



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 06:57 AM 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 ⓘ symbol.

The types of validation reports are described at

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

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

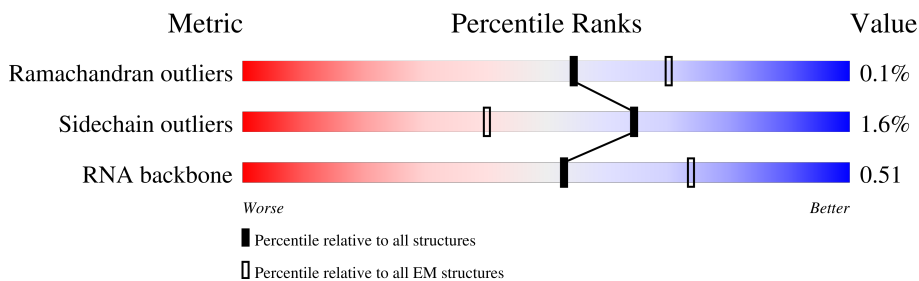
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	5	3597	
2	7	120	
3	8	151	
4	A	248	
5	B	394	
6	C	362	
7	D	293	
8	E	291	

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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

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
14	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 15 is a protein called eL14.

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

- Molecule 16 is a protein called eL15.

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

- Molecule 17 is a protein called uL13.

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

- Molecule 18 is a protein called uL22.

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

- Molecule 19 is a protein called eL18.

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

- Molecule 20 is a protein called eL19.

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

- 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
28	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 29 is a protein called uL15.

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

- Molecule 30 is a protein called eL29.

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

- Molecule 31 is a protein called eL30.

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

- Molecule 32 is a protein called eL31.

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

- Molecule 33 is a protein called eL32.

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

- Molecule 34 is a protein called eL33.

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

- Molecule 35 is a protein called eL34.

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

- Molecule 36 is a protein called uL29.

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

- Molecule 37 is a protein called eL36.

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

- Molecule 38 is a protein called eL37.

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

- Molecule 39 is a protein called eL38.

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

- Molecule 40 is a protein called eL39.

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

- Molecule 41 is a protein called eL40.

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

- Molecule 42 is a protein called eL41.

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

- Molecule 43 is a protein called eL42.

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

- Molecule 44 is a protein called eL43.

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

- Molecule 45 is a protein called eL28.

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

- Molecule 46 is a protein called uL10.

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

- Molecule 47 is a protein called eL11.

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

- Molecule 48 is a protein called uL1.

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

- 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
56	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- 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
70	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 71 is a protein called eS19.

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- 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
85	5	200	Total	Mg	0
			200	200	
85	7	7	Total	Mg	0
			7	7	
85	8	6	Total	Mg	0
			6	6	
85	A	1	Total	Mg	0
			1	1	
85	P	1	Total	Mg	0
			1	1	
85	V	1	Total	Mg	0
			1	1	
85	a	1	Total	Mg	0
			1	1	
85	g	1	Total	Mg	0
			1	1	
85	v	1	Total	Mg	0
			1	1	
85	9	73	Total	Mg	0
			73	73	
85	SS	2	Total	Mg	0
			2	2	
85	TT	1	Total	Mg	0
			1	1	
85	aa	1	Total	Mg	0
			1	1	
85	dd	1	Total	Mg	0
			1	1	

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

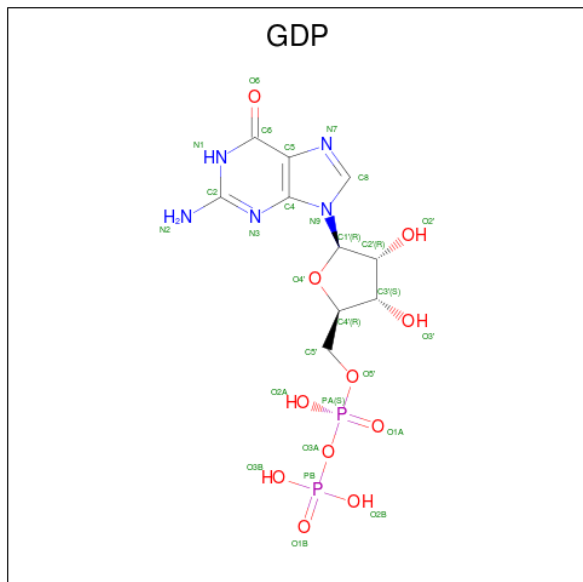
Mol	Chain	Residues	Atoms		AltConf
86	g	1	Total	Zn	0
			1	1	
86	j	1	Total	Zn	0
			1	1	
86	m	1	Total	Zn	0
			1	1	

Continued on next page...

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

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

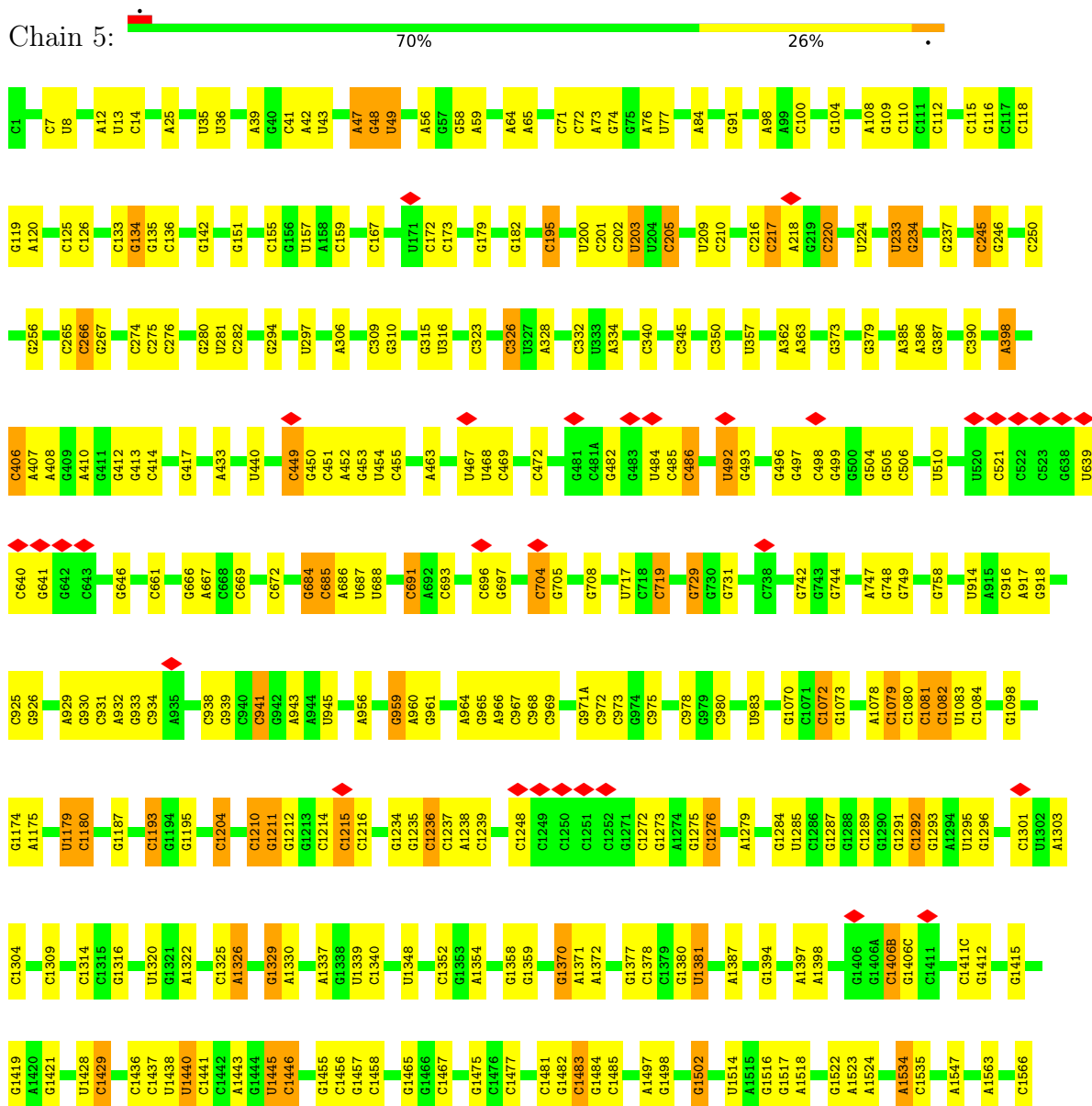


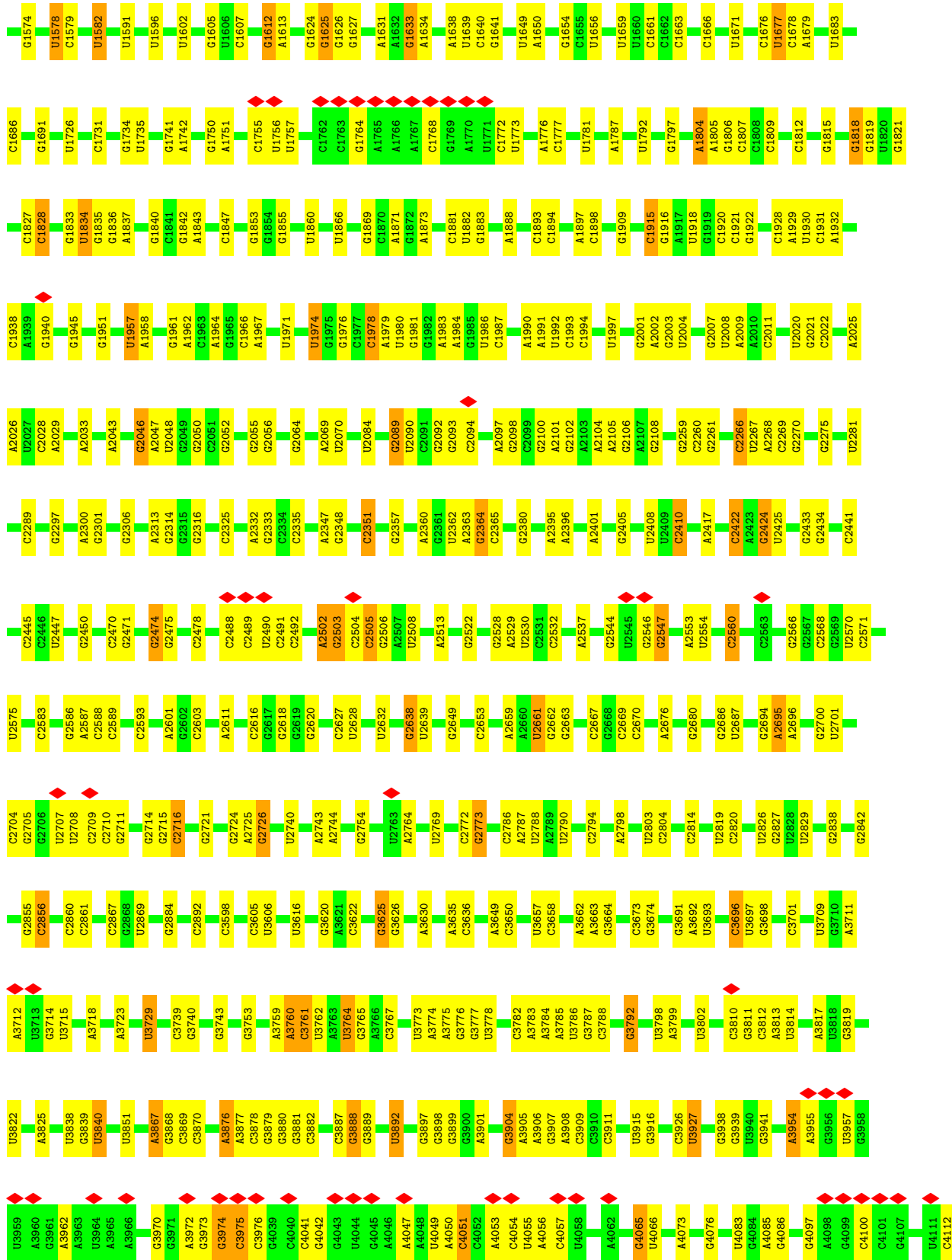
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
87	v	1	28	10	5	11	2	0

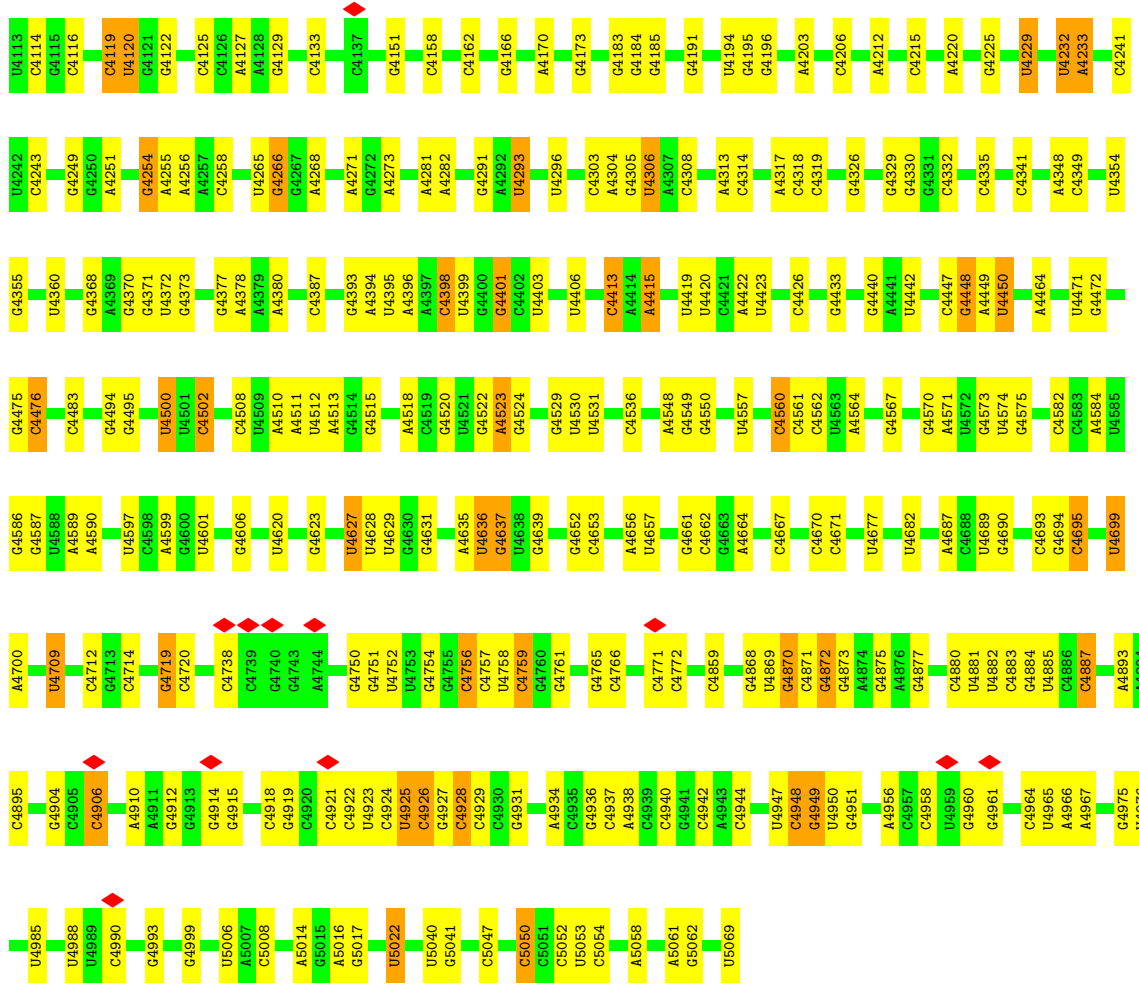
3 Residue-property plots [i](#)

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.

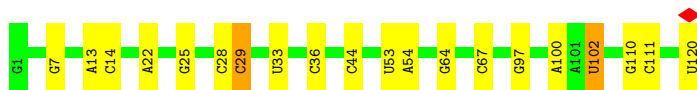
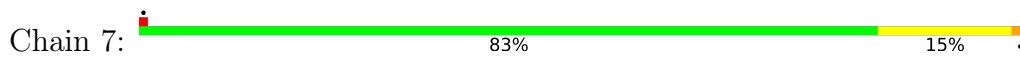
- Molecule 1: 28S rRNA



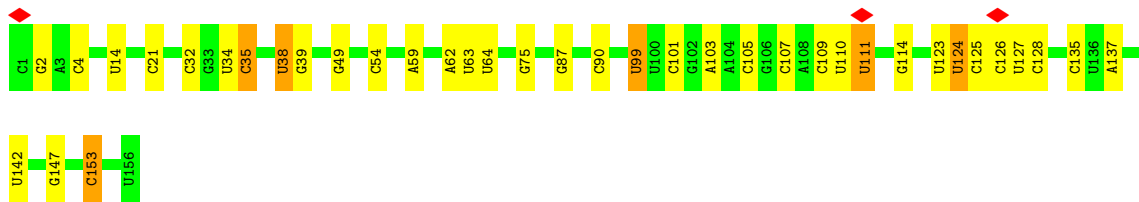
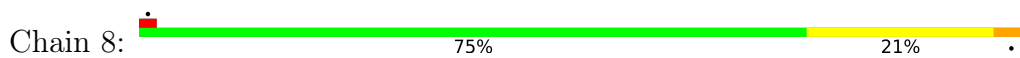




• Molecule 2: 5S rRNA

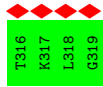


• Molecule 3: 5.8S rRNA

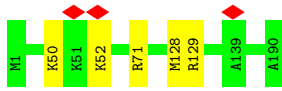


• Molecule 4: uL2

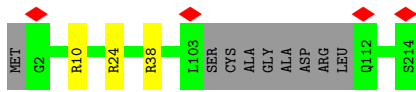




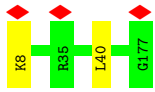
- Molecule 11: uL6



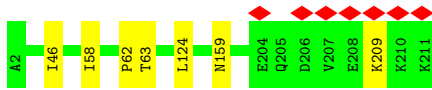
- Molecule 12: uL16



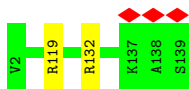
- Molecule 13: uL5



- Molecule 14: eL13



- Molecule 15: eL14

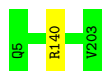


- Molecule 16: eL15



- Molecule 17: uL13

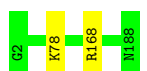




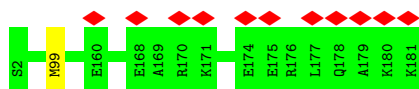
- Molecule 18: uL22



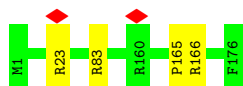
- Molecule 19: eL18



- Molecule 20: eL19



- Molecule 21: eL20



- Molecule 22: eL21

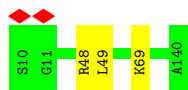


- Molecule 23: eL22

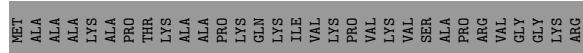
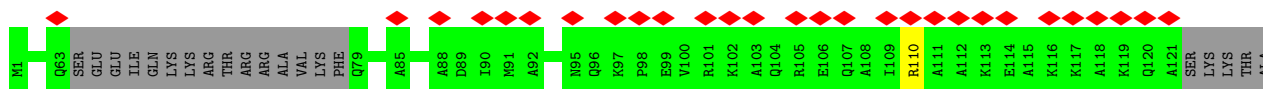


- Molecule 24: uL14

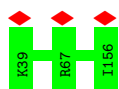




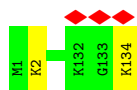
• Molecule 25: eL24



• Molecule 26: uL23



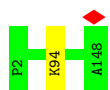
• Molecule 27: uL24



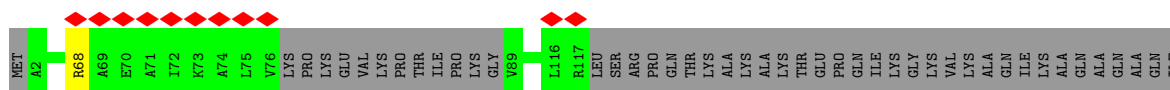
• Molecule 28: eL27



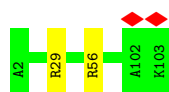
• Molecule 29: uL15



• Molecule 30: eL29

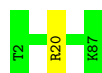


Chain i:  98%



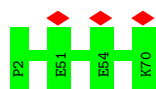
• Molecule 38: eL37

Chain j:  99%



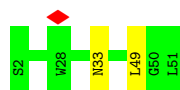
• Molecule 39: eL38

Chain k:  100%



• Molecule 40: eL39

Chain l:  96%



• Molecule 41: eL40

Chain m:  96%



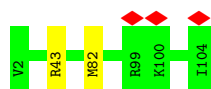
• Molecule 42: eL41

Chain n:  100%



• Molecule 43: eL42

Chain o:  98%



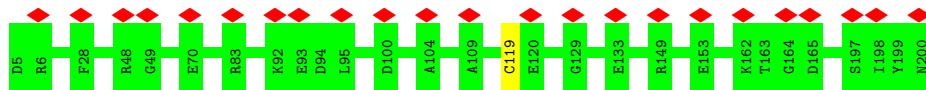
• Molecule 44: eL43



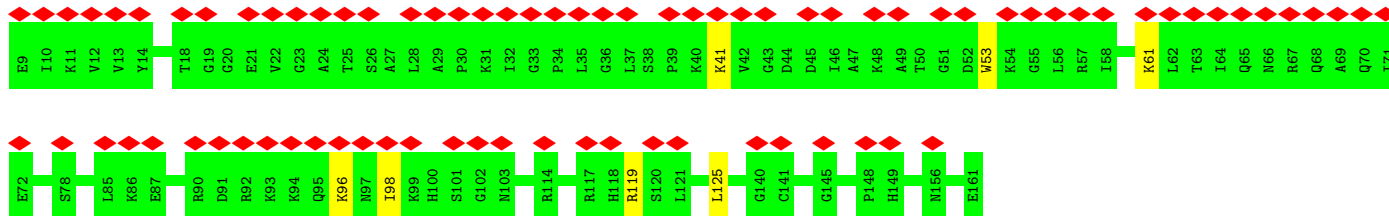
• Molecule 45: eI28



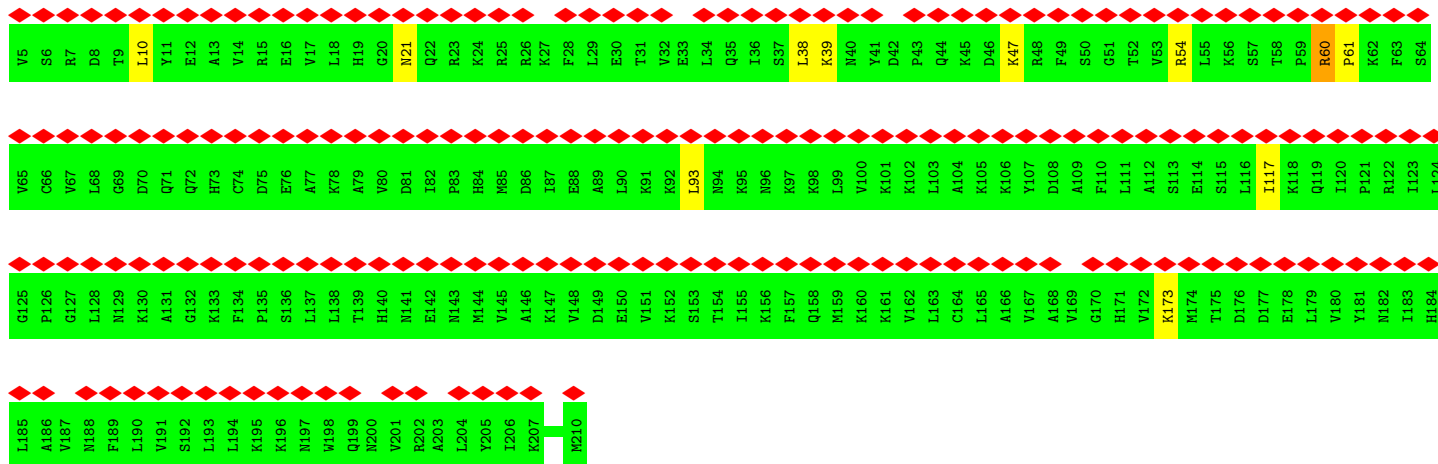
• Molecule 46: uL10



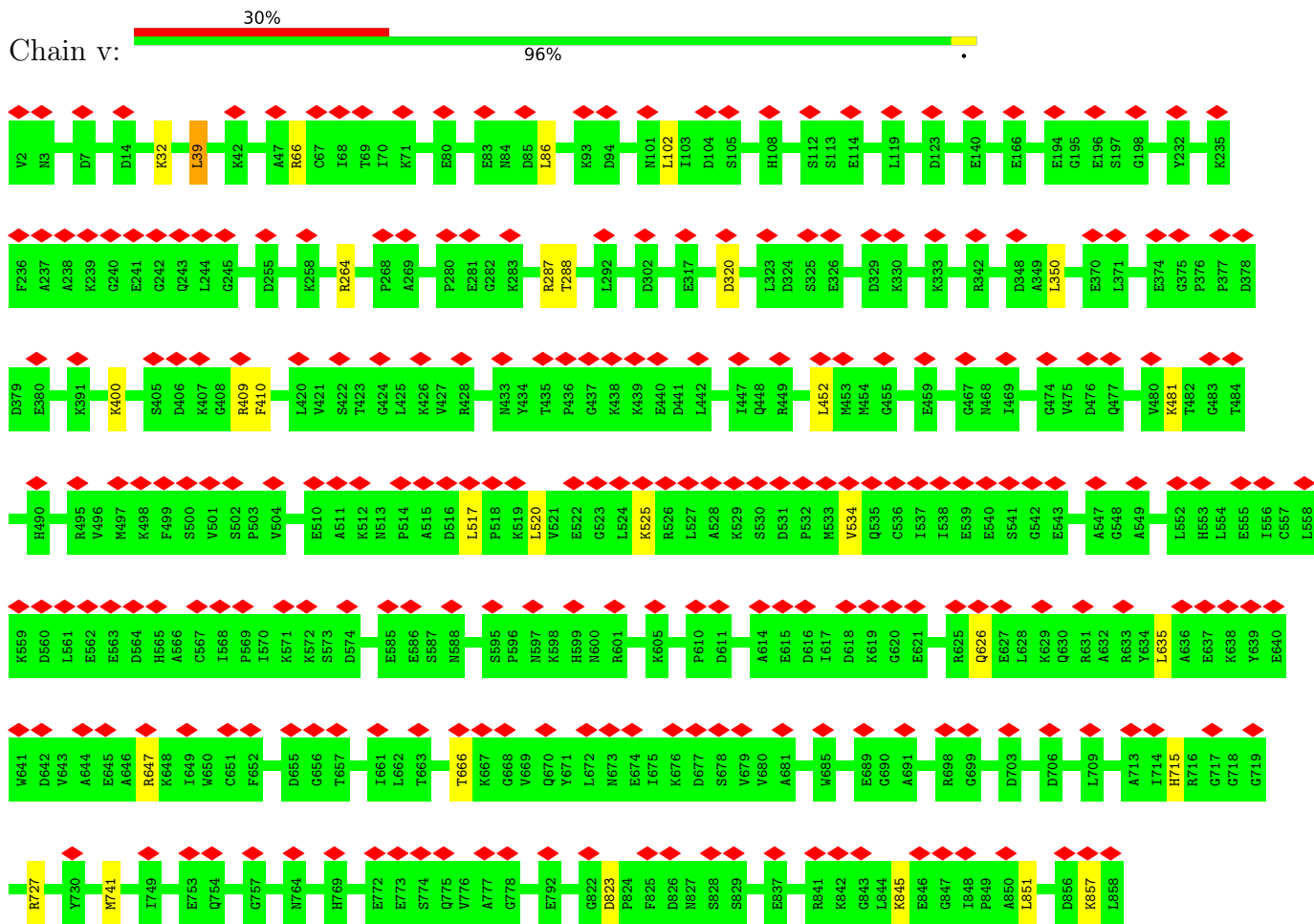
• Molecule 47: eL11



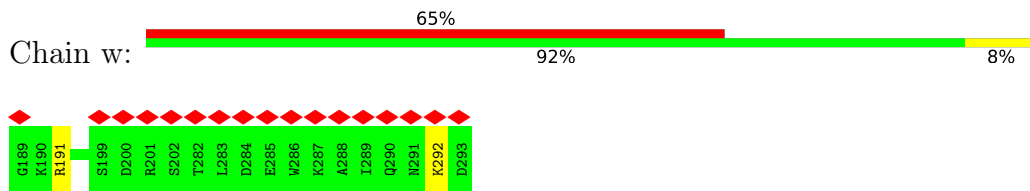
• Molecule 48: uL1



• Molecule 49: eEF2

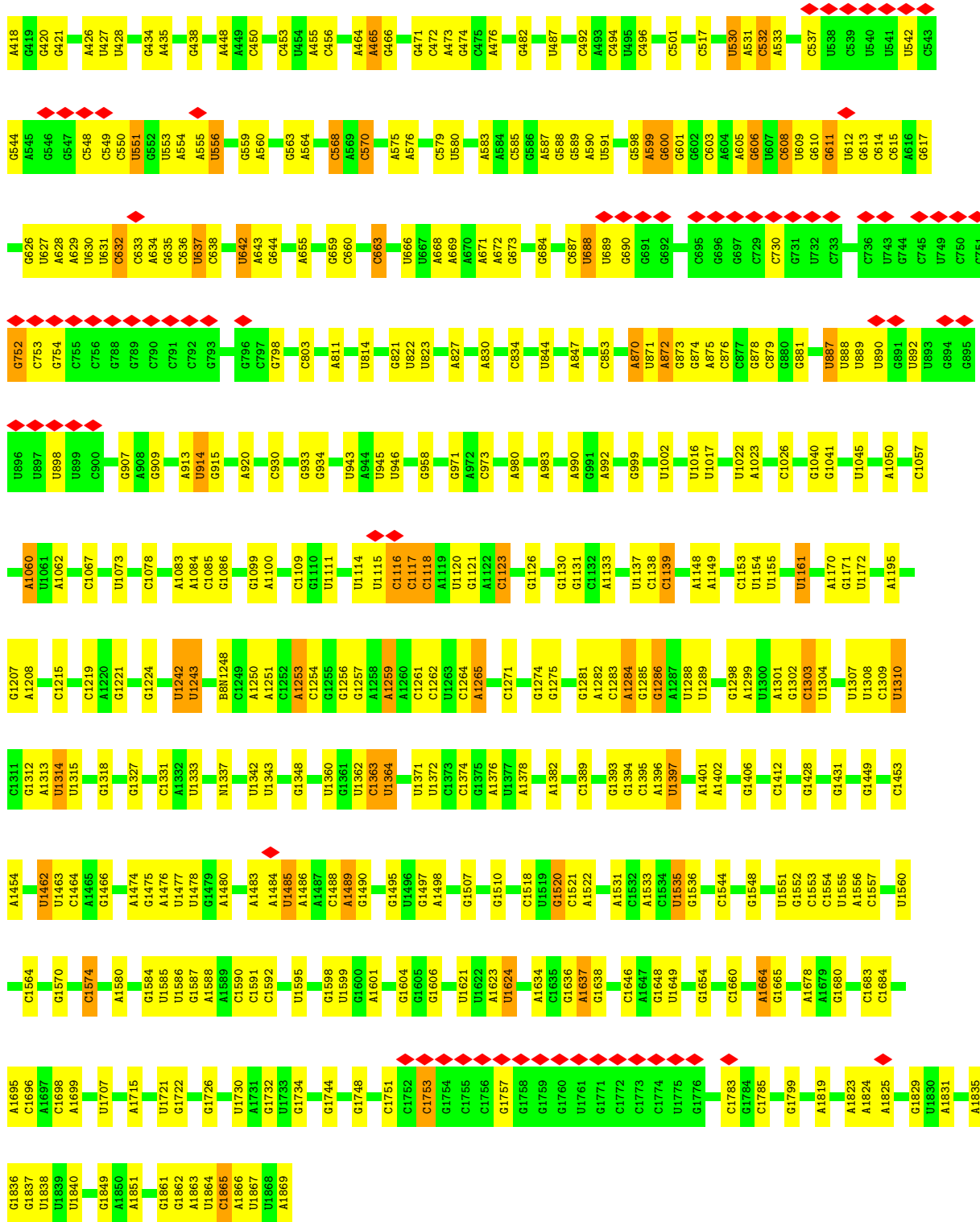


• Molecule 50: SERBP1



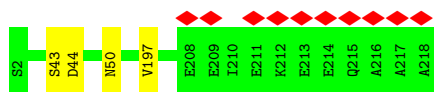
• Molecule 51: 18S rRNA





• Molecule 52: uS2

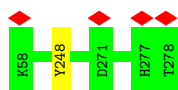




- Molecule 53: eS1



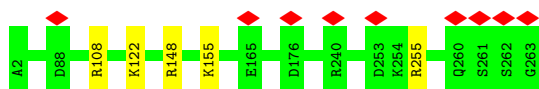
- Molecule 54: uS5



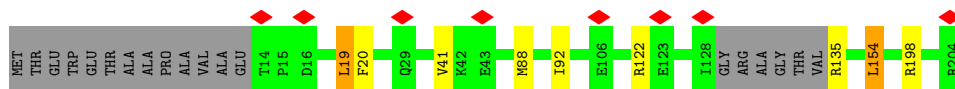
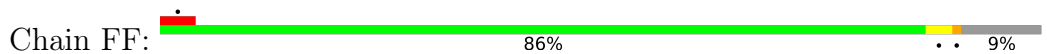
- Molecule 55: uS3



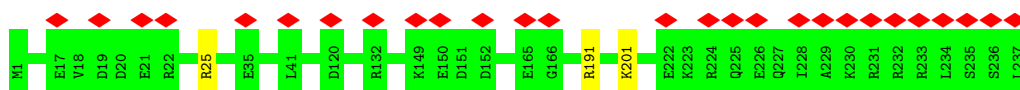
- Molecule 56: eS4



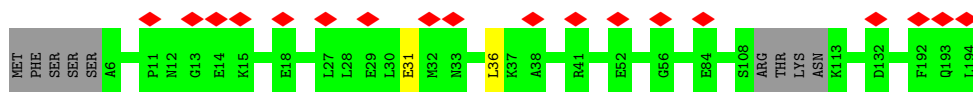
- Molecule 57: uS7



- Molecule 58: eS6



- Molecule 59: eS7



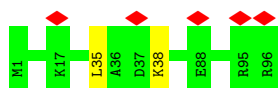
• Molecule 60: eS8



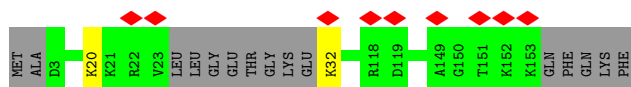
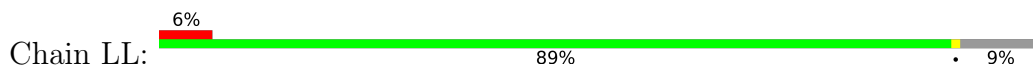
• Molecule 61: uS4



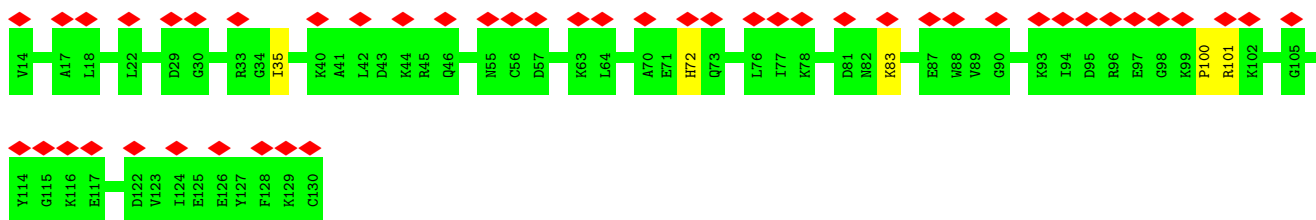
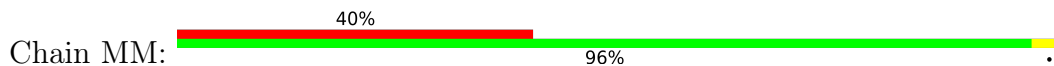
• Molecule 62: eS10



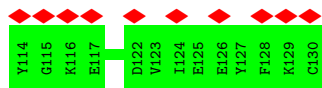
• Molecule 63: uS17

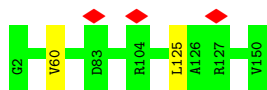


• Molecule 64: eS12

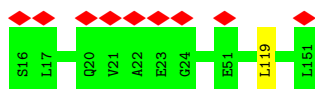


• Molecule 65: uS15

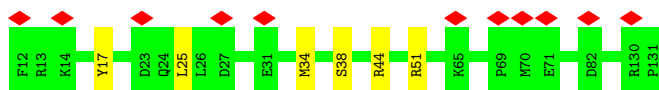




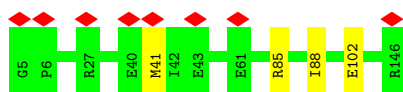
- Molecule 66: uS11



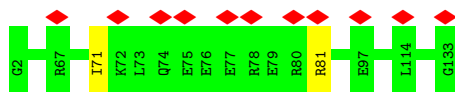
- Molecule 67: uS19



- Molecule 68: uS9



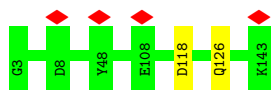
- Molecule 69: eS17



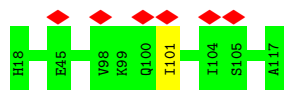
- Molecule 70: uS13



- Molecule 71: eS19



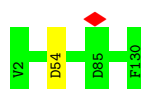
- Molecule 72: uS10



- Molecule 73: eS21



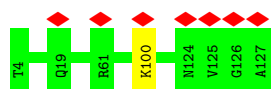
- Molecule 74: uS8



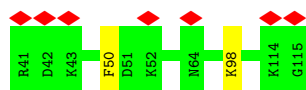
- Molecule 75: uS12



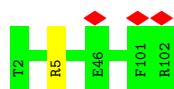
- Molecule 76: eS24



- Molecule 77: eS25



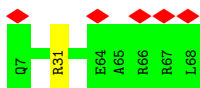
- Molecule 78: eS26



- Molecule 79: eS27



- Molecule 80: eS28

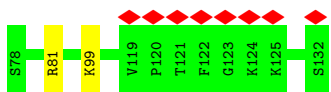


- Molecule 81: uS14

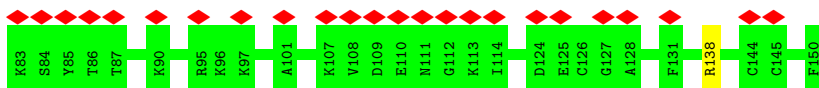


There are no outlier residues recorded for this chain.

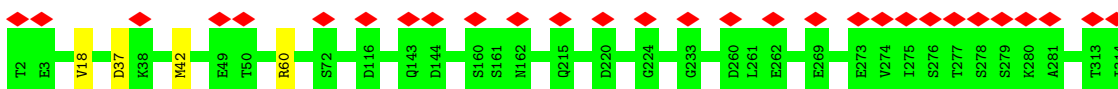
- Molecule 82: eS30



- Molecule 83: eS31



- Molecule 84: RACK1



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 (\AA)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: B8T, DDE, UR3, ZN, P7G, 7MG, B8H, B9B, PSU, 2MG, I4U, A2M, B9H, B8Q, OMG, B8K, M7A, E7G, P4U, 5MC, GDP, MG, E6G, 4AC, BGH, 6MZ, B8W, 5MU, MLZ, OMU, B8N, OMC, MHG, 1MA

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(°)	Ideal(°)
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%)	25	57
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%)	19	51
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%)	7	32
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%)	22	54
48	u	204/206 (99%)	178 (87%)	24 (12%)	2 (1%)	15	46
49	v	834/839 (99%)	754 (90%)	78 (9%)	2 (0%)	47	77
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%)	25	57
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%)	29	61
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%)	6	30
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%)	54	81

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%)	39	67
5	B	342/342 (100%)	337 (98%)	5 (2%)	65	81
6	C	301/301 (100%)	296 (98%)	5 (2%)	60	78
7	D	247/247 (100%)	243 (98%)	4 (2%)	62	79
8	E	190/251 (76%)	187 (98%)	3 (2%)	62	79
9	F	196/196 (100%)	196 (100%)	0	100	100
10	G	200/272 (74%)	193 (96%)	7 (4%)	36	64
11	H	169/169 (100%)	166 (98%)	3 (2%)	59	78
12	I	175/181 (97%)	172 (98%)	3 (2%)	60	78
13	J	143/143 (100%)	142 (99%)	1 (1%)	84	90
14	L	175/175 (100%)	170 (97%)	5 (3%)	42	69
15	M	117/117 (100%)	115 (98%)	2 (2%)	60	78
16	N	171/171 (100%)	168 (98%)	3 (2%)	59	78
17	O	171/171 (100%)	170 (99%)	1 (1%)	86	91
18	P	134/134 (100%)	132 (98%)	2 (2%)	65	81
19	Q	164/164 (100%)	162 (99%)	2 (1%)	71	83
20	R	159/159 (100%)	159 (100%)	0	100	100
21	S	157/157 (100%)	155 (99%)	2 (1%)	69	82
22	T	139/139 (100%)	139 (100%)	0	100	100
23	U	89/89 (100%)	86 (97%)	3 (3%)	37	65
24	V	101/101 (100%)	99 (98%)	2 (2%)	55	76
25	W	86/126 (68%)	85 (99%)	1 (1%)	71	83
26	X	106/106 (100%)	106 (100%)	0	100	100
27	Y	124/124 (100%)	122 (98%)	2 (2%)	62	79
28	Z	117/117 (100%)	114 (97%)	3 (3%)	46	71
29	a	119/119 (100%)	118 (99%)	1 (1%)	81	89
30	b	84/184 (46%)	83 (99%)	1 (1%)	71	83
31	c	84/84 (100%)	80 (95%)	4 (5%)	25	56
32	d	98/98 (100%)	98 (100%)	0	100	100
33	e	114/114 (100%)	113 (99%)	1 (1%)	78	87
34	f	88/88 (100%)	86 (98%)	2 (2%)	50	73
35	g	98/98 (100%)	96 (98%)	2 (2%)	55	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	h	109/109 (100%)	108 (99%)	1 (1%)	78	87
37	i	86/86 (100%)	84 (98%)	2 (2%)	50	73
38	j	73/73 (100%)	72 (99%)	1 (1%)	67	82
39	k	64/64 (100%)	64 (100%)	0	100	100
40	l	47/47 (100%)	46 (98%)	1 (2%)	53	75
41	m	47/47 (100%)	46 (98%)	1 (2%)	53	75
42	n	24/24 (100%)	24 (100%)	0	100	100
43	o	91/91 (100%)	89 (98%)	2 (2%)	52	74
44	p	74/74 (100%)	74 (100%)	0	100	100
45	r	108/108 (100%)	105 (97%)	3 (3%)	43	70
46	s	164/164 (100%)	164 (100%)	0	100	100
47	t	126/126 (100%)	122 (97%)	4 (3%)	39	67
48	u	186/186 (100%)	179 (96%)	7 (4%)	33	62
49	v	713/713 (100%)	699 (98%)	14 (2%)	55	76
50	w	23/23 (100%)	21 (91%)	2 (9%)	10	34
52	AA	180/181 (99%)	179 (99%)	1 (1%)	86	91
53	BB	194/194 (100%)	193 (100%)	1 (0%)	88	93
54	CC	187/187 (100%)	186 (100%)	1 (0%)	88	93
55	DD	190/190 (100%)	184 (97%)	6 (3%)	39	67
56	EE	224/224 (100%)	220 (98%)	4 (2%)	59	78
57	FF	158/170 (93%)	153 (97%)	5 (3%)	39	67
58	GG	207/207 (100%)	204 (99%)	3 (1%)	67	82
59	HH	165/174 (95%)	163 (99%)	2 (1%)	71	83
60	II	178/178 (100%)	178 (100%)	0	100	100
61	JJ	161/161 (100%)	157 (98%)	4 (2%)	47	72
62	KK	87/87 (100%)	87 (100%)	0	100	100
63	LL	130/142 (92%)	128 (98%)	2 (2%)	65	81
64	MM	99/99 (100%)	96 (97%)	3 (3%)	41	68
65	NN	130/130 (100%)	129 (99%)	1 (1%)	81	89
66	OO	106/106 (100%)	106 (100%)	0	100	100
67	PP	109/109 (100%)	107 (98%)	2 (2%)	59	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	QQ	117/117 (100%)	113 (97%)	4 (3%)	37	65
69	RR	119/119 (100%)	117 (98%)	2 (2%)	60	78
70	SS	125/125 (100%)	122 (98%)	3 (2%)	49	73
71	TT	111/111 (100%)	110 (99%)	1 (1%)	78	87
72	UU	92/92 (100%)	91 (99%)	1 (1%)	73	85
73	VV	67/67 (100%)	66 (98%)	1 (2%)	65	81
74	WW	112/112 (100%)	112 (100%)	0	100	100
75	XX	113/113 (100%)	112 (99%)	1 (1%)	78	87
76	YY	107/107 (100%)	106 (99%)	1 (1%)	78	87
77	ZZ	66/66 (100%)	65 (98%)	1 (2%)	65	81
78	aa	88/88 (100%)	87 (99%)	1 (1%)	73	85
79	bb	75/75 (100%)	72 (96%)	3 (4%)	31	61
80	cc	55/55 (100%)	54 (98%)	1 (2%)	59	78
81	dd	48/48 (100%)	48 (100%)	0	100	100
82	ee	46/46 (100%)	44 (96%)	2 (4%)	29	59
83	ff	61/61 (100%)	60 (98%)	1 (2%)	62	79
84	gg	272/272 (100%)	269 (99%)	3 (1%)	73	85
All	All	10962/11275 (97%)	10787 (98%)	175 (2%)	64	79

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	1MA	5	1322	1,85	16,25,26	3.73	4 (25%)	18,37,40	1.68	3 (16%)
51	5MC	9	1374	51	18,22,23	3.63	7 (38%)	26,32,35	1.10	2 (7%)
1	OMC	5	2804	1	19,22,23	2.83	7 (36%)	26,31,34	0.80	0
1	B8T	5	4671	1	19,22,23	3.01	8 (42%)	26,31,34	0.94	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	B8Q	5	1456	1	17,22,23	2.70	5 (29%)	22,32,35	2.05	5 (22%)
1	MHG	5	4371	1	29,32,33	3.94	11 (37%)	34,46,49	2.38	12 (35%)
1	7MG	5	4550	1	22,26,27	3.50	10 (45%)	29,39,42	1.96	8 (27%)
1	A2M	5	3785	1	18,25,26	4.59	9 (50%)	18,36,39	2.44	3 (16%)
1	A2M	5	4571	1	18,25,26	4.79	9 (50%)	18,36,39	2.60	4 (22%)
1	PSU	5	4403	1	18,21,22	1.00	1 (5%)	22,30,33	1.73	5 (22%)
51	PSU	9	1243	51	18,21,22	1.17	1 (5%)	22,30,33	1.33	4 (18%)
1	A2M	5	2401	1,85	18,25,26	4.73	9 (50%)	18,36,39	2.66	3 (16%)
1	P7G	5	1909	1	24,28,29	4.13	11 (45%)	27,41,44	1.74	4 (14%)
1	B8H	5	3762	1	19,22,23	6.80	6 (31%)	22,32,35	2.39	5 (22%)
6	MLZ	C	333	6	8,9,10	0.84	0	4,9,11	0.70	0
1	OMG	5	1316	1	18,26,27	2.46	8 (44%)	19,38,41	1.66	4 (21%)
1	OMC	5	3887	1	19,22,23	2.83	7 (36%)	26,31,34	0.89	1 (3%)
1	A2M	5	398	1	18,25,26	4.80	9 (50%)	18,36,39	2.55	3 (16%)
1	OMC	5	2365	1	19,22,23	2.84	7 (36%)	26,31,34	0.68	0
1	P7G	5	3880	1	24,28,29	3.86	10 (41%)	27,41,44	1.60	4 (14%)
1	PSU	5	1677	1	18,21,22	1.10	3 (16%)	22,30,33	1.89	6 (27%)
1	OMG	5	373	1	18,26,27	2.49	8 (44%)	19,38,41	1.64	5 (26%)
51	4AC	9	1337	51	21,24,25	3.16	9 (42%)	29,34,37	1.13	3 (10%)
1	A2M	5	1524	1	18,25,26	4.71	9 (50%)	18,36,39	2.65	3 (16%)
1	OMG	5	3792	1	18,26,27	2.50	8 (44%)	19,38,41	1.58	4 (21%)
1	B9B	5	237	1	21,28,29	6.35	9 (42%)	23,40,43	2.26	5 (21%)
1	PSU	5	4500	1	18,21,22	1.00	1 (5%)	22,30,33	1.90	4 (18%)
1	OMG	5	1883	1	18,26,27	2.49	8 (44%)	19,38,41	1.67	4 (21%)
1	2MG	5	4872	15,1	18,26,27	2.62	7 (38%)	16,38,41	1.72	4 (25%)
1	OMC	5	4536	1	19,22,23	2.84	7 (36%)	26,31,34	0.99	1 (3%)
1	OMG	5	2424	1	18,26,27	2.53	8 (44%)	19,38,41	1.56	4 (21%)
1	OMC	5	3869	1	19,22,23	2.82	7 (36%)	26,31,34	0.70	0
1	B8W	5	4529	1,85	18,26,27	5.28	8 (44%)	21,38,41	6.32	10 (47%)
1	5MC	5	4447	1	18,22,23	3.67	7 (38%)	26,32,35	1.09	1 (3%)
1	2MG	5	729	1	18,26,27	2.45	7 (38%)	16,38,41	1.36	3 (18%)
1	A2M	5	4523	1,85	18,25,26	4.83	9 (50%)	18,36,39	2.58	3 (16%)
1	I4U	5	1659	1	21,24,25	4.92	15 (71%)	27,34,37	1.42	2 (7%)
1	PSU	5	4442	1	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
1	OMG	5	4637	1	18,26,27	2.42	8 (44%)	19,38,41	1.52	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	B8W	5	4185	1	18,26,27	5.15	8 (44%)	21,38,41	5.96	11 (52%)
1	B9B	5	1574	1	21,28,29	6.29	9 (42%)	23,40,43	2.19	6 (26%)
1	UR3	5	1866	1	19,22,23	2.54	6 (31%)	26,32,35	1.35	4 (15%)
1	2MG	5	1517	1	18,26,27	2.52	7 (38%)	16,38,41	1.63	4 (25%)
1	OMU	5	4620	1	19,22,23	2.70	7 (36%)	26,31,34	1.70	5 (19%)
51	A2M	9	1678	51	18,25,26	4.87	9 (50%)	18,36,39	2.63	3 (16%)
49	DDE	v	715	49	14,20,21	1.00	0	14,28,30	1.30	2 (14%)
1	5MU	5	4083	1	19,22,23	4.77	7 (36%)	28,32,35	3.59	10 (35%)
1	OMC	5	2422	1,85	19,22,23	2.91	7 (36%)	26,31,34	0.94	1 (3%)
1	E6G	5	4355	1	20,27,28	5.77	9 (45%)	22,39,42	2.07	7 (31%)
1	OMG	5	2050	1	18,26,27	2.45	8 (44%)	19,38,41	1.49	4 (21%)
3	OMU	8	14	1,3	19,22,23	2.79	7 (36%)	26,31,34	1.98	7 (26%)
1	B8W	5	2380	1	18,26,27	5.23	7 (38%)	21,38,41	6.10	7 (33%)
1	5MC	5	4335	1	18,22,23	3.56	7 (38%)	26,32,35	1.27	3 (11%)
1	P4U	5	1348	1,85	21,24,25	3.37	8 (38%)	27,33,36	1.43	3 (11%)
1	B8W	5	4129	1	18,26,27	5.25	8 (44%)	21,38,41	6.11	9 (42%)
1	7MG	5	2522	1	22,26,27	3.52	10 (45%)	29,39,42	1.98	8 (27%)
1	UR3	5	4530	1	19,22,23	2.65	6 (31%)	26,32,35	1.30	2 (7%)
1	OMU	5	4306	1	19,22,23	2.81	7 (36%)	26,31,34	1.76	5 (19%)
1	B8T	5	4483	1	19,22,23	3.06	8 (42%)	26,31,34	1.01	2 (7%)
1	A2M	5	3867	1	18,25,26	4.63	9 (50%)	18,36,39	2.58	3 (16%)
1	B8K	5	4690	1,11	24,28,29	5.03	17 (70%)	30,42,45	2.59	11 (36%)
1	PSU	5	1683	1	18,21,22	1.11	1 (5%)	22,30,33	1.79	4 (18%)
1	OMC	5	2861	1	19,22,23	2.88	7 (36%)	26,31,34	0.90	1 (3%)
1	OMG	5	2773	1	18,26,27	2.51	8 (44%)	19,38,41	1.49	4 (21%)
1	PSU	5	4628	1	18,21,22	1.12	2 (11%)	22,30,33	1.99	4 (18%)
1	PSU	5	3764	1	18,21,22	1.04	1 (5%)	22,30,33	1.64	4 (18%)
1	OMG	5	4196	1	18,26,27	2.47	8 (44%)	19,38,41	1.57	4 (21%)
1	OMC	5	3909	1	19,22,23	2.84	7 (36%)	26,31,34	0.73	0
1	6MZ	5	4220	1	18,25,26	2.14	4 (22%)	16,36,39	2.07	4 (25%)
1	A2M	5	1326	1	18,25,26	4.67	9 (50%)	18,36,39	2.67	3 (16%)
1	PSU	5	3729	1	18,21,22	1.03	1 (5%)	22,30,33	1.70	4 (18%)
1	M7A	5	4564	1	20,25,26	1.96	3 (15%)	28,37,40	3.86	8 (28%)
1	OMG	5	4623	1	18,26,27	2.48	8 (44%)	19,38,41	1.60	4 (21%)
1	OMG	5	1625	1,85	18,26,27	2.46	8 (44%)	19,38,41	1.51	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	5	4450	1,85	18,21,22	1.06	2 (11%)	22,30,33	1.92	4 (18%)
1	BGH	5	3899	1,85	25,29,30	4.22	16 (64%)	31,43,46	2.51	13 (41%)
1	UR3	5	4597	1	19,22,23	2.62	6 (31%)	26,32,35	1.32	3 (11%)
1	B8H	5	1860	1	19,22,23	6.80	6 (31%)	22,32,35	2.33	5 (22%)
1	OMG	5	4494	1	18,26,27	2.47	8 (44%)	19,38,41	1.58	4 (21%)
1	1MA	5	4415	1	16,25,26	3.94	4 (25%)	18,37,40	1.66	3 (16%)
1	A2M	5	1871	1,85	18,25,26	4.77	9 (50%)	18,36,39	2.72	3 (16%)
1	A2M	5	2363	1,85	18,25,26	4.76	9 (50%)	18,36,39	2.73	4 (22%)
1	PSU	5	3715	1	18,21,22	0.98	1 (5%)	22,30,33	1.64	4 (18%)
1	PSU	5	4531	1	18,21,22	1.03	1 (5%)	22,30,33	1.85	5 (22%)
41	MLZ	m	72	41	8,9,10	0.73	0	4,9,11	0.77	0
1	A2M	5	1534	1,85	18,25,26	4.68	9 (50%)	18,36,39	2.71	4 (22%)
1	OMG	5	2364	1	18,26,27	2.46	8 (44%)	19,38,41	1.58	4 (21%)
1	E7G	5	2297	1	24,27,28	3.48	11 (45%)	30,40,43	2.15	9 (30%)
1	7MG	5	1605	1	22,26,27	3.45	10 (45%)	29,39,42	2.04	9 (31%)
1	OMG	5	1522	1	18,26,27	2.49	8 (44%)	19,38,41	1.60	4 (21%)
1	OMG	5	4870	1	18,26,27	2.44	8 (44%)	19,38,41	1.55	3 (15%)
1	OMG	5	4370	1	18,26,27	2.52	8 (44%)	19,38,41	1.51	4 (21%)
1	B8K	5	3897	1	24,28,29	4.76	17 (70%)	30,42,45	2.56	12 (40%)
51	B8N	9	1248	51	24,29,30	2.79	7 (29%)	29,42,45	1.75	5 (17%)
1	A2M	5	3718	1	18,25,26	4.78	10 (55%)	18,36,39	2.50	3 (16%)
1	PSU	5	2508	1	18,21,22	0.98	1 (5%)	22,30,33	1.62	3 (13%)
1	PSU	5	1582	1	18,21,22	1.15	2 (11%)	22,30,33	1.70	4 (18%)
1	B8H	5	4296	1	19,22,23	6.81	6 (31%)	22,32,35	2.40	5 (22%)
1	PSU	5	4636	1	18,21,22	1.04	2 (11%)	22,30,33	1.93	4 (18%)
51	B8Q	9	1219	51	17,22,23	2.95	4 (23%)	22,32,35	2.80	7 (31%)
1	I4U	5	4194	1	21,24,25	4.96	15 (71%)	27,34,37	1.17	2 (7%)
1	5MC	5	3782	1	18,22,23	3.61	7 (38%)	26,32,35	1.11	1 (3%)
1	A2M	5	3825	1	18,25,26	4.74	7 (38%)	18,36,39	2.69	3 (16%)
1	A2M	5	3723	1	18,25,26	4.84	9 (50%)	18,36,39	2.59	3 (16%)
1	B9H	5	2786	1	20,25,26	3.15	3 (15%)	22,35,38	1.90	3 (13%)
1	B8W	5	4472	1	18,26,27	5.34	8 (44%)	21,38,41	6.01	10 (47%)
1	PSU	5	4293	1	18,21,22	1.06	1 (5%)	22,30,33	1.84	4 (18%)
1	OMC	5	3701	1,85	19,22,23	2.79	7 (36%)	26,31,34	0.75	0
1	B9B	5	2754	1,85	21,28,29	6.35	9 (42%)	23,40,43	1.98	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	E7G	5	1797	1	24,27,28	3.56	11 (45%)	30,40,43	2.18	9 (30%)

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	1MA	5	1322	1,85	-	0/3/25/26	0/3/3/3
51	5MC	9	1374	51	-	0/7/25/26	0/2/2/2
1	OMC	5	2804	1	-	0/9/27/28	0/2/2/2
1	B8T	5	4671	1	-	0/7/27/28	0/2/2/2
1	B8Q	5	1456	1	-	1/7/42/43	0/2/2/2
1	MHG	5	4371	1	-	6/16/46/47	0/3/3/3
1	7MG	5	4550	1	-	0/7/37/38	0/3/3/3
1	A2M	5	3785	1	-	3/5/27/28	0/3/3/3
1	A2M	5	4571	1	-	0/5/27/28	0/3/3/3
1	PSU	5	4403	1	-	2/7/25/26	0/2/2/2
51	PSU	9	1243	51	-	2/7/25/26	0/2/2/2
1	A2M	5	2401	1,85	-	0/5/27/28	0/3/3/3
1	P7G	5	1909	1	-	2/10/40/41	0/3/3/3
1	B8H	5	3762	1	-	3/7/25/26	0/2/2/2
6	MLZ	C	333	6	-	2/7/8/10	-
1	OMG	5	1316	1	-	0/5/27/28	0/3/3/3
1	OMC	5	3887	1	-	1/9/27/28	0/2/2/2
1	A2M	5	398	1	-	2/5/27/28	0/3/3/3
1	OMC	5	2365	1	-	0/9/27/28	0/2/2/2
1	P7G	5	3880	1	-	3/10/40/41	0/3/3/3
1	PSU	5	1677	1	-	0/7/25/26	0/2/2/2
1	OMG	5	373	1	-	1/5/27/28	0/3/3/3
51	4AC	9	1337	51	-	0/11/29/30	0/2/2/2
1	A2M	5	1524	1	-	0/5/27/28	0/3/3/3
1	OMG	5	3792	1	-	2/5/27/28	0/3/3/3
1	B9B	5	237	1	-	4/7/29/30	0/3/3/3
1	PSU	5	4500	1	-	4/7/25/26	0/2/2/2
1	OMG	5	1883	1	-	0/5/27/28	0/3/3/3
1	2MG	5	4872	15,1	-	2/5/27/28	0/3/3/3
1	OMC	5	4536	1	-	0/9/27/28	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	OMC	5	3869	1	-	0/9/27/28	0/2/2/2
1	B8W	5	4529	1,85	-	2/5/27/28	0/3/3/3
1	5MC	5	4447	1	-	4/7/25/26	0/2/2/2
1	2MG	5	729	1	-	1/5/27/28	0/3/3/3
1	A2M	5	4523	1,85	-	2/5/27/28	0/3/3/3
1	I4U	5	1659	1	-	2/9/29/30	0/2/2/2
1	PSU	5	4442	1	-	0/7/25/26	0/2/2/2
1	OMG	5	4637	1	-	2/5/27/28	0/3/3/3
1	B8W	5	4185	1	-	3/5/27/28	0/3/3/3
1	B9B	5	1574	1	-	2/7/29/30	0/3/3/3
1	UR3	5	1866	1	-	2/7/25/26	0/2/2/2
1	2MG	5	1517	1	-	0/5/27/28	0/3/3/3
1	OMU	5	4620	1	-	1/9/27/28	0/2/2/2
51	A2M	9	1678	51	-	0/5/27/28	0/3/3/3
49	DDE	v	715	49	-	13/20/21/23	0/1/1/1
1	5MU	5	4083	1	-	0/7/25/26	0/2/2/2
1	OMC	5	2422	1,85	-	1/9/27/28	0/2/2/2
1	E6G	5	4355	1	-	3/6/28/29	0/3/3/3
1	OMG	5	2050	1	-	0/5/27/28	0/3/3/3
3	OMU	8	14	1,3	-	1/9/27/28	0/2/2/2
1	B8W	5	2380	1	-	5/5/27/28	0/3/3/3
1	5MC	5	4335	1	-	0/7/25/26	0/2/2/2
1	P4U	5	1348	1,85	-	4/10/29/30	0/2/2/2
1	B8W	5	4129	1	-	3/5/27/28	0/3/3/3
1	7MG	5	2522	1	-	0/7/37/38	0/3/3/3
1	UR3	5	4530	1	-	2/7/25/26	0/2/2/2
1	OMU	5	4306	1	-	0/9/27/28	0/2/2/2
1	B8T	5	4483	1	-	0/7/27/28	0/2/2/2
1	A2M	5	3867	1	-	2/5/27/28	0/3/3/3
1	B8K	5	4690	1,11	-	2/11/41/42	0/3/3/3
1	PSU	5	1683	1	-	0/7/25/26	0/2/2/2
1	OMC	5	2861	1	-	0/9/27/28	0/2/2/2
1	OMG	5	2773	1	-	2/5/27/28	0/3/3/3
1	PSU	5	4628	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	4196	1	-	0/5/27/28	0/3/3/3
1	OMC	5	3909	1	-	0/9/27/28	0/2/2/2
1	6MZ	5	4220	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	5	1326	1	-	0/5/27/28	0/3/3/3
1	PSU	5	3729	1	-	2/7/25/26	0/2/2/2
1	M7A	5	4564	1	-	0/7/37/38	0/3/3/3
1	OMG	5	4623	1	-	0/5/27/28	0/3/3/3
1	OMG	5	1625	1,85	-	3/5/27/28	0/3/3/3
1	PSU	5	4450	1,85	-	3/7/25/26	0/2/2/2
1	BGH	5	3899	1,85	-	2/13/43/44	0/3/3/3
1	UR3	5	4597	1	-	0/7/25/26	0/2/2/2
1	B8H	5	1860	1	-	0/7/25/26	0/2/2/2
1	OMG	5	4494	1	-	1/5/27/28	0/3/3/3
1	1MA	5	4415	1	-	2/3/25/26	0/3/3/3
1	A2M	5	1871	1,85	-	0/5/27/28	0/3/3/3
1	A2M	5	2363	1,85	-	0/5/27/28	0/3/3/3
1	PSU	5	3715	1	-	0/7/25/26	0/2/2/2
1	PSU	5	4531	1	-	0/7/25/26	0/2/2/2
41	MLZ	m	72	41	-	3/7/8/10	-
1	A2M	5	1534	1,85	-	2/5/27/28	0/3/3/3
1	OMG	5	2364	1	-	2/5/27/28	0/3/3/3
1	E7G	5	2297	1	-	1/9/39/40	0/3/3/3
1	7MG	5	1605	1	-	0/7/37/38	0/3/3/3
1	OMG	5	1522	1	-	0/5/27/28	0/3/3/3
1	OMG	5	4870	1	-	3/5/27/28	0/3/3/3
1	OMG	5	4370	1	-	2/5/27/28	0/3/3/3
1	B8K	5	3897	1	-	3/11/41/42	0/3/3/3
51	B8N	9	1248	51	-	4/16/34/35	0/2/2/2
1	A2M	5	3718	1	-	0/5/27/28	0/3/3/3
1	PSU	5	2508	1	-	0/7/25/26	0/2/2/2
1	PSU	5	1582	1	-	2/7/25/26	0/2/2/2
1	B8H	5	4296	1	-	0/7/25/26	0/2/2/2
1	PSU	5	4636	1	-	3/7/25/26	0/2/2/2
51	B8Q	9	1219	51	-	1/7/42/43	0/2/2/2
1	I4U	5	4194	1	-	3/9/29/30	0/2/2/2
1	5MC	5	3782	1	-	0/7/25/26	0/2/2/2
1	A2M	5	3825	1	-	0/5/27/28	0/3/3/3
1	A2M	5	3723	1	-	0/5/27/28	0/3/3/3
1	B9H	5	2786	1	-	4/12/47/48	0/2/2/2
1	B8W	5	4472	1	-	2/5/27/28	0/3/3/3
1	PSU	5	4293	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	5	3701	1,85	-	4/9/27/28	0/2/2/2
1	B9B	5	2754	1,85	-	3/7/29/30	0/3/3/3
1	E7G	5	1797	1	-	2/9/39/40	0/3/3/3

The worst 5 of 766 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2754	B9B	C2'-C1'	-18.08	1.26	1.53
1	5	1574	B9B	C2'-C1'	-17.90	1.26	1.53
1	5	237	B9B	C2'-C1'	-17.70	1.26	1.53
1	5	237	B9B	O4'-C1'	17.26	1.65	1.41
1	5	1574	B9B	O4'-C1'	16.74	1.64	1.41

The worst 5 of 475 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4529	B8W	N2-C2-N3	17.01	145.51	117.79
1	5	2380	B8W	N2-C2-N3	16.88	145.29	117.79
1	5	4129	B8W	N2-C2-N3	16.74	145.07	117.79
1	5	4185	B8W	N2-C2-N3	16.50	144.68	117.79
1	5	4472	B8W	N2-C2-N3	16.34	144.42	117.79

There are no chirality outliers.

5 of 159 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 monosaccharides in this entry.

5.6 Ligand geometry

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	-	24,30,30	0.97	1 (4%)	30,47,47	1.30	5 (16%)

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	-2.77	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	v	900	GDP	PA-O3A-PB	-3.68	120.20	132.83
87	v	900	GDP	C3'-C2'-C1'	2.91	105.36	100.98
87	v	900	GDP	C5-C6-N1	2.53	118.42	113.95
87	v	900	GDP	C8-N7-C5	2.16	107.10	102.99
87	v	900	GDP	O6-C6-C5	-2.04	120.38	124.37

There are no chirality outliers.

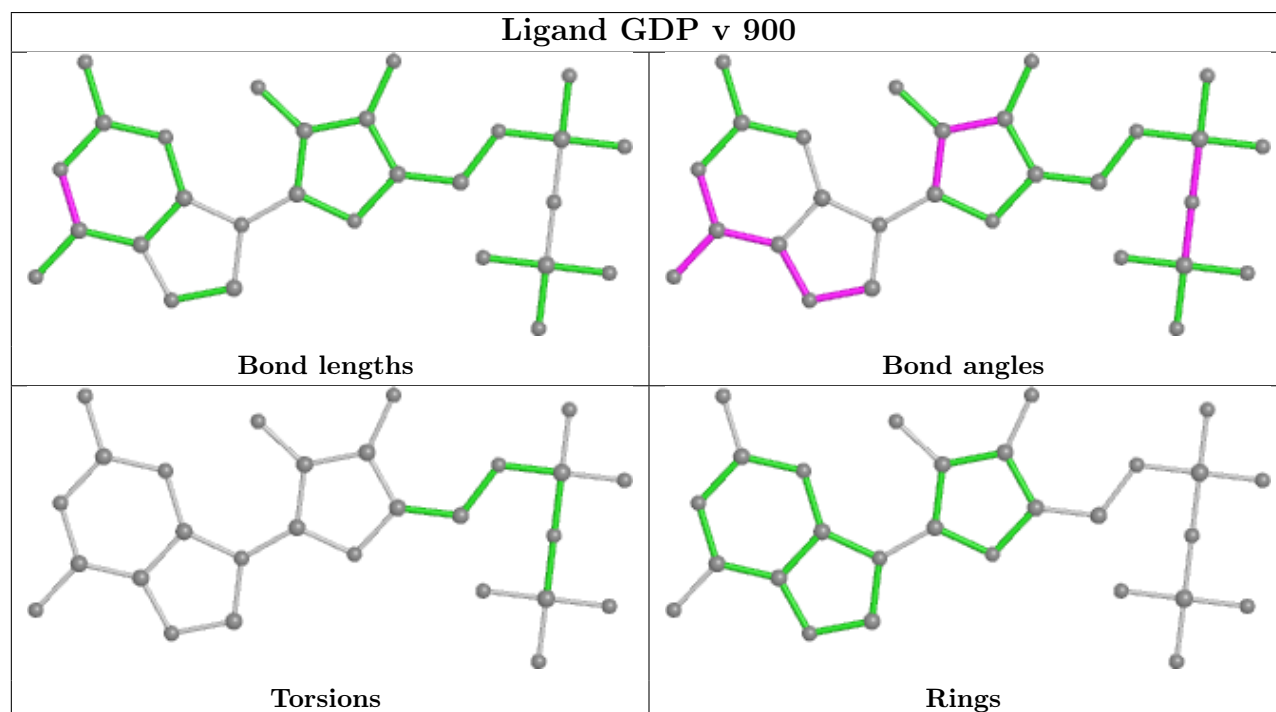
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	47
51	9	19
50	w	1
3	8	1

Continued on next page...

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Mol	Chain	Number of breaks
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

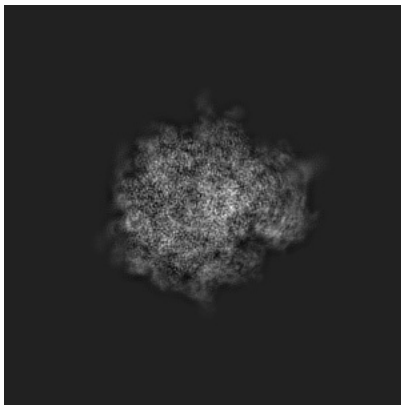
6 Map visualisation [i](#)

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.

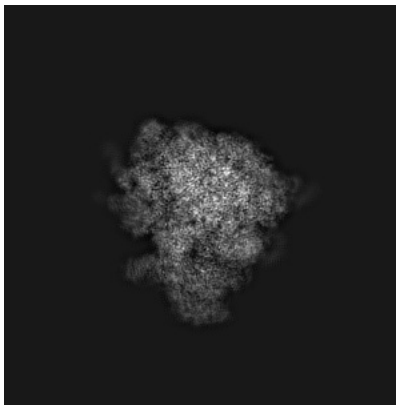
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

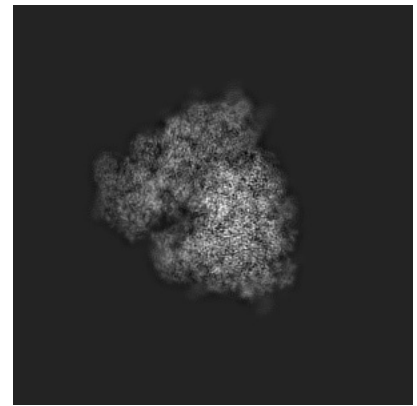
6.1.1 Primary map



X

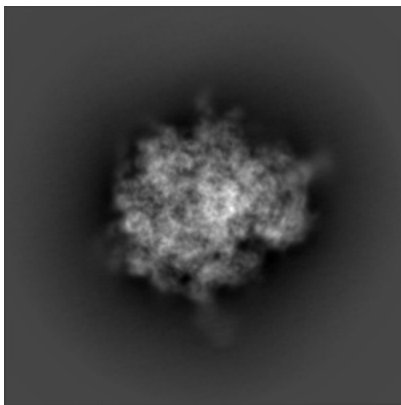


Y

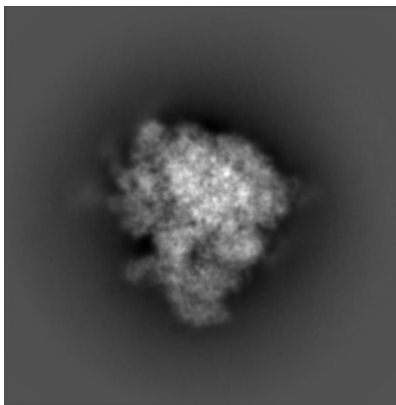


Z

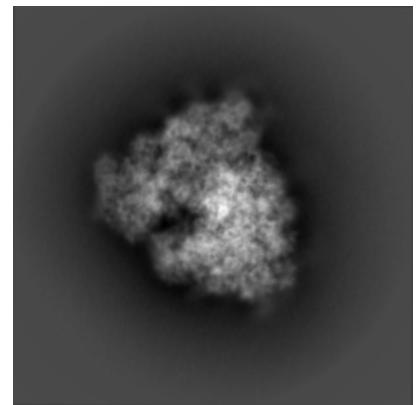
6.1.2 Raw map



X



Y

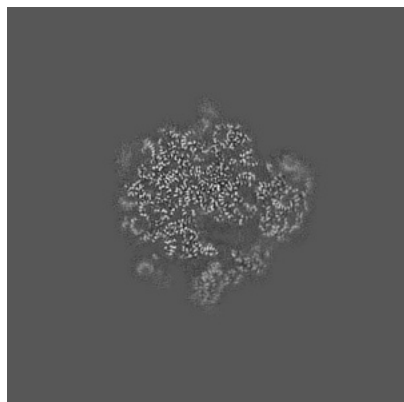


Z

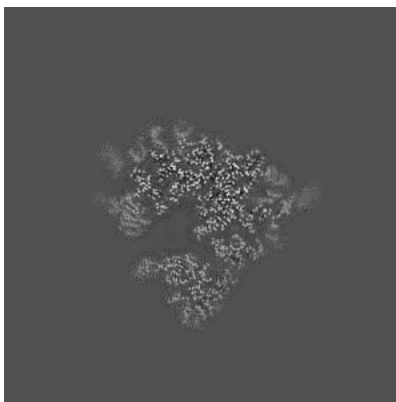
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

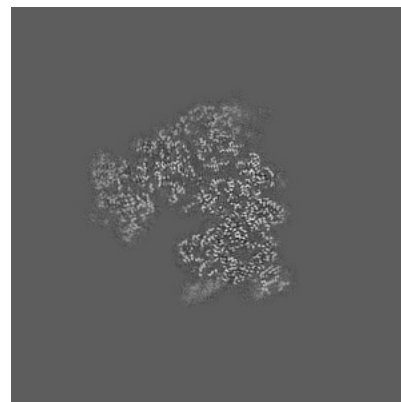
6.2.1 Primary map



X Index: 200

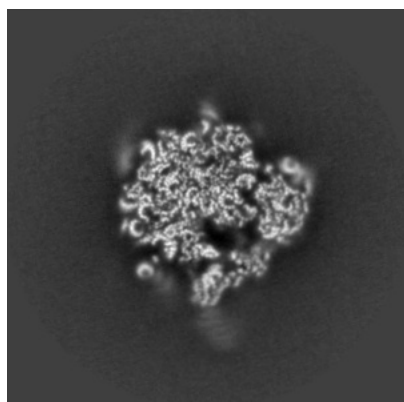


Y Index: 200

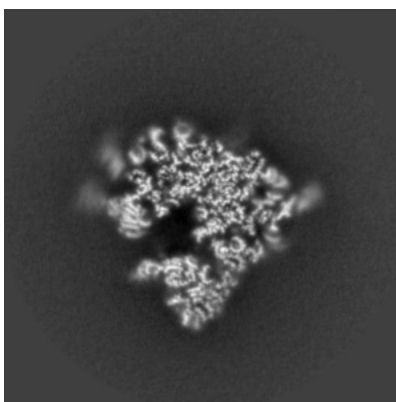


Z Index: 200

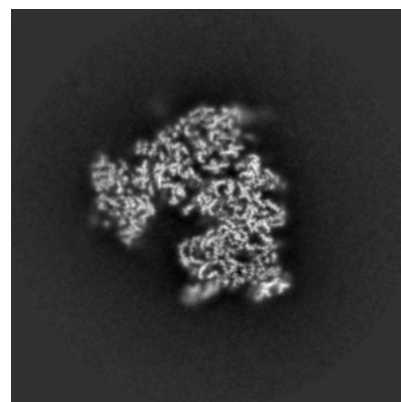
6.2.2 Raw map



X Index: 200



Y Index: 200

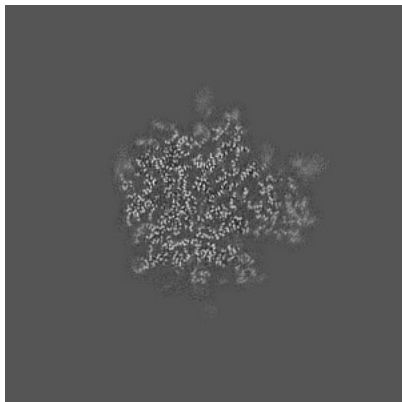


Z Index: 200

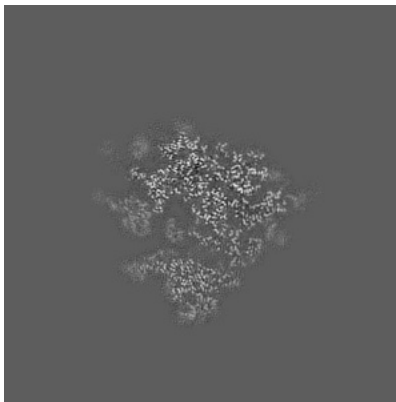
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

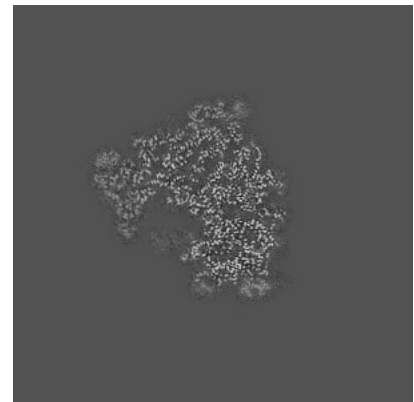
6.3.1 Primary map



X Index: 213

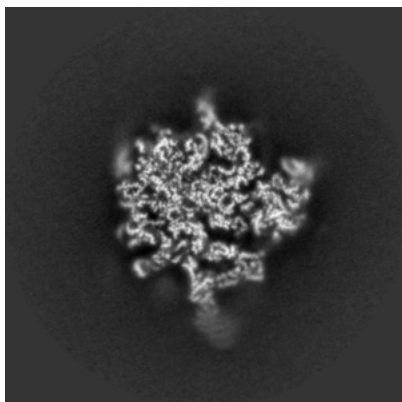


Y Index: 208

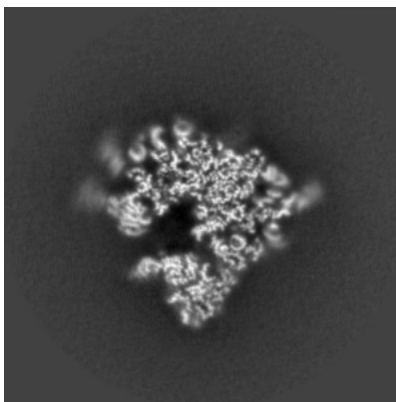


Z Index: 210

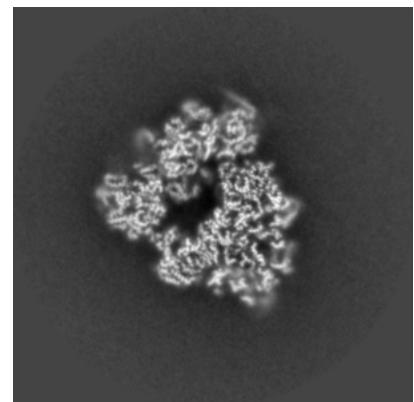
6.3.2 Raw map



X Index: 206



Y Index: 201



Z Index: 176

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

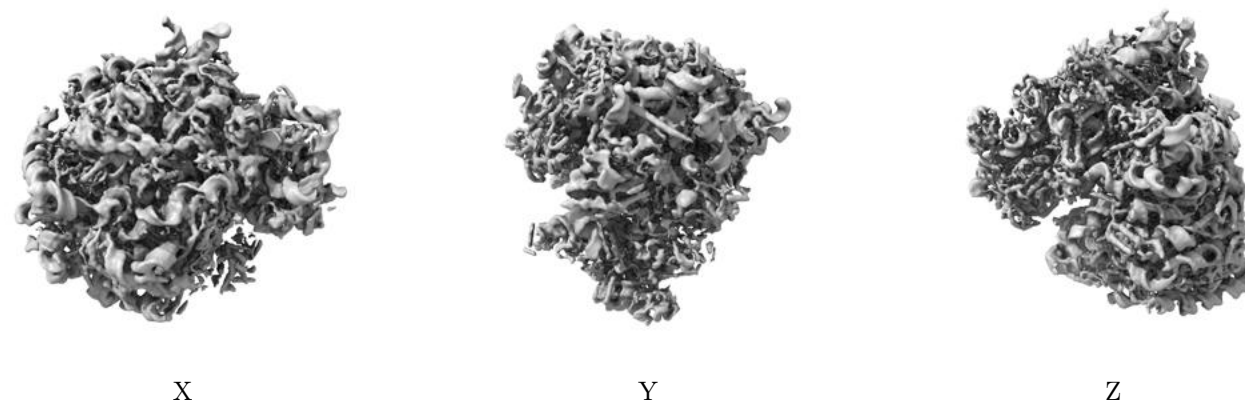
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



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.

6.4.2 Raw map



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

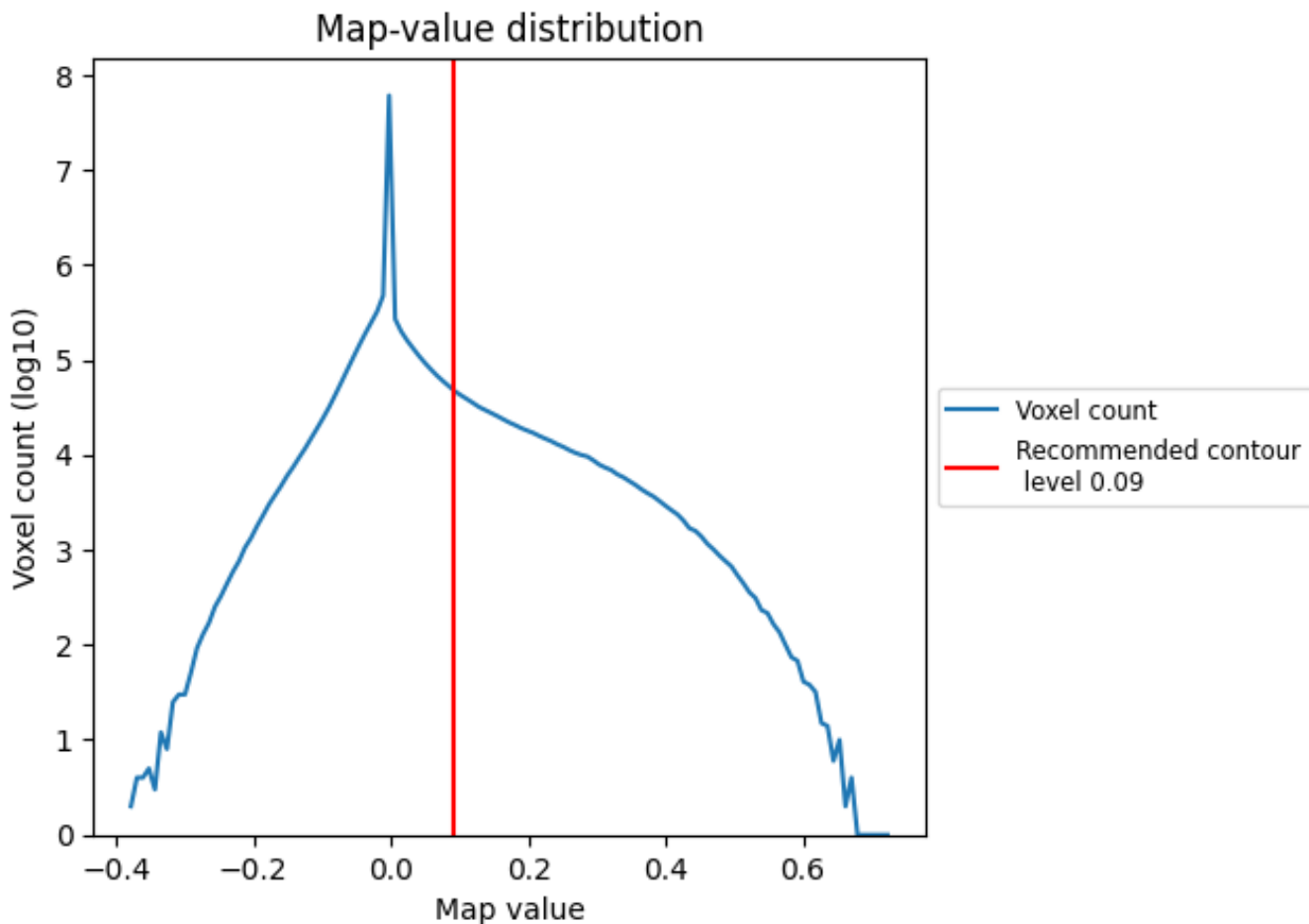
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

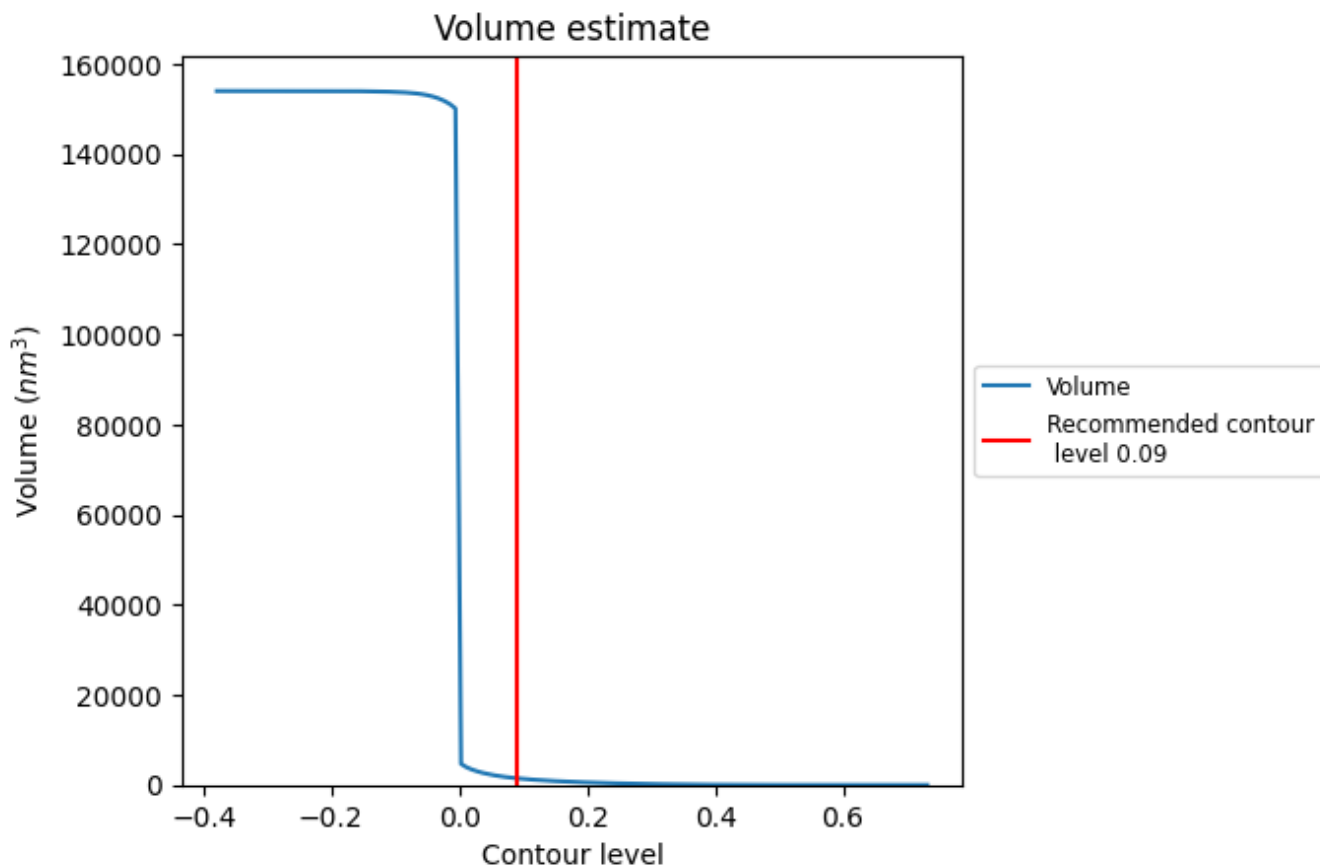
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

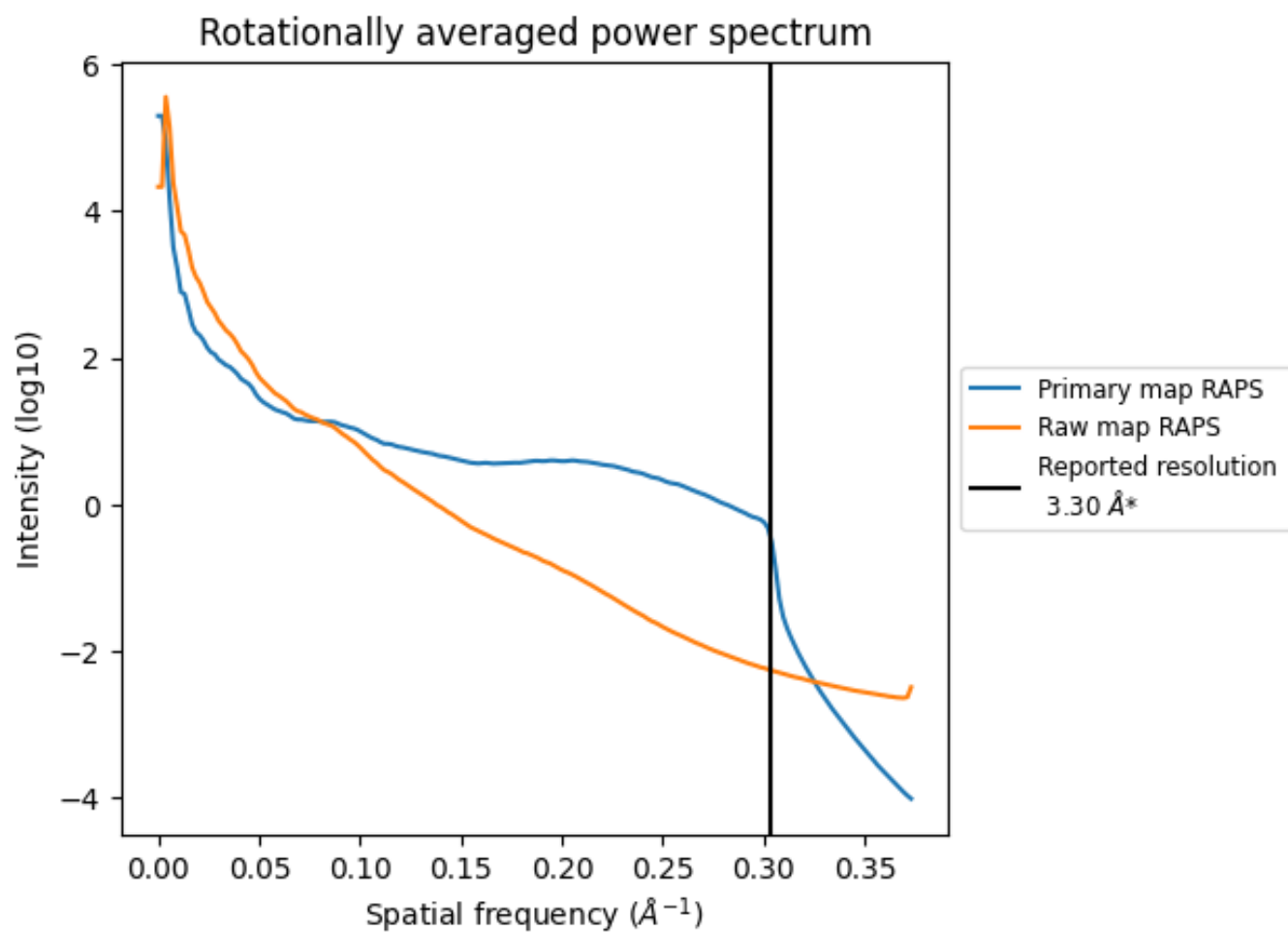
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1483 nm³; 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

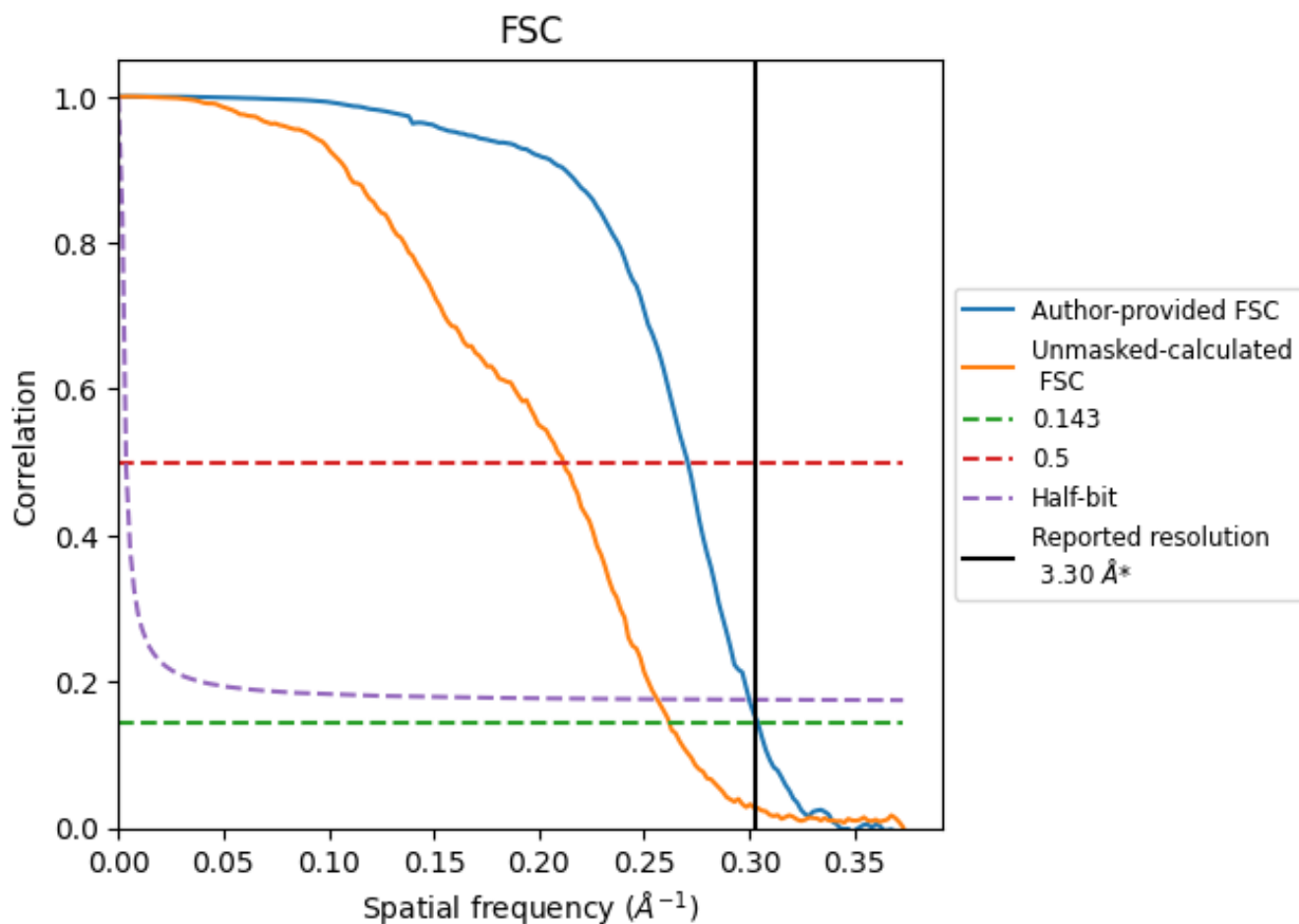


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

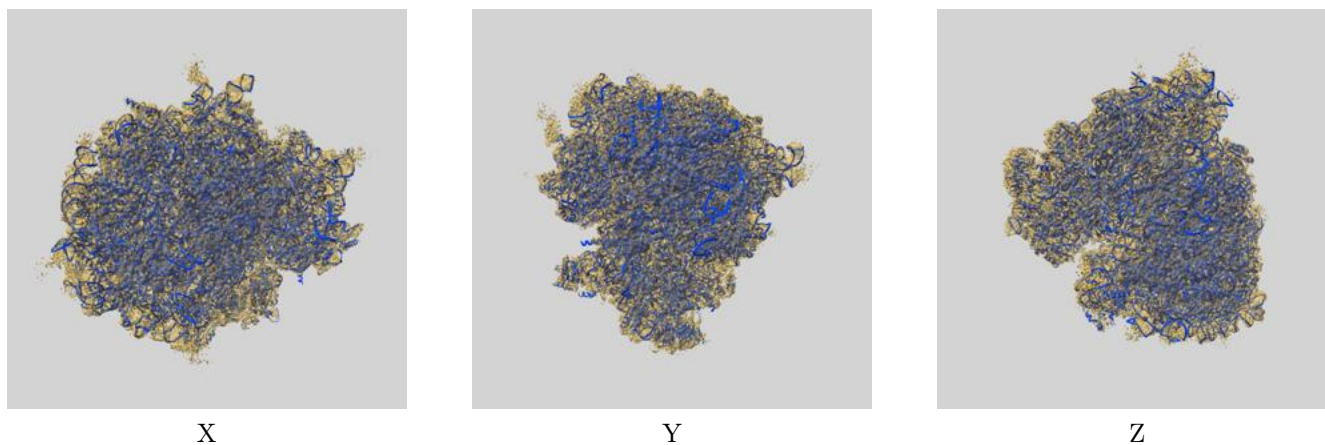
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.69	3.33
Unmasked-calculated*	3.82	4.73	3.90

*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](#)

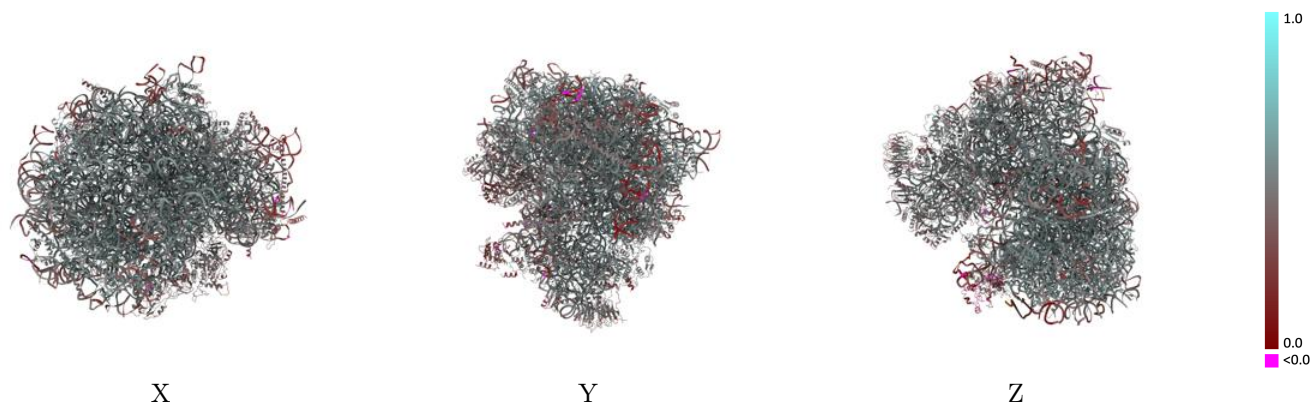
This section contains information regarding the fit between EMDB map EMD-9240 and PDB model 6MTD. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



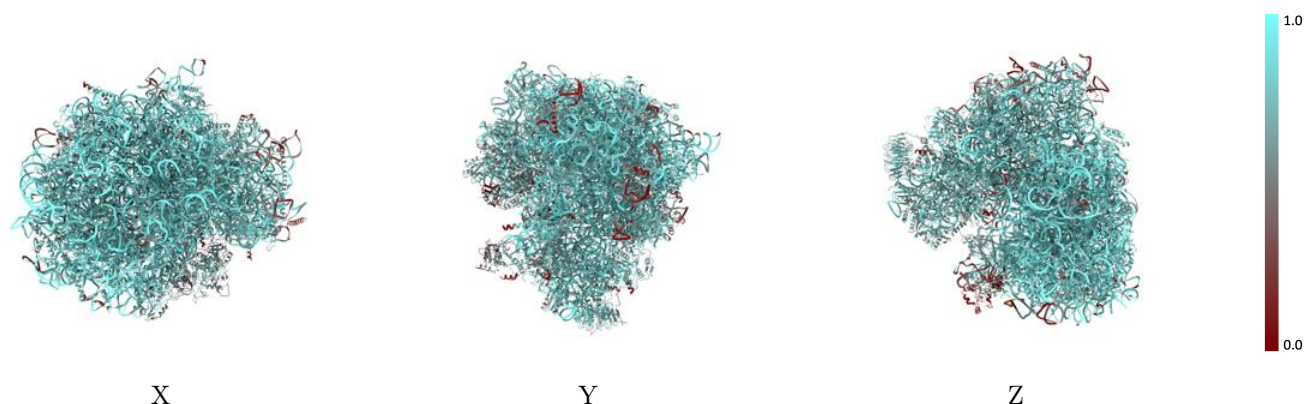
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



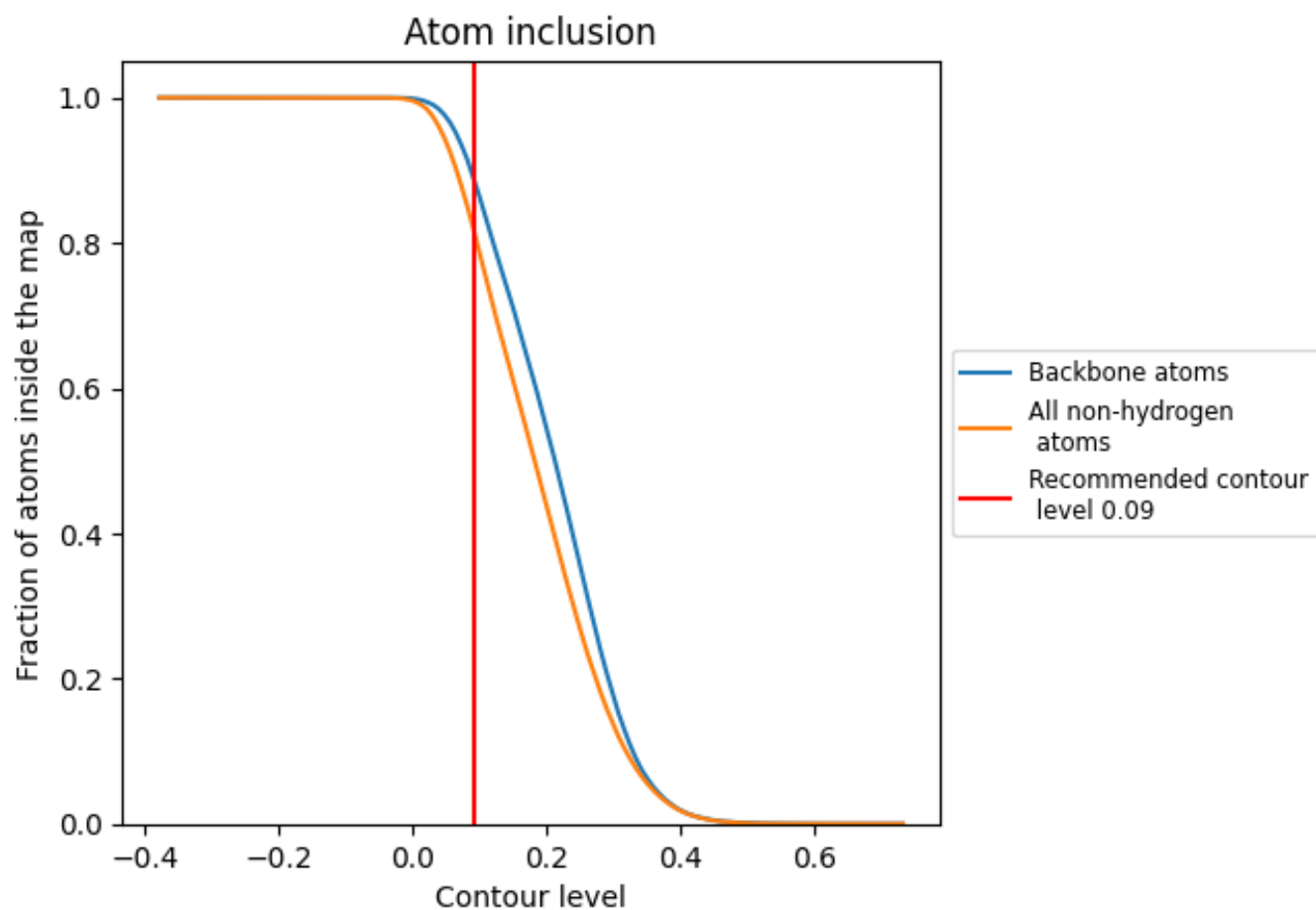
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).







































































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

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	 0.8201	 0.4860
5	 0.8944	 0.4930
7	 0.9462	 0.5210
8	 0.9098	 0.5010
9	 0.8650	 0.4680
A	 0.8393	 0.5480
AA	 0.7711	 0.4910
B	 0.8666	 0.5460
BB	 0.7198	 0.4820
C	 0.8427	 0.5400
CC	 0.7838	 0.5130
D	 0.8323	 0.5040
DD	 0.7009	 0.4740
E	 0.8148	 0.5160
EE	 0.7289	 0.4850
F	 0.8247	 0.5370
FF	 0.6955	 0.4600
G	 0.7726	 0.4990
GG	 0.6593	 0.4410
H	 0.7991	 0.5270
HH	 0.6653	 0.4530
I	 0.8166	 0.5310
II	 0.7474	 0.4970
J	 0.7835	 0.4970
JJ	 0.7208	 0.4760
KK	 0.7228	 0.4450
L	 0.8158	 0.5210
LL	 0.7711	 0.5210
M	 0.8444	 0.5210
MM	 0.4206	 0.2910
N	 0.8765	 0.5560
NN	 0.7667	 0.5110
O	 0.8529	 0.5390
OO	 0.7427	 0.4930
P	 0.8368	 0.5370



















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Chain	Atom inclusion	Q-score
PP	0.7098	0.4520
Q	0.8531	0.5460
QQ	0.7363	0.4780
R	0.7828	0.5120
RR	0.6927	0.4710
S	0.8558	0.5410
SS	0.6983	0.4540
T	0.8092	0.5320
TT	0.7303	0.4610
U	0.7623	0.4700
UU	0.7274	0.4580
V	0.8205	0.5440
VV	0.7540	0.4930
W	0.6414	0.4420
WW	0.7911	0.5150
X	0.8021	0.5220
XX	0.7526	0.5140
Y	0.8145	0.5270
YY	0.6983	0.4510
Z	0.8322	0.5160
ZZ	0.6381	0.4220
a	0.8671	0.5540
aa	0.7739	0.5120
b	0.7117	0.4810
bb	0.6995	0.4820
c	0.8078	0.5110
cc	0.6596	0.4710
d	0.8133	0.5170
dd	0.8397	0.5150
e	0.8151	0.5450
ee	0.6291	0.4480
f	0.8694	0.5590
ff	0.4917	0.3380
g	0.8002	0.5260
gg	0.6683	0.4220
h	0.7926	0.5170
i	0.7990	0.5110
j	0.8722	0.5460
k	0.7271	0.4800
l	0.8173	0.5300
m	0.8345	0.5360
n	0.7615	0.5090

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Chain	Atom inclusion	Q-score
o	 0.8017	 0.5420
p	 0.7794	 0.5290
r	 0.8506	 0.5360
s	 0.6148	 0.4070
t	 0.3699	 0.2830
u	 0.1321	 0.2110
v	 0.5364	 0.3910
w	 0.3158	 0.3470