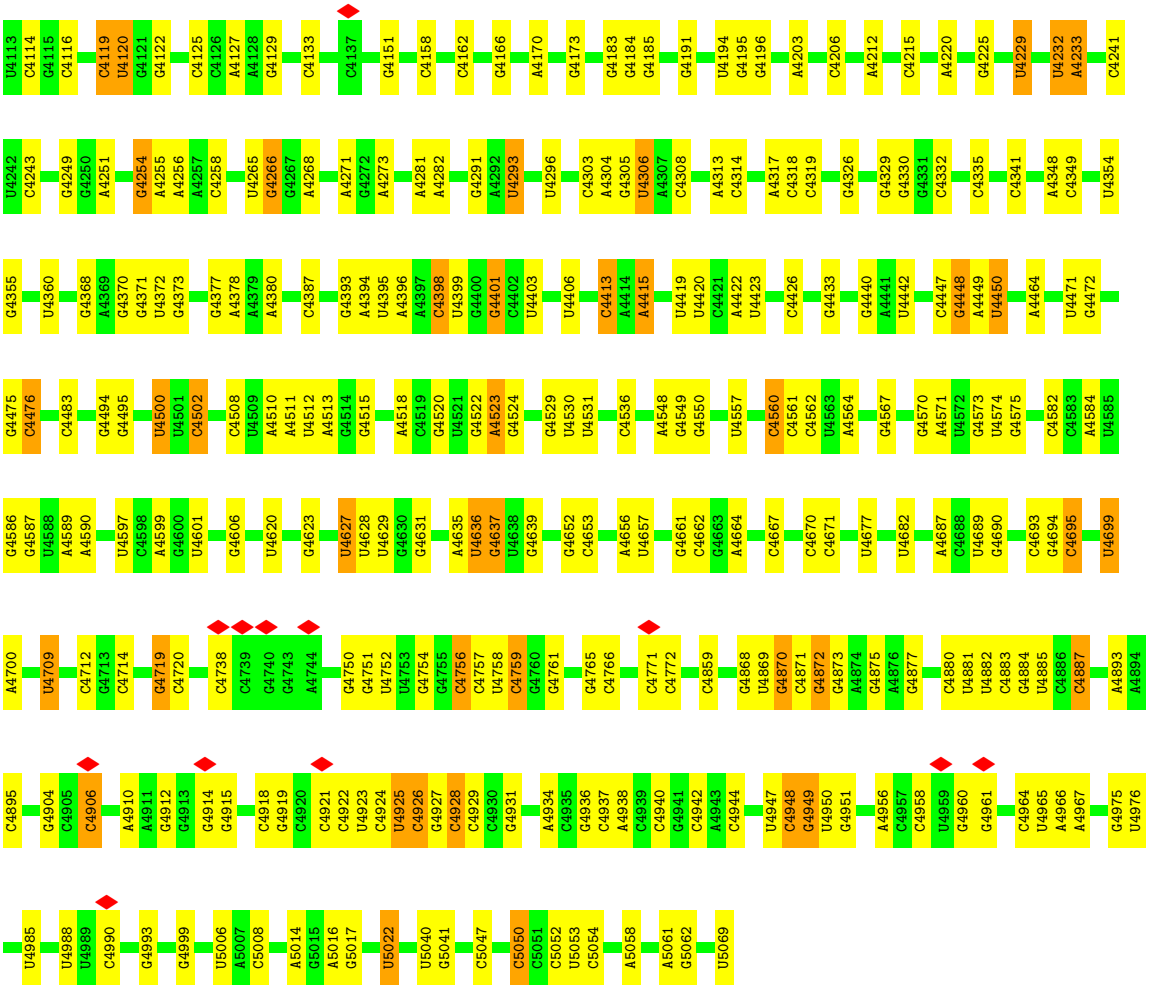
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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:

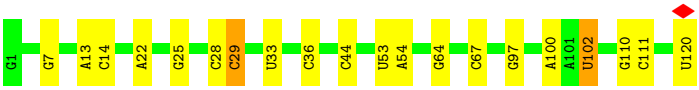



G1574 U1578 C1579 U1582 U1591 U1596 U1602 G1605 U1606 C1607 G1612 A1613 G1624 G1625 G1626 G1627 A1631 A1632 G1633 A1634 A1638 U1639 C1640 G1641 U1649 A1650 G1654 C1655 U1656 U1659 U1660 C1661 C1662 C1663 C1666 U1671 C1676 U1677 C1678 A1679 U1683
C1686 G1691 U1726 C1731 G1734 U1735 G1741 A1742 G1750 A1751 C1755 U1756 U1757 C1762 C1763 G1764 A1765 A1766 A1767 C1768 G1769 A1770 U1771 C1772 U1773 A1776 C1777 U1781 A1787 U1792 G1797 A1804 A1805 G1806 C1807 C1808 C1809 C1812 G1815 G1818 G1819 U1820 G1821
C1827 C1828 G1833 U1834 G1835 G1836 A1837 G1840 C1841 G1842 A1843 C1847 G1853 G1854 G1855 U1860 U1866 G1869 C1870 A1871 G1872 A1873 C1881 U1882 G1883 A1888 C1893 C1894 A1897 C1898 G1909 C1915 G1916 A1917 U1918 G1919 C1920 C1921 G1922 C1928 A1929 U1930 C1931 A1932
C1938 A1939 G1940 G1945 G1951 U1957 A1958 G1961 A1962 C1963 A1964 G1965 C1966 A1967 U1971 U1974 G1975 G1976 C1977 C1978 A1979 U1980 G1981 G1982 A1983 A1984 G1985 U1986 C1987 A1990 A1991 U1992 C1993 C1994 U1997 G2001 A2002 G2003 U2004 G2007 U2008 A2009 A2010 C2011 U2020 G2021 C2022 A2025
A2026 U2027 C2028 A2029 A2033 A2043 G2046 A2047 U2048 G2049 G2050 C2051 G2052 G2055 G2056 G2064 A2069 U2070 U2084 G2089 U2090 C2091 G2092 G2093 C2094 A2097 G2098 C2099 C2100 A2101 G2102 A2103 A2104 A2105 G2106 A2107 G2108 G2259 C2260 G2261 C2266 U2267 A2268 C2269 G2270 G2275 U2281
C2289 G2297 A2300 G2301 G2306 A2313 G2314 G2315 G2316 C2325 A2332 G2333 C2334 C2335 A2347 G2348 C2351 G2357 A2360 G2361 U2362 A2363 G2364 C2365 G2380 A2395 A2396 A2401 G2405 U2408 U2409 C2410 A2417 C2422 A2423 G2424 U2425 G2433 G2434 C2441
C2445 C2446 U2447 G2450 C2470 G2471 G2474 G2475 C2478 C2488 C2489 U2490 C2491 C2492 A2502 G2503 C2504 C2505 G2506 A2507 U2508 A2513 G2522 G2528 A2529 U2530 C2531 C2532 A2537 G2544 U2545 G2546 G2547 A2553 U2554 C2560 C2563 G2566 G2567 C2568 G2569 U2570 C2571
U2575 C2583 G2586 A2587 C2588 C2589 C2593 A2601 G2602 C2603 A2611 C2616 G2617 G2618 C2619 G2620 C2627 U2628 U2632 G2638 U2639 G2649 C2653 A2659 A2660 U2661 G2662 G2663 C2667 G2668 C2669 C2670 A2676 G2680 G2686 U2687 G2694 A2695 A2696 G2700 U2701
C2704 G2705 G2706 U2707 U2708 C2709 C2710 G2711 G2714 G2715 C2716 G2721 G2724 A2725 G2726 U2740 A2743 A2744 G2754 U2763 A2764 U2769 C2772 G2773 C2786 A2787 U2788 A2789 U2790 C2794 A2798 U2803 C2804 C2814 U2819 C2820 U2826 G2827 U2828 U2829 G2838 G2842
G2855 C2856 C2860 C2861 C2867 G2868 U2869 G2884 C2892 C3598 C3605 U3606 U3616 G3620 A3621 C3622 G3625 G3626 A3630 A3635 C3636 A3649 C3650 U3657 C3658 A3662 A3663 G3664 C3673 G3674 G3691 A3692 U3693 C3696 U3697 G3698 C3701 U3709 G3710 A3711
A3712 U3713 G3714 U3715 A3718 A3723 U3729 C3739 G3740 G3743 G3753 A3759 A3760 C3761 U3762 A3763 U3764 G3765 A3766 C3767 U3773 A3774 A3775 G3776 G3777 U3778 C3782 A3783 A3784 A3785 U3786 G3787 C3788 G3792 U3798 A3799 U3802 C3810 G3811 C3812 A3813 U3814 A3817 U3818 G3819
U3822 A3825 U3838 G3839 U3840 U3851 A3867 G3868 C3869 C3870 A3876 A3877 C3878 G3879 G3880 G3881 C3882 C3887 G3888 G3889 U3892 G3897 G3898 G3899 G3900 A3901 G3904 A3905 A3906 G3907 A3908 C3909 C3910 C3911 U3915 G3916 C3926 U3927 G3938 G3939 U3940 G3941 A3954 A3955 G3956 U3957 G3958
U3959 A3960 G3961 A3962 A3963 U3964 A3965 A3966 G3970 G3971 A3972 G3973 G3974 C3975 C3976 G4039 C4040 C4041 G4042 G4043 U4044 G4045 A4046 A4047 A4048 U4049 A4050 C4051 C4052 A4053 C4054 U4055 A4056 C4057 U4058 A4062 G4065 U4066 A4073 G4076 U4083 G4084 A4085 G4086 G4097 A4098 G4099 C4100 C4101 G4107 U4111 C4112



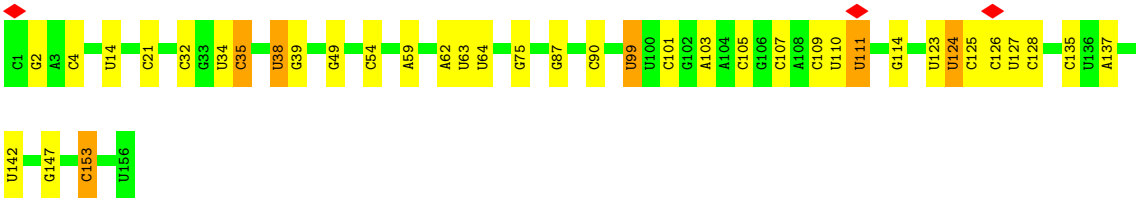
- Molecule 2: 5S rRNA

Chain 7: 83% 15%



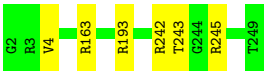
- Molecule 3: 5.8S rRNA

Chain 8: 75% 21%



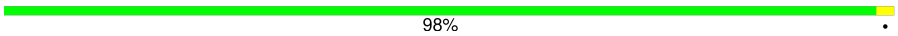
- Molecule 4: uL2

Chain A: 98%



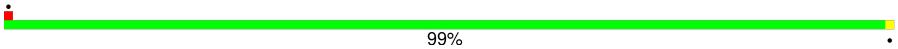
• Molecule 5: uL3

Chain B:



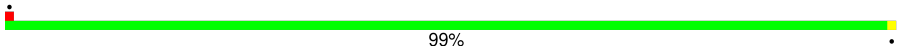
• Molecule 6: uL4

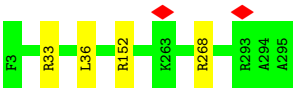
Chain C:



• Molecule 7: uL18

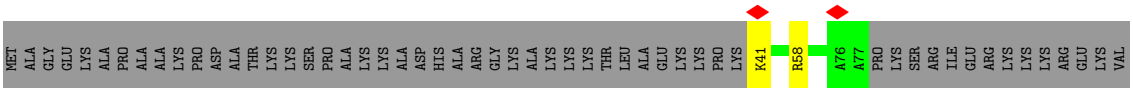
Chain D:

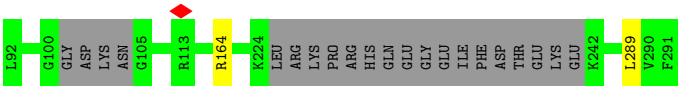




• Molecule 8: eL6

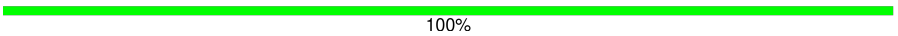
Chain E:





• Molecule 9: uL30

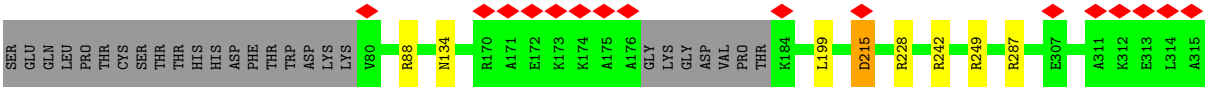
Chain F:

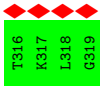


There are no outlier residues recorded for this chain.

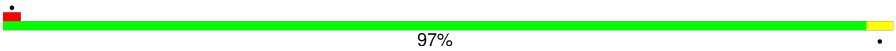
• Molecule 10: eL8

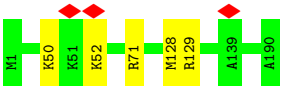
Chain G:



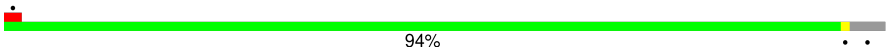


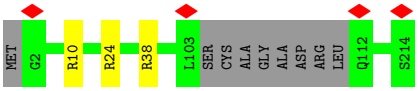
• Molecule 11: uL6

Chain H: 

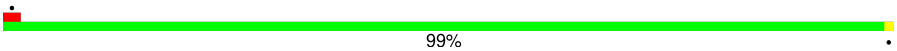


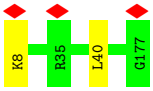
• Molecule 12: uL16

Chain I: 

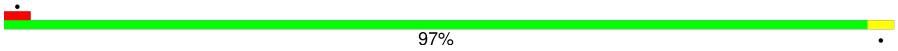


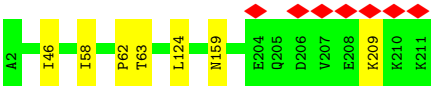
• Molecule 13: uL5

Chain J: 

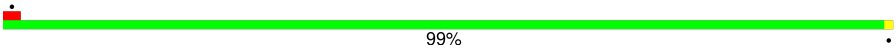


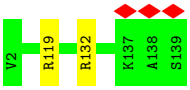
• Molecule 14: eL13

Chain L: 

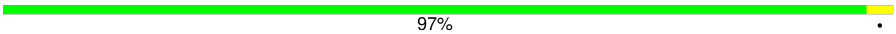


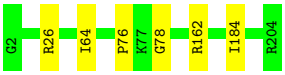
• Molecule 15: eL14

Chain M: 

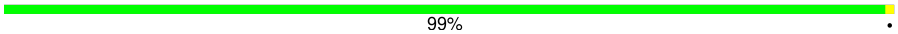


• Molecule 16: eL15

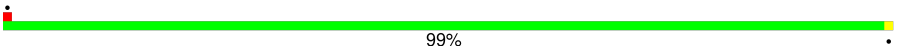
Chain N: 

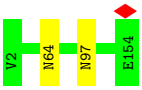


• Molecule 17: uL13

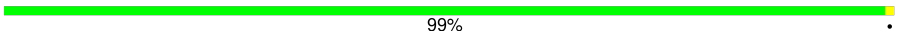
Chain O: 

• Molecule 18: uL22

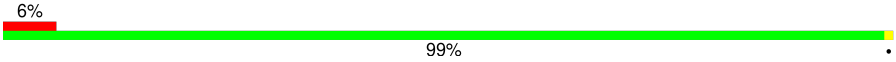
Chain P: 

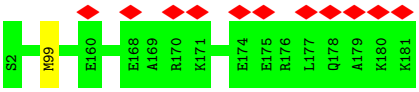


• Molecule 19: eL18

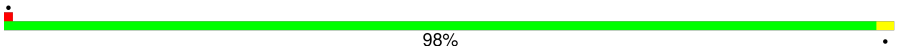
Chain Q: 

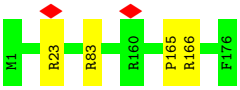
• Molecule 20: eL19

Chain R: 

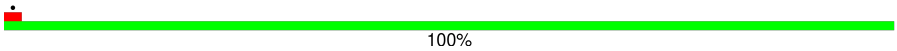


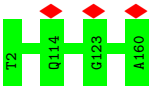
• Molecule 21: eL20

Chain S: 

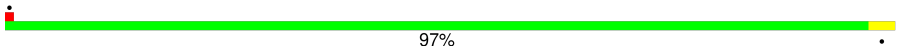


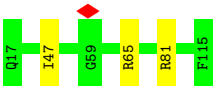
• Molecule 22: eL21

Chain T: 

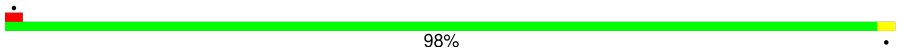


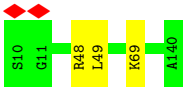
• Molecule 23: eL22

Chain U: 



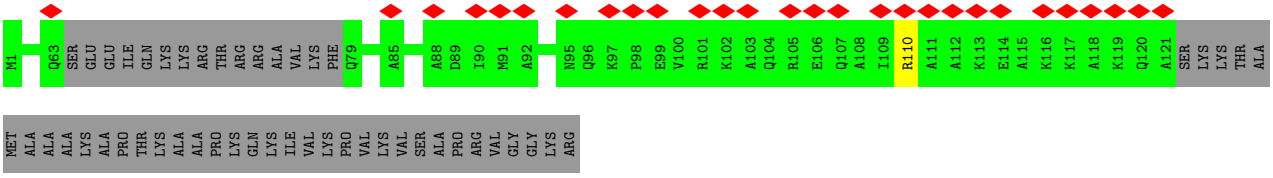
• Molecule 24: uL14

Chain V: 



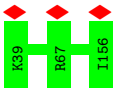
• Molecule 25: eL24

Chain W:



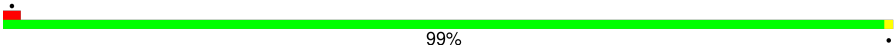
• Molecule 26: uL23

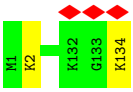
Chain X:



• Molecule 27: uL24

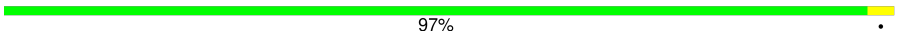
Chain Y:





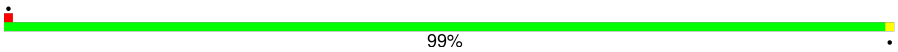
• Molecule 28: eL27

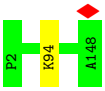
Chain Z:



• Molecule 29: uL15

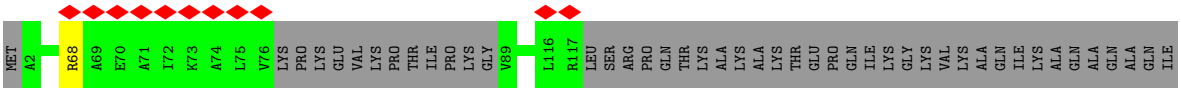
Chain a:





• Molecule 30: eL29

Chain b:

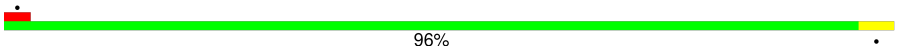


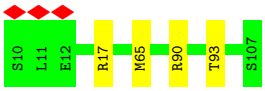
LYS SER LYS GLY LYS GLY LYS ALA GLN ALA GLU THR LYS PRO LYS ALA GLN ALA GLU THR LYS PRO LYS ALA GLN ALA GLN ALA ALA LYS PRO LYS ALA GLN ALA GLN GLY LYS PRO LYS ALA GLN ALA GLN GLY LYS PRO LYS ALA GLN ALA GLN ALA LYS PRO LYS ALA GLN ALA GLN ALA GLN GLN

LYS PRO LYS ALA GLN ALA GLN THR LYS PRO LYS ALA GLN ALA THR PRO ALA ALA PRO VAL PRO ALA GLN ALA PRO PRO LYS GLY ALA GLN PRO PRO ALA LYS ALA PRO

- Molecule 31: eL30

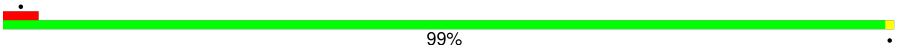
Chain c:

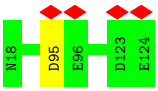




- Molecule 32: eL31

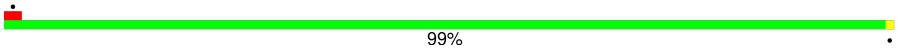
Chain d:

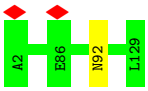




- Molecule 33: eL32

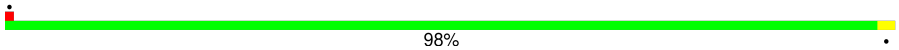
Chain e:





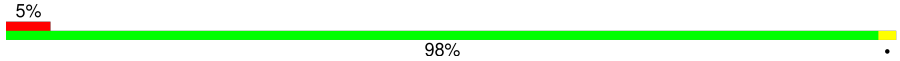
- Molecule 34: eL33

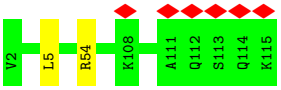
Chain f:



- Molecule 35: eL34

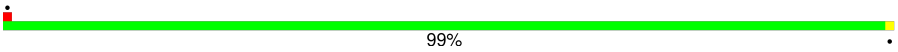
Chain g:

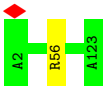




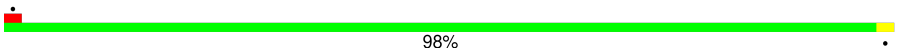
- Molecule 36: uL29

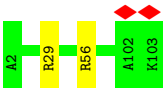
Chain h:



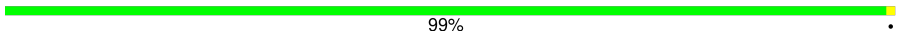


- Molecule 37: eL36

Chain i: 

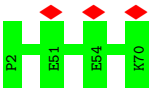


• Molecule 38: eL37

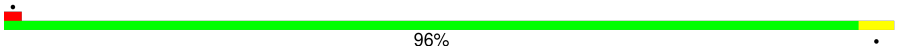
Chain j: 

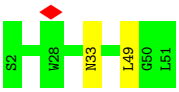
• Molecule 39: eL38

Chain k:

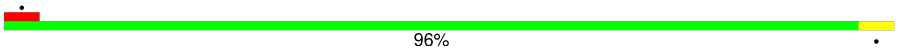


• Molecule 40: eL39

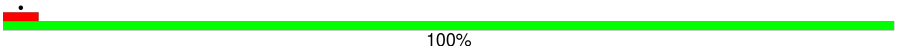
Chain l: 



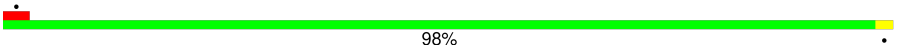
• Molecule 41: eL40

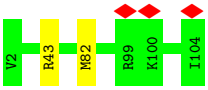
Chain m: 

• Molecule 42: eL41

Chain n: 

• Molecule 43: eL42

Chain o: 



- Molecule 44: eL43

Chain p: 100%

A2 D91 Q92

- Molecule 45: el28

Chain r: 97%

S2 L17 L106 R107 R119 M125

- Molecule 46: uL10

Chain s: 12% 99%

D5 R6 F28 R48 G49 E70 R83 K92 E93 D94 L95 D100 A104 A109 C119 E120 G129 E133 R149 E153 K162 T163 G164 D165 S197 I198 Y199 N200

- Molecule 47: eL11

Chain t: 52% 95% 5%

E9 I10 K11 V12 V13 Y14 T18 G19 G20 E21 V22 G23 A24 T25 S26 A27 L28 A29 P30 K31 I32 G33 P34 L35 G36 L37 S38 P39 K40 K41 V42 G43 D44 D45 I46 A47 K48 A49 T50 G51 D52 W53 K54 G55 L56 R57 I58 K61 L62 T63 I64 Q65 N66 R67 Q68 A69 Q70 I71

E72 S78 L85 K86 E87 R90 D91 R92 K93 K94 Q95 K96 N97 I98 K99 H100 S101 G102 N103 R114 R117 H118 R119 S120 L121 L125 G140 C141 G145 P148 H149 N156 E161

- Molecule 48: uL1

Chain u: 96% 95% 5%

V5 S6 R7 D8 T9 L10 Y11 E12 A13 V14 R15 E16 V17 L18 H19 G20 N21 Q22 R23 K24 R25 R26 K27 F28 L29 E30 T31 V32 E33 L34 Q35 T36 S37 L38 K39 N40 Y41 D42 P43 Q44 K45 D46 K47 R48 F49 S50 G51 T52 V53 R54 L55 K56 S57 T58 P59 R60 P61 K62 F63 S64

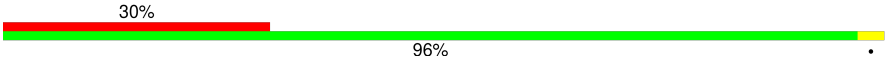
V65 C66 V67 L68 G69 D70 Q71 Q72 H73 C74 D75 E76 A77 K78 A79 V80 D81 I82 P83 H84 M85 D86 I87 E88 A89 L90 K91 K92 L93 N94 K95 N96 K97 K98 L99 V100 K101 K102 L103 A104 K105 K106 Y107 D108 A109 F110 L111 A112 S113 E114 S115 L116 I117 K118 Q119 I120 P121 R122 I123 L124

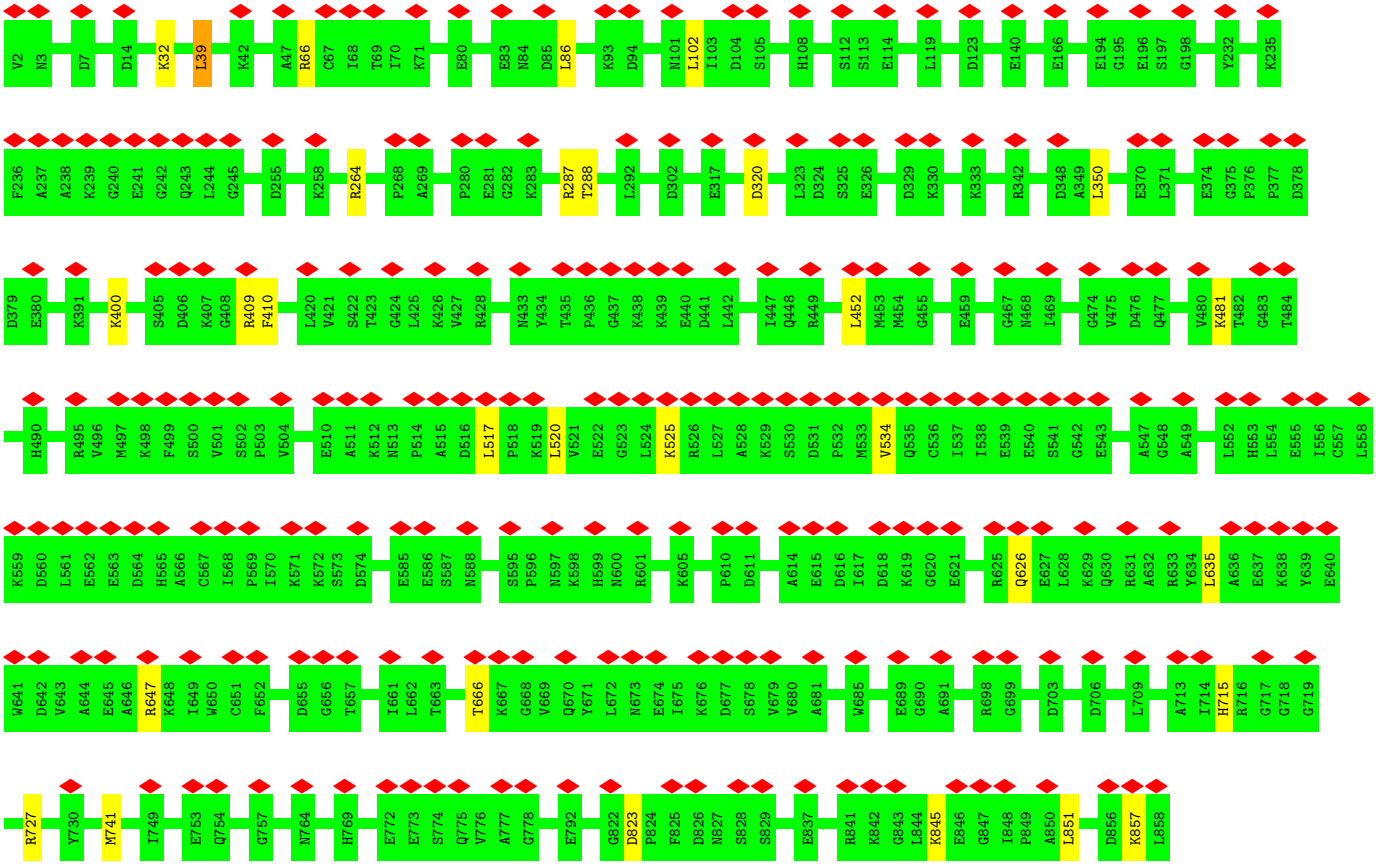
G125 P126 G127 L128 N129 K130 A131 G132 K133 F134 P135 S136 L137 L138 T139 H140 N141 E142 N143 M144 V145 A146 K147 V148 D149 E150 V151 K152 S153 T154 I155 K156 F157 Q158 M159 K160 K161 V162 L163 C164 L165 A166 V167 A168 V169 G170 H171 V172 K173 M174 T175 D176 D177 E178 L179 V180 Y181 N182 I183 H184

L185 A186 V187 N188 F189 L190 V191 S192 L193 L194 K195 K196 N197 W198 Q199 N200 V201 R202 A203 L204 Y205 I206 K207 M210

- Molecule 49: eEF2

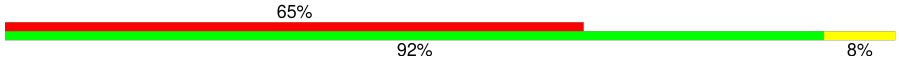
Chain v:

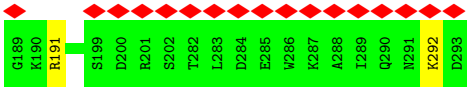




- Molecule 50: SERBP1

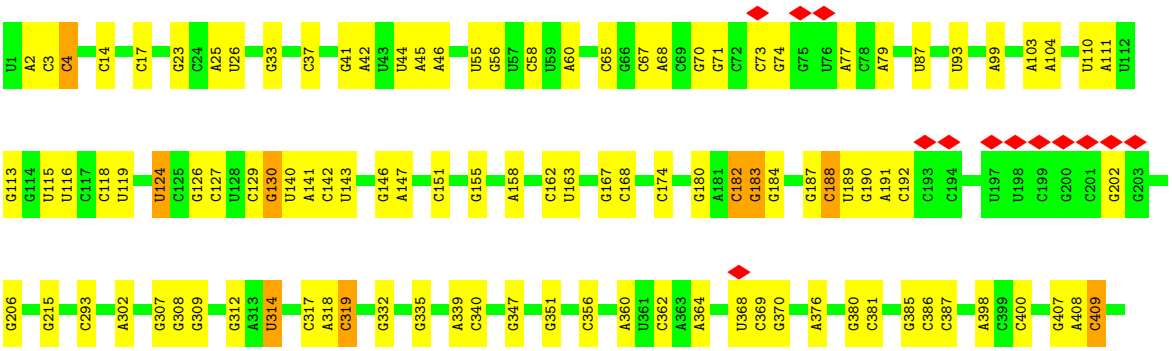
Chain w:

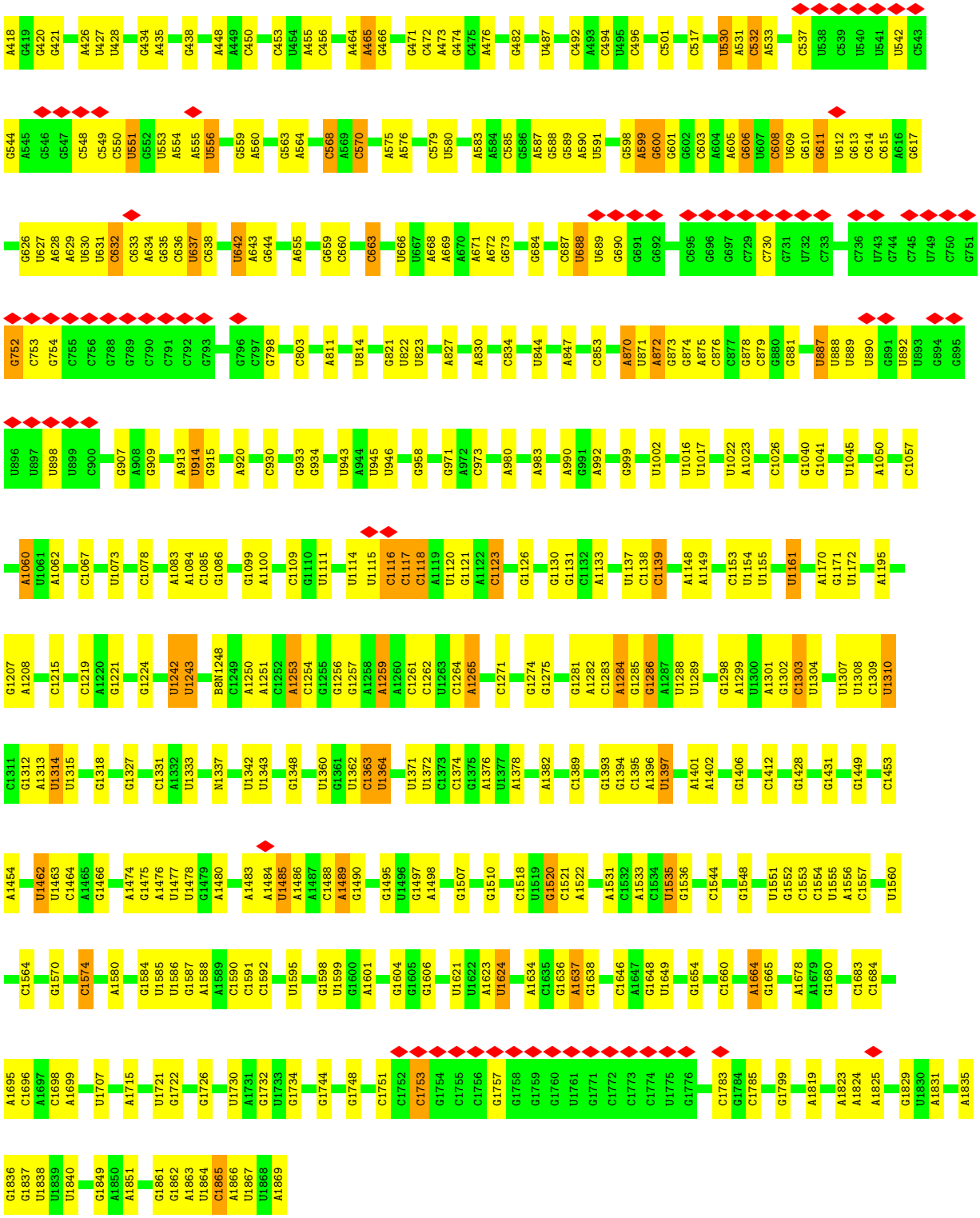




- Molecule 51: 18S rRNA

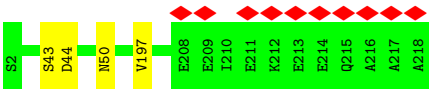
Chain 9:





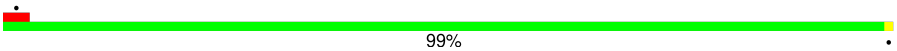
- Molecule 52: uS2

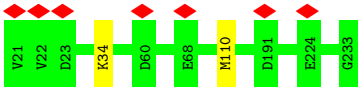
Chain AA: 5% 98%



- Molecule 53: eS1

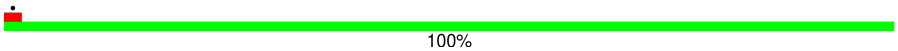
Chain BB:





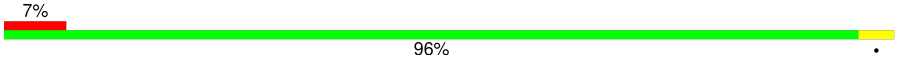
- Molecule 54: uS5

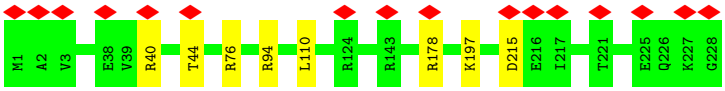
Chain CC:



- Molecule 55: uS3

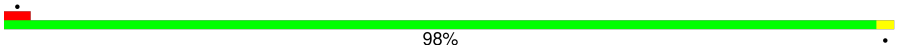
Chain DD:

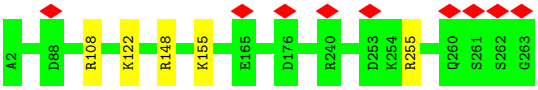




- Molecule 56: eS4

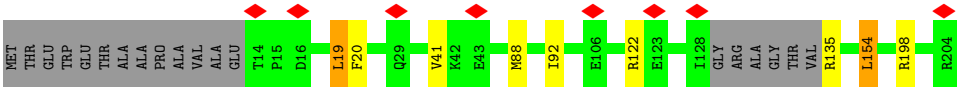
Chain EE:





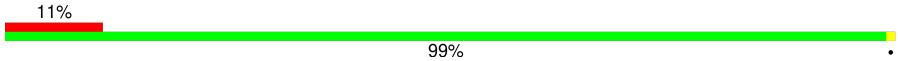
- Molecule 57: uS7

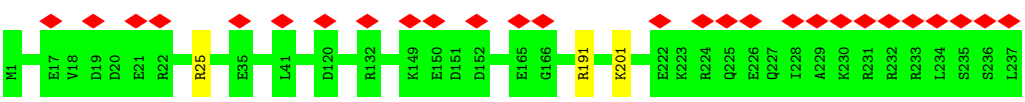
Chain FF:



- Molecule 58: eS6

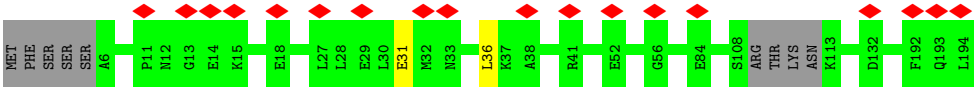
Chain GG:





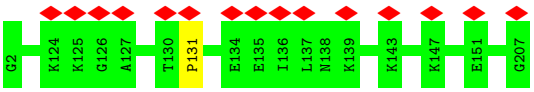
- Molecule 59: eS7

Chain HH: 9% 94% 5%



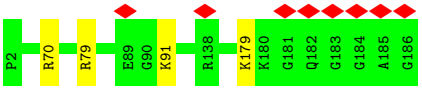
- Molecule 60: eS8

Chain II: 7% 100%



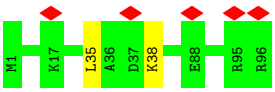
- Molecule 61: uS4

Chain JJ: 98%



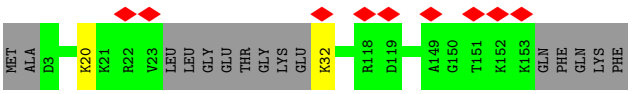
- Molecule 62: eS10

Chain KK: 5% 98%



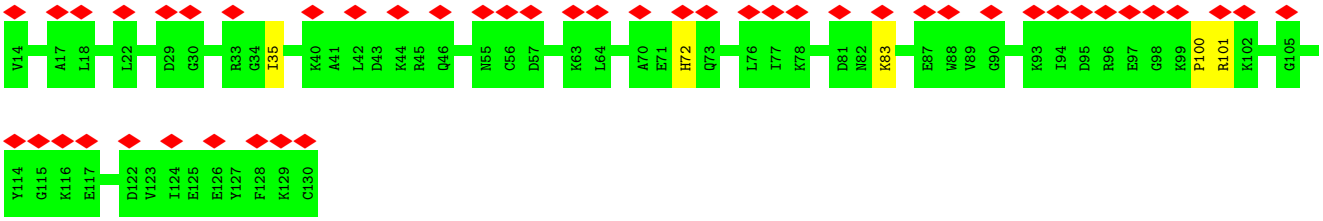
- Molecule 63: uS17

Chain LL: 6% 89% 9%



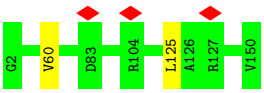
- Molecule 64: eS12

Chain MM: 40% 96%



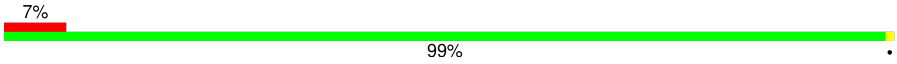
- Molecule 65: uS15

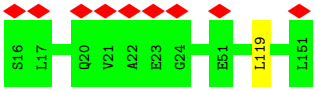
Chain NN: 99%



- Molecule 66: uS11

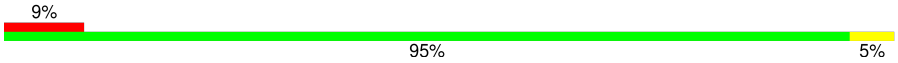
Chain OO:

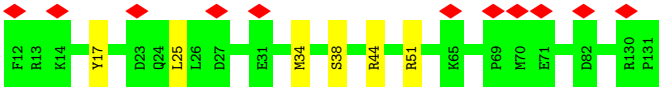




- Molecule 67: uS19

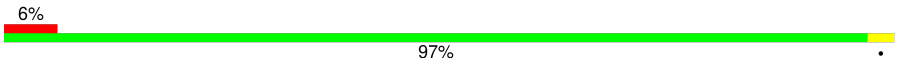
Chain PP:

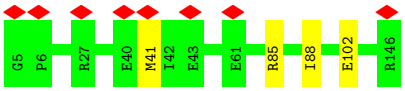




- Molecule 68: uS9

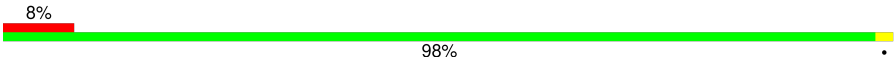
Chain QQ:

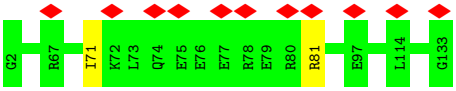




- Molecule 69: eS17

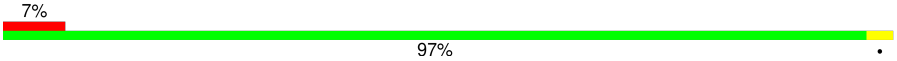
Chain RR:

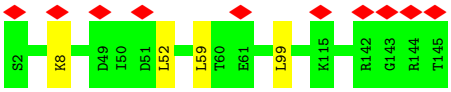




- Molecule 70: uS13

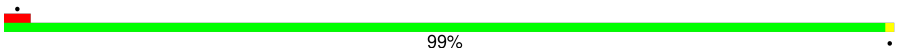
Chain SS:

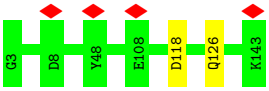




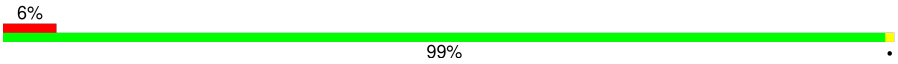
- Molecule 71: eS19

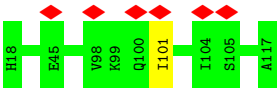
Chain TT:



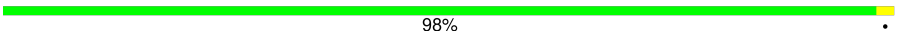


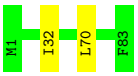
- Molecule 72: uS10

Chain UU: 

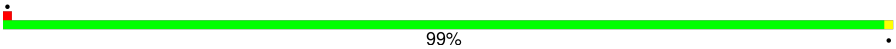


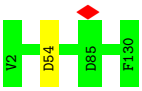
- Molecule 73: eS21

Chain VV: 

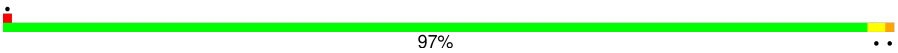


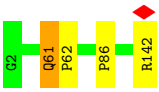
- Molecule 74: uS8

Chain WW: 

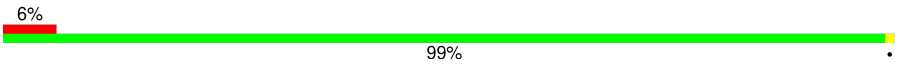


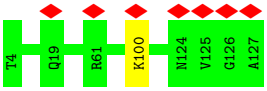
- Molecule 75: uS12

Chain XX: 

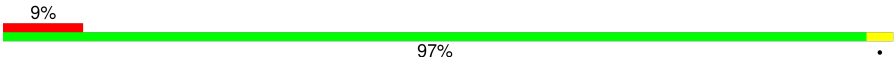


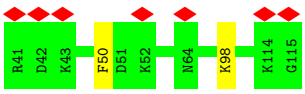
- Molecule 76: eS24

Chain YY: 

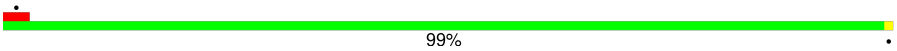


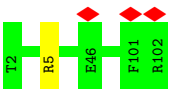
- Molecule 77: eS25

Chain ZZ: 



- Molecule 78: eS26

Chain aa: 

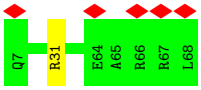


- Molecule 79: eS27

Chain bb: 6% 96%

• Molecule 80: eS28

Chain cc: 8% 98%



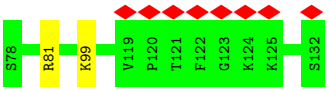
• Molecule 81: uS14

Chain dd: 100%

There are no outlier residues recorded for this chain.

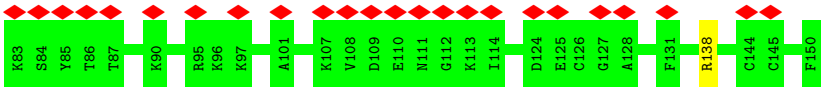
• Molecule 82: eS30

Chain ee: 15% 96%



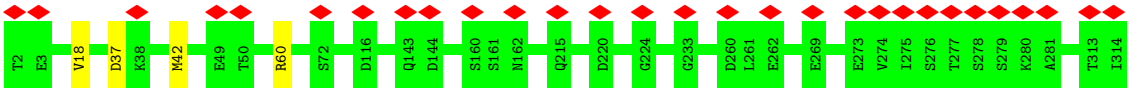
• Molecule 83: eS31

Chain ff: 35% 99%



• Molecule 84: RACK1

Chain gg: 9% 99%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146801	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	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.732	Depositor
Minimum map value	-0.379	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.09	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: MG, B9H, OMC, B8T, 5MU, I4U, B8W, E7G, P4U, M7A, UR3, OMU, 2MG, 1MA, 4AC, DDE, B8N, 7MG, B8H, 5MC, E6G, 6MZ, B9B, BGH, MHG, PSU, A2M, GDP, ZN, B8K, OMG, MLZ, B8Q, P7G

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	0.75	0/83821	1.14	578/130598 (0.4%)
2	7	0.73	0/2858	1.08	13/4455 (0.3%)
3	8	0.73	0/3559	1.15	24/5543 (0.4%)
4	A	0.48	0/1936	0.63	0/2596
5	B	0.52	0/3240	0.65	1/4339 (0.0%)
6	C	0.44	0/2927	0.58	0/3932
7	D	0.42	0/2437	0.57	0/3264
8	E	0.38	0/1762	0.60	1/2362 (0.0%)
9	F	0.46	0/1911	0.60	0/2549
10	G	0.42	0/1910	0.64	1/2569 (0.0%)
11	H	0.46	0/1535	0.67	0/2063
12	I	0.44	0/1702	0.58	0/2272
13	J	0.40	0/1385	0.65	1/1852 (0.1%)
14	L	0.42	0/1733	0.61	0/2316
15	M	0.47	0/1158	0.61	0/1547
16	N	0.51	0/1746	0.62	0/2338
17	O	0.49	0/1662	0.63	0/2222
18	P	0.46	0/1268	0.63	0/1700
19	Q	0.46	0/1539	0.65	0/2054
20	R	0.42	0/1524	0.66	2/2013 (0.1%)
21	S	0.49	0/1501	0.61	0/2012
22	T	0.46	0/1326	0.59	0/1770
23	U	0.41	0/823	0.67	0/1104
24	V	0.48	0/993	0.66	1/1332 (0.1%)
25	W	0.45	0/873	0.58	0/1158
26	X	0.40	0/984	0.59	0/1323
27	Y	0.42	0/1132	0.59	0/1504
28	Z	0.44	0/1130	0.59	0/1507
29	a	0.49	0/1191	0.59	0/1590
30	b	0.33	0/861	0.55	0/1138

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	c	0.45	0/771	0.62	0/1034
32	d	0.45	0/903	0.65	0/1216
33	e	0.45	0/1071	0.56	0/1429
34	f	0.49	0/895	0.60	0/1198
35	g	0.44	0/916	0.60	0/1220
36	h	0.38	0/1021	0.60	0/1348
37	i	0.39	0/841	0.58	0/1112
38	j	0.45	0/720	0.64	0/952
39	k	0.38	0/575	0.57	0/761
40	l	0.38	0/459	0.60	1/608 (0.2%)
41	m	0.45	0/425	0.67	0/561
42	n	0.34	0/240	0.60	0/305
43	o	0.42	0/855	0.55	0/1128
44	p	0.46	0/718	0.58	0/953
45	r	0.46	0/1010	0.64	1/1354 (0.1%)
46	s	0.31	0/1530	0.62	0/2064
47	t	0.30	0/1174	0.70	0/1582
48	u	0.30	0/1680	0.71	1/2255 (0.0%)
49	v	0.35	0/6651	0.72	11/8982 (0.1%)
50	w	0.34	0/218	0.60	0/287
51	9	0.75	17/40385 (0.0%)	1.93	419/62909 (0.7%)
52	AA	0.42	1/1747 (0.1%)	0.67	2/2374 (0.1%)
53	BB	0.36	0/1756	0.62	1/2350 (0.0%)
54	CC	0.41	0/1753	0.61	0/2369
55	DD	0.39	0/1796	0.67	2/2417 (0.1%)
56	EE	0.36	0/2118	0.61	0/2849
57	FF	0.36	0/1492	0.63	3/2005 (0.1%)
58	GG	0.32	0/1946	0.58	0/2590
59	HH	0.36	0/1510	0.62	0/2022
60	II	0.38	0/1715	0.61	0/2287
61	JJ	0.34	0/1550	0.55	0/2069
62	KK	0.43	0/834	0.67	1/1125 (0.1%)
63	LL	0.42	0/1195	0.56	0/1597
64	MM	0.31	0/918	0.66	0/1233
65	NN	0.37	0/1226	0.61	1/1649 (0.1%)
66	OO	0.39	0/1029	0.61	1/1380 (0.1%)
67	PP	0.36	0/1017	0.68	2/1358 (0.1%)
68	QQ	0.38	0/1146	0.63	0/1534
69	RR	0.35	0/1082	0.63	0/1452
70	SS	0.37	0/1208	0.62	0/1618
71	TT	0.36	0/1115	0.63	1/1493 (0.1%)
72	UU	0.35	0/805	0.60	0/1081
73	VV	0.40	0/643	0.63	0/860

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	WW	0.41	0/1051	0.64	0/1406
75	XX	0.38	0/1116	0.62	0/1490
76	YY	0.32	0/1028	0.57	0/1366
77	ZZ	0.30	0/604	0.60	0/810
78	aa	0.42	0/828	0.60	0/1109
79	bb	0.33	0/665	0.56	0/891
80	cc	0.34	0/490	0.65	0/656
81	dd	0.43	0/470	0.58	0/623
82	ee	0.36	0/447	0.61	0/587
83	ff	0.32	0/567	0.57	0/753
84	gg	0.33	0/2493	0.65	0/3394
All	All	0.62	18/234845 (0.0%)	1.17	1069/343077 (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
5	B	0	1
10	G	0	1
11	H	0	2
14	L	0	2
16	N	0	3
21	S	0	1
32	d	0	1
46	s	0	1
47	t	0	2
48	u	0	2
49	v	0	3
52	AA	0	1
56	EE	0	1
57	FF	0	2
62	KK	0	1
64	MM	0	2
67	PP	0	2
70	SS	0	1
73	VV	0	1
74	WW	0	1
75	XX	0	1
77	ZZ	0	1
84	gg	0	1
All	All	0	34

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1284	A	N9-C4	41.96	1.63	1.37
51	9	1286	G	N9-C8	-31.95	1.15	1.37
51	9	1286	G	N9-C4	31.85	1.63	1.38
51	9	1284	A	N9-C8	-25.69	1.17	1.37
51	9	1284	A	N3-C4	19.97	1.46	1.34

The worst 5 of 1069 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	1286	G	C4-C5-N7	-172.13	41.95	110.80
51	9	1284	A	N7-C8-N9	-146.83	40.38	113.80
51	9	1286	G	N7-C8-N9	-144.28	40.96	113.10
51	9	1284	A	C4-C5-N7	-138.38	41.51	110.70
51	9	1286	G	C8-N9-C4	-132.00	53.60	106.40

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	55	HIS	Peptide
10	G	215	ASP	Peptide
11	H	129	ARG	Peptide
11	H	50	LYS	Peptide
14	L	46	ILE	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%)	225 (92%)	21 (8%)	0	100	100
5	B	392/394 (100%)	367 (94%)	25 (6%)	0	100	100
6	C	359/362 (99%)	342 (95%)	17 (5%)	0	100	100
7	D	291/293 (99%)	277 (95%)	14 (5%)	0	100	100
8	E	208/291 (72%)	195 (94%)	13 (6%)	0	100	100
9	F	223/225 (99%)	212 (95%)	11 (5%)	0	100	100
10	G	229/319 (72%)	218 (95%)	11 (5%)	0	100	100
11	H	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
12	I	201/214 (94%)	192 (96%)	9 (4%)	0	100	100
13	J	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
14	L	208/210 (99%)	202 (97%)	6 (3%)	0	100	100
15	M	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
16	N	201/203 (99%)	188 (94%)	13 (6%)	0	100	100
17	O	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
18	P	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
19	Q	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
20	R	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
21	S	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	22	53
22	T	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
23	U	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
24	V	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
25	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
26	X	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
27	Y	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
28	Z	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	46
29	a	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
30	b	100/245 (41%)	94 (94%)	6 (6%)	0	100	100
31	c	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
32	d	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
33	e	126/128 (98%)	116 (92%)	10 (8%)	0	100	100
34	f	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
35	g	112/114 (98%)	109 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	h	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
37	i	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
38	j	84/86 (98%)	75 (89%)	9 (11%)	0	100	100
39	k	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
40	l	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
41	m	49/52 (94%)	43 (88%)	5 (10%)	1 (2%)	6	28
42	n	23/25 (92%)	23 (100%)	0	0	100	100
43	o	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
44	p	89/91 (98%)	89 (100%)	0	0	100	100
45	r	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
46	s	194/196 (99%)	176 (91%)	18 (9%)	0	100	100
47	t	151/153 (99%)	132 (87%)	18 (12%)	1 (1%)	19	50
48	u	204/206 (99%)	178 (87%)	24 (12%)	2 (1%)	13	42
49	v	834/839 (99%)	754 (90%)	78 (9%)	2 (0%)	44	71
50	w	22/26 (85%)	22 (100%)	0	0	100	100
52	AA	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
53	BB	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
54	CC	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
55	DD	226/228 (99%)	216 (96%)	10 (4%)	0	100	100
56	EE	260/262 (99%)	248 (95%)	12 (5%)	0	100	100
57	FF	181/204 (89%)	165 (91%)	15 (8%)	1 (1%)	22	53
58	GG	235/237 (99%)	230 (98%)	5 (2%)	0	100	100
59	HH	181/194 (93%)	174 (96%)	7 (4%)	0	100	100
60	II	204/206 (99%)	191 (94%)	12 (6%)	1 (0%)	25	56
61	JJ	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
62	KK	94/96 (98%)	85 (90%)	9 (10%)	0	100	100
63	LL	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
64	MM	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
65	NN	147/149 (99%)	142 (97%)	5 (3%)	0	100	100
66	OO	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
67	PP	118/120 (98%)	111 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	QQ	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
69	RR	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
70	SS	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
71	TT	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
72	UU	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
73	VV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
74	WW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
75	XX	139/141 (99%)	133 (96%)	3 (2%)	3 (2%)	5	26
76	YY	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
77	ZZ	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
78	aa	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
79	bb	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
80	cc	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
81	dd	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
82	ee	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/68 (97%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/313 (99%)	283 (91%)	28 (9%)	0	100	100
All	All	12576/13168 (96%)	11879 (94%)	684 (5%)	13 (0%)	50	76

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	m	73	CYS
48	u	61	PRO
49	v	288	THR
21	S	166	ARG
49	v	481	LYS

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%)	184 (97%)	6 (3%)	34	61
5	B	342/342 (100%)	337 (98%)	5 (2%)	60	77
6	C	301/301 (100%)	296 (98%)	5 (2%)	56	74
7	D	247/247 (100%)	243 (98%)	4 (2%)	58	76
8	E	190/251 (76%)	187 (98%)	3 (2%)	58	76
9	F	196/196 (100%)	196 (100%)	0	100	100
10	G	200/272 (74%)	193 (96%)	7 (4%)	31	58
11	H	169/169 (100%)	166 (98%)	3 (2%)	54	74
12	I	175/181 (97%)	172 (98%)	3 (2%)	56	74
13	J	143/143 (100%)	142 (99%)	1 (1%)	81	88
14	L	175/175 (100%)	170 (97%)	5 (3%)	37	63
15	M	117/117 (100%)	115 (98%)	2 (2%)	56	74
16	N	171/171 (100%)	168 (98%)	3 (2%)	54	74
17	O	171/171 (100%)	170 (99%)	1 (1%)	84	90
18	P	134/134 (100%)	132 (98%)	2 (2%)	60	77
19	Q	164/164 (100%)	162 (99%)	2 (1%)	67	80
20	R	159/159 (100%)	159 (100%)	0	100	100
21	S	157/157 (100%)	155 (99%)	2 (1%)	65	79
22	T	139/139 (100%)	139 (100%)	0	100	100
23	U	89/89 (100%)	86 (97%)	3 (3%)	32	59
24	V	101/101 (100%)	99 (98%)	2 (2%)	50	71
25	W	86/126 (68%)	85 (99%)	1 (1%)	67	80
26	X	106/106 (100%)	106 (100%)	0	100	100
27	Y	124/124 (100%)	122 (98%)	2 (2%)	58	76
28	Z	117/117 (100%)	114 (97%)	3 (3%)	41	66
29	a	119/119 (100%)	118 (99%)	1 (1%)	79	87
30	b	84/184 (46%)	83 (99%)	1 (1%)	67	80
31	c	84/84 (100%)	80 (95%)	4 (5%)	21	50
32	d	98/98 (100%)	98 (100%)	0	100	100
33	e	114/114 (100%)	113 (99%)	1 (1%)	75	85
34	f	88/88 (100%)	86 (98%)	2 (2%)	45	68
35	g	98/98 (100%)	96 (98%)	2 (2%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	h	109/109 (100%)	108 (99%)	1 (1%)	75	85
37	i	86/86 (100%)	84 (98%)	2 (2%)	45	68
38	j	73/73 (100%)	72 (99%)	1 (1%)	62	78
39	k	64/64 (100%)	64 (100%)	0	100	100
40	l	47/47 (100%)	46 (98%)	1 (2%)	48	70
41	m	47/47 (100%)	46 (98%)	1 (2%)	48	70
42	n	24/24 (100%)	24 (100%)	0	100	100
43	o	91/91 (100%)	89 (98%)	2 (2%)	47	69
44	p	74/74 (100%)	74 (100%)	0	100	100
45	r	108/108 (100%)	105 (97%)	3 (3%)	38	64
46	s	164/164 (100%)	164 (100%)	0	100	100
47	t	126/126 (100%)	122 (97%)	4 (3%)	34	61
48	u	186/186 (100%)	179 (96%)	7 (4%)	28	56
49	v	713/713 (100%)	699 (98%)	14 (2%)	50	71
50	w	23/23 (100%)	21 (91%)	2 (9%)	8	29
52	AA	180/181 (99%)	179 (99%)	1 (1%)	84	90
53	BB	194/194 (100%)	193 (100%)	1 (0%)	86	91
54	CC	187/187 (100%)	186 (100%)	1 (0%)	86	91
55	DD	190/190 (100%)	184 (97%)	6 (3%)	34	61
56	EE	224/224 (100%)	220 (98%)	4 (2%)	54	74
57	FF	158/170 (93%)	153 (97%)	5 (3%)	34	61
58	GG	207/207 (100%)	204 (99%)	3 (1%)	62	78
59	HH	165/174 (95%)	163 (99%)	2 (1%)	67	80
60	II	178/178 (100%)	178 (100%)	0	100	100
61	JJ	161/161 (100%)	157 (98%)	4 (2%)	42	67
62	KK	87/87 (100%)	87 (100%)	0	100	100
63	LL	130/142 (92%)	128 (98%)	2 (2%)	60	77
64	MM	99/99 (100%)	96 (97%)	3 (3%)	36	62
65	NN	130/130 (100%)	129 (99%)	1 (1%)	79	87
66	OO	106/106 (100%)	106 (100%)	0	100	100
67	PP	109/109 (100%)	107 (98%)	2 (2%)	54	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	QQ	117/117 (100%)	113 (97%)	4 (3%)	32	59
69	RR	119/119 (100%)	117 (98%)	2 (2%)	56	74
70	SS	125/125 (100%)	122 (98%)	3 (2%)	44	68
71	TT	111/111 (100%)	110 (99%)	1 (1%)	75	85
72	UU	92/92 (100%)	91 (99%)	1 (1%)	70	82
73	VV	67/67 (100%)	66 (98%)	1 (2%)	60	77
74	WW	112/112 (100%)	112 (100%)	0	100	100
75	XX	113/113 (100%)	112 (99%)	1 (1%)	75	85
76	YY	107/107 (100%)	106 (99%)	1 (1%)	75	85
77	ZZ	66/66 (100%)	65 (98%)	1 (2%)	60	77
78	aa	88/88 (100%)	87 (99%)	1 (1%)	70	82
79	bb	75/75 (100%)	72 (96%)	3 (4%)	27	55
80	cc	55/55 (100%)	54 (98%)	1 (2%)	54	74
81	dd	48/48 (100%)	48 (100%)	0	100	100
82	ee	46/46 (100%)	44 (96%)	2 (4%)	25	53
83	ff	61/61 (100%)	60 (98%)	1 (2%)	58	76
84	gg	272/272 (100%)	269 (99%)	3 (1%)	70	82
All	All	10962/11275 (97%)	10787 (98%)	175 (2%)	58	76

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	BB	110	MET
64	MM	35	ILE
55	DD	76	ARG
57	FF	154	LEU
68	QQ	85	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
18	P	64	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3522/3597 (97%)	832 (23%)	64 (1%)
2	7	119/120 (99%)	15 (12%)	0
3	8	149/151 (98%)	26 (17%)	1 (0%)
51	9	1675/1698 (98%)	406 (24%)	30 (1%)
All	All	5465/5566 (98%)	1279 (23%)	95 (1%)

5 of 1279 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	8	U
1	5	12	A
1	5	13	U
1	5	25	A
1	5	35	U

5 of 95 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	4448	G
51	9	555	A
1	5	4719	G
51	9	110	U
51	9	688	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	5	3715	1	18,21,22	1.01	1 (5%)	21,30,33	1.77	4 (19%)
1	PSU	5	3764	1	18,21,22	1.07	1 (5%)	21,30,33	1.77	4 (19%)
1	OMG	5	1316	1	19,26,27	2.41	8 (42%)	21,38,41	1.59	4 (19%)
1	1MA	5	4415	1	17,25,26	3.85	4 (23%)	17,37,40	1.74	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMG	5	4637	1	19,26,27	2.37	8 (42%)	21,38,41	1.47	4 (19%)
51	5MC	9	1374	51	19,22,23	3.84	8 (42%)	26,32,35	1.10	2 (7%)
1	E6G	5	4355	1	19,27,28	4.71	7 (36%)	18,39,42	2.31	5 (27%)
1	PSU	5	4500	1	18,21,22	1.03	2 (11%)	21,30,33	2.05	4 (19%)
1	PSU	5	2508	1	18,21,22	1.00	1 (5%)	21,30,33	1.74	3 (14%)
1	A2M	5	4571	1	18,25,26	5.01	8 (44%)	20,36,39	2.62	5 (25%)
1	B9B	5	2754	1,85	20,28,29	5.07	8 (40%)	19,40,43	2.23	6 (31%)
1	B8H	5	1860	1	19,22,23	6.84	6 (31%)	21,32,35	2.46	5 (23%)
1	A2M	5	3718	1	18,25,26	5.00	10 (55%)	20,36,39	2.48	3 (15%)
1	E7G	5	2297	1	24,27,28	3.14	11 (45%)	28,40,43	2.28	9 (32%)
1	PSU	5	4403	1	18,21,22	1.02	1 (5%)	21,30,33	1.87	5 (23%)
41	MLZ	m	72	41	8,9,10	0.74	0	4,9,11	0.78	0
1	PSU	5	4450	1,85	18,21,22	1.08	2 (11%)	21,30,33	2.07	5 (23%)
1	2MG	5	4872	1	18,26,27	2.66	7 (38%)	16,38,41	3.52	6 (37%)
6	MLZ	C	333	6	8,9,10	0.84	0	4,9,11	0.72	0
1	7MG	5	2522	1	23,26,27	3.30	10 (43%)	27,39,42	2.12	10 (37%)
1	UR3	5	4597	1	19,22,23	2.65	7 (36%)	26,32,35	1.59	4 (15%)
1	B9B	5	237	1	20,28,29	5.15	8 (40%)	19,40,43	2.45	6 (31%)
51	PSU	9	1243	51	18,21,22	1.19	1 (5%)	21,30,33	1.44	4 (19%)
1	7MG	5	4550	1	23,26,27	3.28	10 (43%)	27,39,42	2.10	10 (37%)
1	OMG	5	373	1	19,26,27	2.44	8 (42%)	21,38,41	1.58	5 (23%)
1	A2M	5	4523	1,85	18,25,26	5.05	9 (50%)	20,36,39	2.71	5 (25%)
1	PSU	5	1683	1	18,21,22	1.13	2 (11%)	21,30,33	1.93	4 (19%)
1	OMC	5	2365	1	19,22,23	2.86	7 (36%)	25,31,34	0.68	0
1	B8H	5	3762	1	19,22,23	6.84	6 (31%)	21,32,35	2.54	5 (23%)
51	B8N	9	1248	51	25,29,30	3.08	8 (32%)	28,42,45	2.06	7 (25%)
1	OMG	5	2424	1	19,26,27	2.48	8 (42%)	21,38,41	1.49	4 (19%)
1	P7G	5	1909	1	24,28,29	3.74	11 (45%)	25,41,44	1.47	2 (8%)
1	A2M	5	3867	1	18,25,26	4.85	9 (50%)	20,36,39	2.66	5 (25%)
1	B8K	5	4690	1	24,28,29	4.93	17 (70%)	29,42,45	2.72	12 (41%)
1	B8Q	5	1456	1	18,22,23	2.71	5 (27%)	21,32,35	1.92	5 (23%)
1	OMU	5	4620	1	19,22,23	2.73	7 (36%)	25,31,34	1.81	5 (20%)
1	P7G	5	3880	1	24,28,29	3.52	10 (41%)	25,41,44	1.36	2 (8%)
1	OMG	5	2050	1	19,26,27	2.40	8 (42%)	21,38,41	1.44	4 (19%)
1	A2M	5	3785	1	18,25,26	4.80	10 (55%)	20,36,39	2.80	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	A2M	5	2401	1,85	18,25,26	4.96	8 (44%)	20,36,39	2.76	4 (20%)
1	PSU	5	4636	1	18,21,22	1.07	2 (11%)	21,30,33	2.08	5 (23%)
1	B8H	5	4296	1	19,22,23	6.85	6 (31%)	21,32,35	2.55	5 (23%)
1	OMC	5	2804	1	19,22,23	2.84	7 (36%)	25,31,34	0.82	0
1	MHG	5	4371	1	29,32,33	3.65	11 (37%)	34,46,49	2.46	12 (35%)
1	A2M	5	3825	1	18,25,26	4.96	7 (38%)	20,36,39	2.75	4 (20%)
1	OMG	5	4623	1	19,26,27	2.42	8 (42%)	21,38,41	1.54	4 (19%)
1	B8W	5	2380	1	18,26,27	4.22	6 (33%)	17,38,41	7.11	9 (52%)
1	B8W	5	4185	1	18,26,27	4.18	7 (38%)	17,38,41	7.06	11 (64%)
1	A2M	5	1524	1	18,25,26	4.93	8 (44%)	20,36,39	3.17	4 (20%)
1	PSU	5	1677	1	18,21,22	1.11	3 (16%)	21,30,33	2.03	6 (28%)
1	A2M	5	1326	1	18,25,26	4.88	9 (50%)	20,36,39	2.65	4 (20%)
49	DDE	v	715	49	15,20,21	0.97	0	11,28,30	1.10	1 (9%)
1	2MG	5	729	1	18,26,27	2.50	7 (38%)	16,38,41	1.37	3 (18%)
1	OMG	5	1522	1	19,26,27	2.44	8 (42%)	21,38,41	1.55	4 (19%)
1	OMG	5	2773	1	19,26,27	2.46	8 (42%)	21,38,41	1.44	4 (19%)
1	PSU	5	3729	1	18,21,22	1.06	1 (5%)	21,30,33	1.85	4 (19%)
1	7MG	5	1605	1	23,26,27	3.25	10 (43%)	27,39,42	2.17	10 (37%)
1	OMC	5	3909	1	19,22,23	2.86	7 (36%)	25,31,34	0.74	0
1	5MC	5	4335	1	19,22,23	3.84	8 (42%)	26,32,35	1.24	3 (11%)
1	PSU	5	4442	1	18,21,22	1.10	2 (11%)	21,30,33	1.98	4 (19%)
1	B8T	5	4483	1	19,22,23	3.08	8 (42%)	25,31,34	1.03	2 (8%)
1	UR3	5	1866	1	19,22,23	2.57	6 (31%)	26,32,35	1.56	5 (19%)
1	UR3	5	4530	1	19,22,23	2.68	7 (36%)	26,32,35	1.57	4 (15%)
51	4AC	9	1337	51	21,24,25	3.15	10 (47%)	28,34,37	1.17	4 (14%)
1	OMC	5	3869	1	19,22,23	2.83	7 (36%)	25,31,34	0.72	0
1	A2M	5	2363	1,85	18,25,26	4.97	9 (50%)	20,36,39	2.79	5 (25%)
1	OMC	5	2422	1,85	19,22,23	2.93	7 (36%)	25,31,34	0.95	2 (8%)
1	PSU	5	1582	1	18,21,22	1.17	3 (16%)	21,30,33	1.83	4 (19%)
1	OMG	5	4494	1	19,26,27	2.42	8 (42%)	21,38,41	1.54	4 (19%)
1	B9B	5	1574	1	20,28,29	5.03	8 (40%)	19,40,43	2.41	6 (31%)
1	A2M	5	1871	1,85	18,25,26	4.99	9 (50%)	20,36,39	2.76	4 (20%)
1	PSU	5	4293	1	18,21,22	1.08	2 (11%)	21,30,33	1.99	4 (19%)
1	OMG	5	2364	1	19,26,27	2.41	8 (42%)	21,38,41	1.52	4 (19%)
1	OMC	5	3887	1	19,22,23	2.84	7 (36%)	25,31,34	0.91	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	BGH	5	3899	1,85	25,29,30	4.19	15 (60%)	30,43,46	2.62	13 (43%)
1	B8W	5	4472	1	18,26,27	4.27	7 (38%)	17,38,41	7.03	9 (52%)
1	1MA	5	1322	1,85	17,25,26	3.65	4 (23%)	17,37,40	1.73	3 (17%)
1	PSU	5	4628	1	18,21,22	1.14	3 (16%)	21,30,33	2.15	5 (23%)
1	E7G	5	1797	1	24,27,28	3.22	11 (45%)	28,40,43	2.31	10 (35%)
1	PSU	5	4531	1	18,21,22	1.06	1 (5%)	21,30,33	1.99	5 (23%)
1	OMG	5	3792	1	19,26,27	2.45	8 (42%)	21,38,41	1.52	4 (19%)
1	B9H	5	2786	1	21,25,26	3.15	3 (14%)	22,35,38	2.07	4 (18%)
1	A2M	5	1534	1,85	18,25,26	4.89	10 (55%)	20,36,39	2.73	5 (25%)
51	B8Q	9	1219	51	18,22,23	2.95	4 (22%)	21,32,35	2.81	7 (33%)
1	B8W	5	4129	1	18,26,27	4.31	6 (33%)	17,38,41	7.04	8 (47%)
1	A2M	5	398	1	18,25,26	5.02	9 (50%)	20,36,39	2.54	3 (15%)
1	A2M	5	3723	1	18,25,26	5.07	9 (50%)	20,36,39	2.65	4 (20%)
1	OMG	5	4370	1	19,26,27	2.47	8 (42%)	21,38,41	1.45	4 (19%)
1	P4U	5	1348	1,85	21,24,25	3.28	7 (33%)	28,33,36	1.98	4 (14%)
1	B8K	5	3897	1	24,28,29	4.71	17 (70%)	29,42,45	2.69	12 (41%)
1	B8T	5	4671	1	19,22,23	3.04	8 (42%)	25,31,34	0.93	1 (4%)
1	OMG	5	1883	1	19,26,27	2.43	8 (42%)	21,38,41	1.60	4 (19%)
51	A2M	9	1678	51	18,25,26	5.10	9 (50%)	20,36,39	2.76	4 (20%)
1	OMU	5	4306	1	19,22,23	2.85	8 (42%)	25,31,34	1.87	5 (20%)
1	5MC	5	3782	1	19,22,23	3.80	8 (42%)	26,32,35	1.10	1 (3%)
1	OMC	5	3701	1,85	19,22,23	2.81	7 (36%)	25,31,34	0.75	0
1	5MC	5	4447	1	19,22,23	3.81	8 (42%)	26,32,35	1.15	2 (7%)
1	I4U	5	4194	1	20,24,25	5.00	14 (70%)	27,34,37	1.90	3 (11%)
3	OMU	8	14	1,3	19,22,23	2.83	7 (36%)	25,31,34	2.10	7 (28%)
1	OMC	5	2861	1	19,22,23	2.90	7 (36%)	25,31,34	0.92	1 (4%)
1	6MZ	5	4220	1	17,25,26	1.83	3 (17%)	15,36,39	2.30	4 (26%)
1	M7A	5	4564	1	19,25,26	1.61	2 (10%)	25,37,40	4.07	8 (32%)
1	OMG	5	4196	1	19,26,27	2.41	8 (42%)	21,38,41	1.50	4 (19%)
1	OMG	5	1625	1,85	19,26,27	2.42	8 (42%)	21,38,41	1.49	4 (19%)
1	I4U	5	1659	1	20,24,25	4.97	13 (65%)	27,34,37	2.07	3 (11%)
1	5MU	5	4083	1	19,22,23	4.82	7 (36%)	27,32,35	3.59	10 (37%)
1	B8W	5	4529	1,85	18,26,27	4.28	7 (38%)	17,38,41	7.26	10 (58%)
1	2MG	5	1517	1	18,26,27	2.57	7 (38%)	16,38,41	2.02	5 (31%)
1	OMG	5	4870	1	19,26,27	2.41	8 (42%)	21,38,41	1.54	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMC	5	4536	1	19,22,23	2.86	7 (36%)	25,31,34	1.02	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	5	3715	1	-	0/7/25/26	0/2/2/2
1	PSU	5	3764	1	-	1/7/25/26	0/2/2/2
1	OMG	5	1316	1	-	0/5/27/28	0/3/3/3
1	1MA	5	4415	1	-	2/3/25/26	0/3/3/3
1	OMG	5	4637	1	-	2/5/27/28	0/3/3/3
51	5MC	9	1374	51	-	0/7/25/26	0/2/2/2
1	E6G	5	4355	1	-	3/6/28/29	0/3/3/3
1	PSU	5	4500	1	-	4/7/25/26	0/2/2/2
1	PSU	5	2508	1	-	0/7/25/26	0/2/2/2
1	A2M	5	4571	1	-	0/5/27/28	0/3/3/3
1	B9B	5	2754	1,85	-	3/7/29/30	0/3/3/3
1	B8H	5	1860	1	-	0/7/25/26	0/2/2/2
1	A2M	5	3718	1	-	0/5/27/28	0/3/3/3
1	E7G	5	2297	1	-	1/9/39/40	0/3/3/3
1	PSU	5	4403	1	-	2/7/25/26	0/2/2/2
41	MLZ	m	72	41	-	3/7/8/10	-
1	PSU	5	4450	1,85	-	3/7/25/26	0/2/2/2
1	2MG	5	4872	1	-	2/5/27/28	0/3/3/3
6	MLZ	C	333	6	-	2/7/8/10	-
1	7MG	5	2522	1	-	0/7/37/38	0/3/3/3
1	UR3	5	4597	1	-	0/7/25/26	0/2/2/2
1	B9B	5	237	1	-	4/7/29/30	0/3/3/3
51	PSU	9	1243	51	-	2/7/25/26	0/2/2/2
1	7MG	5	4550	1	-	0/7/37/38	0/3/3/3
1	OMG	5	373	1	-	1/5/27/28	0/3/3/3
1	A2M	5	4523	1,85	-	2/5/27/28	0/3/3/3
1	PSU	5	1683	1	-	0/7/25/26	0/2/2/2
1	OMC	5	2365	1	-	0/9/27/28	0/2/2/2
1	B8H	5	3762	1	-	3/7/25/26	0/2/2/2
51	B8N	9	1248	51	-	3/16/34/35	0/2/2/2
1	OMG	5	2424	1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	P7G	5	1909	1	-	2/10/40/41	0/3/3/3
1	A2M	5	3867	1	-	2/5/27/28	0/3/3/3
1	B8K	5	4690	1	-	2/11/41/42	0/3/3/3
1	B8Q	5	1456	1	-	2/7/42/43	0/2/2/2
1	OMU	5	4620	1	-	1/9/27/28	0/2/2/2
1	P7G	5	3880	1	-	3/10/40/41	0/3/3/3
1	OMG	5	2050	1	-	0/5/27/28	0/3/3/3
1	A2M	5	3785	1	-	2/5/27/28	0/3/3/3
1	A2M	5	2401	1,85	-	0/5/27/28	0/3/3/3
1	PSU	5	4636	1	-	3/7/25/26	0/2/2/2
1	B8H	5	4296	1	-	0/7/25/26	0/2/2/2
1	OMC	5	2804	1	-	0/9/27/28	0/2/2/2
1	MHG	5	4371	1	-	7/16/46/47	0/3/3/3
1	A2M	5	3825	1	-	0/5/27/28	0/3/3/3
1	OMG	5	4623	1	-	0/5/27/28	0/3/3/3
1	B8W	5	2380	1	-	5/5/27/28	0/3/3/3
1	B8W	5	4185	1	-	3/5/27/28	0/3/3/3
1	A2M	5	1524	1	-	0/5/27/28	0/3/3/3
1	PSU	5	1677	1	-	0/7/25/26	0/2/2/2
1	A2M	5	1326	1	-	0/5/27/28	0/3/3/3
49	DDE	v	715	49	-	12/20/21/23	0/1/1/1
1	2MG	5	729	1	-	1/5/27/28	0/3/3/3
1	OMG	5	1522	1	-	0/5/27/28	0/3/3/3
1	OMG	5	2773	1	-	2/5/27/28	0/3/3/3
1	PSU	5	3729	1	-	2/7/25/26	0/2/2/2
1	7MG	5	1605	1	-	0/7/37/38	0/3/3/3
1	OMC	5	3909	1	-	0/9/27/28	0/2/2/2
1	5MC	5	4335	1	-	0/7/25/26	0/2/2/2
1	PSU	5	4442	1	-	0/7/25/26	0/2/2/2
1	B8T	5	4483	1	-	0/7/27/28	0/2/2/2
1	UR3	5	1866	1	-	1/7/25/26	0/2/2/2
1	UR3	5	4530	1	-	2/7/25/26	0/2/2/2
51	4AC	9	1337	51	-	0/11/29/30	0/2/2/2
1	OMC	5	3869	1	-	0/9/27/28	0/2/2/2
1	A2M	5	2363	1,85	-	0/5/27/28	0/3/3/3
1	OMC	5	2422	1,85	-	0/9/27/28	0/2/2/2
1	PSU	5	1582	1	-	2/7/25/26	0/2/2/2
1	OMG	5	4494	1	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B9B	5	1574	1	-	2/7/29/30	0/3/3/3
1	A2M	5	1871	1,85	-	0/5/27/28	0/3/3/3
1	PSU	5	4293	1	-	0/7/25/26	0/2/2/2
1	OMG	5	2364	1	-	2/5/27/28	0/3/3/3
1	OMC	5	3887	1	-	1/9/27/28	0/2/2/2
1	BGH	5	3899	1,85	-	2/13/43/44	0/3/3/3
1	B8W	5	4472	1	-	2/5/27/28	0/3/3/3
1	1MA	5	1322	1,85	-	0/3/25/26	0/3/3/3
1	PSU	5	4628	1	-	0/7/25/26	0/2/2/2
1	E7G	5	1797	1	-	2/9/39/40	0/3/3/3
1	PSU	5	4531	1	-	0/7/25/26	0/2/2/2
1	OMG	5	3792	1	-	2/5/27/28	0/3/3/3
1	B9H	5	2786	1	-	4/12/47/48	0/2/2/2
1	A2M	5	1534	1,85	-	1/5/27/28	0/3/3/3
51	B8Q	9	1219	51	-	1/7/42/43	0/2/2/2
1	B8W	5	4129	1	-	3/5/27/28	0/3/3/3
1	A2M	5	398	1	-	2/5/27/28	0/3/3/3
1	A2M	5	3723	1	-	0/5/27/28	0/3/3/3
1	OMG	5	4370	1	-	1/5/27/28	0/3/3/3
1	P4U	5	1348	1,85	-	4/10/29/30	0/2/2/2
1	B8K	5	3897	1	-	3/11/41/42	0/3/3/3
1	B8T	5	4671	1	-	0/7/27/28	0/2/2/2
1	OMG	5	1883	1	-	0/5/27/28	0/3/3/3
51	A2M	9	1678	51	-	0/5/27/28	0/3/3/3
1	OMU	5	4306	1	-	0/9/27/28	0/2/2/2
1	5MC	5	3782	1	-	0/7/25/26	0/2/2/2
1	OMC	5	3701	1,85	-	4/9/27/28	0/2/2/2
1	5MC	5	4447	1	-	4/7/25/26	0/2/2/2
1	I4U	5	4194	1	-	3/9/29/30	0/2/2/2
3	OMU	8	14	1,3	-	1/9/27/28	0/2/2/2
1	OMC	5	2861	1	-	0/9/27/28	0/2/2/2
1	6MZ	5	4220	1	-	0/5/27/28	0/3/3/3
1	M7A	5	4564	1	-	0/7/37/38	0/3/3/3
1	OMG	5	4196	1	-	0/5/27/28	0/3/3/3
1	OMG	5	1625	1,85	-	3/5/27/28	0/3/3/3
1	I4U	5	1659	1	-	2/9/29/30	0/2/2/2
1	5MU	5	4083	1	-	0/7/25/26	0/2/2/2
1	B8W	5	4529	1,85	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	5	1517	1	-	0/5/27/28	0/3/3/3
1	OMG	5	4870	1	-	3/5/27/28	0/3/3/3
1	OMC	5	4536	1	-	1/9/27/28	0/2/2/2

The worst 5 of 762 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	237	B9B	O4'-C1'	18.49	1.65	1.40
1	5	1574	B9B	O4'-C1'	17.94	1.64	1.40
1	5	2754	B9B	O4'-C1'	17.92	1.64	1.40
1	5	4523	A2M	O4'-C1'	17.82	1.64	1.40
1	5	3723	A2M	O4'-C1'	17.70	1.64	1.40

The worst 5 of 512 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4529	B8W	N2-C2-N3	17.76	145.51	117.79
1	5	2380	B8W	N2-C2-N3	17.62	145.29	117.79
1	5	4129	B8W	N2-C2-N3	17.48	145.07	117.79
1	5	4185	B8W	N2-C2-N3	17.22	144.68	117.79
1	5	4472	B8W	N2-C2-N3	17.06	144.42	117.79

There are no chirality outliers.

5 of 155 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	333	MLZ	N-CA-CB-CG
6	C	333	MLZ	C-CA-CB-CG
49	v	715	DDE	O-C-CA-CB
49	v	715	DDE	CA-CB-CG-ND1
49	v	715	DDE	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 306 ligands modelled in this entry, 305 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	$\#\|Z\| > 2$
87	GDP	v	900	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)

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
87	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)
87	v	900	GDP	C6-N1	-2.64	1.33	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	v	900	GDP	C8-N7-C5	2.67	107.10	102.55
87	v	900	GDP	C5-C6-N1	2.28	118.42	114.07

There are no chirality outliers.

There are no torsion outliers.

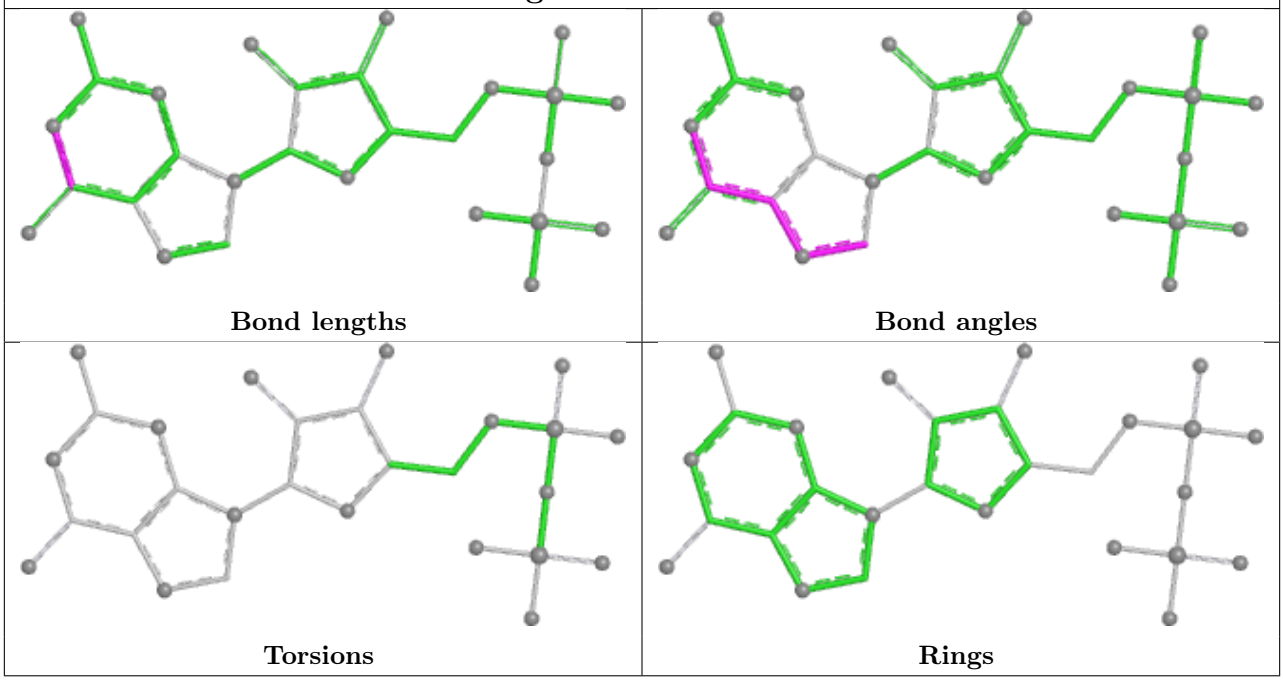
There are no ring outliers.

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.

Ligand GDP v 900



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	47
51	9	19
50	w	1
3	8	1
49	v	1

The worst 5 of 69 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	202:SER	C	282:THR	N	64.88
1	5	2113:G	O3'	2258:C	P	39.97
1	5	1252:C	O3'	1271:G	P	34.48
1	5	1406(C):G	O3'	1411:C	P	20.81
1	5	1405:C	O3'	1406:G	P	20.70

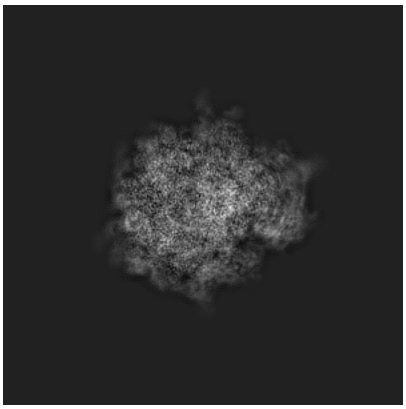
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9240. These allow visual inspection of the internal detail of the map and identification of artifacts.

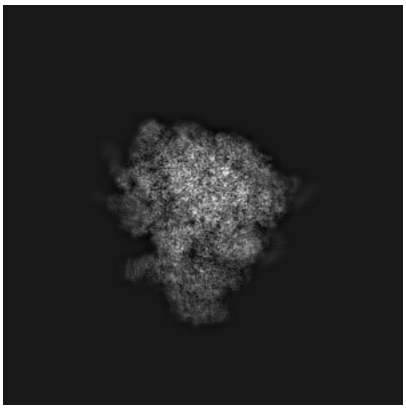
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

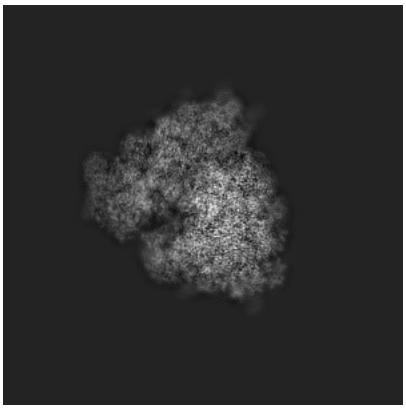
6.1.1 Primary map



X

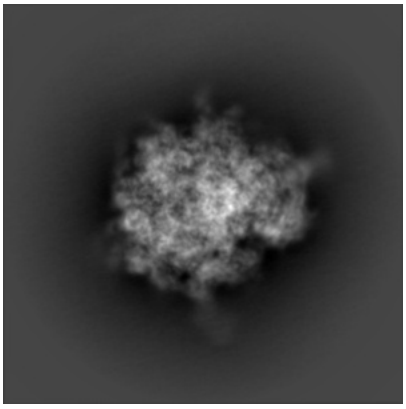


Y

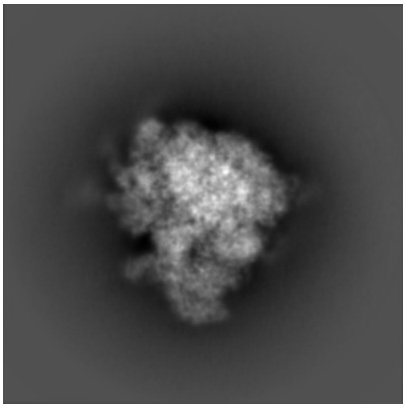


Z

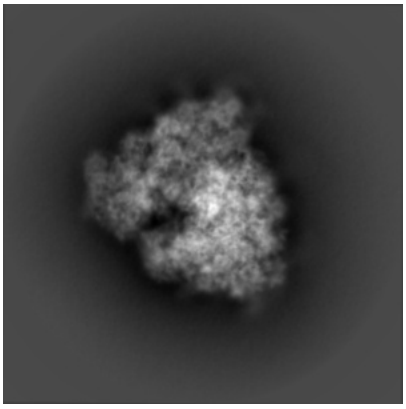
6.1.2 Raw map



X



Y

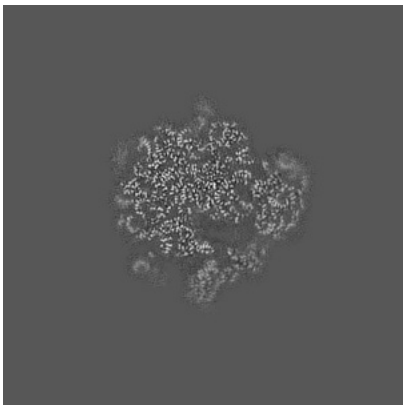


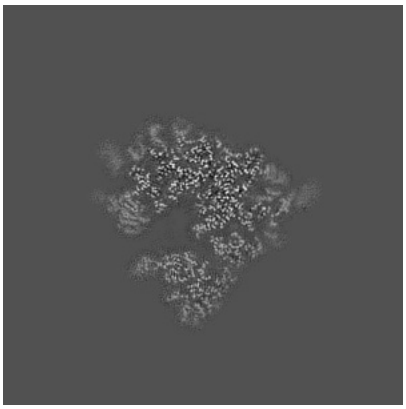
Z

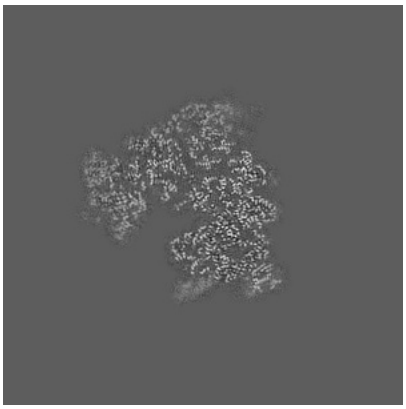
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

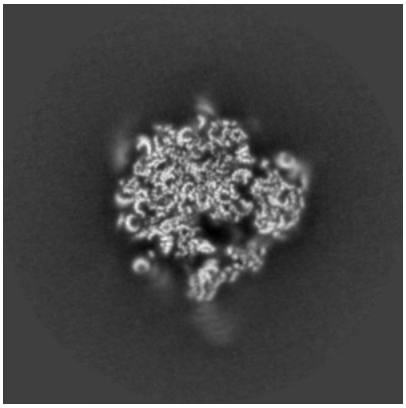
6.2.1 Primary map

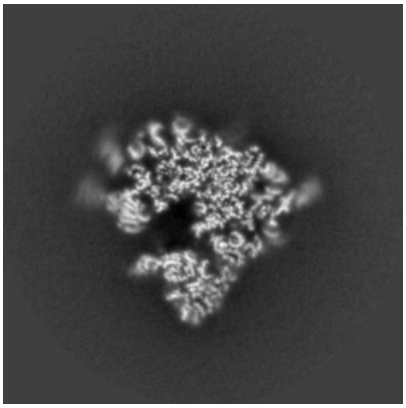

X Index: 200

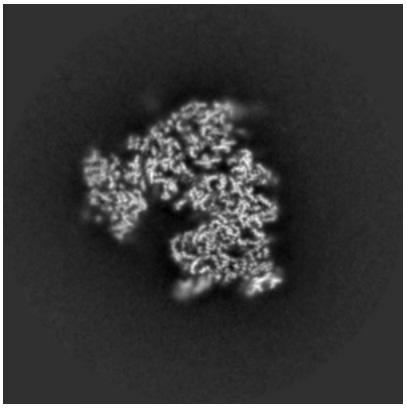

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

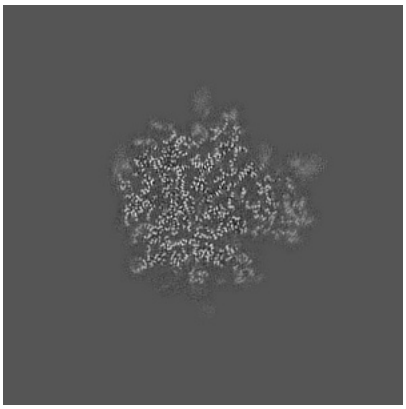

Y Index: 200


Z Index: 200

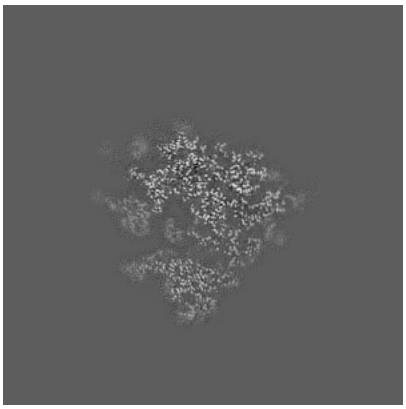
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

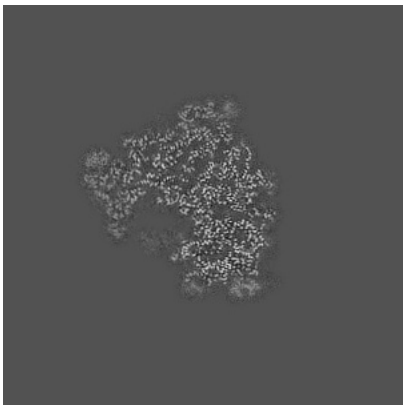
6.3.1 Primary map



X Index: 213

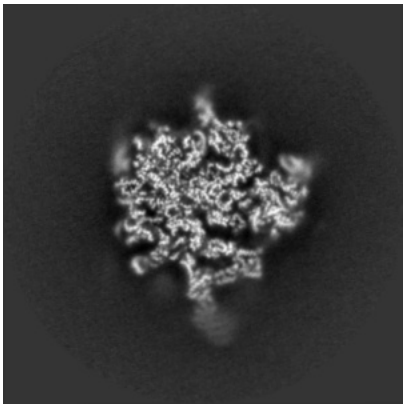


Y Index: 208

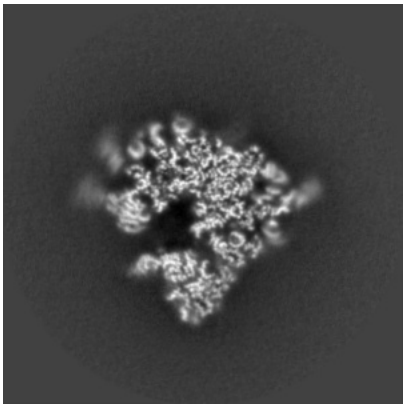


Z Index: 210

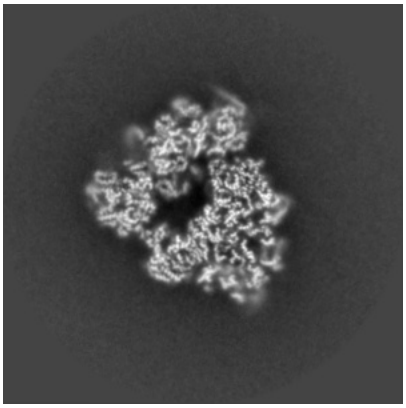
6.3.2 Raw map



X Index: 206



Y Index: 201

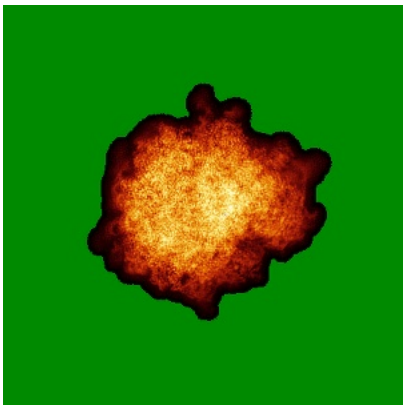


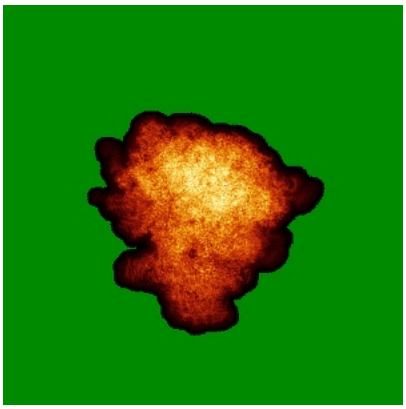
Z Index: 176

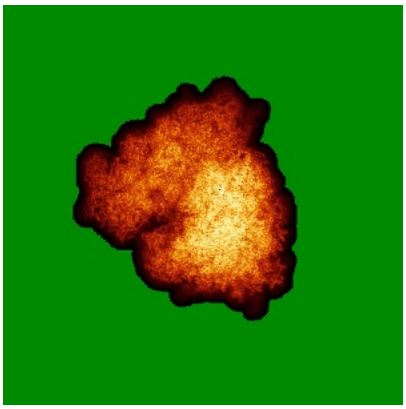
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

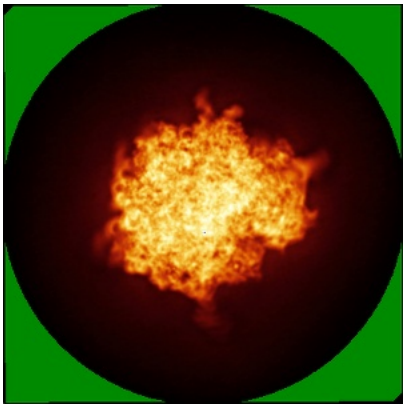
6.4.1 Primary map

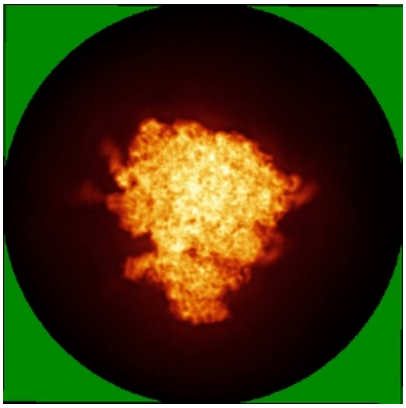

X

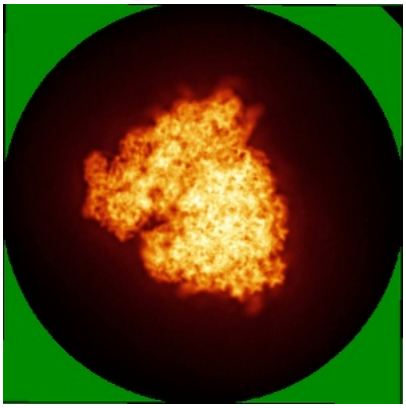

Y


Z

6.4.2 Raw map


X

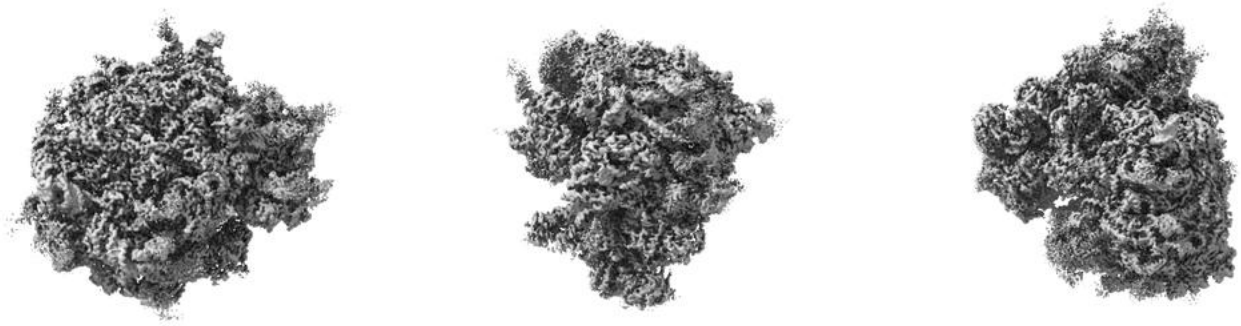

Y


Z

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

6.5 Orthogonal surface views (i)

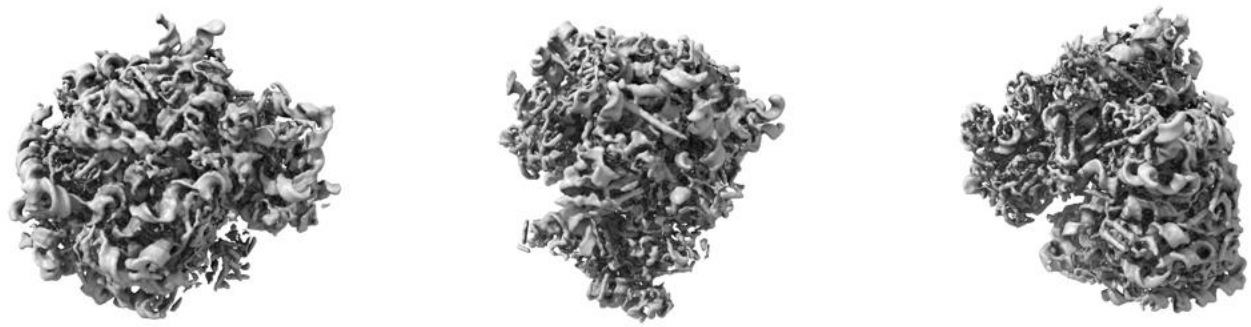
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

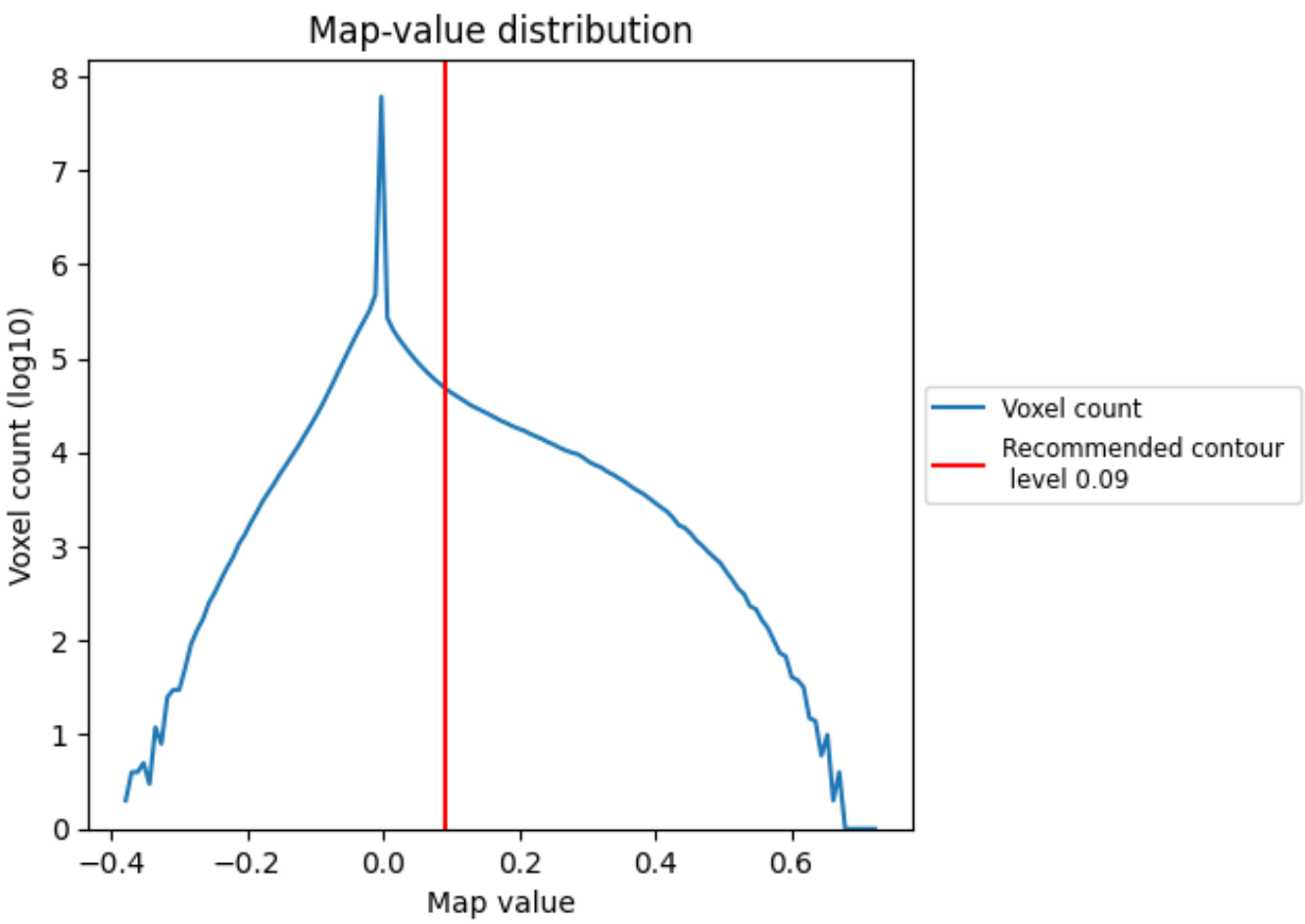
6.6 Mask visualisation (i)

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

7 Map analysis (i)

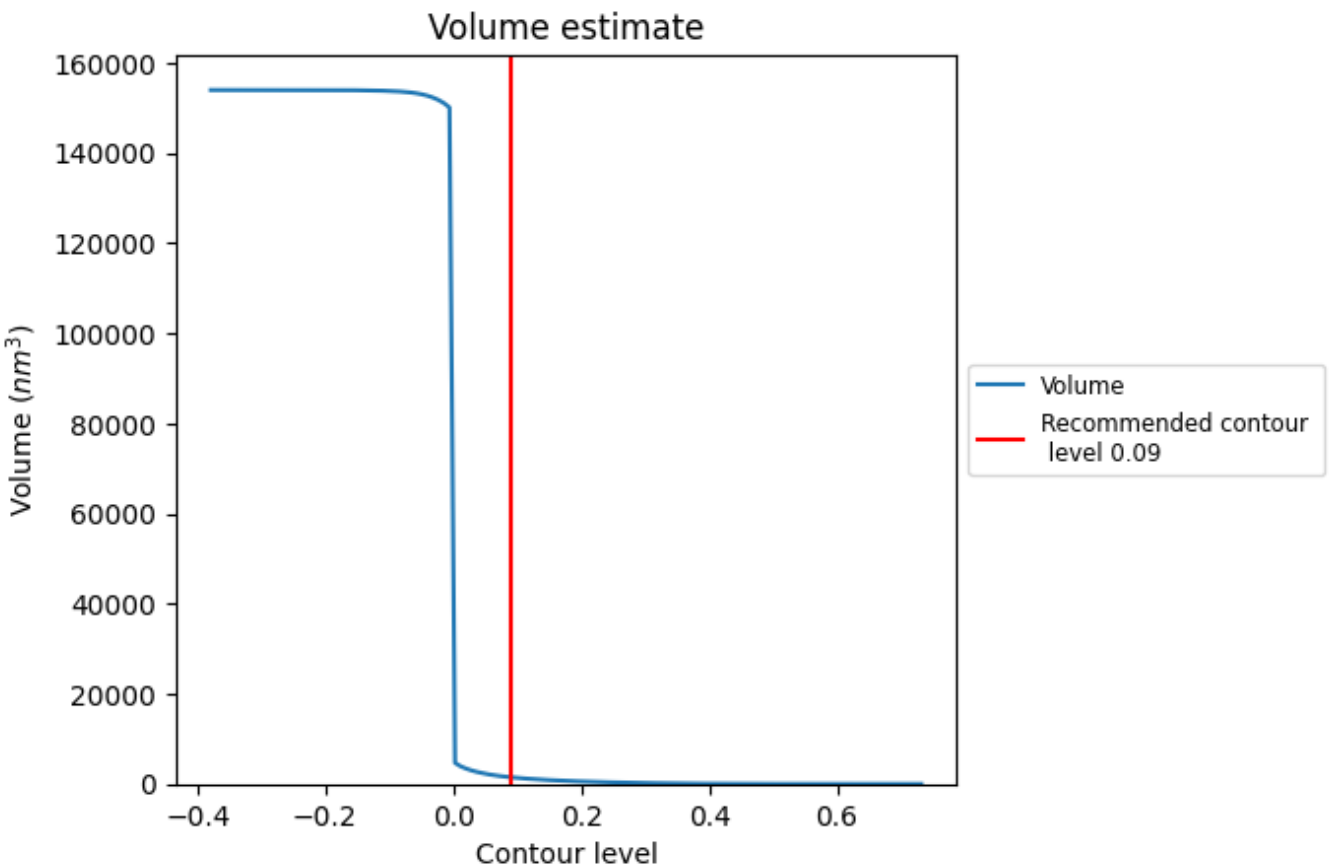
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

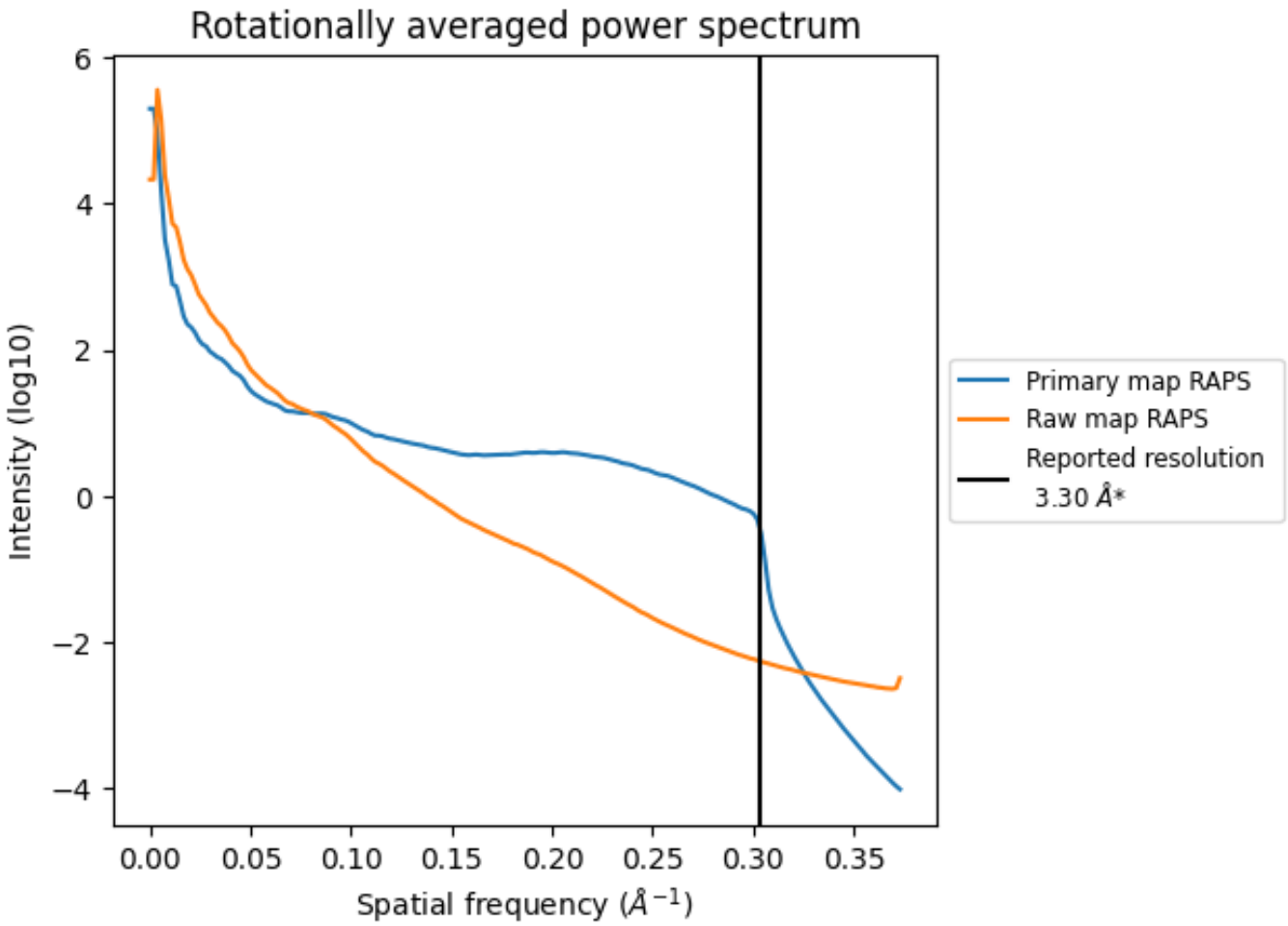
7.2 Volume estimate (i)



The volume at the recommended contour level is 1483 nm^3; this corresponds to an approximate mass of 1340 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)

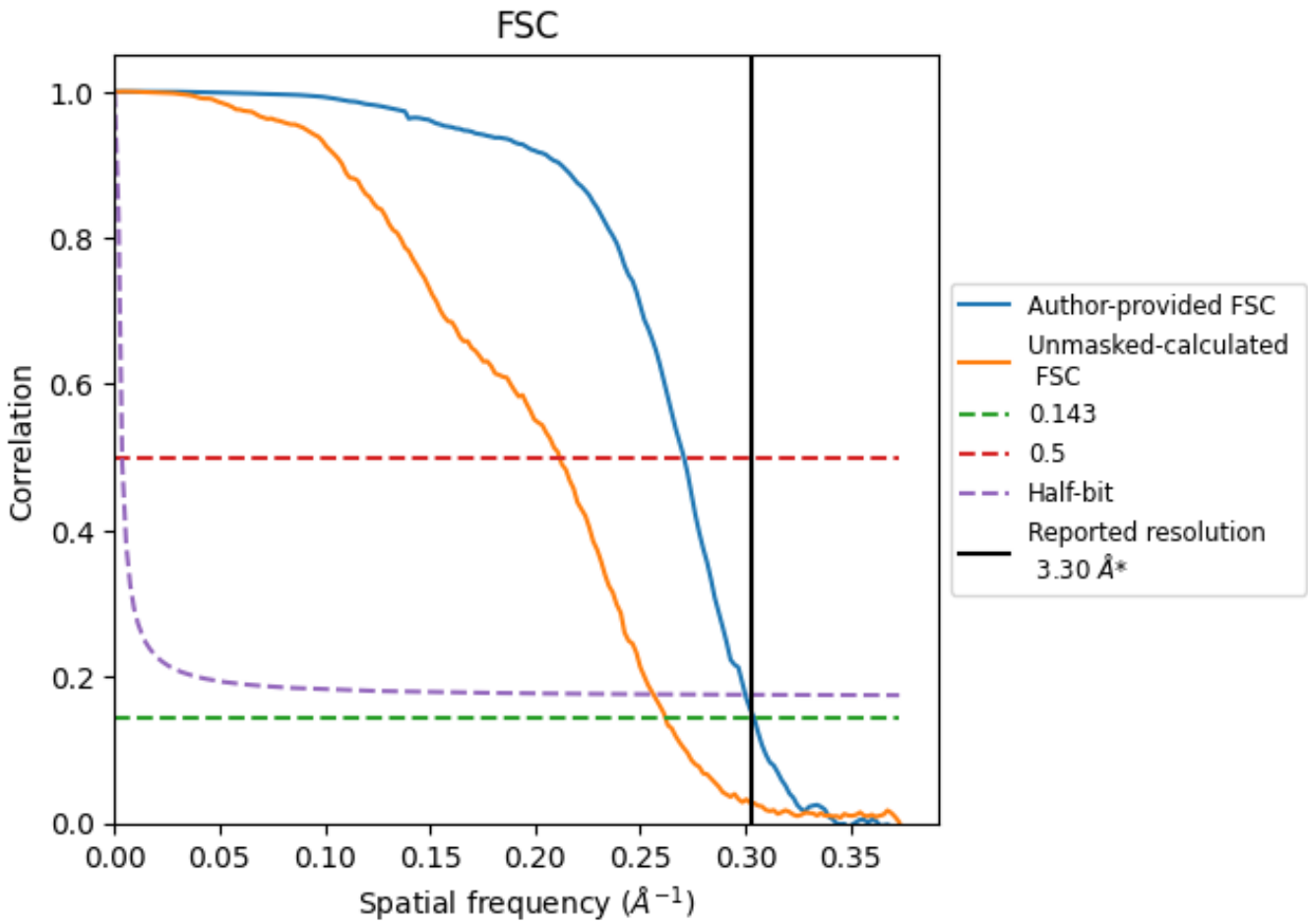


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

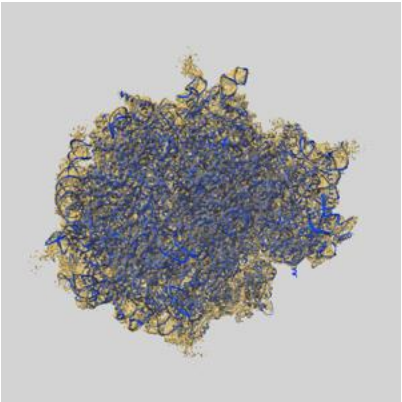
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.69	3.33
Unmasked-calculated*	3.82	4.73	3.90

*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 3.82 differs from the reported value 3.3 by more than 10 %

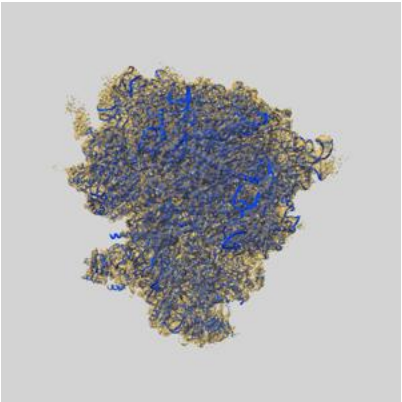
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9240 and PDB model 6MTD. Per-residue inclusion information can be found in section 3 on page 21.

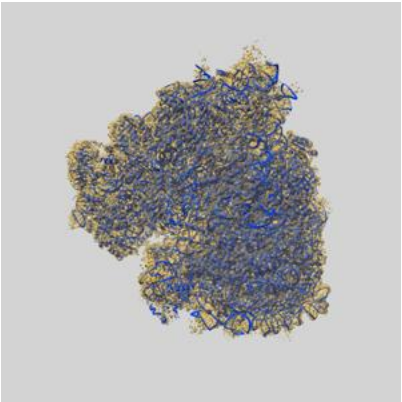
9.1 Map-model overlay (i)



X



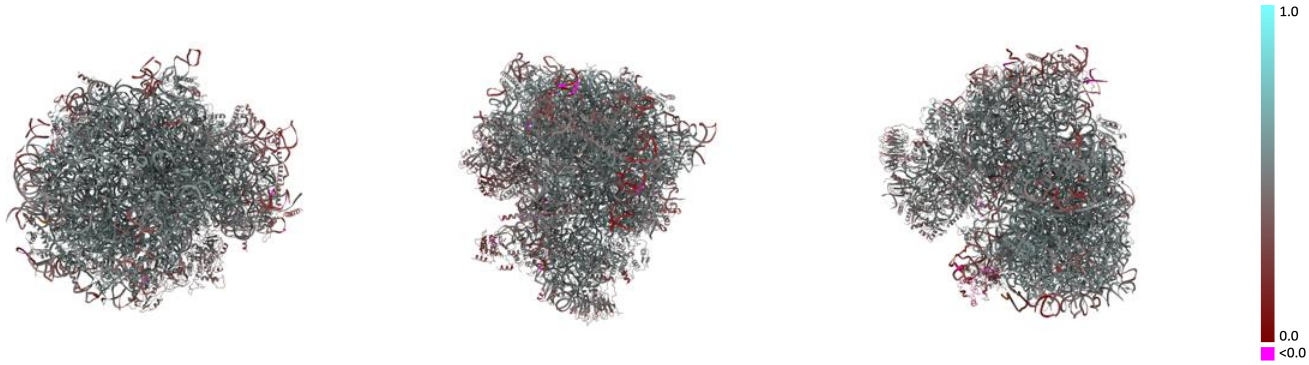
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

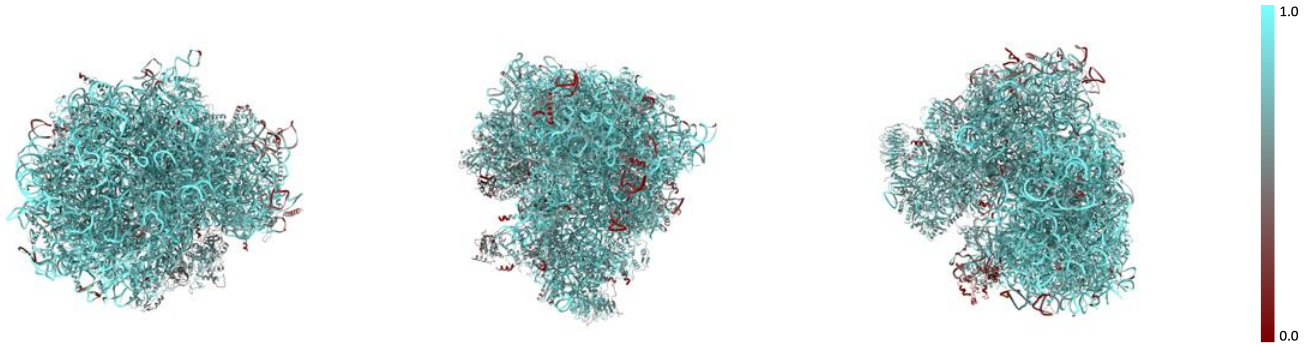
9.2 Q-score mapped to coordinate model (i)



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.

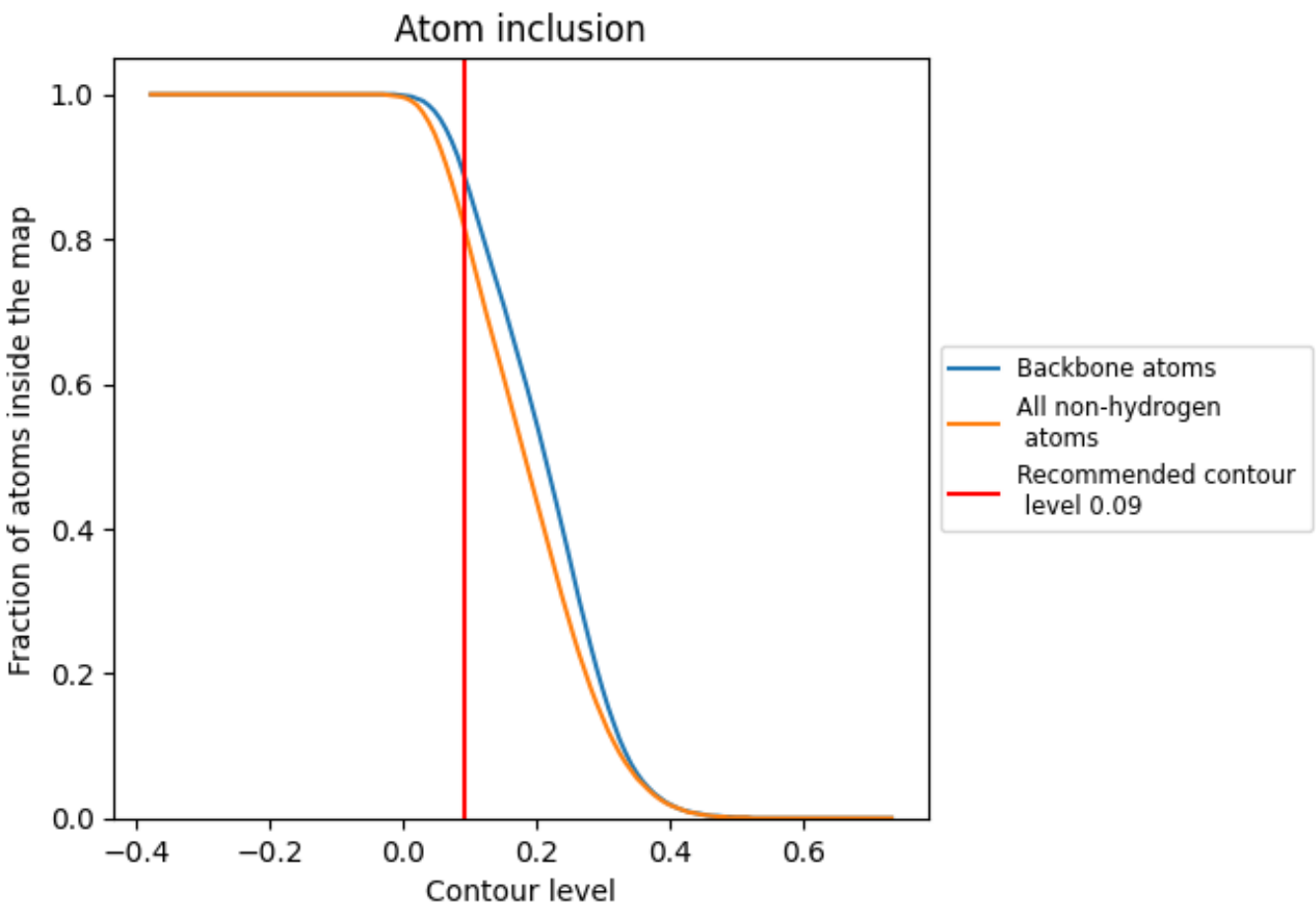
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8200	0.4860
5	0.8940	0.4930
7	0.9460	0.5210
8	0.9100	0.5010
9	0.8650	0.4680
A	0.8390	0.5480
AA	0.7710	0.4910
B	0.8670	0.5460
BB	0.7200	0.4820
C	0.8430	0.5400
CC	0.7840	0.5130
D	0.8320	0.5040
DD	0.7010	0.4740
E	0.8150	0.5160
EE	0.7290	0.4850
F	0.8250	0.5370
FF	0.6960	0.4600
G	0.7730	0.4990
GG	0.6590	0.4410
H	0.7990	0.5270
HH	0.6650	0.4530
I	0.8170	0.5310
II	0.7470	0.4970
J	0.7830	0.4970
JJ	0.7210	0.4760
KK	0.7230	0.4450
L	0.8160	0.5210
LL	0.7710	0.5210
M	0.8440	0.5210
MM	0.4210	0.2910
N	0.8760	0.5560
NN	0.7670	0.5110
O	0.8530	0.5390
OO	0.7430	0.4930
P	0.8370	0.5370

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Chain	Atom inclusion	Q-score
PP	0.7100	0.4520
Q	0.8530	0.5460
QQ	0.7360	0.4780
R	0.7830	0.5120
RR	0.6930	0.4710
S	0.8560	0.5410
SS	0.6980	0.4540
T	0.8090	0.5320
TT	0.7300	0.4610
U	0.7620	0.4700
UU	0.7270	0.4580
V	0.8210	0.5440
VV	0.7540	0.4930
W	0.6410	0.4420
WW	0.7910	0.5150
X	0.8020	0.5220
XX	0.7530	0.5140
Y	0.8150	0.5270
YY	0.6980	0.4510
Z	0.8320	0.5160
ZZ	0.6380	0.4220
a	0.8670	0.5540
aa	0.7740	0.5120
b	0.7120	0.4810
bb	0.7000	0.4820
c	0.8080	0.5110
cc	0.6600	0.4710
d	0.8130	0.5170
dd	0.8400	0.5150
e	0.8150	0.5450
ee	0.6290	0.4480
f	0.8690	0.5590
ff	0.4920	0.3380
g	0.8000	0.5260
gg	0.6680	0.4220
h	0.7930	0.5170
i	0.7990	0.5110
j	0.8720	0.5460
k	0.7270	0.4800
l	0.8170	0.5300
m	0.8350	0.5360
n	0.7610	0.5090

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Chain	Atom inclusion	Q-score
o	0.8020	0.5420
p	0.7790	0.5290
r	0.8510	0.5360
s	0.6150	0.4070
t	0.3700	0.2830
u	0.1320	0.2110
v	0.5360	0.3910
w	0.3160	0.3470