



# wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 05:02 PM EST

PDB ID : 6MTC  
EMDB ID : EMD-9239  
Title : Rabbit 80S ribosome with Z-site tRNA and IFRD2 (unrotated state)  
Authors : Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.  
Deposited on : 2018-10-19  
Resolution : 3.40 Å(reported)  
Based on initial model : 5LZV

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

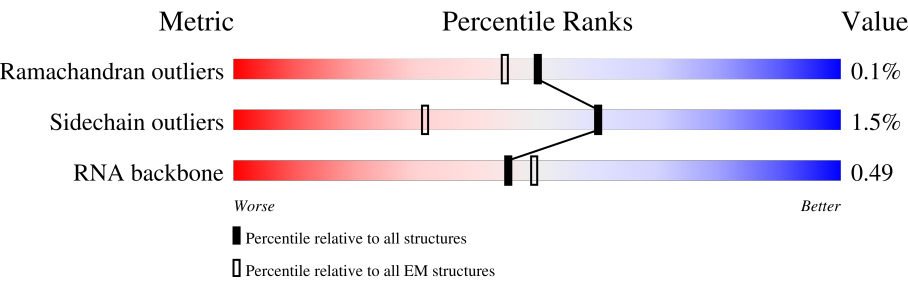
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson 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 3.40 Å.

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




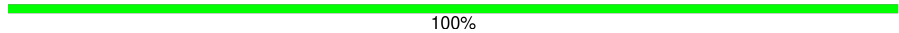

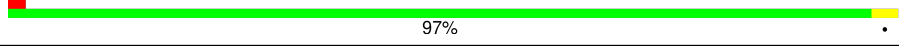
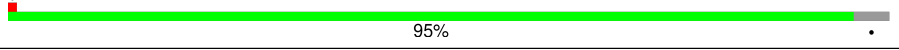
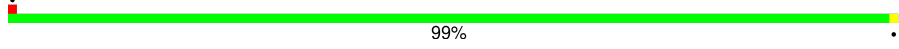
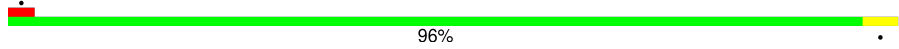
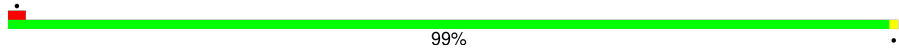
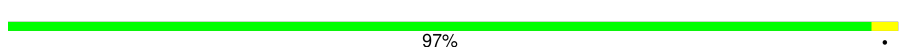
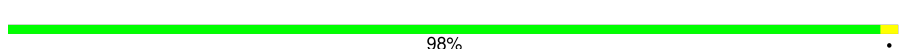
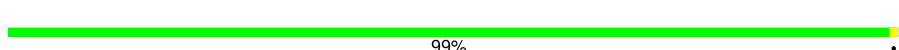

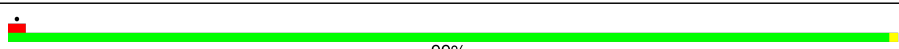
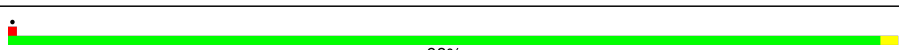
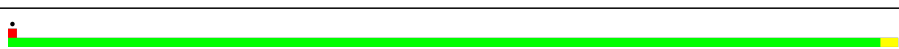

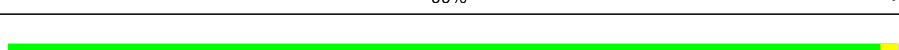
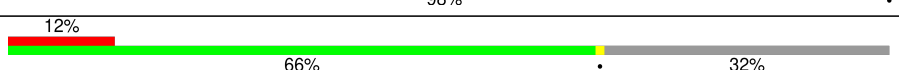

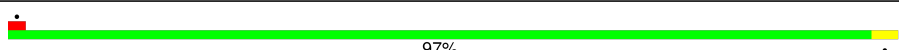
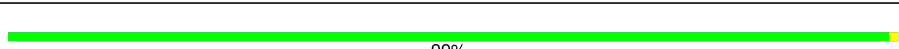

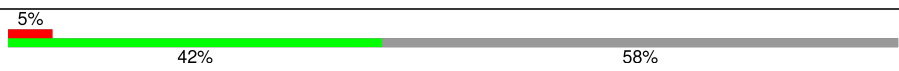
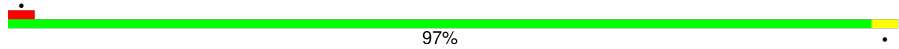
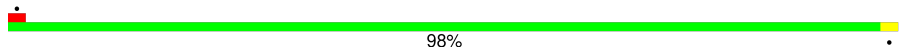
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	4	75	<div><div>5%</div><div>45%</div><div>51%</div><div>.</div></div>
2	5	3597	<div><div>.</div><div>67%</div><div>28%</div><div>5%</div><div>.</div></div>
3	7	120	<div><div>.</div><div>81%</div><div>18%</div><div>.</div></div>
4	8	151	<div><div>.</div><div>74%</div><div>25%</div><div>.</div></div>
5	A	248	<div><div>98%</div><div>.</div></div>
6	B	394	<div><div>98%</div><div>.</div></div>
7	C	362	<div><div>.</div><div>98%</div><div>.</div></div>
8	D	293	<div><div>99%</div><div>.</div></div>

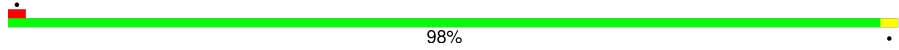
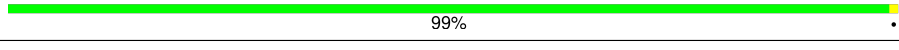
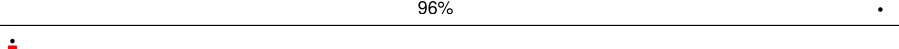
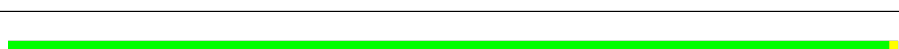
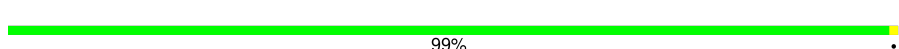
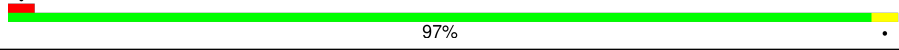
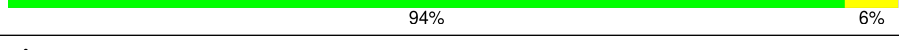
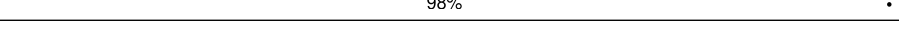

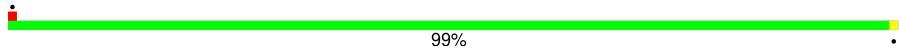
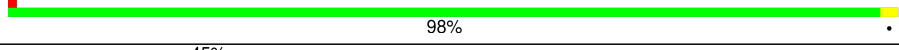
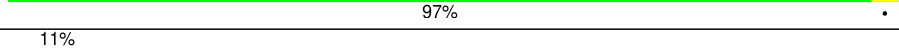

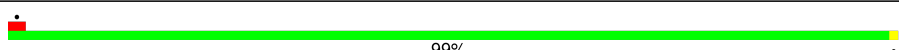
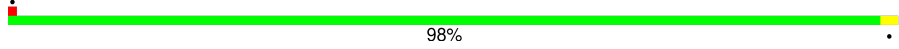
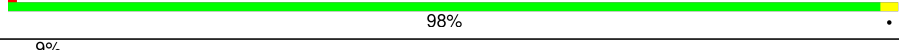
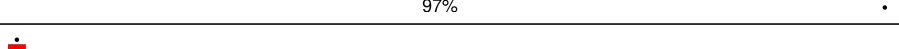


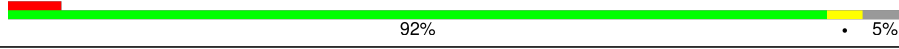
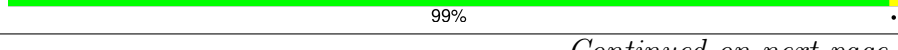



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Mol	Chain	Length	Quality of chain
9	E	291	
10	F	225	
11	G	319	
12	H	190	
13	I	214	
14	J	170	
15	L	210	
16	M	138	
17	N	203	
18	O	199	
19	P	153	
20	Q	187	
21	R	180	
22	S	176	
23	T	159	
24	U	99	
25	V	131	
26	W	157	
27	X	118	
28	Y	134	
29	Z	135	
30	a	147	
31	b	245	
32	c	98	
33	d	107	

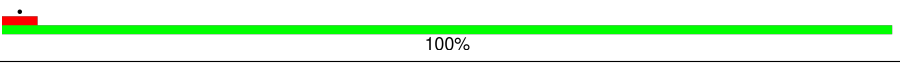
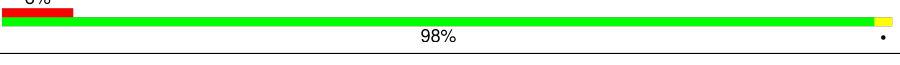
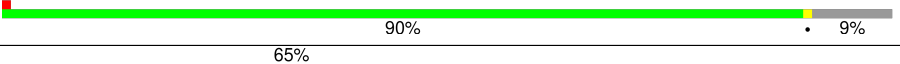
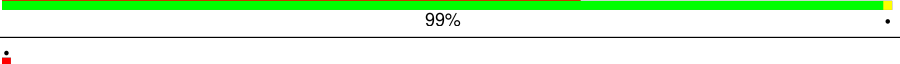
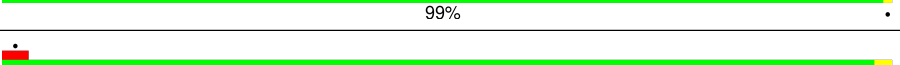
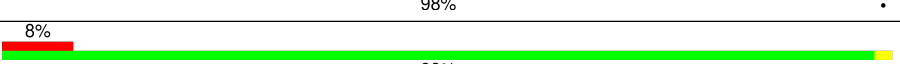
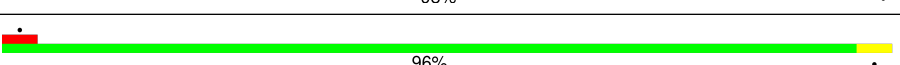
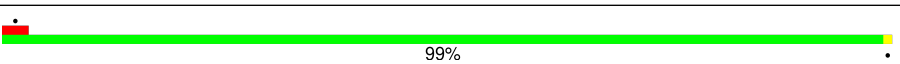
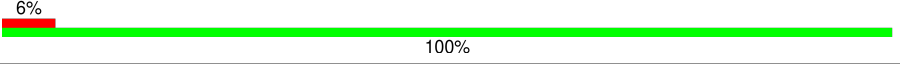
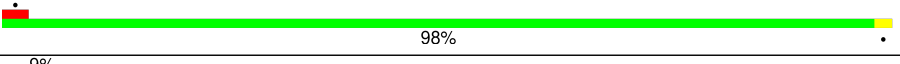
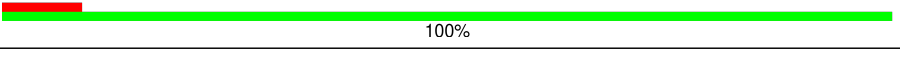
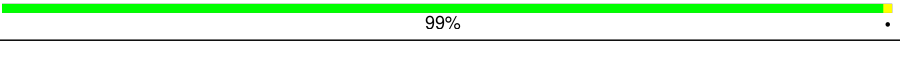
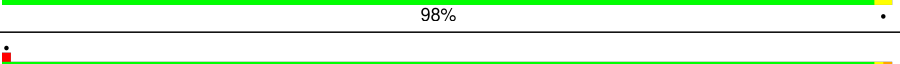
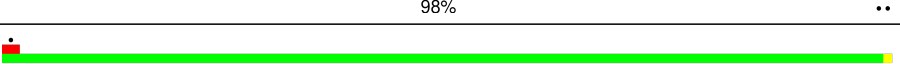
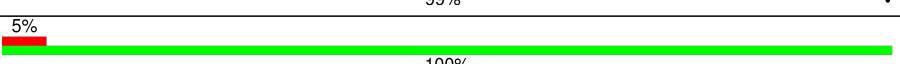
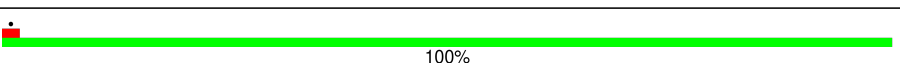
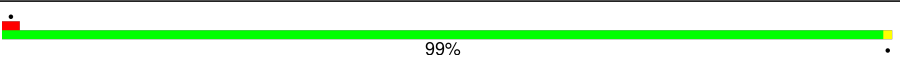
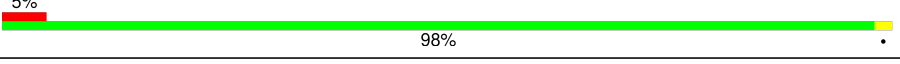
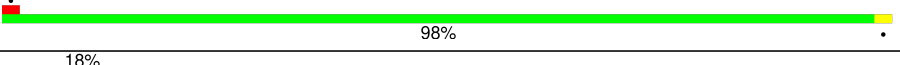
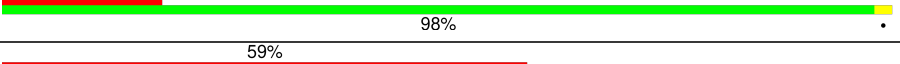
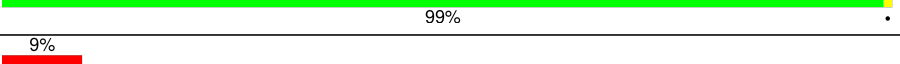
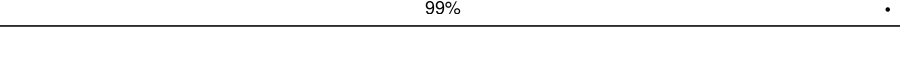


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Mol	Chain	Length	Quality of chain
34	e	128	
35	f	109	
36	g	114	
37	h	122	
38	i	102	
39	j	86	
40	k	69	
41	l	50	
42	m	52	
43	n	25	
44	o	103	
45	p	91	
46	r	124	
47	u	206	
48	v	441	
49	9	1698	
50	AA	217	
51	BB	213	
52	CC	221	
53	DD	228	
54	EE	262	
55	FF	204	
56	GG	237	
57	HH	194	
58	II	206	

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Mol	Chain	Length	Quality of chain
59	JJ	185	
60	KK	96	
61	LL	158	
62	MM	117	
63	NN	149	
64	OO	136	
65	PP	120	
66	QQ	142	
67	RR	132	
68	SS	144	
69	TT	141	
70	UU	100	
71	VV	83	
72	WW	129	
73	XX	141	
74	YY	124	
75	ZZ	75	
76	aa	101	
77	bb	83	
78	cc	62	
79	dd	55	
80	ee	55	
81	ff	68	
82	gg	313	

## 2 Entry composition [i](#)

There are 84 unique types of molecules in this entry. The entry contains 216975 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 Z-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	3597	Total	C	N	O	P	0	0
			77254	34469	14127	25061	3597		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	151	Total	C	N	O	P	0	0
			3209	1433	564	1062	150		

- Molecule 5 is a protein called 60S ribosomal protein L8.

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

- Molecule 6 is a protein called 60S ribosomal protein L3.

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

- Molecule 7 is a protein called 60S ribosomal protein L4.

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

- Molecule 8 is a protein called 60S ribosomal protein L5.

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

- Molecule 9 is a protein called 60S ribosomal protein L6.

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

- Molecule 10 is a protein called 60S ribosomal protein L7.

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

- Molecule 11 is a protein called 60S ribosomal protein L7a.

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

- Molecule 12 is a protein called 60S ribosomal protein L9.

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

- Molecule 13 is a protein called 60S ribosomal protein L10.

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

- Molecule 14 is a protein called 60S ribosomal protein L11.

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

- Molecule 15 is a protein called 60S ribosomal protein L13.

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

- Molecule 16 is a protein called 60S ribosomal protein L14.

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

- Molecule 17 is a protein called 60S Ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

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

- Molecule 19 is a protein called 60S ribosomal protein L17.

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

- Molecule 20 is a protein called 60S ribosomal protein L18.

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

- Molecule 21 is a protein called 60S ribosomal protein L19.

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

- Molecule 22 is a protein called 60S ribosomal protein L18a.

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

- Molecule 23 is a protein called 60S ribosomal protein L21.

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

- Molecule 24 is a protein called 60S ribosomal protein L22.

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

- Molecule 25 is a protein called 60S ribosomal protein L23.

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

- Molecule 26 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 27 is a protein called 60S ribosomal protein L23a.

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

- Molecule 28 is a protein called 60S ribosomal protein L26.

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

- Molecule 29 is a protein called 60S ribosomal protein L27.

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

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

- Molecule 31 is a protein called 60S ribosomal protein L29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

- Molecule 33 is a protein called 60S ribosomal protein L31.

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

- Molecule 34 is a protein called 60S ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

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

- Molecule 36 is a protein called 60S ribosomal protein L34.

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

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

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

- Molecule 39 is a protein called 60S ribosomal protein L37.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

- Molecule 41 is a protein called 60S ribosomal protein L39.

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

- Molecule 42 is a protein called 60S ribosomal protein L40.

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

- Molecule 43 is a protein called 60S ribosomal protein L41.

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

- Molecule 44 is a protein called 60S ribosomal protein L36a.

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

- Molecule 45 is a protein called 60S ribosomal protein L37a.

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

- Molecule 46 is a protein called 60S ribosomal protein L28.

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

- Molecule 47 is a protein called 60S ribosomal protein L10a.

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

- Molecule 48 is a protein called Interferon-related developmental regulator 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	354	Total	C	N	O	S	0	0
			2737	1725	493	506	13		

- Molecule 49 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	9	1698	Total	C	N	O	P	0	0
			36291	16217	6509	11868	1697		

- Molecule 50 is a protein called 40S ribosomal protein SA.

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

- Molecule 51 is a protein called 40S ribosomal protein S3a.

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

- Molecule 52 is a protein called 40S ribosomal protein S2.

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

- Molecule 53 is a protein called 40S ribosomal protein S3.

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

- Molecule 54 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 55 is a protein called 40S ribosomal protein S5.

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

- Molecule 56 is a protein called 40S ribosomal protein S6.

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

- Molecule 57 is a protein called 40S ribosomal protein S7.

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

- Molecule 58 is a protein called 40S ribosomal protein S8.

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

- Molecule 59 is a protein called 40S ribosomal protein S9.

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

- Molecule 60 is a protein called 40S ribosomal protein S10.

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

- Molecule 61 is a protein called 40S ribosomal protein S11.

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

- Molecule 62 is a protein called 40S ribosomal protein S12.

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

- Molecule 63 is a protein called 40S ribosomal protein S13.

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

- Molecule 64 is a protein called 40S ribosomal protein S14.

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

- Molecule 65 is a protein called 40S ribosomal protein S15.

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

- Molecule 66 is a protein called 40S ribosomal protein S16.

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

- Molecule 67 is a protein called 40S ribosomal protein S17.

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

- Molecule 68 is a protein called 40S ribosomal protein S18.

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

- Molecule 69 is a protein called 40S ribosomal protein S19.

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

- Molecule 70 is a protein called 40S ribosomal protein S20.

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

- Molecule 71 is a protein called 40S ribosomal protein S21.

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

- Molecule 72 is a protein called 40S ribosomal protein S15a.

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

- Molecule 73 is a protein called 40S ribosomal protein S23.

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

- Molecule 74 is a protein called 40S ribosomal protein S24.

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

- Molecule 75 is a protein called 40S ribosomal protein S25.

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

- Molecule 76 is a protein called 40S ribosomal protein S26.

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

- Molecule 77 is a protein called 40S ribosomal protein S27.

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

- Molecule 78 is a protein called 40S ribosomal protein S28.

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

- Molecule 79 is a protein called 40S ribosomal protein S29.

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

- Molecule 80 is a protein called 40S ribosomal protein S30.

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

- Molecule 81 is a protein called 40S ribosomal protein S27a.

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

- Molecule 82 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	5	199	Total	Mg	0
			199	199	
83	7	7	Total	Mg	0
			7	7	
83	8	6	Total	Mg	0
			6	6	

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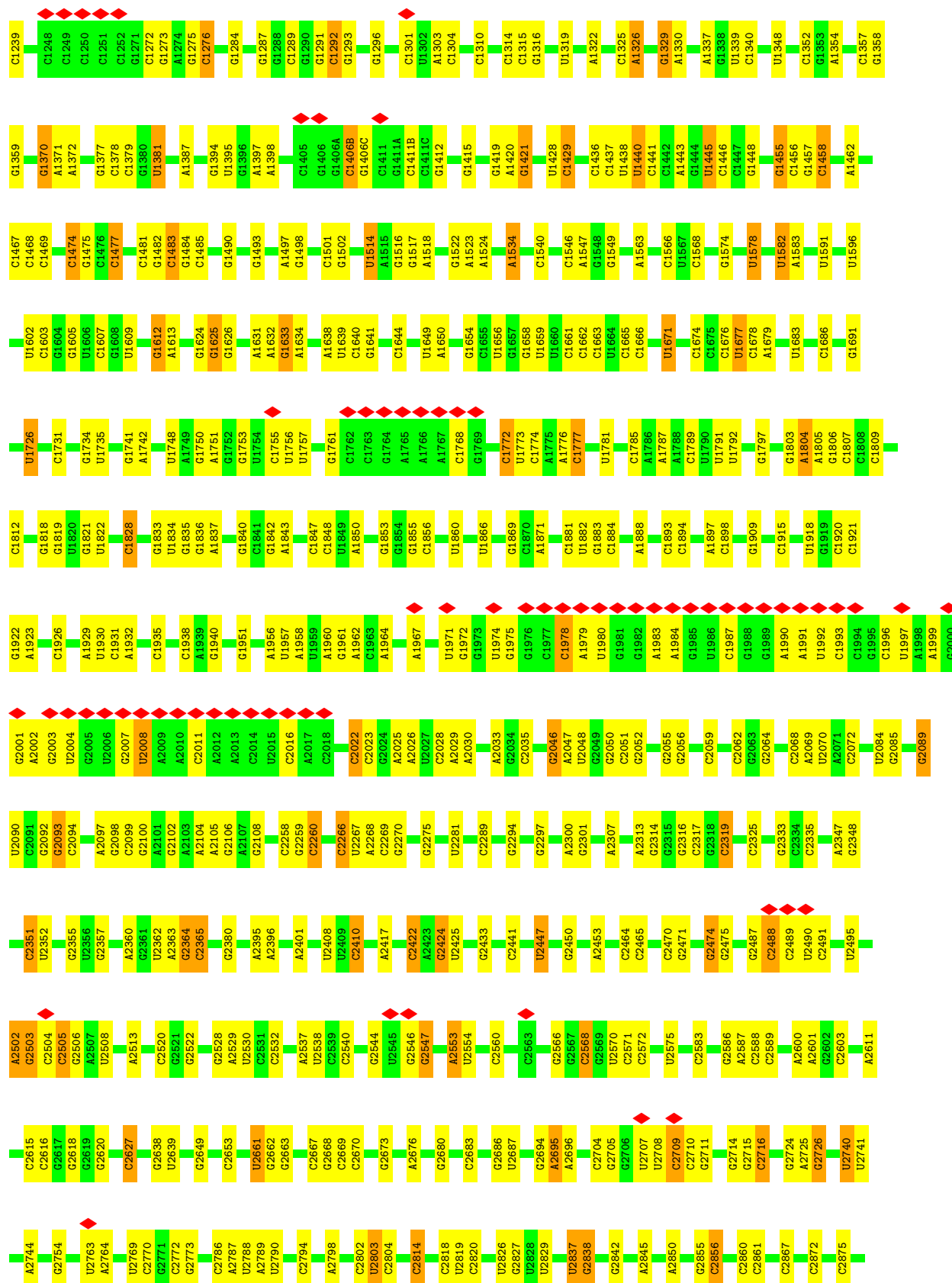
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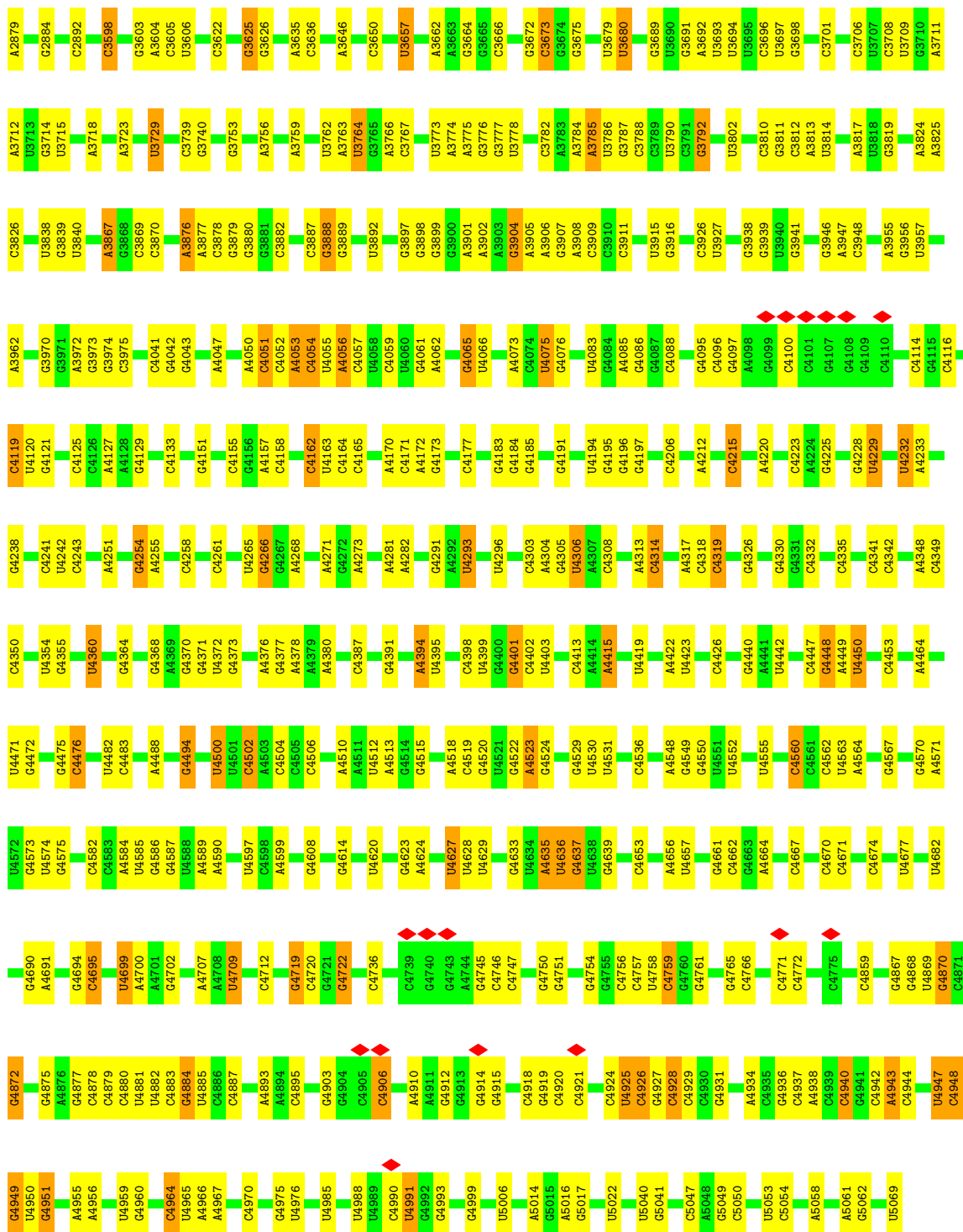
Mol	Chain	Residues	Atoms		AltConf
83	A	1	Total 1	Mg 1	0
83	B	1	Total 1	Mg 1	0
83	P	2	Total 2	Mg 2	0
83	V	1	Total 1	Mg 1	0
83	j	1	Total 1	Mg 1	0
83	9	77	Total 77	Mg 77	0
83	LL	1	Total 1	Mg 1	0
83	TT	1	Total 1	Mg 1	0

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

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







• Molecule 3: 5S rRNA

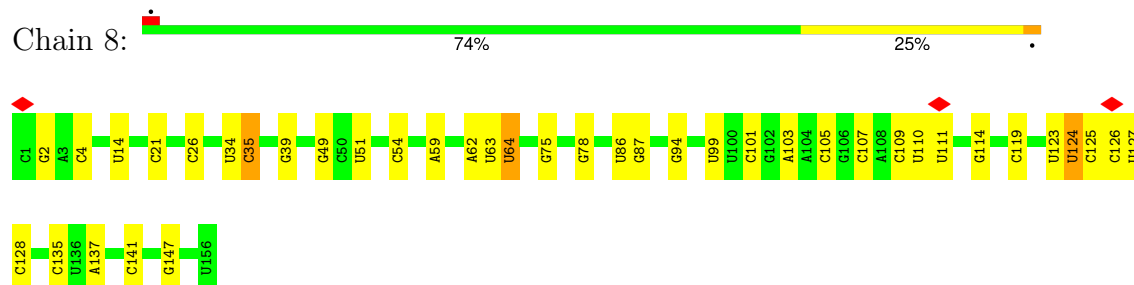
Chain 7:

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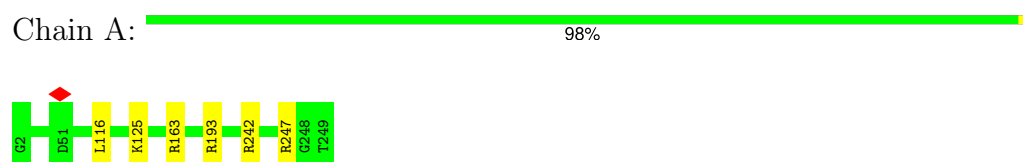
18%



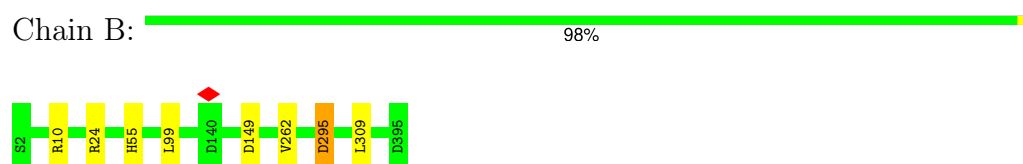
- Molecule 4: 5.8S rRNA



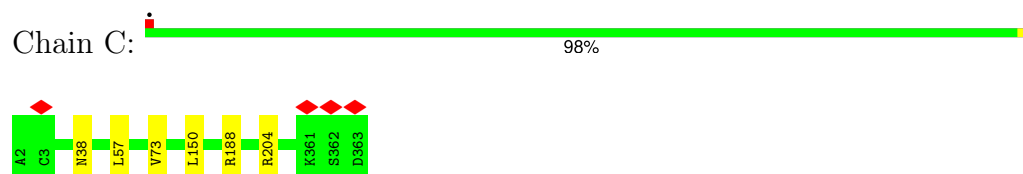
- Molecule 5: 60S ribosomal protein L8



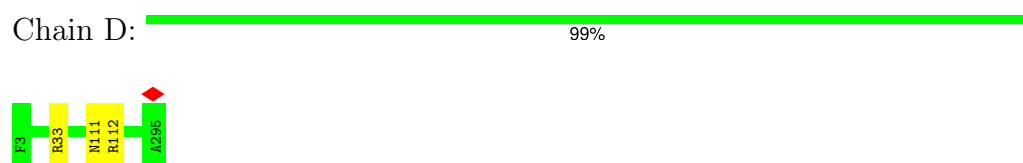
- Molecule 6: 60S ribosomal protein L3



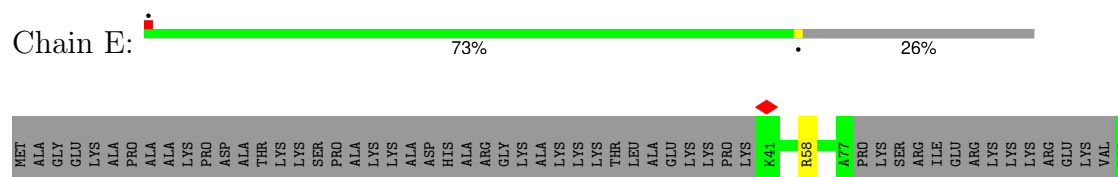
- Molecule 7: 60S ribosomal protein L4

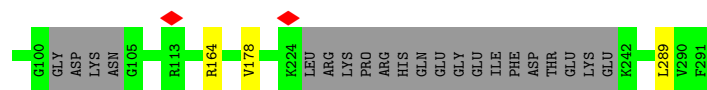


- Molecule 8: 60S ribosomal protein L5



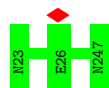
- Molecule 9: 60S ribosomal protein L6





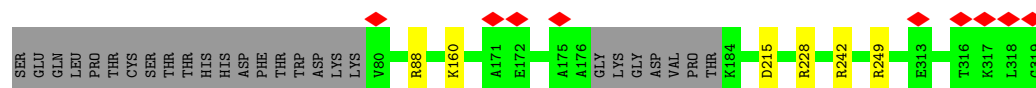
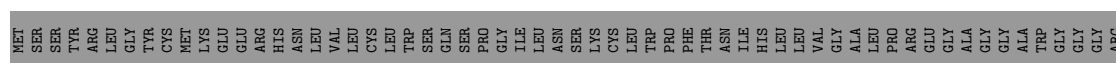
- Molecule 10: 60S ribosomal protein L7

Chain F: 100%



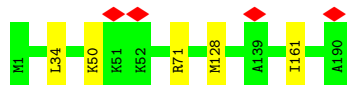
- Molecule 11: 60S ribosomal protein L7a

Chain G: 71% 27%



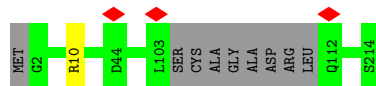
- Molecule 12: 60S ribosomal protein L9

Chain H: 97%



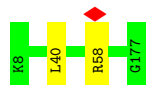
- Molecule 13: 60S ribosomal protein L10

Chain I: 95%



- Molecule 14: 60S ribosomal protein L11

Chain J: 99%



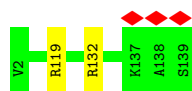
- Molecule 15: 60S ribosomal protein L13

Chain L: 96%



- Molecule 16: 60S ribosomal protein L14

Chain M: 99%



- Molecule 17: 60S Ribosomal protein L15

Chain N: 97%



- Molecule 18: 60S ribosomal protein L13a

Chain O: 98%



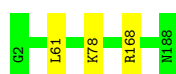
- Molecule 19: 60S ribosomal protein L17

Chain P: 99%



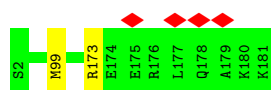
- Molecule 20: 60S ribosomal protein L18

Chain Q: 98%



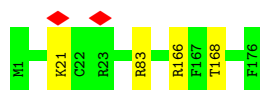
- Molecule 21: 60S ribosomal protein L19

Chain R: 99%



- Molecule 22: 60S ribosomal protein L18a

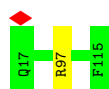
Chain S: 98%



- Molecule 23: 60S ribosomal protein L21



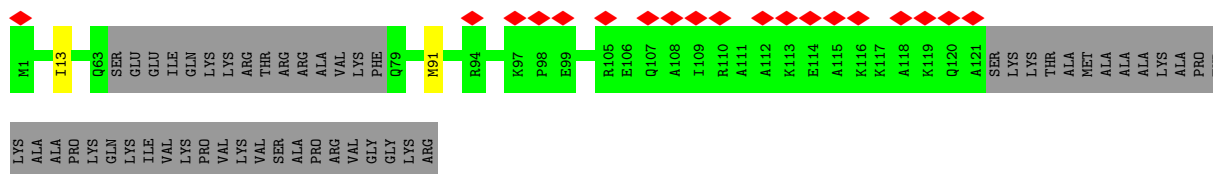
- Molecule 24: 60S ribosomal protein L22



- Molecule 25: 60S ribosomal protein L23



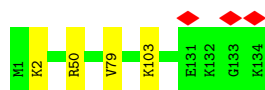
- Molecule 26: 60S ribosomal protein L24



- Molecule 27: 60S ribosomal protein L23a



- Molecule 28: 60S ribosomal protein L26



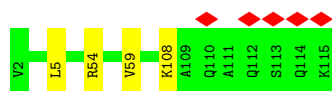


Chain f:  99%



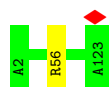
- Molecule 36: 60S ribosomal protein L34

Chain g:  96%



- Molecule 37: 60S ribosomal protein L35

Chain h:  99%



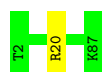
- Molecule 38: 60S ribosomal protein L36

Chain i:  99%



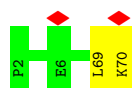
- Molecule 39: 60S ribosomal protein L37

Chain j:  99%



- Molecule 40: 60S ribosomal protein L38

Chain k:  97%



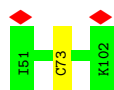
- Molecule 41: 60S ribosomal protein L39

Chain l:  94%



- Molecule 42: 60S ribosomal protein L40

Chain m:  98%



- Molecule 43: 60S ribosomal protein L41

Chain n:  100%

There are no outlier residues recorded for this chain.

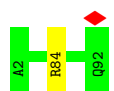
- Molecule 44: 60S ribosomal protein L36a

Chain o:  98%



- Molecule 45: 60S ribosomal protein L37a

Chain p:  99%



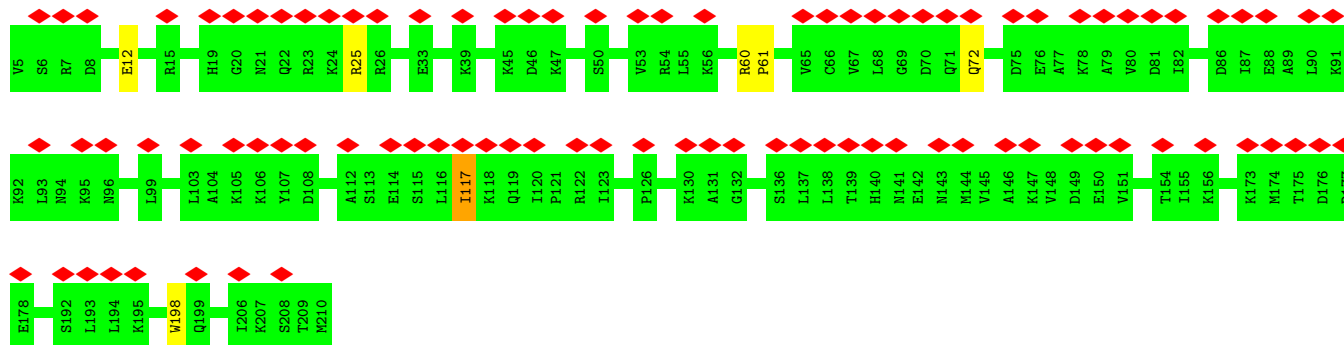
- Molecule 46: 60S ribosomal protein L28

Chain r:  98%



- Molecule 47: 60S ribosomal protein L10a

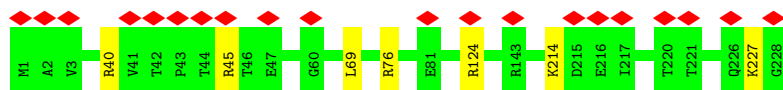
Chain u:  45% 97%



- Molecule 48: Interferon-related developmental regulator 2







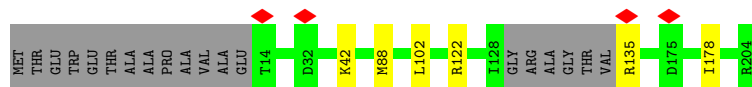
- Molecule 54: 40S ribosomal protein S4, X isoform

Chain EE: 98%



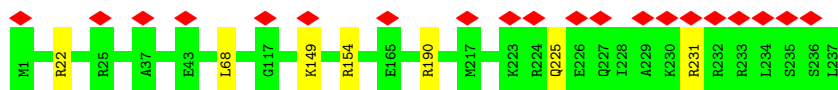
- Molecule 55: 40S ribosomal protein S5

Chain FF: 88% 9%



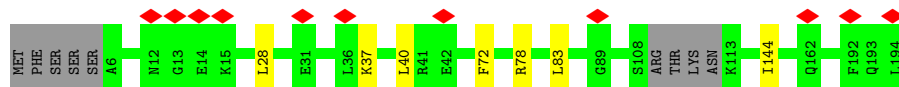
- Molecule 56: 40S ribosomal protein S6

Chain GG: 8% 97%



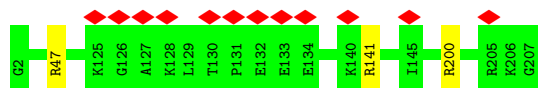
- Molecule 57: 40S ribosomal protein S7

Chain HH: 6% 92% 5%



- Molecule 58: 40S ribosomal protein S8

Chain II: 6% 99%

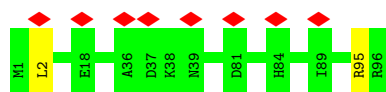


- Molecule 59: 40S ribosomal protein S9

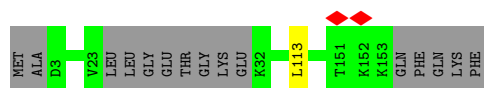
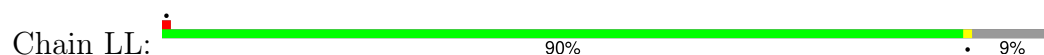
Chain JJ: 100%



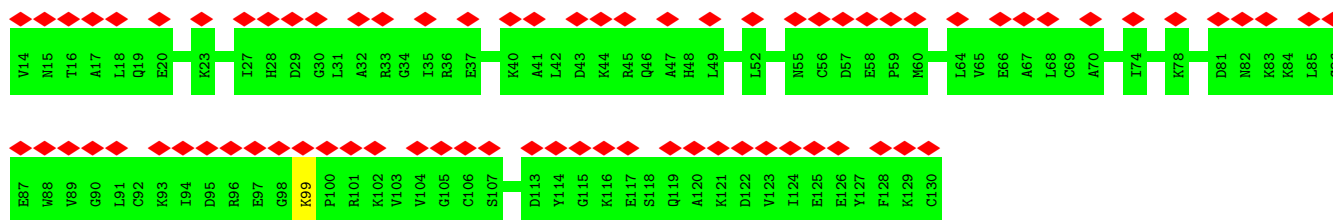
- Molecule 60: 40S ribosomal protein S10



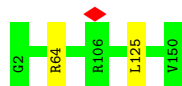
- Molecule 61: 40S ribosomal protein S11



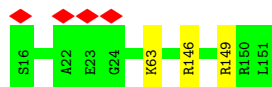
- Molecule 62: 40S ribosomal protein S12



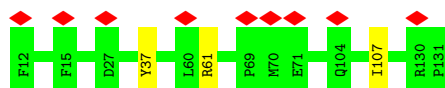
- Molecule 63: 40S ribosomal protein S13



- Molecule 64: 40S ribosomal protein S14

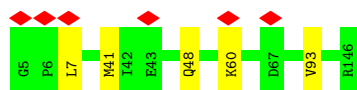


- Molecule 65: 40S ribosomal protein S15



- Molecule 66: 40S ribosomal protein S16





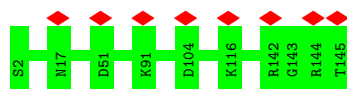
- Molecule 67: 40S ribosomal protein S17

Chain RR: 99%



- Molecule 68: 40S ribosomal protein S18

Chain SS: 6% 100%



- Molecule 69: 40S ribosomal protein S19

Chain TT: 98%



- Molecule 70: 40S ribosomal protein S20

Chain UU: 9% 100%



- Molecule 71: 40S ribosomal protein S21

Chain VV: 99%



- Molecule 72: 40S ribosomal protein S15a

Chain WW: 98%



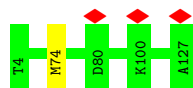
- Molecule 73: 40S ribosomal protein S23

Chain XX:  98% ..



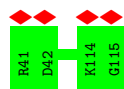
- Molecule 74: 40S ribosomal protein S24

Chain YY:  99% .



- Molecule 75: 40S ribosomal protein S25

Chain ZZ:  5% 100%



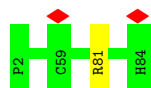
- Molecule 76: 40S ribosomal protein S26

Chain aa:  100%



- Molecule 77: 40S ribosomal protein S27

Chain bb:  99% .



- Molecule 78: 40S ribosomal protein S28

Chain cc:  5% 98% .

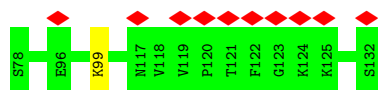


- Molecule 79: 40S ribosomal protein S29

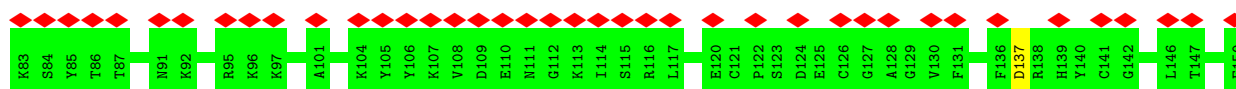
Chain dd:  98% .



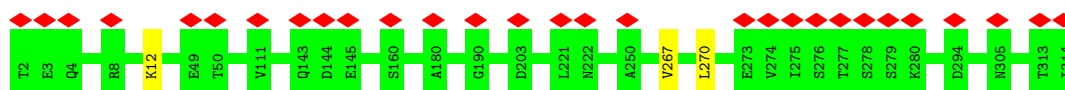
## • Molecule 80: 40S ribosomal protein S30



## • Molecule 81: 40S ribosomal protein S27a



## • Molecule 82: Receptor of activated protein C kinase 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74031	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	1.018	Depositor
Minimum map value	-0.622	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.1	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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	4	0.42	0/1779	1.19	17/2771 (0.6%)
2	5	0.90	0/83825	1.21	704/130614 (0.5%)
3	7	0.87	0/2858	1.14	15/4455 (0.3%)
4	8	0.90	0/3559	1.20	27/5543 (0.5%)
5	A	0.59	0/1936	0.72	1/2596 (0.0%)
6	B	0.55	0/3240	0.70	4/4339 (0.1%)
7	C	0.52	0/2927	0.64	0/3932
8	D	0.48	0/2437	0.58	0/3264
9	E	0.43	0/1762	0.64	1/2362 (0.0%)
10	F	0.54	0/1911	0.65	0/2549
11	G	0.47	0/1910	0.64	0/2569
12	H	0.48	0/1535	0.67	1/2063 (0.0%)
13	I	0.49	0/1702	0.60	0/2272
14	J	0.44	0/1385	0.68	1/1852 (0.1%)
15	L	0.46	0/1733	0.64	0/2316
16	M	0.51	0/1158	0.63	0/1547
17	N	0.60	0/1746	0.65	0/2338
18	O	0.54	0/1662	0.66	0/2222
19	P	0.56	0/1268	0.63	0/1700
20	Q	0.52	0/1539	0.67	0/2054
21	R	0.49	0/1524	0.70	2/2013 (0.1%)
22	S	0.56	0/1501	0.65	0/2012
23	T	0.54	0/1326	0.64	0/1770
24	U	0.41	0/823	0.67	0/1104
25	V	0.52	0/993	0.66	1/1332 (0.1%)
26	W	0.48	0/873	0.63	1/1158 (0.1%)
27	X	0.47	0/984	0.61	0/1323
28	Y	0.50	0/1132	0.65	0/1504
29	Z	0.52	0/1130	0.61	0/1507
30	a	0.56	0/1191	0.63	0/1590

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	b	0.40	0/861	0.61	0/1138
32	c	0.55	0/771	0.69	0/1034
33	d	0.50	0/903	0.65	0/1216
34	e	0.52	0/1071	0.58	0/1429
35	f	0.57	0/895	0.65	0/1198
36	g	0.51	0/916	0.66	0/1220
37	h	0.45	0/1021	0.62	0/1348
38	i	0.46	0/841	0.61	0/1112
39	j	0.55	0/720	0.68	0/952
40	k	0.43	0/575	0.61	0/761
41	l	0.51	0/459	0.67	1/608 (0.2%)
42	m	0.50	0/425	0.68	0/561
43	n	0.44	0/240	0.72	0/305
44	o	0.49	0/855	0.60	0/1128
45	p	0.57	0/718	0.62	0/953
46	r	0.55	0/1010	0.68	0/1354
47	u	0.33	0/1680	0.72	1/2255 (0.0%)
48	v	0.37	0/2779	0.71	5/3751 (0.1%)
49	9	0.76	0/39723	1.19	338/61870 (0.5%)
50	AA	0.48	0/1747	0.68	0/2374
51	BB	0.46	0/1756	0.67	0/2350
52	CC	0.49	0/1753	0.69	0/2369
53	DD	0.38	0/1796	0.67	1/2417 (0.0%)
54	EE	0.44	1/2118 (0.0%)	0.65	1/2849 (0.0%)
55	FF	0.42	0/1492	0.64	1/2005 (0.0%)
56	GG	0.38	0/1946	0.64	1/2590 (0.0%)
57	HH	0.40	0/1510	0.69	1/2022 (0.0%)
58	II	0.46	0/1715	0.63	0/2287
59	JJ	0.41	0/1550	0.61	0/2069
60	KK	0.37	0/834	0.65	1/1125 (0.1%)
61	LL	0.52	0/1195	0.63	1/1597 (0.1%)
62	MM	0.35	0/918	0.70	0/1233
63	NN	0.46	0/1226	0.68	1/1649 (0.1%)
64	OO	0.49	0/1029	0.65	0/1380
65	PP	0.39	0/1017	0.62	1/1358 (0.1%)
66	QQ	0.41	0/1146	0.65	1/1534 (0.1%)
67	RR	0.38	0/1082	0.65	0/1452
68	SS	0.36	0/1208	0.66	0/1618
69	TT	0.37	0/1115	0.60	1/1493 (0.1%)
70	UU	0.36	0/805	0.63	0/1081
71	VV	0.46	0/643	0.60	0/860
72	WW	0.50	0/1051	0.69	0/1406
73	XX	0.45	0/1116	0.67	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
74	YY	0.40	0/1028	0.56	0/1366
75	ZZ	0.35	0/604	0.62	0/810
76	aa	0.48	0/828	0.62	0/1109
77	bb	0.40	0/665	0.62	0/891
78	cc	0.40	0/490	0.61	0/656
79	dd	0.47	0/470	0.59	0/623
80	ee	0.38	0/447	0.59	0/587
81	ff	0.33	0/567	0.56	0/753
82	gg	0.35	0/2493	0.64	0/3394
All	All	0.72	1/229172 (0.0%)	1.02	1131/335661 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	B	0	1
7	C	0	1
11	G	0	1
12	H	0	1
15	L	0	2
17	N	0	3
18	O	0	1
23	T	0	1
31	b	0	1
33	d	0	1
40	k	0	1
47	u	0	2
52	CC	0	1
54	EE	0	1
71	VV	0	1
72	WW	0	1
73	XX	0	1
81	ff	0	1
All	All	0	22

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	EE	237	SER	C-N	-5.43	1.21	1.34

The worst 5 of 1131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	9	501	C	C2-N1-C1'	12.91	133.00	118.80
2	5	1978	C	N1-C2-O2	12.32	126.29	118.90
49	9	501	C	N1-C2-O2	12.10	126.16	118.90
2	5	2505	C	N1-C2-O2	12.03	126.11	118.90
2	5	4056	A	OP1-P-O3'	-11.92	78.98	105.20

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	55	HIS	Peptide
7	C	73	VAL	Peptide
11	G	215	ASP	Peptide
12	H	50	LYS	Peptide
15	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	
5	A	246/248 (99%)	218 (89%)	28 (11%)	0	100	100
6	B	392/394 (100%)	364 (93%)	27 (7%)	1 (0%)	37	66
7	C	359/362 (99%)	343 (96%)	16 (4%)	0	100	100
8	D	291/293 (99%)	277 (95%)	14 (5%)	0	100	100
9	E	208/291 (72%)	193 (93%)	15 (7%)	0	100	100
10	F	223/225 (99%)	215 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	G	229/319 (72%)	221 (96%)	8 (4%)	0	100	100
12	H	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
13	I	201/214 (94%)	194 (96%)	7 (4%)	0	100	100
14	J	168/170 (99%)	166 (99%)	2 (1%)	0	100	100
15	L	208/210 (99%)	200 (96%)	7 (3%)	1 (0%)	25	54
16	M	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
17	N	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
18	O	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
19	P	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
20	Q	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
21	R	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
22	S	174/176 (99%)	164 (94%)	9 (5%)	1 (1%)	22	50
23	T	157/159 (99%)	148 (94%)	9 (6%)	0	100	100
24	U	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
25	V	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
26	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
27	X	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
28	Y	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
29	Z	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	44
30	a	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
31	b	100/245 (41%)	93 (93%)	7 (7%)	0	100	100
32	c	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
33	d	105/107 (98%)	95 (90%)	9 (9%)	1 (1%)	13	39
34	e	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
35	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
36	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
37	h	120/122 (98%)	120 (100%)	0	0	100	100
38	i	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
39	j	84/86 (98%)	75 (89%)	9 (11%)	0	100	100
40	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
41	l	48/50 (96%)	41 (85%)	7 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	m	49/52 (94%)	43 (88%)	5 (10%)	1 (2%)	6	25
43	n	23/25 (92%)	23 (100%)	0	0	100	100
44	o	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
45	p	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
46	r	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
47	u	204/206 (99%)	173 (85%)	29 (14%)	2 (1%)	13	39
48	v	348/441 (79%)	320 (92%)	28 (8%)	0	100	100
50	AA	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
51	BB	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
52	CC	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
53	DD	226/228 (99%)	217 (96%)	9 (4%)	0	100	100
54	EE	260/262 (99%)	243 (94%)	17 (6%)	0	100	100
55	FF	181/204 (89%)	172 (95%)	9 (5%)	0	100	100
56	GG	235/237 (99%)	226 (96%)	9 (4%)	0	100	100
57	HH	181/194 (93%)	172 (95%)	9 (5%)	0	100	100
58	II	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
59	JJ	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
60	KK	94/96 (98%)	86 (92%)	8 (8%)	0	100	100
61	LL	139/158 (88%)	132 (95%)	7 (5%)	0	100	100
62	MM	115/117 (98%)	102 (89%)	13 (11%)	0	100	100
63	NN	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
64	OO	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
65	PP	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
66	QQ	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
67	RR	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
68	SS	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
69	TT	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
70	UU	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
71	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
72	WW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
73	XX	139/141 (99%)	130 (94%)	7 (5%)	2 (1%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	YY	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
75	ZZ	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
76	aa	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
77	bb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
78	cc	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
79	dd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
80	ee	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
81	ff	66/68 (97%)	58 (88%)	8 (12%)	0	100	100
82	gg	311/313 (99%)	279 (90%)	32 (10%)	0	100	100
All	All	11723/12395 (95%)	11060 (94%)	653 (6%)	10 (0%)	50	78

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	m	73	CYS
6	B	295	ASP
33	d	96	GLU
47	u	61	PRO
47	u	198	TRP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	190/190 (100%)	185 (97%)	5 (3%)	41	64
6	B	342/342 (100%)	339 (99%)	3 (1%)	75	86
7	C	301/301 (100%)	296 (98%)	5 (2%)	56	74
8	D	247/247 (100%)	244 (99%)	3 (1%)	67	80
9	E	190/251 (76%)	187 (98%)	3 (2%)	58	75
10	F	196/196 (100%)	196 (100%)	0	100	100
11	G	200/272 (74%)	195 (98%)	5 (2%)	42	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	H	169/169 (100%)	166 (98%)	3 (2%)	54	73
13	I	175/181 (97%)	174 (99%)	1 (1%)	84	90
14	J	143/143 (100%)	142 (99%)	1 (1%)	81	88
15	L	175/175 (100%)	170 (97%)	5 (3%)	37	61
16	M	117/117 (100%)	115 (98%)	2 (2%)	56	74
17	N	171/171 (100%)	168 (98%)	3 (2%)	54	73
18	O	171/171 (100%)	169 (99%)	2 (1%)	67	80
19	P	134/134 (100%)	133 (99%)	1 (1%)	81	88
20	Q	164/164 (100%)	161 (98%)	3 (2%)	54	73
21	R	159/159 (100%)	158 (99%)	1 (1%)	84	90
22	S	157/157 (100%)	154 (98%)	3 (2%)	52	71
23	T	139/139 (100%)	137 (99%)	2 (1%)	62	77
24	U	89/89 (100%)	88 (99%)	1 (1%)	70	81
25	V	101/101 (100%)	100 (99%)	1 (1%)	73	83
26	W	86/126 (68%)	85 (99%)	1 (1%)	67	80
27	X	106/106 (100%)	106 (100%)	0	100	100
28	Y	124/124 (100%)	120 (97%)	4 (3%)	34	59
29	Z	117/117 (100%)	117 (100%)	0	100	100
30	a	119/119 (100%)	119 (100%)	0	100	100
31	b	84/184 (46%)	84 (100%)	0	100	100
32	c	84/84 (100%)	81 (96%)	3 (4%)	30	56
33	d	98/98 (100%)	98 (100%)	0	100	100
34	e	114/114 (100%)	111 (97%)	3 (3%)	41	64
35	f	88/88 (100%)	87 (99%)	1 (1%)	70	81
36	g	98/98 (100%)	94 (96%)	4 (4%)	26	51
37	h	109/109 (100%)	108 (99%)	1 (1%)	75	86
38	i	86/86 (100%)	85 (99%)	1 (1%)	67	80
39	j	73/73 (100%)	72 (99%)	1 (1%)	62	77
40	k	64/64 (100%)	63 (98%)	1 (2%)	58	75
41	l	47/47 (100%)	45 (96%)	2 (4%)	25	50
42	m	47/47 (100%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	n	24/24 (100%)	24 (100%)	0	100	100
44	o	91/91 (100%)	89 (98%)	2 (2%)	47	68
45	p	74/74 (100%)	73 (99%)	1 (1%)	62	77
46	r	108/108 (100%)	106 (98%)	2 (2%)	52	71
47	u	186/186 (100%)	183 (98%)	3 (2%)	58	75
48	v	289/355 (81%)	284 (98%)	5 (2%)	56	74
50	AA	180/181 (99%)	178 (99%)	2 (1%)	70	81
51	BB	194/194 (100%)	190 (98%)	4 (2%)	48	69
52	CC	187/187 (100%)	184 (98%)	3 (2%)	58	75
53	DD	190/190 (100%)	184 (97%)	6 (3%)	34	59
54	EE	224/224 (100%)	221 (99%)	3 (1%)	65	78
55	FF	158/170 (93%)	153 (97%)	5 (3%)	34	59
56	GG	207/207 (100%)	201 (97%)	6 (3%)	37	61
57	HH	165/174 (95%)	159 (96%)	6 (4%)	30	56
58	II	178/178 (100%)	175 (98%)	3 (2%)	56	74
59	JJ	161/161 (100%)	161 (100%)	0	100	100
60	KK	87/87 (100%)	86 (99%)	1 (1%)	70	81
61	LL	130/142 (92%)	130 (100%)	0	100	100
62	MM	99/99 (100%)	98 (99%)	1 (1%)	73	83
63	NN	130/130 (100%)	129 (99%)	1 (1%)	79	87
64	OO	106/106 (100%)	103 (97%)	3 (3%)	38	62
65	PP	109/109 (100%)	107 (98%)	2 (2%)	54	73
66	QQ	117/117 (100%)	113 (97%)	4 (3%)	32	57
67	RR	119/119 (100%)	118 (99%)	1 (1%)	79	87
68	SS	125/125 (100%)	125 (100%)	0	100	100
69	TT	111/111 (100%)	109 (98%)	2 (2%)	54	73
70	UU	92/92 (100%)	92 (100%)	0	100	100
71	VV	67/67 (100%)	67 (100%)	0	100	100
72	WW	112/112 (100%)	111 (99%)	1 (1%)	75	86
73	XX	113/113 (100%)	112 (99%)	1 (1%)	75	86
74	YY	107/107 (100%)	106 (99%)	1 (1%)	75	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	ZZ	66/66 (100%)	66 (100%)	0	100	100
76	aa	88/88 (100%)	88 (100%)	0	100	100
77	bb	75/75 (100%)	74 (99%)	1 (1%)	65	78
78	cc	55/55 (100%)	54 (98%)	1 (2%)	54	73
79	dd	48/48 (100%)	47 (98%)	1 (2%)	48	69
80	ee	46/46 (100%)	45 (98%)	1 (2%)	47	68
81	ff	61/61 (100%)	61 (100%)	0	100	100
82	gg	272/272 (100%)	269 (99%)	3 (1%)	70	81
All	All	10225/10604 (96%)	10074 (98%)	151 (2%)	60	76

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	GG	225	GLN
74	YY	74	MET
57	HH	72	PHE
64	OO	146	ARG
82	gg	270	LEU

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

Mol	Chain	Res	Type
19	P	64	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	4	74/75 (98%)	35 (47%)	1 (1%)
2	5	3526/3597 (98%)	884 (25%)	68 (1%)
3	7	119/120 (99%)	14 (11%)	0
4	8	149/151 (98%)	27 (18%)	1 (0%)
49	9	1671/1698 (98%)	388 (23%)	20 (1%)
All	All	5539/5641 (98%)	1348 (24%)	90 (1%)

5 of 1348 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	4	2	C
1	4	3	C
1	4	4	C
1	4	8	U
1	4	9	A

5 of 90 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	4075	U
49	9	140	U
2	5	4232	U
2	5	4884	G
49	9	553	U

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

137 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$
2	P7G	5	3880	2	24,28,29	3.54	10 (41%)	25,41,44	1.48	3 (12%)
49	A2M	9	484	49	18,25,26	4.91	9 (50%)	20,36,39	2.76	4 (20%)
49	M7A	9	1806	49	19,25,26	1.62	2 (10%)	25,37,40	3.88	8 (32%)
2	OMG	5	2364	2	19,26,27	2.37	8 (42%)	21,38,41	1.57	4 (19%)
2	B8Q	5	1456	2	18,22,23	2.77	5 (27%)	21,32,35	1.95	5 (23%)
2	A2M	5	398	2	18,25,26	4.99	10 (55%)	20,36,39	2.60	4 (20%)
2	OMG	5	4370	2	19,26,27	2.41	8 (42%)	21,38,41	1.48	4 (19%)
2	OMG	5	4637	2	19,26,27	2.31	8 (42%)	21,38,41	1.51	3 (14%)
49	OMC	9	517	49	19,22,23	2.86	7 (36%)	25,31,34	1.01	1 (4%)
2	UR3	5	4530	2	19,22,23	2.69	7 (36%)	26,32,35	1.67	6 (23%)
2	P4U	5	1348	2,83	21,24,25	3.29	7 (33%)	28,33,36	1.87	3 (10%)
2	2MG	5	729	2	18,26,27	2.49	7 (38%)	16,38,41	1.34	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	MA6	9	1850	49	19,26,27	1.71	2 (10%)	18,38,41	3.06	3 (16%)
2	I4U	5	1659	2	20,24,25	4.95	13 (65%)	27,34,37	2.02	3 (11%)
49	OMG	9	644	49	19,26,27	2.38	8 (42%)	21,38,41	1.52	4 (19%)
2	A2M	5	2363	2,83	18,25,26	4.98	10 (55%)	20,36,39	2.70	5 (25%)
4	OMU	8	14	2,4	19,22,23	2.83	7 (36%)	25,31,34	2.05	6 (24%)
2	UR3	5	1866	2	19,22,23	2.46	6 (31%)	26,32,35	1.56	5 (19%)
2	OMG	5	1883	2	19,26,27	2.46	8 (42%)	21,38,41	1.61	5 (23%)
2	PSU	5	3764	2	18,21,22	1.03	1 (5%)	21,30,33	1.70	4 (19%)
2	PSU	5	1582	2	18,21,22	1.18	2 (11%)	21,30,33	1.94	4 (19%)
49	PSU	9	1081	49	18,21,22	1.09	3 (16%)	21,30,33	1.78	4 (19%)
2	OMG	5	4196	2	19,26,27	2.34	8 (42%)	21,38,41	1.48	4 (19%)
2	PSU	5	4531	2	18,21,22	1.11	2 (11%)	21,30,33	2.01	5 (23%)
2	B8W	5	4529	2,83	18,26,27	4.18	7 (38%)	17,38,41	7.43	10 (58%)
2	5MC	5	3782	2	19,22,23	3.65	8 (42%)	26,32,35	1.13	2 (7%)
2	OMC	5	3701	2,83	19,22,23	2.77	7 (36%)	25,31,34	0.83	0
2	B8K	5	3897	2	24,28,29	4.73	17 (70%)	29,42,45	2.73	14 (48%)
2	OMU	5	4620	2	19,22,23	2.72	7 (36%)	25,31,34	2.05	6 (24%)
2	OMG	5	2773	2	19,26,27	2.40	8 (42%)	21,38,41	1.44	4 (19%)
49	4AC	9	1842	49	21,24,25	3.07	10 (47%)	28,34,37	1.34	4 (14%)
2	OMG	5	4870	2	19,26,27	2.45	7 (36%)	21,38,41	1.48	4 (19%)
2	PSU	5	4450	2,83	18,21,22	1.07	2 (11%)	21,30,33	2.24	6 (28%)
2	OMC	5	3869	2	19,22,23	2.78	7 (36%)	25,31,34	0.81	0
2	PSU	5	4500	2	18,21,22	1.05	3 (16%)	21,30,33	2.07	6 (28%)
49	B8N	9	1248	49	25,29,30	3.08	7 (28%)	28,42,45	2.05	7 (25%)
49	PSU	9	119	49	18,21,22	0.97	1 (5%)	21,30,33	1.73	4 (19%)
49	A2M	9	159	49	18,25,26	5.09	8 (44%)	20,36,39	2.65	5 (25%)
2	A2M	5	3867	2	18,25,26	4.92	8 (44%)	20,36,39	2.54	3 (15%)
49	PSU	9	823	49	18,21,22	1.06	2 (11%)	21,30,33	1.82	4 (19%)
2	A2M	5	4571	2	18,25,26	5.00	8 (44%)	20,36,39	2.71	4 (20%)
2	7MG	5	4550	2	23,26,27	3.20	10 (43%)	27,39,42	2.16	11 (40%)
2	UR3	5	4597	2	19,22,23	2.62	6 (31%)	26,32,35	1.57	5 (19%)
49	OMG	9	509	49,83	19,26,27	2.36	8 (42%)	21,38,41	1.46	4 (19%)
42	MLZ	m	72	42	8,9,10	0.79	0	4,9,11	0.85	0
49	OMG	9	683	49	19,26,27	2.45	8 (42%)	21,38,41	1.56	5 (23%)
49	UR3	9	1830	49	19,22,23	2.60	6 (31%)	26,32,35	1.88	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	5MU	9	814	49	19,22,23	4.84	7 (36%)	27,32,35	3.53	11 (40%)
2	PSU	5	4628	2	18,21,22	1.08	3 (16%)	21,30,33	2.25	5 (23%)
2	PSU	5	3715	2	18,21,22	1.03	1 (5%)	21,30,33	1.76	4 (19%)
2	OMC	5	4536	2	19,22,23	2.77	7 (36%)	25,31,34	1.02	1 (4%)
2	E6G	5	4355	2	19,27,28	4.65	7 (36%)	18,39,42	2.50	6 (33%)
2	E7G	5	2297	2	24,27,28	3.15	11 (45%)	28,40,43	2.25	9 (32%)
2	A2M	5	3825	2	18,25,26	4.88	7 (38%)	20,36,39	2.91	6 (30%)
49	E3C	9	568	49	19,23,24	3.45	6 (31%)	21,33,36	2.81	6 (28%)
2	2MG	5	4872	2	18,26,27	2.71	7 (38%)	16,38,41	3.37	6 (37%)
2	OMU	5	4306	2	19,22,23	2.69	7 (36%)	25,31,34	1.94	5 (20%)
2	A2M	5	4523	2,83	18,25,26	4.99	9 (50%)	20,36,39	2.86	6 (30%)
2	B8T	5	4483	2	19,22,23	3.01	8 (42%)	25,31,34	1.15	2 (8%)
49	A2M	9	1678	49	18,25,26	5.00	9 (50%)	20,36,39	2.82	5 (25%)
2	B8H	5	1860	2	19,22,23	6.83	6 (31%)	21,32,35	2.45	5 (23%)
2	A2M	5	2401	2,83	18,25,26	4.94	9 (50%)	20,36,39	2.74	4 (20%)
2	OMG	5	373	2	19,26,27	2.42	7 (36%)	21,38,41	1.63	6 (28%)
49	OMU	9	116	49	19,22,23	2.82	7 (36%)	25,31,34	1.87	5 (20%)
49	5MC	9	1374	49	19,22,23	3.73	8 (42%)	26,32,35	1.04	1 (3%)
2	5MC	5	4335	2	19,22,23	3.82	8 (42%)	26,32,35	1.22	3 (11%)
49	B8Q	9	1219	49,83	18,22,23	2.89	5 (27%)	21,32,35	2.63	7 (33%)
2	BGH	5	3899	2,83	25,29,30	4.11	15 (60%)	30,43,46	2.70	16 (53%)
2	OMC	5	2804	2	19,22,23	2.84	7 (36%)	25,31,34	0.91	1 (4%)
2	OMG	5	3792	2	19,26,27	2.41	8 (42%)	21,38,41	1.54	4 (19%)
2	PSU	5	4293	2	18,21,22	1.09	2 (11%)	21,30,33	1.89	4 (19%)
2	2MG	5	1517	2	18,26,27	2.58	7 (38%)	16,38,41	1.84	4 (25%)
2	B8H	5	4296	2	19,22,23	6.89	7 (36%)	21,32,35	2.62	5 (23%)
2	A2M	5	3723	2	18,25,26	5.07	9 (50%)	20,36,39	2.68	4 (20%)
2	A2M	5	1534	2,83	18,25,26	4.87	10 (55%)	20,36,39	2.86	6 (30%)
2	OMG	5	2424	2	19,26,27	2.47	8 (42%)	21,38,41	1.57	4 (19%)
49	OMC	9	174	49	19,22,23	2.90	7 (36%)	25,31,34	0.72	0
49	OMC	9	1710	49	19,22,23	2.93	7 (36%)	25,31,34	1.15	2 (8%)
2	B9B	5	1574	2	20,28,29	4.99	8 (40%)	19,40,43	2.35	7 (36%)
2	OMC	5	2422	2,83	19,22,23	2.91	7 (36%)	25,31,34	0.78	1 (4%)
2	PSU	5	2508	2	18,21,22	1.01	1 (5%)	21,30,33	1.69	4 (19%)
49	A2M	9	668	49,83	18,25,26	4.86	8 (44%)	20,36,39	3.22	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	B8T	5	4671	2	19,22,23	3.05	8 (42%)	25,31,34	0.89	1 (4%)
2	B8W	5	4129	2	18,26,27	4.21	7 (38%)	17,38,41	6.92	10 (58%)
2	OMG	5	1625	2,83	19,26,27	2.32	8 (42%)	21,38,41	1.49	4 (19%)
2	P7G	5	1909	2	24,28,29	3.70	10 (41%)	25,41,44	1.56	3 (12%)
2	A2M	5	3718	2	18,25,26	5.00	10 (55%)	20,36,39	2.51	4 (20%)
49	MA6	9	1851	49	19,26,27	1.67	2 (10%)	18,38,41	2.82	3 (16%)
2	B8K	5	4690	2	24,28,29	4.92	17 (70%)	29,42,45	2.80	13 (44%)
2	1MA	5	1322	2,83	17,25,26	3.61	4 (23%)	17,37,40	1.87	3 (17%)
49	OMU	9	121	49	19,22,23	2.89	7 (36%)	25,31,34	1.99	6 (24%)
2	7MG	5	2522	2	23,26,27	3.17	10 (43%)	27,39,42	2.18	9 (33%)
2	M7A	5	4564	2	19,25,26	1.60	2 (10%)	25,37,40	4.04	7 (28%)
49	PSU	9	1243	49	18,21,22	1.22	2 (11%)	21,30,33	1.43	4 (19%)
2	MHG	5	4371	2	29,32,33	3.66	11 (37%)	34,46,49	2.46	12 (35%)
2	OMC	5	3909	2	19,22,23	2.83	7 (36%)	25,31,34	0.66	0
2	7MG	5	1605	2	23,26,27	3.23	10 (43%)	27,39,42	2.17	9 (33%)
2	A2M	5	3785	2	18,25,26	4.76	10 (55%)	20,36,39	2.93	5 (25%)
2	B8W	5	4472	2	18,26,27	4.17	6 (33%)	17,38,41	6.87	8 (47%)
2	OMG	5	2050	2	19,26,27	2.37	8 (42%)	21,38,41	1.43	4 (19%)
2	OMG	5	4623	2	19,26,27	2.39	8 (42%)	21,38,41	1.51	4 (19%)
2	OMC	5	2365	2	19,22,23	2.88	7 (36%)	25,31,34	0.94	0
7	MLZ	C	333	7	8,9,10	0.87	0	4,9,11	0.78	0
2	B8W	5	2380	2	18,26,27	4.23	6 (33%)	17,38,41	7.22	9 (52%)
2	PSU	5	1683	2	18,21,22	1.22	2 (11%)	21,30,33	1.99	4 (19%)
49	PSU	9	612	49	18,21,22	0.98	2 (11%)	21,30,33	1.79	5 (23%)
49	A2M	9	166	49	18,25,26	5.08	8 (44%)	20,36,39	2.75	6 (30%)
2	PSU	5	4442	2	18,21,22	1.08	2 (11%)	21,30,33	2.08	5 (23%)
49	PSU	9	822	49	18,21,22	1.04	1 (5%)	21,30,33	1.94	5 (23%)
2	1MA	5	4415	2	17,25,26	3.83	4 (23%)	17,37,40	1.79	3 (17%)
2	OMG	5	1316	2	19,26,27	2.45	8 (42%)	21,38,41	1.66	5 (23%)
49	A2M	9	1031	49	18,25,26	5.02	9 (50%)	20,36,39	2.58	4 (20%)
2	B8W	5	4185	2	18,26,27	4.19	6 (33%)	17,38,41	7.04	10 (58%)
2	B8H	5	3762	2	19,22,23	6.84	6 (31%)	21,32,35	2.54	5 (23%)
2	B9B	5	237	2	20,28,29	5.16	8 (40%)	19,40,43	2.55	6 (31%)
2	5MC	5	4447	2	19,22,23	3.85	8 (42%)	26,32,35	1.20	2 (7%)
2	A2M	5	1871	2,83	18,25,26	4.88	9 (50%)	20,36,39	2.77	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	6MZ	9	1832	49,83	17,25,26	1.45	3 (17%)	15,36,39	2.21	4 (26%)
2	OMG	5	4494	2	19,26,27	2.45	8 (42%)	21,38,41	1.63	6 (28%)
2	6MZ	5	4220	2	17,25,26	2.01	3 (17%)	15,36,39	2.18	5 (33%)
2	PSU	5	3729	2	18,21,22	1.08	2 (11%)	21,30,33	1.84	4 (19%)
2	OMC	5	2861	2	19,22,23	2.85	7 (36%)	25,31,34	1.07	2 (8%)
49	OMC	9	1703	49	19,22,23	2.95	7 (36%)	25,31,34	0.73	0
2	PSU	5	4403	2	18,21,22	0.99	1 (5%)	21,30,33	2.00	6 (28%)
2	B9H	5	2786	2	21,25,26	2.91	3 (14%)	22,35,38	1.83	3 (13%)
2	OMG	5	1522	2	19,26,27	2.39	8 (42%)	21,38,41	1.56	4 (19%)
2	A2M	5	1524	2	18,25,26	4.88	10 (55%)	20,36,39	3.11	5 (25%)
2	PSU	5	4636	2	18,21,22	1.14	2 (11%)	21,30,33	2.11	5 (23%)
2	B9B	5	2754	2,83	20,28,29	5.02	8 (40%)	19,40,43	2.28	6 (31%)
2	A2M	5	1326	2	18,25,26	4.84	10 (55%)	20,36,39	2.70	3 (15%)
2	E7G	5	1797	2	24,27,28	3.23	11 (45%)	28,40,43	2.31	9 (32%)
2	OMC	5	3887	2	19,22,23	2.74	7 (36%)	25,31,34	0.88	1 (4%)
2	PSU	5	1677	2	18,21,22	1.19	3 (16%)	21,30,33	2.07	5 (23%)
49	4AC	9	1337	49	21,24,25	3.14	10 (47%)	28,34,37	1.18	4 (14%)
2	I4U	5	4194	2	20,24,25	4.96	13 (65%)	27,34,37	1.88	5 (18%)
49	A2M	9	27	49,83	18,25,26	4.98	10 (55%)	20,36,39	2.61	3 (15%)
2	5MU	5	4083	2	19,22,23	4.71	7 (36%)	27,32,35	3.76	11 (40%)

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
2	P7G	5	3880	2	-	3/10/40/41	0/3/3/3
49	A2M	9	484	49	-	0/5/27/28	0/3/3/3
49	M7A	9	1806	49	-	0/7/37/38	0/3/3/3
2	OMG	5	2364	2	-	2/5/27/28	0/3/3/3
2	B8Q	5	1456	2	-	0/7/42/43	0/2/2/2
2	A2M	5	398	2	-	2/5/27/28	0/3/3/3
2	OMG	5	4370	2	-	0/5/27/28	0/3/3/3
2	OMG	5	4637	2	-	2/5/27/28	0/3/3/3
49	OMC	9	517	49	-	1/9/27/28	0/2/2/2
2	UR3	5	4530	2	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P4U	5	1348	2,83	-	2/10/29/30	0/2/2/2
2	2MG	5	729	2	-	2/5/27/28	0/3/3/3
49	MA6	9	1850	49	-	1/7/29/30	0/3/3/3
2	I4U	5	1659	2	-	2/9/29/30	0/2/2/2
49	OMG	9	644	49	-	1/5/27/28	0/3/3/3
2	A2M	5	2363	2,83	-	0/5/27/28	0/3/3/3
4	OMU	8	14	2,4	-	1/9/27/28	0/2/2/2
2	UR3	5	1866	2	-	1/7/25/26	0/2/2/2
2	OMG	5	1883	2	-	0/5/27/28	0/3/3/3
2	PSU	5	3764	2	-	1/7/25/26	0/2/2/2
2	PSU	5	1582	2	-	2/7/25/26	0/2/2/2
49	PSU	9	1081	49	-	1/7/25/26	0/2/2/2
2	OMG	5	4196	2	-	0/5/27/28	0/3/3/3
2	PSU	5	4531	2	-	0/7/25/26	0/2/2/2
2	B8W	5	4529	2,83	-	3/5/27/28	0/3/3/3
2	5MC	5	3782	2	-	0/7/25/26	0/2/2/2
2	OMC	5	3701	2,83	-	5/9/27/28	0/2/2/2
2	B8K	5	3897	2	-	3/11/41/42	0/3/3/3
2	OMU	5	4620	2	-	1/9/27/28	0/2/2/2
2	OMG	5	2773	2	-	0/5/27/28	0/3/3/3
49	4AC	9	1842	49	-	0/11/29/30	0/2/2/2
2	OMG	5	4870	2	-	3/5/27/28	0/3/3/3
2	PSU	5	4450	2,83	-	2/7/25/26	0/2/2/2
2	OMC	5	3869	2	-	0/9/27/28	0/2/2/2
2	PSU	5	4500	2	-	3/7/25/26	0/2/2/2
49	B8N	9	1248	49	-	4/16/34/35	0/2/2/2
49	PSU	9	119	49	-	1/7/25/26	0/2/2/2
49	A2M	9	159	49	-	3/5/27/28	0/3/3/3
2	A2M	5	3867	2	-	2/5/27/28	0/3/3/3
49	PSU	9	823	49	-	0/7/25/26	0/2/2/2
2	A2M	5	4571	2	-	0/5/27/28	0/3/3/3
2	7MG	5	4550	2	-	0/7/37/38	0/3/3/3
2	UR3	5	4597	2	-	0/7/25/26	0/2/2/2
49	OMG	9	509	49,83	-	1/5/27/28	0/3/3/3
42	MLZ	m	72	42	-	3/7/8/10	-
49	OMG	9	683	49	-	2/5/27/28	0/3/3/3
49	UR3	9	1830	49	-	2/7/25/26	0/2/2/2
49	5MU	9	814	49	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	5	4628	2	-	0/7/25/26	0/2/2/2
2	PSU	5	3715	2	-	0/7/25/26	0/2/2/2
2	OMC	5	4536	2	-	0/9/27/28	0/2/2/2
2	E6G	5	4355	2	-	4/6/28/29	0/3/3/3
2	E7G	5	2297	2	-	2/9/39/40	0/3/3/3
2	A2M	5	3825	2	-	0/5/27/28	0/3/3/3
49	E3C	9	568	49	-	6/9/44/45	0/2/2/2
2	2MG	5	4872	2	-	2/5/27/28	0/3/3/3
2	OMU	5	4306	2	-	0/9/27/28	0/2/2/2
2	A2M	5	4523	2,83	-	2/5/27/28	0/3/3/3
2	B8T	5	4483	2	-	0/7/27/28	0/2/2/2
49	A2M	9	1678	49	-	0/5/27/28	0/3/3/3
2	B8H	5	1860	2	-	0/7/25/26	0/2/2/2
2	A2M	5	2401	2,83	-	0/5/27/28	0/3/3/3
2	OMG	5	373	2	-	1/5/27/28	0/3/3/3
49	OMU	9	116	49	-	2/9/27/28	0/2/2/2
49	5MC	9	1374	49	-	0/7/25/26	0/2/2/2
2	5MC	5	4335	2	-	0/7/25/26	0/2/2/2
49	B8Q	9	1219	49,83	-	1/7/42/43	0/2/2/2
2	BGH	5	3899	2,83	-	3/13/43/44	0/3/3/3
2	OMC	5	2804	2	-	0/9/27/28	0/2/2/2
2	OMG	5	3792	2	-	2/5/27/28	0/3/3/3
2	PSU	5	4293	2	-	1/7/25/26	0/2/2/2
2	2MG	5	1517	2	-	0/5/27/28	0/3/3/3
2	B8H	5	4296	2	-	0/7/25/26	0/2/2/2
2	A2M	5	3723	2	-	0/5/27/28	0/3/3/3
2	A2M	5	1534	2,83	-	1/5/27/28	0/3/3/3
2	OMG	5	2424	2	-	2/5/27/28	0/3/3/3
49	OMC	9	174	49	-	0/9/27/28	0/2/2/2
49	OMC	9	1710	49	-	0/9/27/28	0/2/2/2
2	B9B	5	1574	2	-	3/7/29/30	0/3/3/3
2	OMC	5	2422	2,83	-	0/9/27/28	0/2/2/2
2	PSU	5	2508	2	-	0/7/25/26	0/2/2/2
49	A2M	9	668	49,83	-	2/5/27/28	0/3/3/3
2	B8T	5	4671	2	-	0/7/27/28	0/2/2/2
2	B8W	5	4129	2	-	3/5/27/28	0/3/3/3
2	OMG	5	1625	2,83	-	3/5/27/28	0/3/3/3
2	P7G	5	1909	2	-	2/10/40/41	0/3/3/3
2	A2M	5	3718	2	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	MA6	9	1851	49	-	4/7/29/30	0/3/3/3
2	B8K	5	4690	2	-	0/11/41/42	0/3/3/3
2	1MA	5	1322	2,83	-	0/3/25/26	0/3/3/3
49	OMU	9	121	49	-	2/9/27/28	0/2/2/2
2	7MG	5	2522	2	-	0/7/37/38	0/3/3/3
2	M7A	5	4564	2	-	0/7/37/38	0/3/3/3
49	PSU	9	1243	49	-	2/7/25/26	0/2/2/2
2	MHG	5	4371	2	-	8/16/46/47	0/3/3/3
2	OMC	5	3909	2	-	0/9/27/28	0/2/2/2
2	7MG	5	1605	2	-	0/7/37/38	0/3/3/3
2	A2M	5	3785	2	-	3/5/27/28	0/3/3/3
2	B8W	5	4472	2	-	2/5/27/28	0/3/3/3
2	OMG	5	2050	2	-	0/5/27/28	0/3/3/3
2	OMG	5	4623	2	-	0/5/27/28	0/3/3/3
2	OMC	5	2365	2	-	2/9/27/28	0/2/2/2
7	MLZ	C	333	7	-	2/7/8/10	-
2	B8W	5	2380	2	-	4/5/27/28	0/3/3/3
2	PSU	5	1683	2	-	0/7/25/26	0/2/2/2
49	PSU	9	612	49	-	0/7/25/26	0/2/2/2
49	A2M	9	166	49	-	2/5/27/28	0/3/3/3
2	PSU	5	4442	2	-	0/7/25/26	0/2/2/2
49	PSU	9	822	49	-	2/7/25/26	0/2/2/2
2	1MA	5	4415	2	-	2/3/25/26	0/3/3/3
2	OMG	5	1316	2	-	0/5/27/28	0/3/3/3
49	A2M	9	1031	49	-	0/5/27/28	0/3/3/3
2	B8W	5	4185	2	-	4/5/27/28	0/3/3/3
2	B8H	5	3762	2	-	2/7/25/26	0/2/2/2
2	B9B	5	237	2	-	5/7/29/30	0/3/3/3
2	5MC	5	4447	2	-	4/7/25/26	0/2/2/2
2	A2M	5	1871	2,83	-	0/5/27/28	0/3/3/3
49	6MZ	9	1832	49,83	-	2/5/27/28	0/3/3/3
2	OMG	5	4494	2	-	3/5/27/28	0/3/3/3
2	6MZ	5	4220	2	-	2/5/27/28	0/3/3/3
2	PSU	5	3729	2	-	2/7/25/26	0/2/2/2
2	OMC	5	2861	2	-	1/9/27/28	0/2/2/2
49	OMC	9	1703	49	-	2/9/27/28	0/2/2/2
2	PSU	5	4403	2	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B9H	5	2786	2	-	2/12/47/48	0/2/2/2
2	OMG	5	1522	2	-	0/5/27/28	0/3/3/3
2	A2M	5	1524	2	-	1/5/27/28	0/3/3/3
2	PSU	5	4636	2	-	3/7/25/26	0/2/2/2
2	B9B	5	2754	2,83	-	3/7/29/30	0/3/3/3
2	A2M	5	1326	2	-	0/5/27/28	0/3/3/3
2	E7G	5	1797	2	-	3/9/39/40	0/3/3/3
2	OMC	5	3887	2	-	1/9/27/28	0/2/2/2
2	PSU	5	1677	2	-	0/7/25/26	0/2/2/2
49	4AC	9	1337	49	-	1/11/29/30	0/2/2/2
2	I4U	5	4194	2	-	3/9/29/30	0/2/2/2
49	A2M	9	27	49,83	-	0/5/27/28	0/3/3/3
2	5MU	5	4083	2	-	0/7/25/26	0/2/2/2

The worst 5 of 929 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	237	B9B	O4'-C1'	18.35	1.65	1.40
2	5	2754	B9B	O4'-C1'	17.82	1.64	1.40
49	9	166	A2M	O4'-C1'	17.79	1.64	1.40
49	9	159	A2M	O4'-C1'	17.67	1.64	1.40
2	5	1574	B9B	O4'-C1'	17.60	1.64	1.40

The worst 5 of 657 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	2380	B8W	N2-C2-N3	17.95	145.81	117.79
2	5	4529	B8W	N2-C2-N3	17.69	145.41	117.79
2	5	4185	B8W	N2-C2-N3	17.35	144.87	117.79
2	5	4472	B8W	N2-C2-N3	16.93	144.22	117.79
2	5	4129	B8W	N2-C2-N3	16.88	144.15	117.79

There are no chirality outliers.

5 of 187 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	333	MLZ	N-CA-CB-CG
7	C	333	MLZ	C-CA-CB-CG
2	5	237	B9B	C5-C6-O6-C61
2	5	237	B9B	N1-C6-O6-C61

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Mol	Chain	Res	Type	Atoms
2	5	237	B9B	O4'-C4'-C5'-O5'

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 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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
2	5	43
49	9	18
4	8	1

The worst 5 of 62 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.50

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1252:C	O3'	1271:G	P	34.93
1	5	1219:G	O3'	1233:G	P	21.40
1	5	1405:C	O3'	1406:G	P	20.69
1	5	1406(C):G	O3'	1411:C	P	20.19

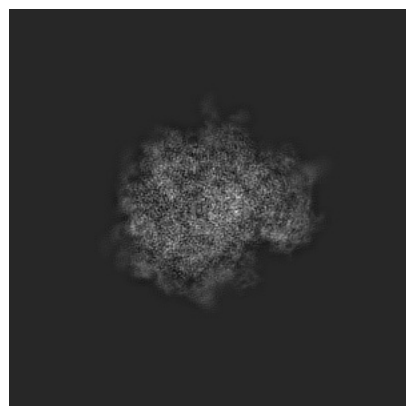
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9239. These allow visual inspection of the internal detail of the map and identification of artifacts.

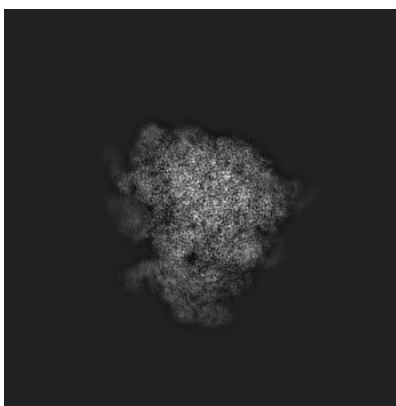
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

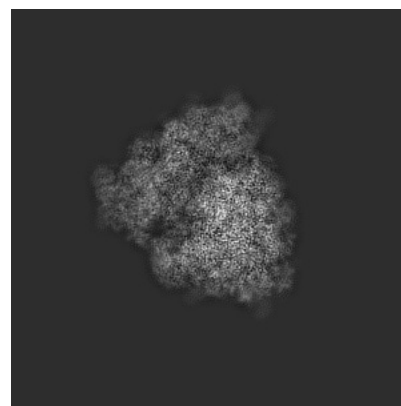
#### 6.1.1 Primary map



X

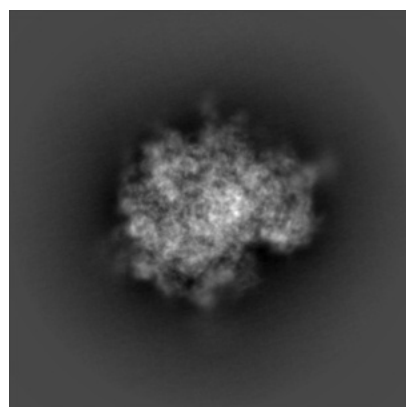


Y

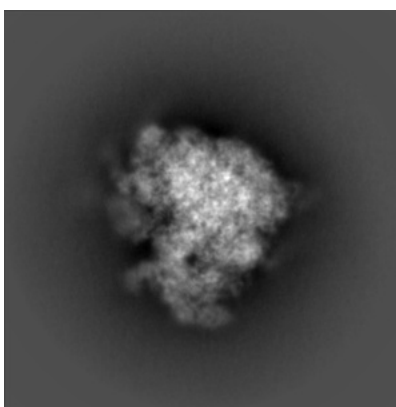


Z

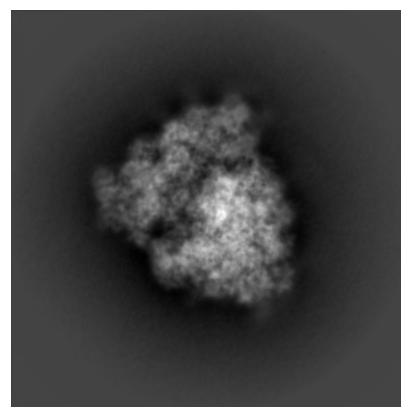
#### 6.1.2 Raw map



X



Y

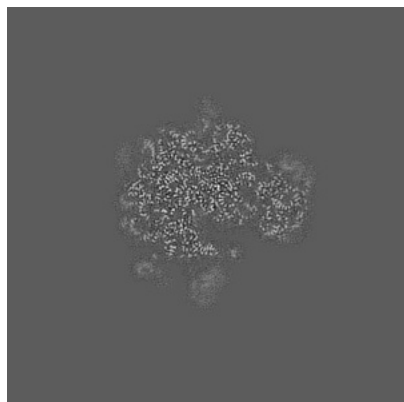


Z

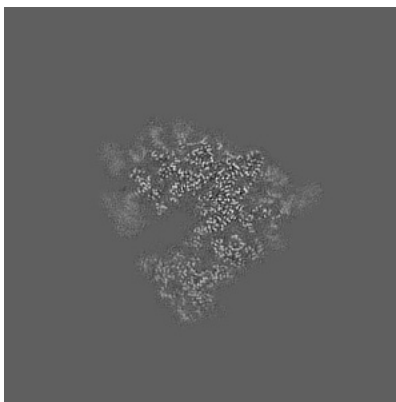
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

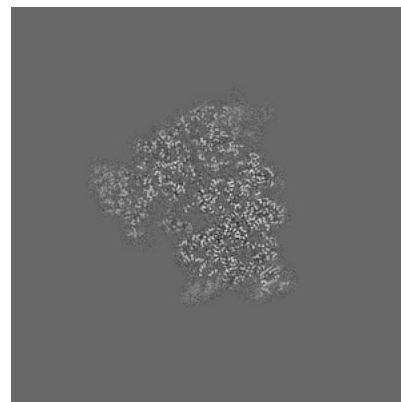
### 6.2.1 Primary map



X Index: 200

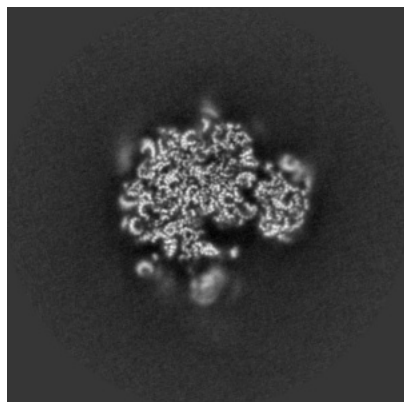


Y Index: 200

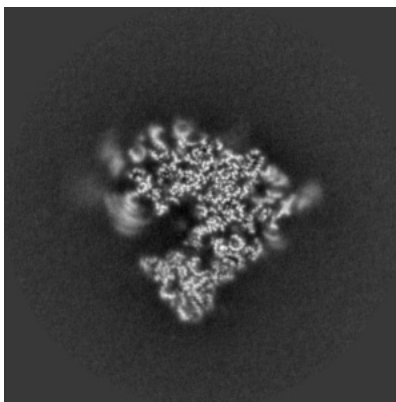


Z Index: 200

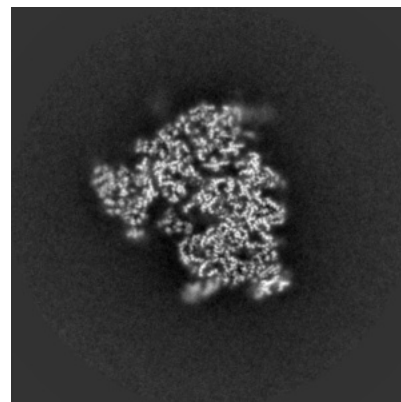
### 6.2.2 Raw map



X Index: 200



Y Index: 200

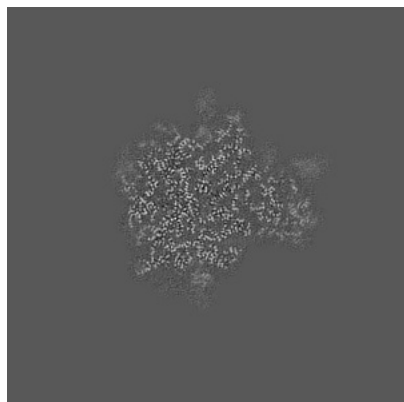


Z Index: 200

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

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

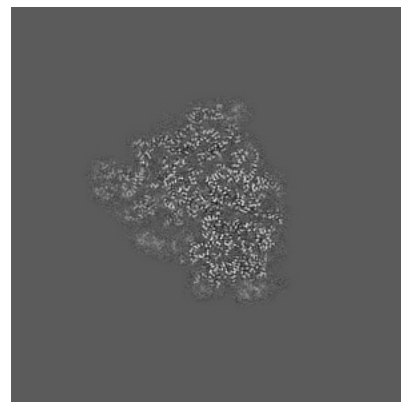
### 6.3.1 Primary map



X Index: 213

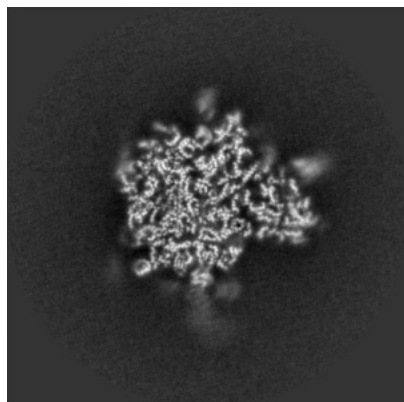


Y Index: 160

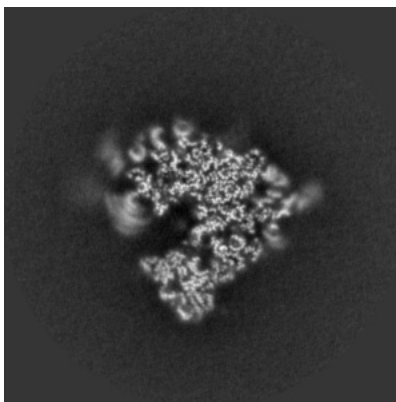


Z Index: 211

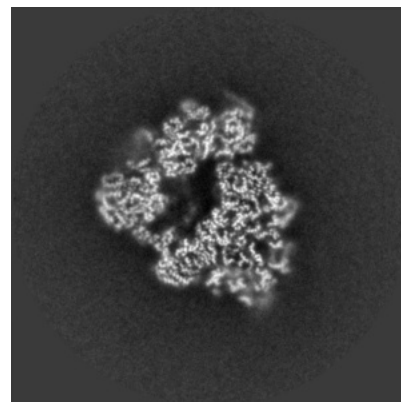
### 6.3.2 Raw map



X Index: 213



Y Index: 201

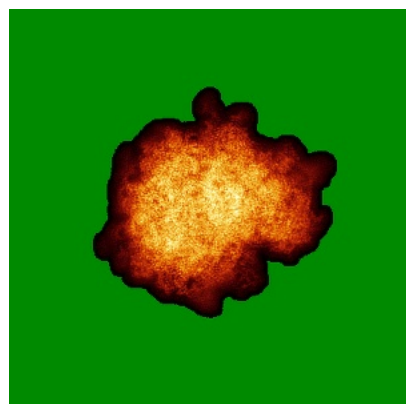


Z Index: 176

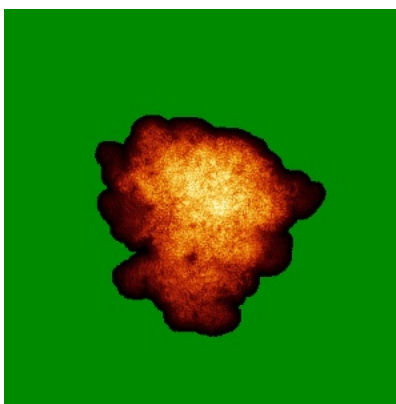
The images above show the largest variance slices of the map in three orthogonal directions.

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

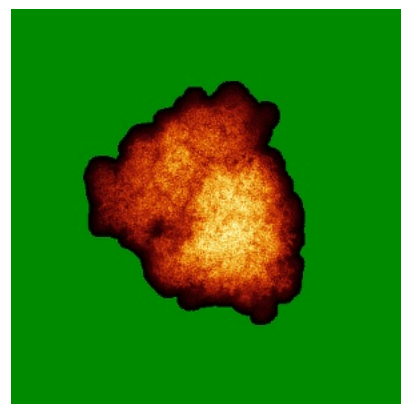
### 6.4.1 Primary map



X

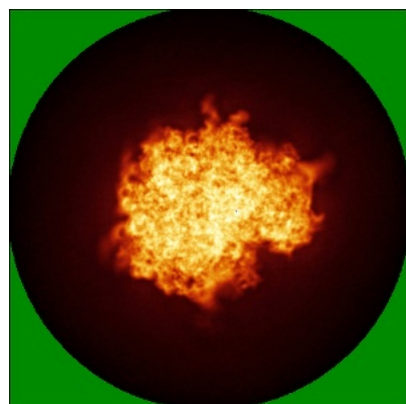


Y

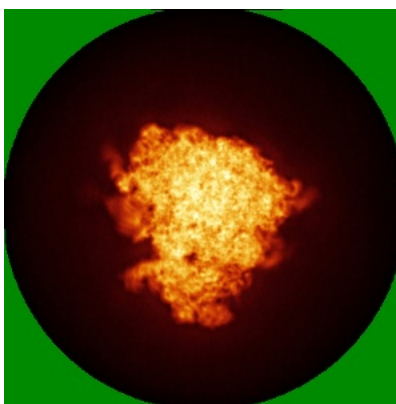


Z

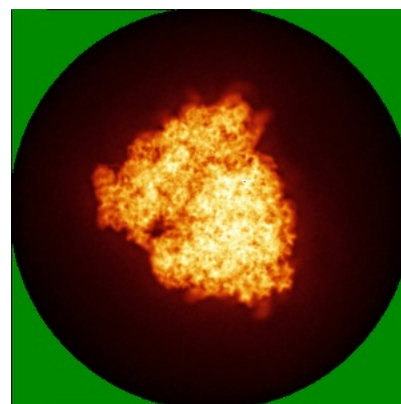
### 6.4.2 Raw map



X



Y

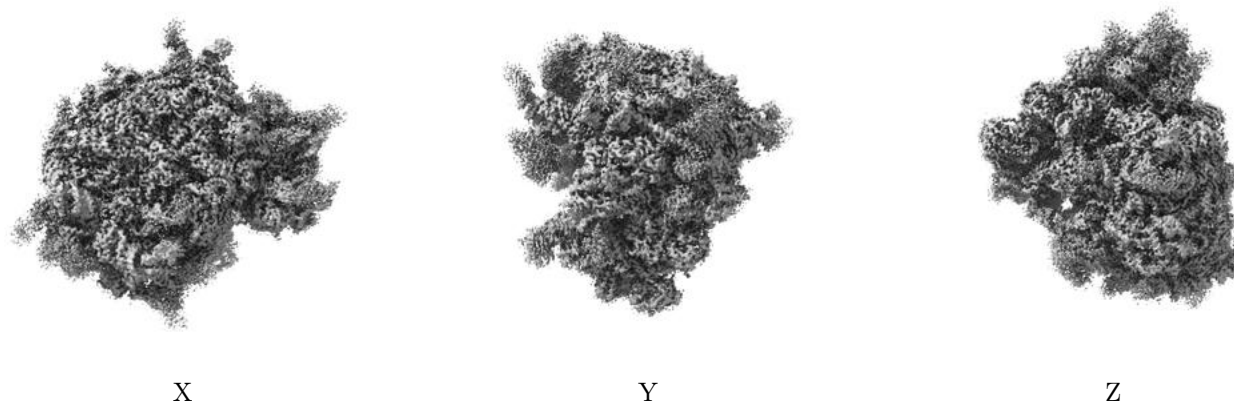


Z

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.

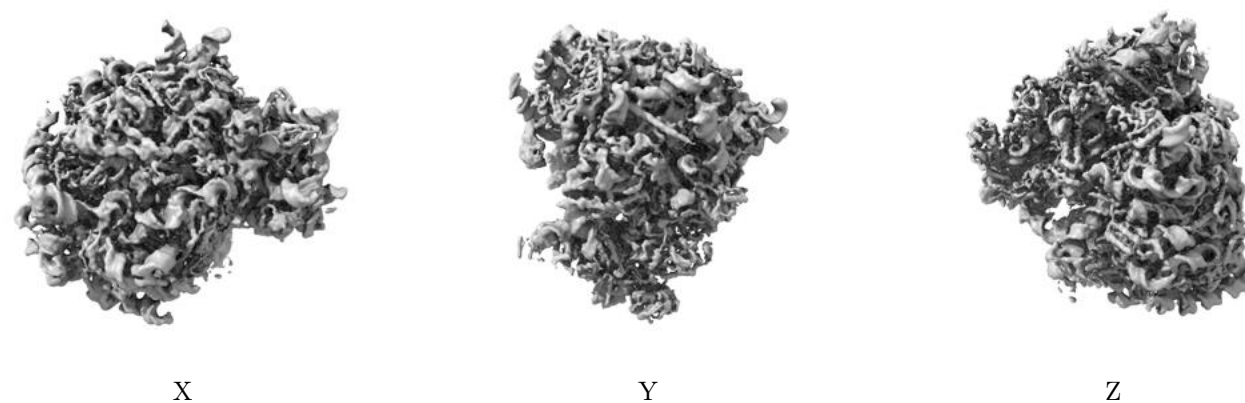
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

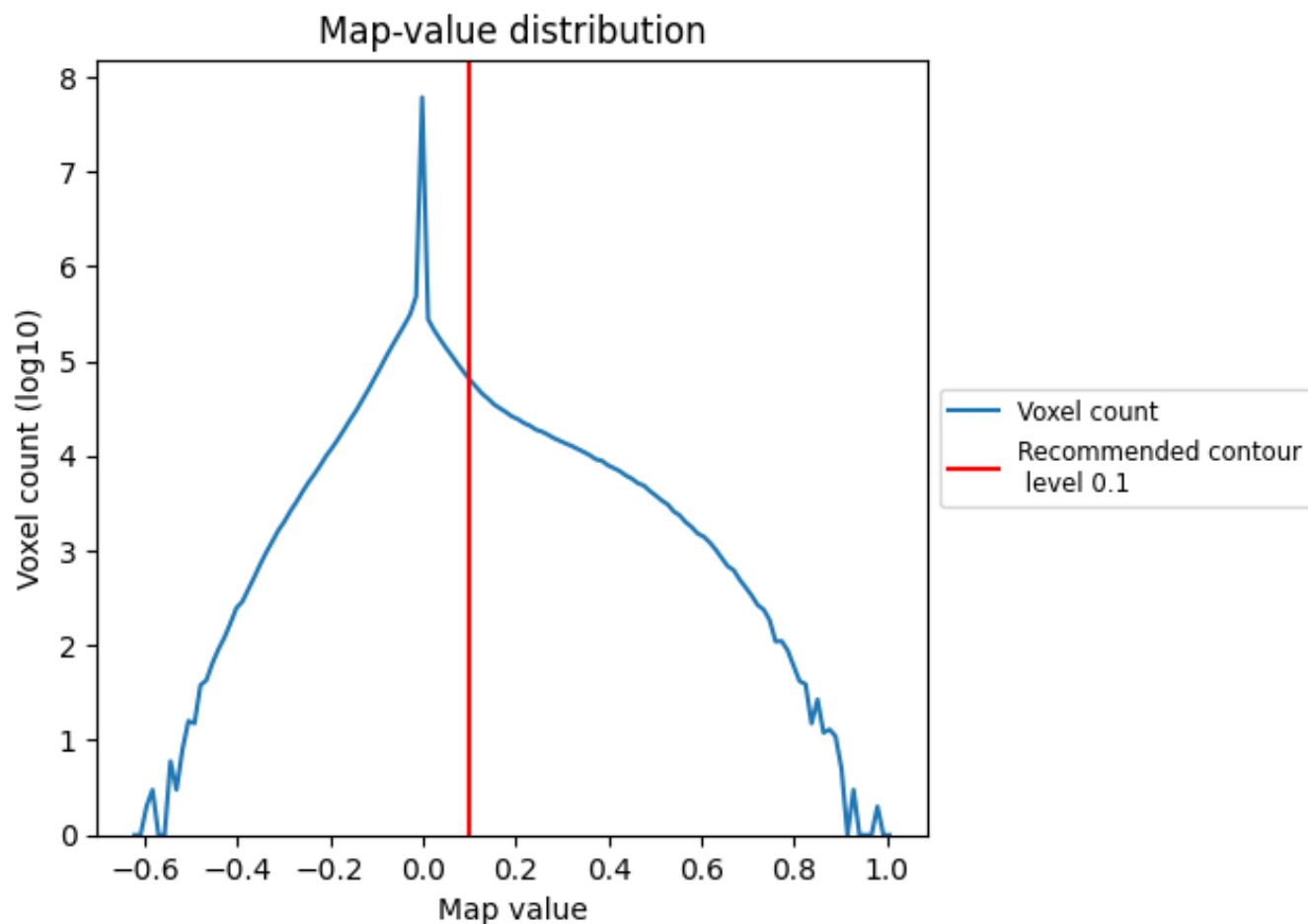
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

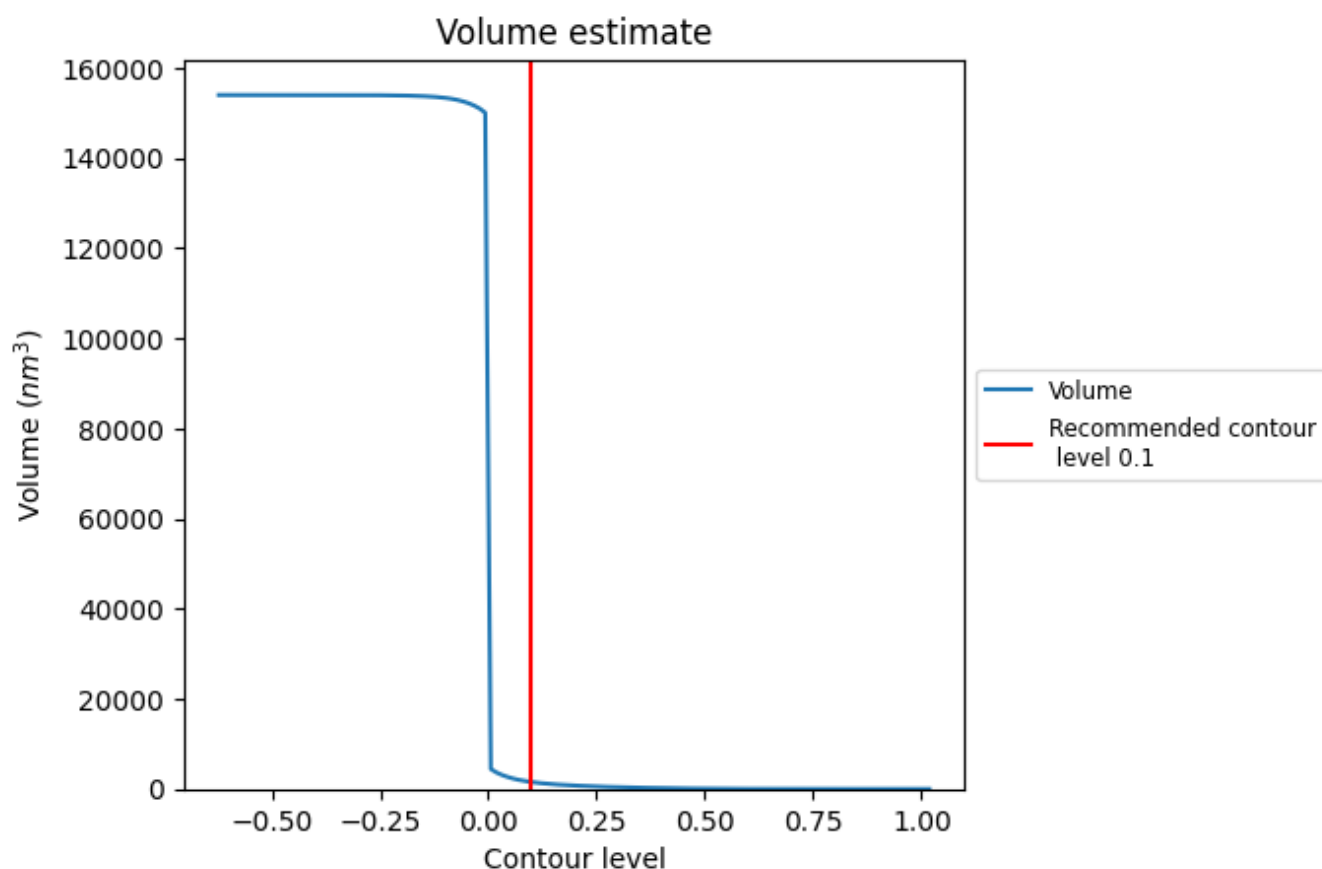
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

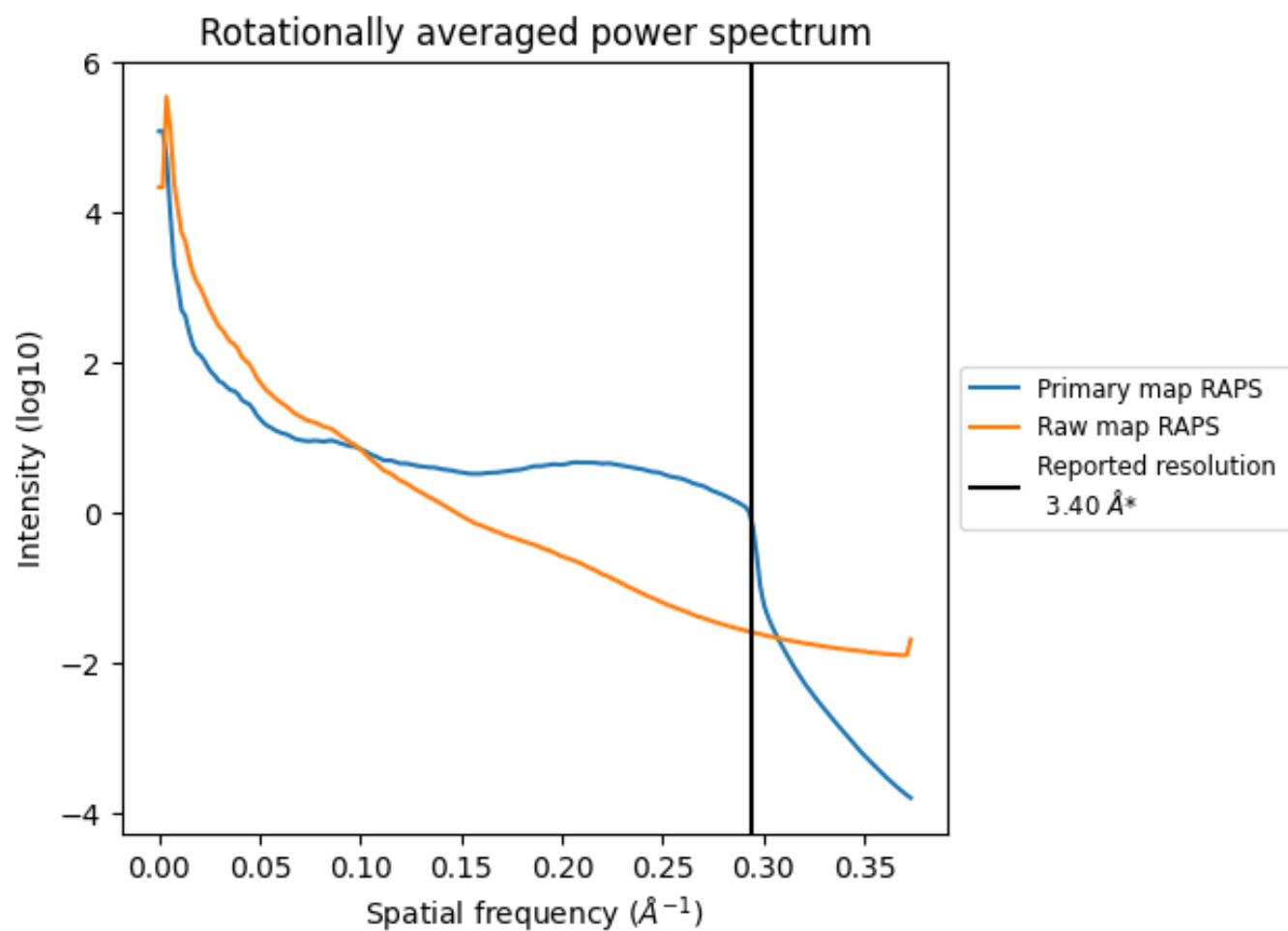
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1528 nm<sup>3</sup>; this corresponds to an approximate mass of 1381 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

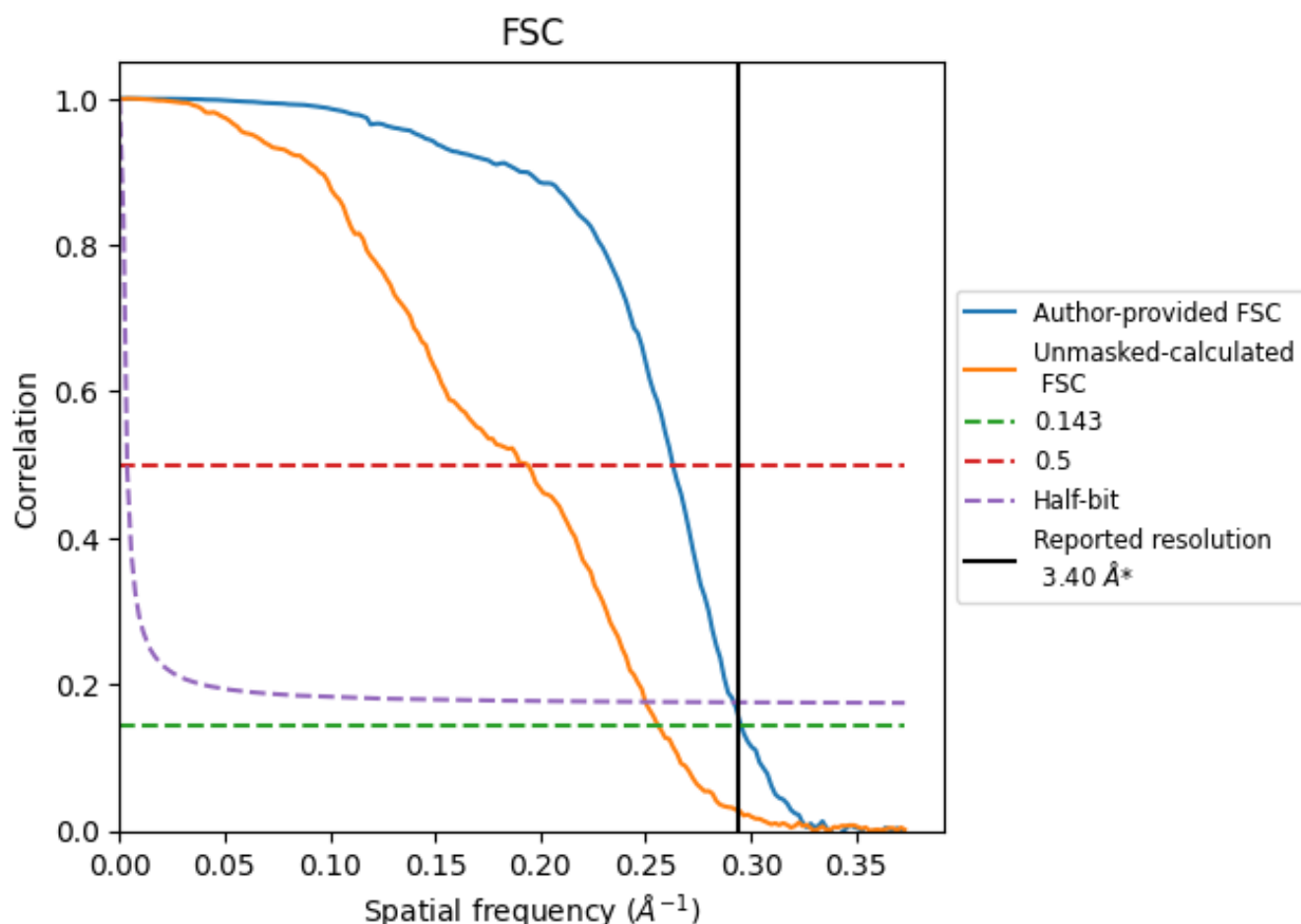


\*Reported resolution corresponds to spatial frequency of  $0.294 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

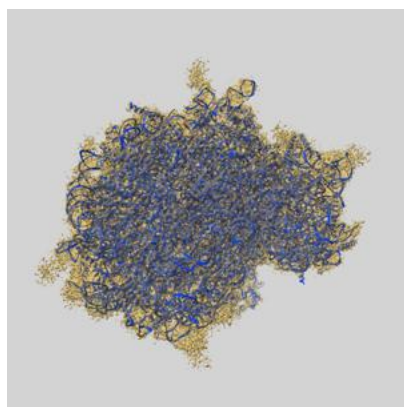
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.81	3.43
Unmasked-calculated*	3.91	5.16	4.00

\*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 3.91 differs from the reported value 3.4 by more than 10 %

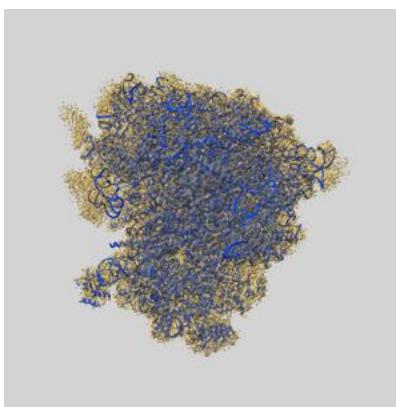
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9239 and PDB model 6MTC. Per-residue inclusion information can be found in section [3](#) on page [19](#).

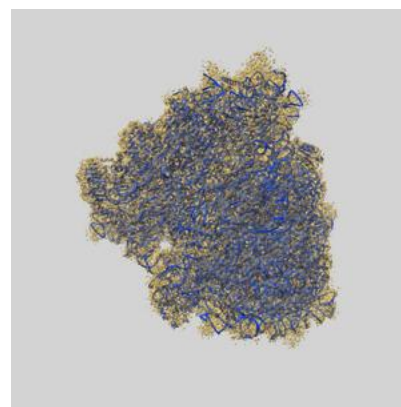
### 9.1 Map-model overlay [i](#)



X



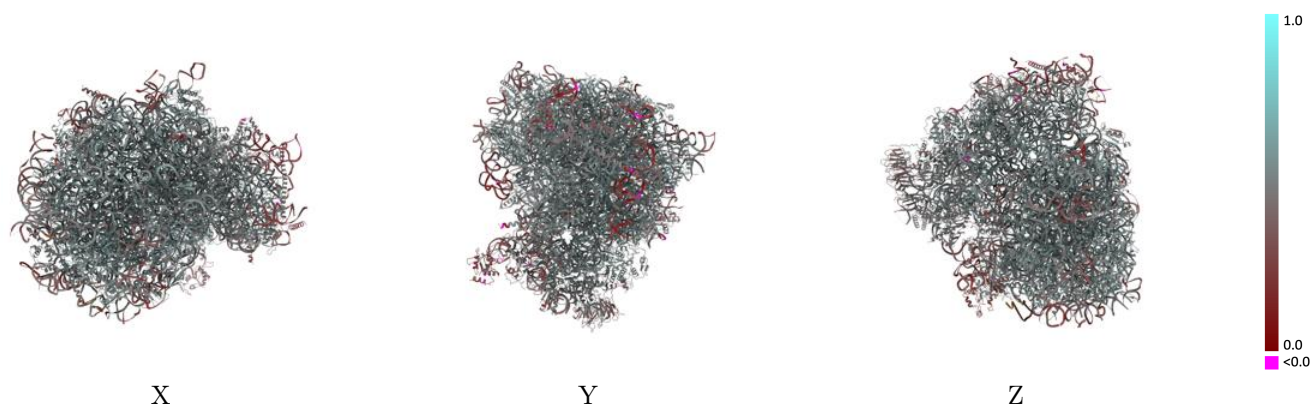
Y



Z

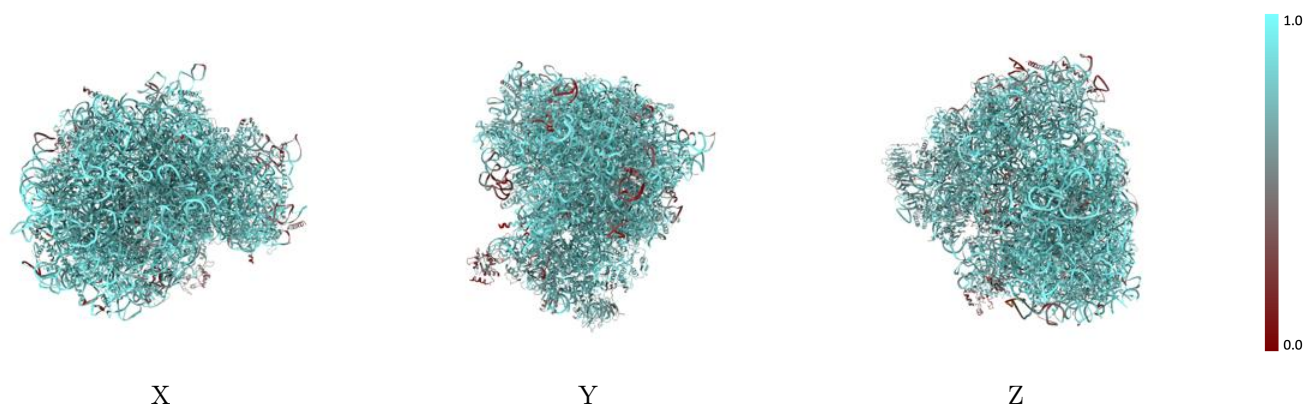
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



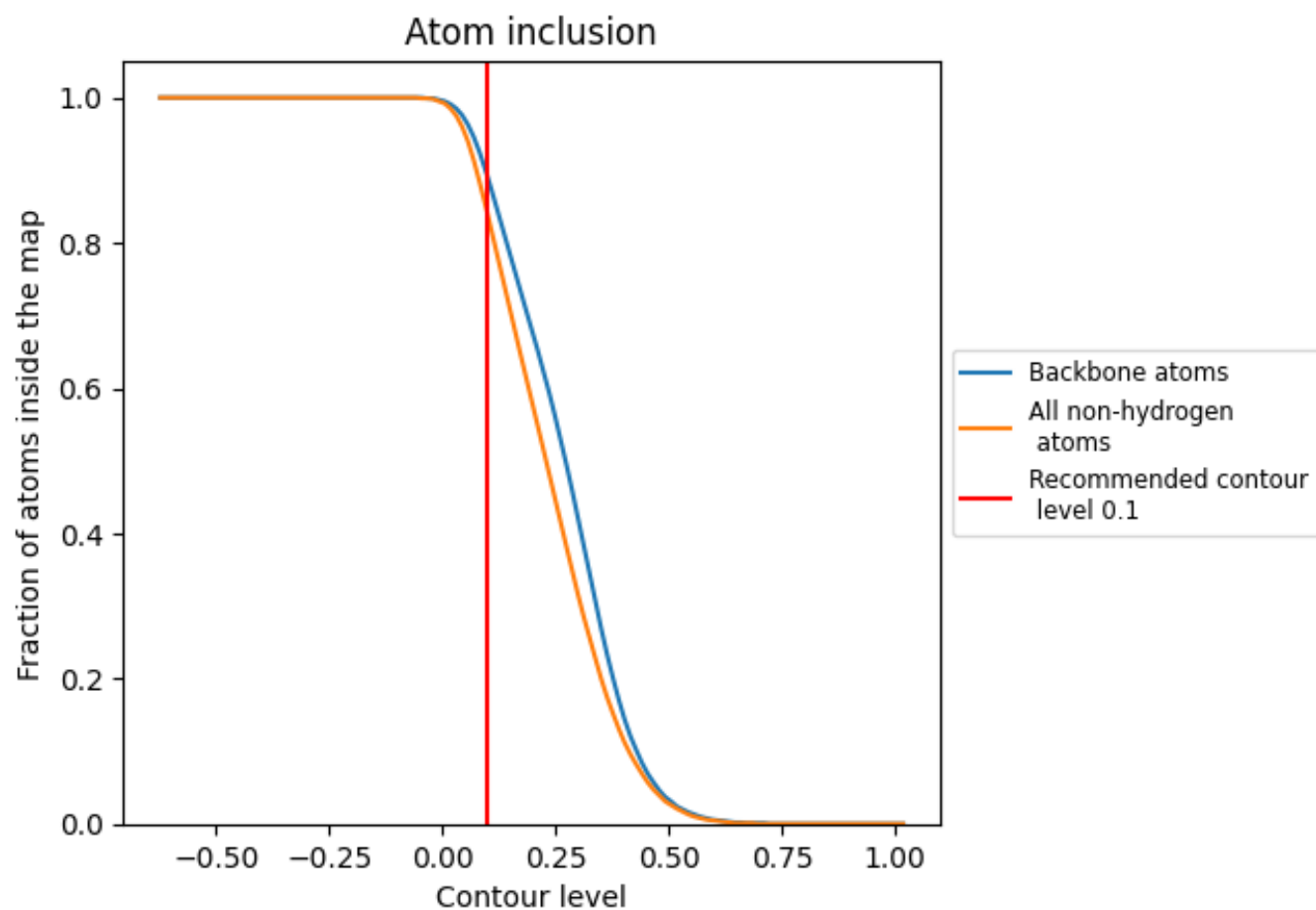
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.4970
4	 0.7290	 0.3350
5	 0.8830	 0.4920
7	 0.9390	 0.5210
8	 0.9060	 0.5060
9	 0.8690	 0.4760
A	 0.8870	 0.5620
AA	 0.8130	 0.5150
B	 0.8750	 0.5500
BB	 0.8030	 0.5210
C	 0.8650	 0.5490
CC	 0.8270	 0.5240
D	 0.8500	 0.5240
DD	 0.6920	 0.4640
E	 0.8410	 0.5280
EE	 0.8100	 0.5260
F	 0.8570	 0.5460
FF	 0.7740	 0.4930
G	 0.7970	 0.5110
GG	 0.7180	 0.4660
H	 0.8200	 0.5310
HH	 0.7300	 0.4720
I	 0.8510	 0.5440
II	 0.7890	 0.5150
J	 0.7900	 0.5020
JJ	 0.8080	 0.5050
KK	 0.6710	 0.4350
L	 0.8270	 0.5300
LL	 0.8150	 0.5350
M	 0.8470	 0.5280
MM	 0.3100	 0.2620
N	 0.8930	 0.5620
NN	 0.8410	 0.5300
O	 0.8540	 0.5430
OO	 0.8070	 0.5220















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Chain	Atom inclusion	Q-score
P	 0.8640	 0.5490
PP	 0.6710	 0.4330
Q	 0.8690	 0.5540
QQ	 0.7400	 0.4770
R	 0.8120	 0.5210
RR	 0.7500	 0.4860
S	 0.8660	 0.5520
SS	 0.7220	 0.4680
T	 0.8460	 0.5380
TT	 0.7430	 0.4740
U	 0.7830	 0.4850
UU	 0.6810	 0.4460
V	 0.8580	 0.5550
VV	 0.8020	 0.5250
W	 0.6940	 0.4530
WW	 0.8550	 0.5380
X	 0.8300	 0.5330
XX	 0.8230	 0.5300
Y	 0.8530	 0.5390
YY	 0.7810	 0.4960
Z	 0.8610	 0.5320
ZZ	 0.7050	 0.4620
a	 0.8730	 0.5560
aa	 0.8330	 0.5420
b	 0.7490	 0.4890
bb	 0.7870	 0.5180
c	 0.8360	 0.5290
cc	 0.7380	 0.5060
d	 0.8310	 0.5300
dd	 0.8080	 0.4980
e	 0.8730	 0.5590
ee	 0.6950	 0.4890
f	 0.8910	 0.5620
ff	 0.3810	 0.3280
g	 0.8310	 0.5430
gg	 0.6390	 0.4170
h	 0.8260	 0.5280
i	 0.8350	 0.5250
j	 0.9020	 0.5550
k	 0.7680	 0.5130
l	 0.8430	 0.5460
m	 0.8540	 0.5360

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Chain	Atom inclusion	Q-score
n	 0.7940	 0.5270
o	 0.8530	 0.5500
p	 0.8390	 0.5540
r	 0.8840	 0.5490
u	 0.4540	 0.3420
v	 0.6270	 0.4620