



## Full wwPDB EM Validation Report ⓘ

Nov 12, 2024 – 10:10 am GMT

PDB ID : 8P8W  
EMDB ID : EMD-17145  
Title : Mycoplasma pneumoniae di-ribosome in chloramphenicol-treated cells (following 70S)  
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.  
Deposited on : 2023-06-02  
Resolution : 8.70 Å (reported)  
Based on initial models : 7OOD, 7OOC

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

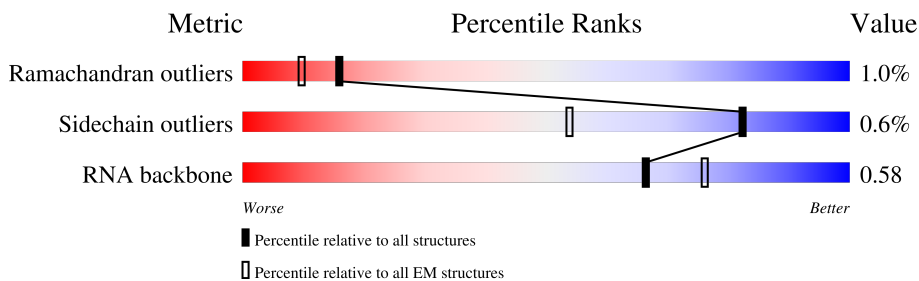
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 8.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	48	12% (red), 98% (green), 0% (yellow), 0% (orange), 0% (grey)
2	1	59	17% (red), 100% (green), 0% (yellow), 0% (orange), 0% (grey)
3	2	37	14% (red), 100% (green), 0% (yellow), 0% (orange), 0% (grey)
4	3	2907	0% (red), 81% (green), 19% (yellow), 0% (orange), 0% (grey)
5	4	108	0% (red), 73% (green), 27% (yellow), 0% (orange), 0% (grey)
6	5	1520	0% (red), 82% (green), 17% (yellow), 0% (orange), 0% (grey)
7	6	76	68% (red), 67% (green), 28% (yellow), 5% (orange), 0% (grey)
8	7	75	0% (red), 69% (green), 31% (yellow), 0% (orange), 0% (grey)

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Mol	Chain	Length	Quality of chain
9	A	294	30% 88% 9%
10	B	273	21% 81% 18%
11	C	205	16% 96% .
11	U	205	93% 91% 8%
12	D	219	28% 76% 21%
13	E	215	23% 75% 22%
14	F	155	22% 95% 5%
15	G	142	23% 98% .
16	H	132	18% 97% ..
17	I	108	35% 94% ..
18	J	121	16% 94% 6%
19	K	139	22% 93% ..
20	L	124	23% 97% ..
21	M	61	16% 98% .
22	N	86	12% 99% .
23	O	94	15% 90% 7%
24	P	85	18% 99% .
25	Q	104	22% 73% 25%
26	R	87	17% 98% ..
27	S	87	. 90% 9%
28	T	60	20% 97% ..
29	X	444	5% 7% 93%
30	Y	29	21% 45% 55%
31	Z	36	67% 100%
32	a	287	24% 99% .

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Mol	Chain	Length	Quality of chain
33	b	287	19% 79% 20%
34	c	212	42% 100%
35	d	180	46% 99%
36	e	184	35% 95%
37	f	149	90% 99%
38	g	161	48% 76% 22%
39	h	137	74% 93% 7%
40	i	146	13% 98%
41	j	122	38% 98%
42	k	151	34% 99%
43	l	139	20% 97%
44	m	124	9% 95%
45	n	116	47% 100%
46	o	119	28% 99%
47	p	127	17% 93% 7%
48	q	100	45% 99%
49	r	159	13% 87% 11%
50	s	237	8% 40% 60%
51	t	111	45% 99%
52	u	104	17% 93%
53	v	65	25% 97%
54	w	111	50% 99%
55	x	97	61% 90% 8%
56	y	57	19% 95%
57	z	53	40% 94% 6%

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 151559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	47	380	236	81	61	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	59	477	300	99	77	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	37	304	189	65	46	4	0	0

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	2893	61995	27704	11293	20105	2893	0	0

- Molecule 5 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	4	108	2305	1030	415	752	108	0	0

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	5	1507	32258	14420	5847	10484	1507	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1003	A	G	conflict	GB 26117688

- Molecule 7 is a RNA chain called tRNA-Ala (E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	6	76	1620	723	287	534	76	0	0

- Molecule 8 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	7	75	1599	712	279	533	75	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	17	G	-	insertion	GB 26117688
7	55	C	U	conflict	GB 26117688

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	268	2152	1368	379	396	9	0	0

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	225	1773	1121	328	319	5	0	0

- Molecule 11 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	204	1669	1057	316	292	4	0	0
11	U	204	1669	1057	316	292	4	0	0

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	173	1346	846	265	232	3	0	0

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	167	1362	857	240	263	2	0	0

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	155	1254	790	240	217	7	0	0

- Molecule 15 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	142	1118	728	194	193	3	0	0

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	129	1040	661	195	183	1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	104	832	536	147	148	1	0	0

- Molecule 18 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J	114	829	514	153	156	6	0	0

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	K	135	1071	677	212	180	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	121	975	609	197	169		0	0

- Molecule 21 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	60	474	302	96	72	4	0	0

- Molecule 22 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	N	86	697	441	131	124	1	0	0

- Molecule 23 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O	87	705	453	130	118	4	0	0

- Molecule 24 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	P	85	693	436	138	118	1	0	0

- Molecule 25 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	78	651	417	129	100	5	0	0

- Molecule 26 is a protein called 30S ribosomal protein S19.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	86	700	444	132	122	2	0	0

- Molecule 27 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	S	79	643	391	138	114		0	0

- Molecule 28 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	59	519	326	111	80	2	0	0

- Molecule 29 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	X	30	242	155	43	43	1	0	0

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	Y	29	623	280	120	194	29	0	0

- Molecule 31 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	Z	36	187	112	37	38	0	0

- Molecule 32 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	a	285	2225	1385	437	397	6	0	0

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	231	Total	C	N	O	S	0	0
			1778	1129	320	322	7		

- Molecule 34 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	211	Total	C	N	O	S	0	0
			1654	1053	299	299	3		

- Molecule 35 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	179	Total	C	N	O	S	0	0
			1416	910	251	251	4		

- Molecule 36 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	e	176	Total	C	N	O	0	0
			1396	899	247	250		

- Molecule 37 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	149	Total	C	N	O	S	0	0
			1210	780	212	215	3		

- Molecule 38 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	125	Total	C	N	O	S	0	0
			951	606	165	177	3		

- Molecule 39 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 40 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 41 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 42 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	150	Total	C	N	O	S	0	0
			1170	741	228	200	1		

- Molecule 43 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 44 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 45 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	116	Total	C	N	O	S	0	0
			918	573	181	162	2		

- Molecule 46 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	118	Total	C	N	O	S	0	0
			966	609	186	170	1		

- Molecule 47 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	118	Total	C	N	O	S	0	0
			981	624	194	161	2		

- Molecule 48 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

- Molecule 49 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	142	Total	C	N	O	S	0	0
			1091	677	212	195	7		

- Molecule 50 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	95	Total	C	N	O	S	0	0
			740	486	125	128	1		

- Molecule 51 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	111	Total	C	N	O	S	0	0
			871	550	166	152	3		

- Molecule 52 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	101	Total	C	N	O	S	0	0
			786	498	148	139	1		

- Molecule 53 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	64	Total	C	N	O	S	0	0
			520	320	109	90	1		

- Molecule 54 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	w	110	Total	C	N	O	0	0
			906	576	168	162		

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	x	89	Total	C	N	O	S	0	0
			708	449	124	131	4		

- Molecule 56 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

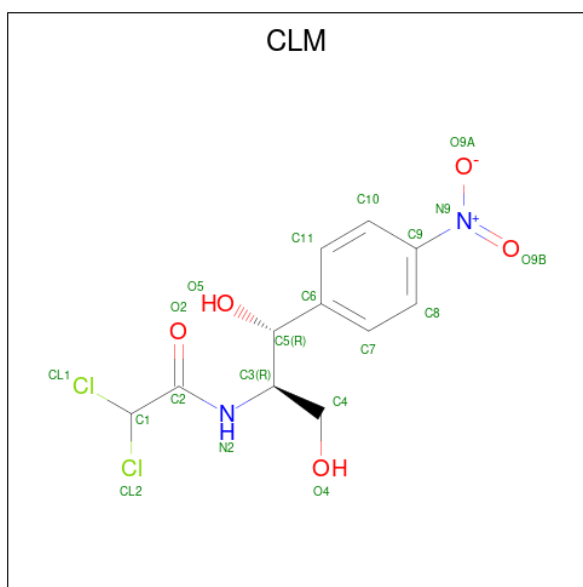
- Molecule 57 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	2	1	Total	Zn	0
			1	1	
58	M	1	Total	Zn	0
			1	1	
58	Q	1	Total	Zn	0
			1	1	
58	x	1	Total	Zn	0
			1	1	
58	y	1	Total	Zn	0
			1	1	
58	z	1	Total	Zn	0
			1	1	

- Molecule 59 is CHLORAMPHENICOL (three-letter code: CLM) (formula: C<sub>11</sub>H<sub>12</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Cl	N		O
59	3	1	20	11	2	2	5	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
60	3	1	1	1	0

- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
61	3	206	206	206	0
61	4	1	1	1	0
61	5	90	90	90	0
61	6	1	1	1	0
61	K	1	1	1	0
61	P	1	1	1	0
61	Y	1	1	1	0

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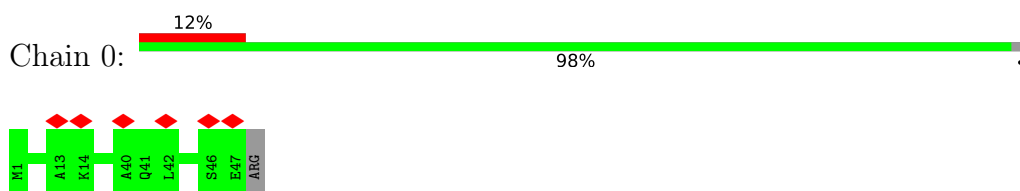
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
61	b	2	Total 2	Mg 2	0
61	i	1	Total 1	Mg 1	0
61	k	2	Total 2	Mg 2	0
61	y	2	Total 2	Mg 2	0

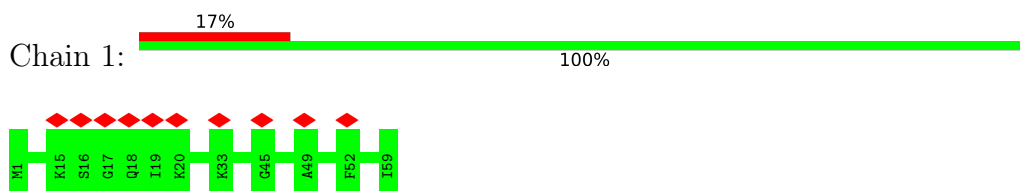
### 3 Residue-property plots [i](#)

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

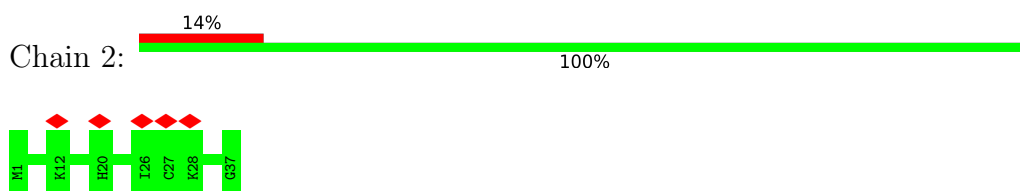
- Molecule 1: 50S ribosomal protein L34



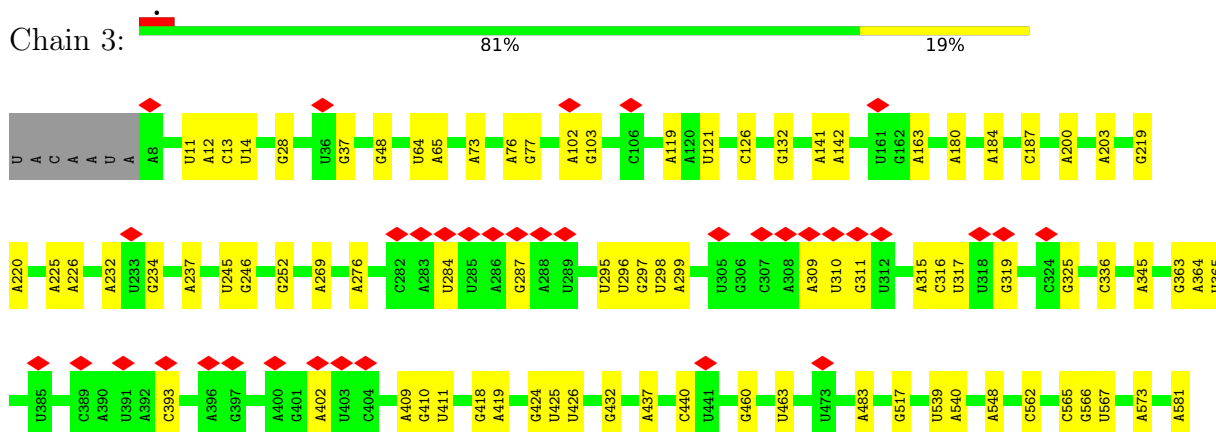
- Molecule 2: 50S ribosomal protein L35



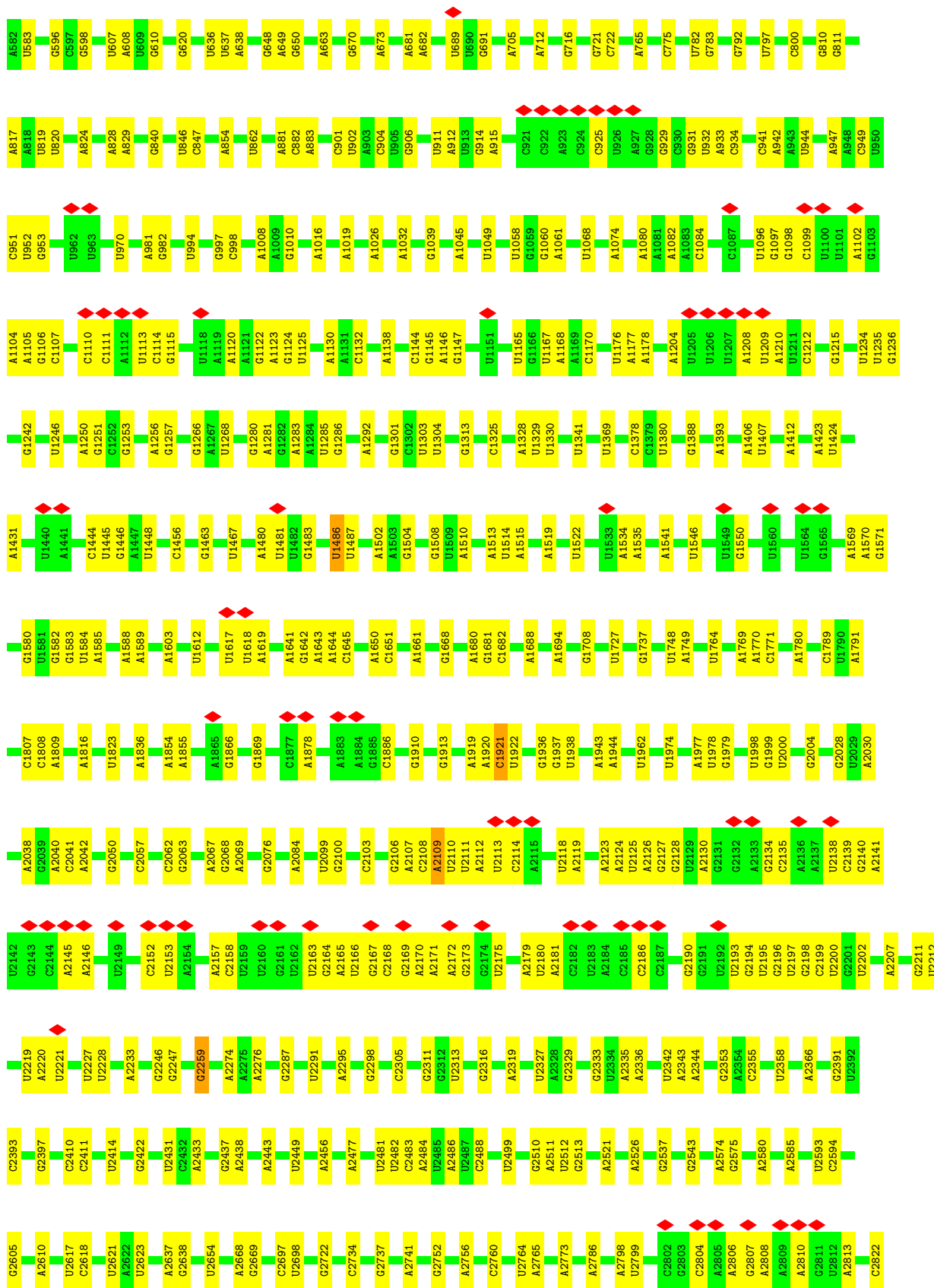
- Molecule 3: 50S ribosomal protein L36

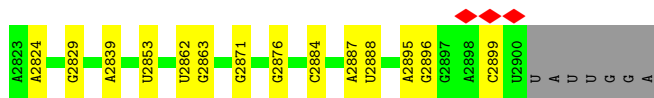


- Molecule 4: 23S ribosomal RNA

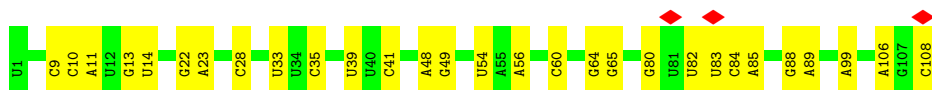




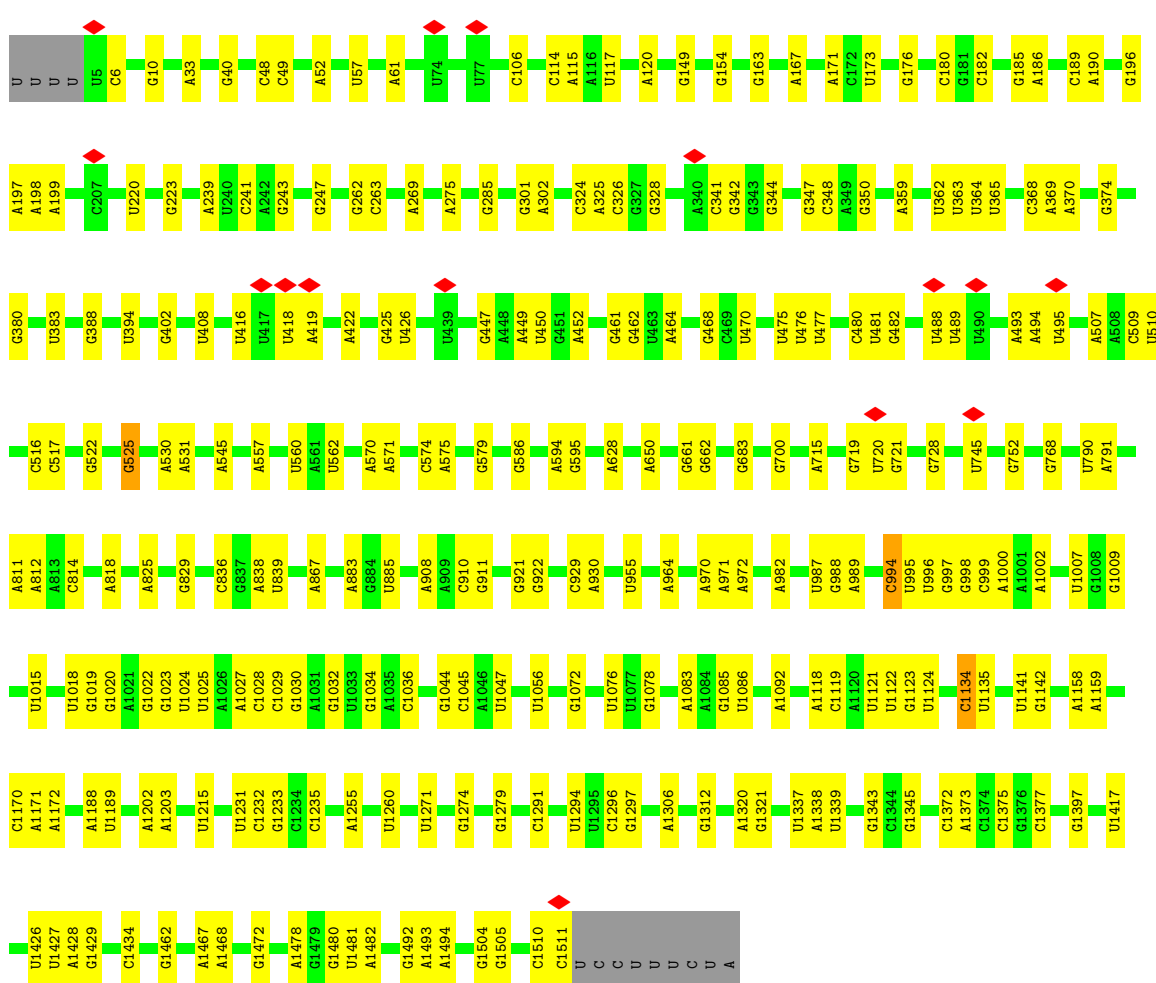
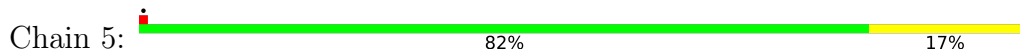




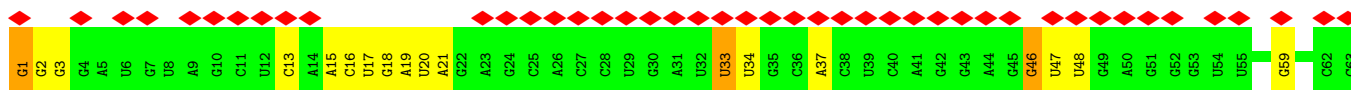
• Molecule 5: 5S ribosomal RNA



• Molecule 6: 16S ribosomal RNA



• Molecule 7: tRNA-Ala (E-site)

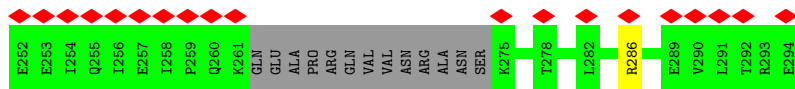
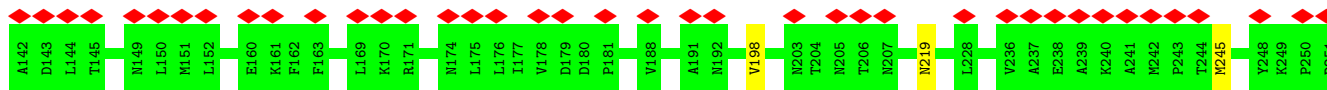
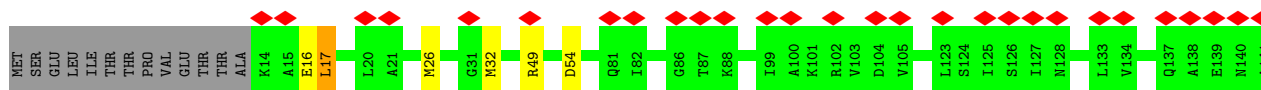
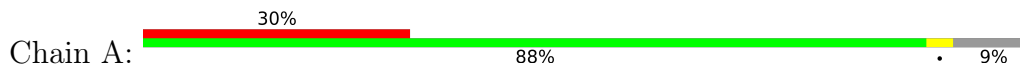




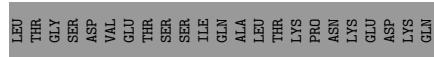
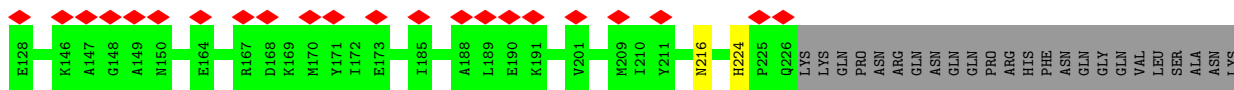
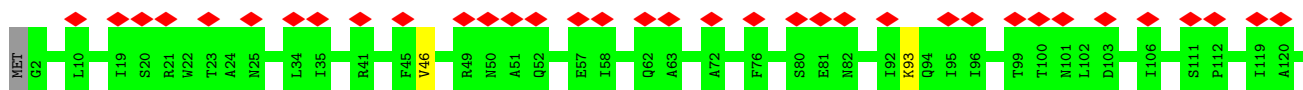
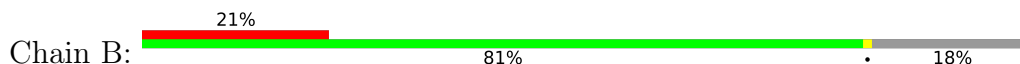
• Molecule 8: tRNA-Asp (P-site)



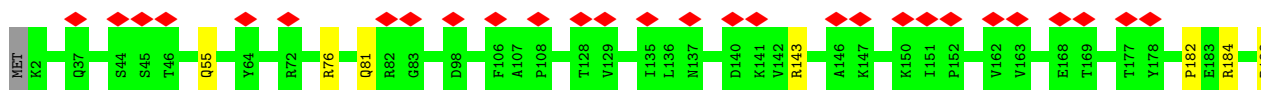
• Molecule 9: 30S ribosomal protein S2



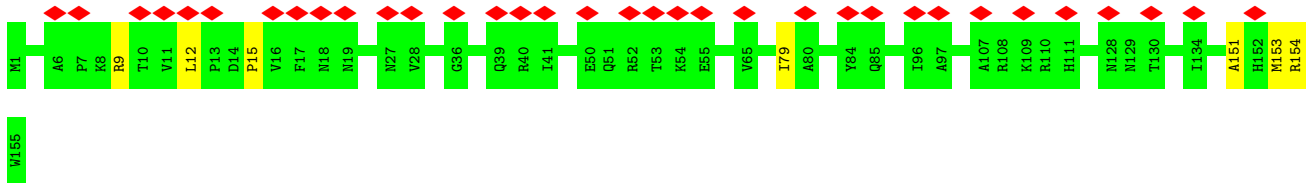
• Molecule 10: 30S ribosomal protein S3



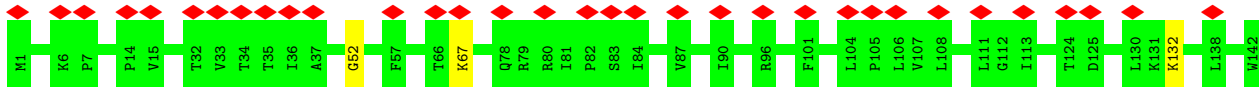
• Molecule 11: 30S ribosomal protein S4



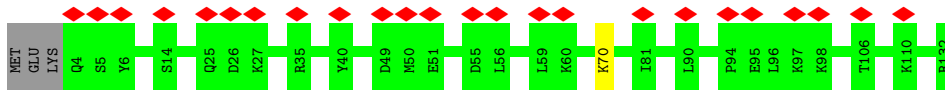




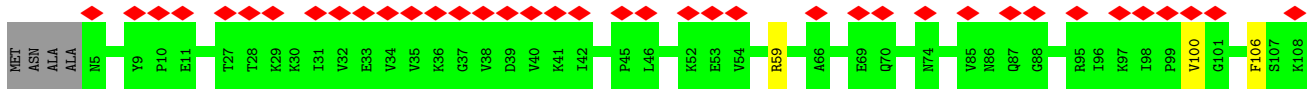
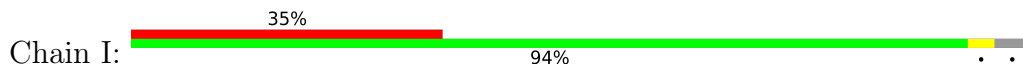
- Molecule 15: 30S ribosomal protein S8



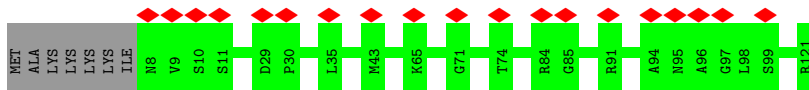
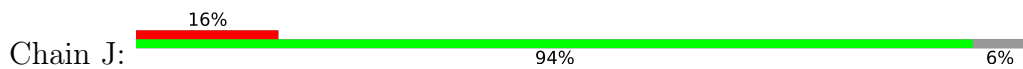
- Molecule 16: 30S ribosomal protein S9



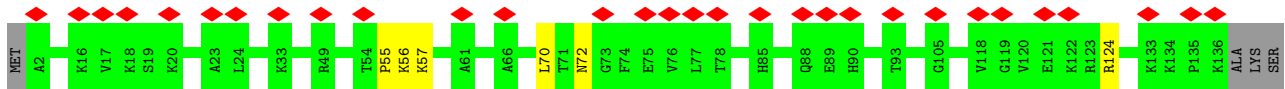
- Molecule 17: 30S ribosomal protein S10



- Molecule 18: 30S ribosomal protein S11

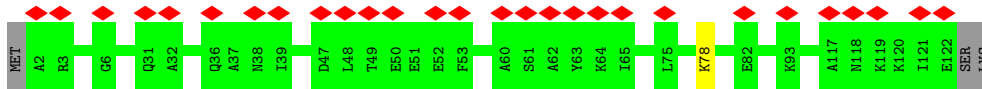


- Molecule 19: 30S ribosomal protein S12

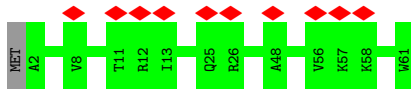


- Molecule 20: 30S ribosomal protein S13

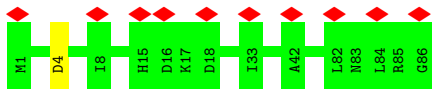




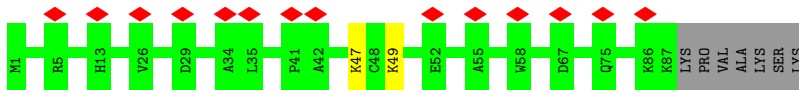
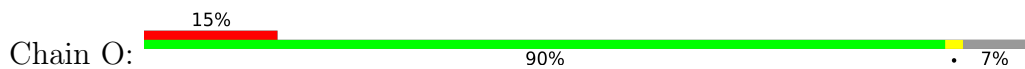
- Molecule 21: 30S ribosomal protein S14 type Z



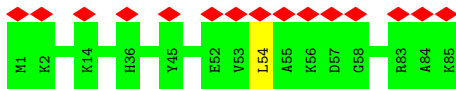
- Molecule 22: 30S ribosomal protein S15



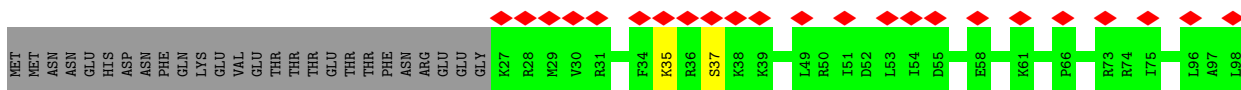
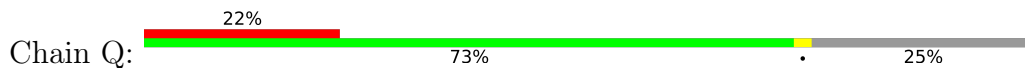
- Molecule 23: 30S ribosomal protein S16



- Molecule 24: 30S ribosomal protein S17



- Molecule 25: 30S ribosomal protein S18

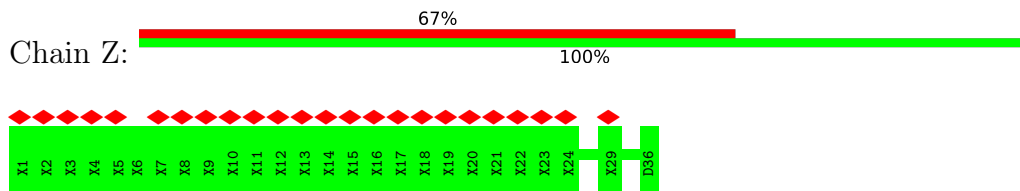


- Molecule 26: 30S ribosomal protein S19

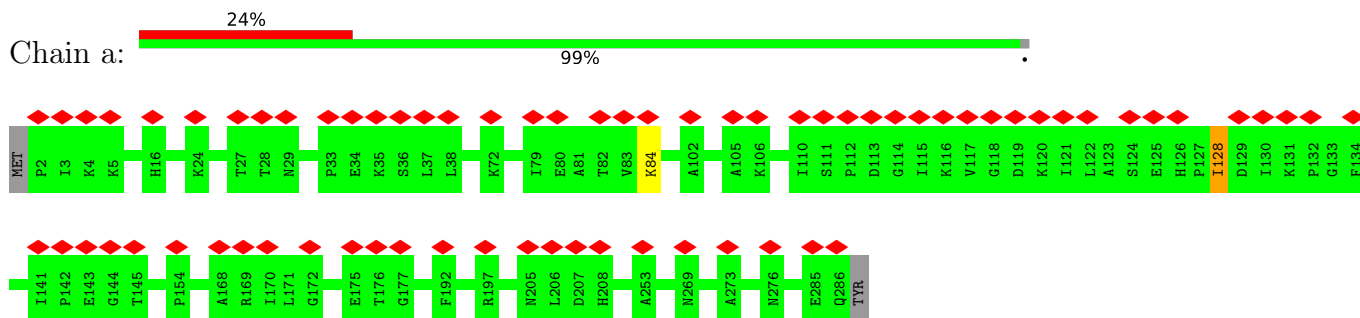




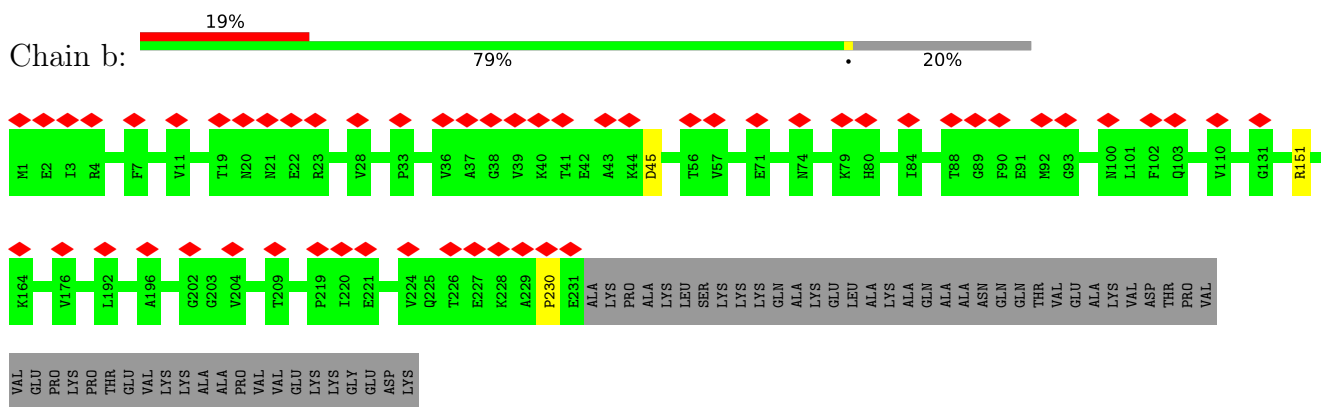
• Molecule 31: Nascent chain



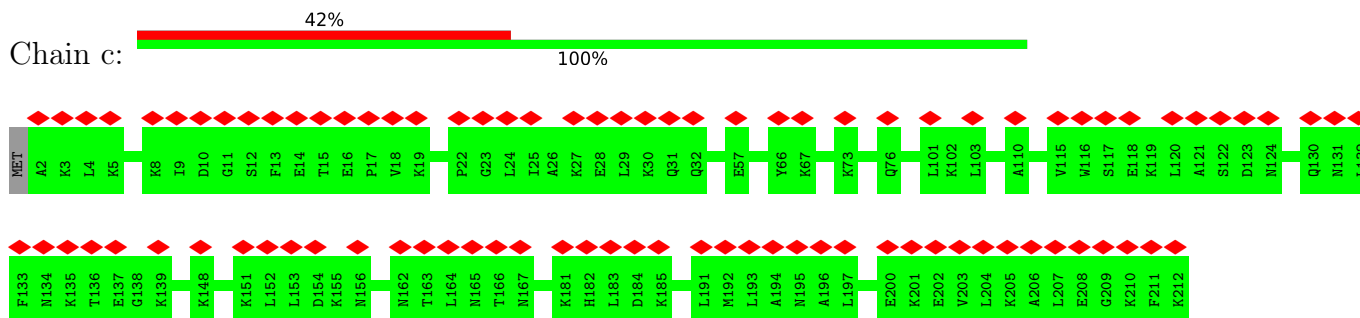
• Molecule 32: 50S ribosomal protein L2



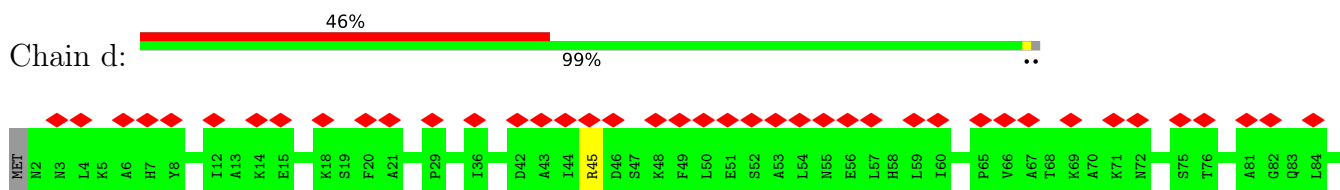
• Molecule 33: 50S ribosomal protein L3



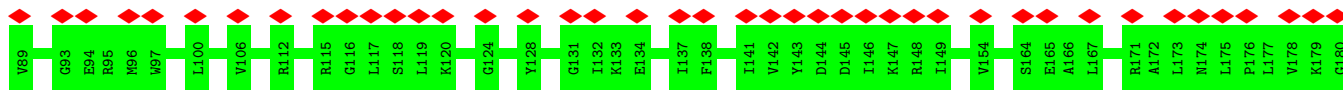
• Molecule 34: 50S ribosomal protein L4



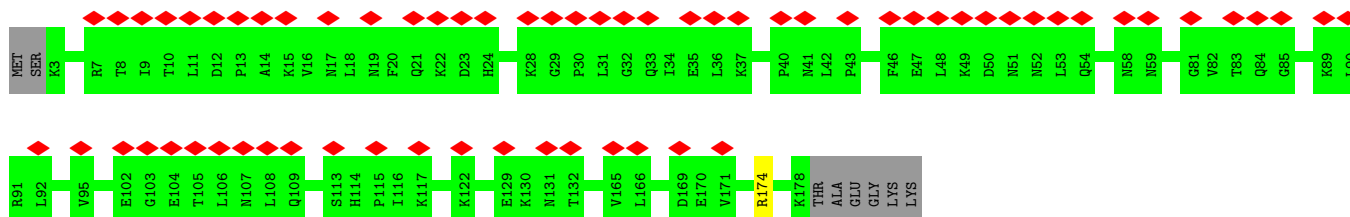
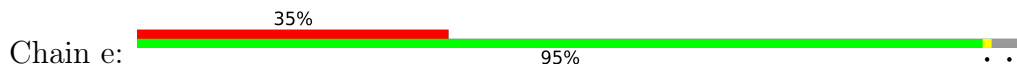
• Molecule 35: 50S ribosomal protein L5



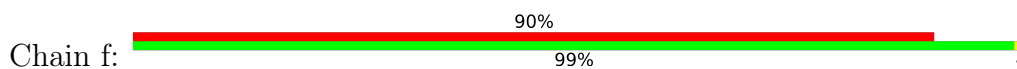




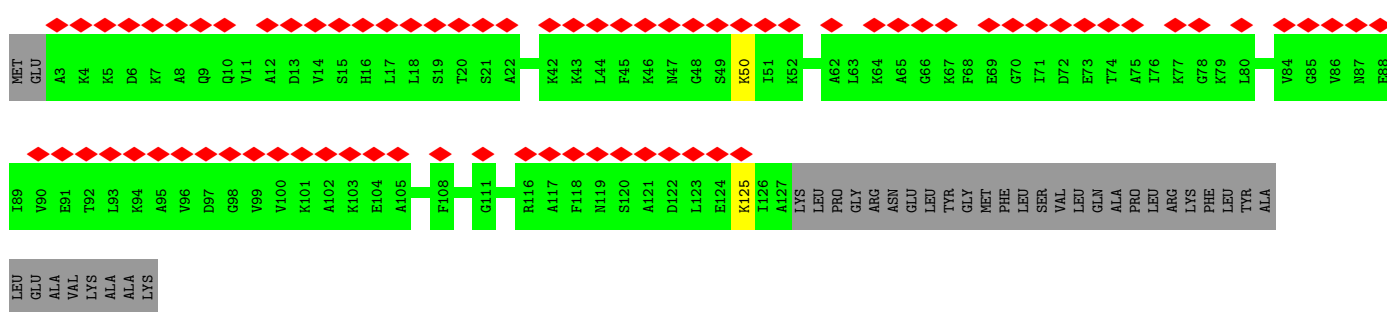
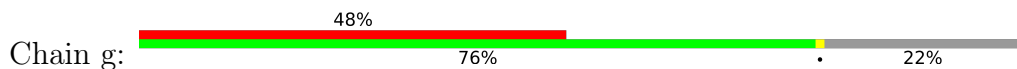
- Molecule 36: 50S ribosomal protein L6



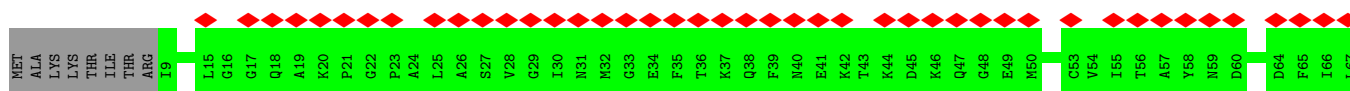
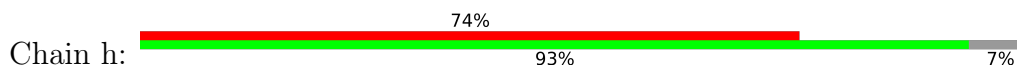
- Molecule 37: 50S ribosomal protein L9

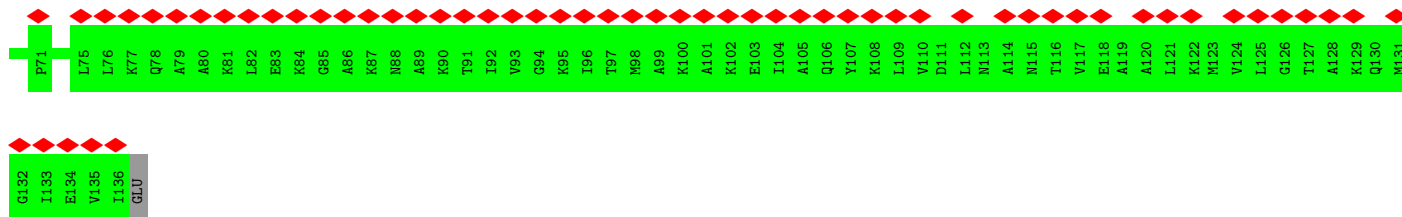


- Molecule 38: 50S ribosomal protein L10

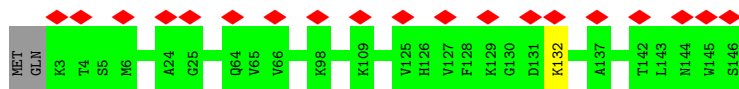


- Molecule 39: 50S ribosomal protein L11

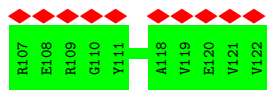
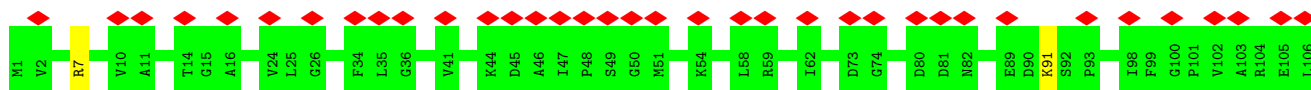




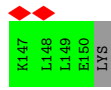
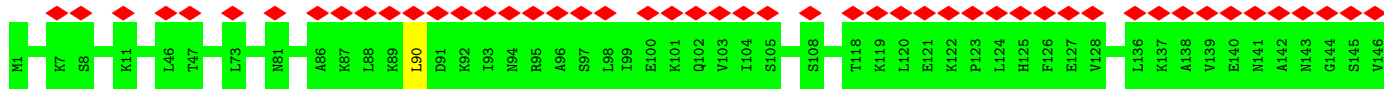
• Molecule 40: 50S ribosomal protein L13



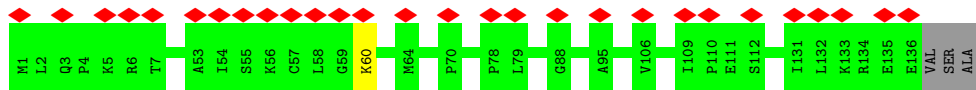
• Molecule 41: 50S ribosomal protein L14



• Molecule 42: 50S ribosomal protein L15

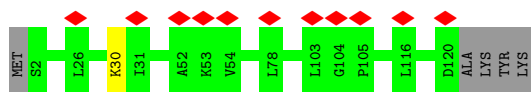


• Molecule 43: 50S ribosomal protein L16

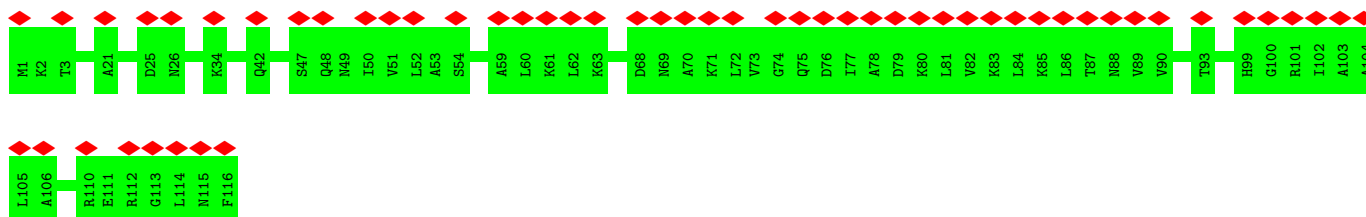


• Molecule 44: 50S ribosomal protein L17

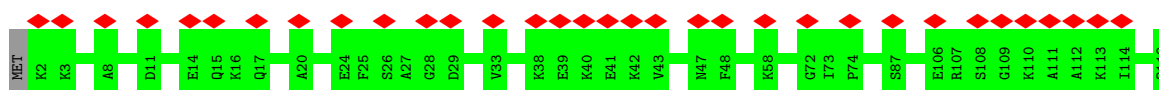




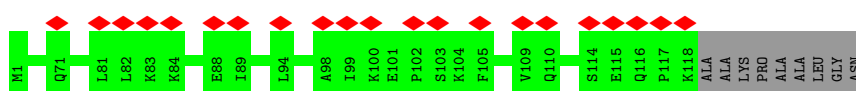
- Molecule 45: 50S ribosomal protein L18



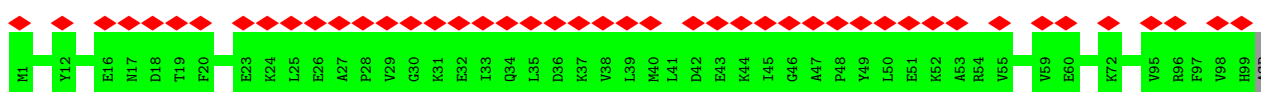
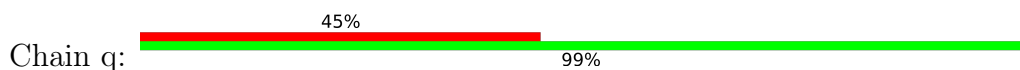
- Molecule 46: 50S ribosomal protein L19



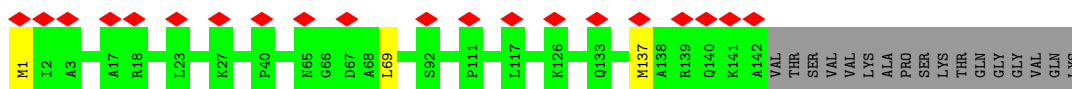
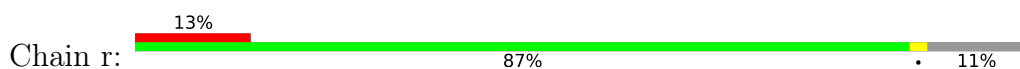
- Molecule 47: 50S ribosomal protein L20



- Molecule 48: 50S ribosomal protein L21

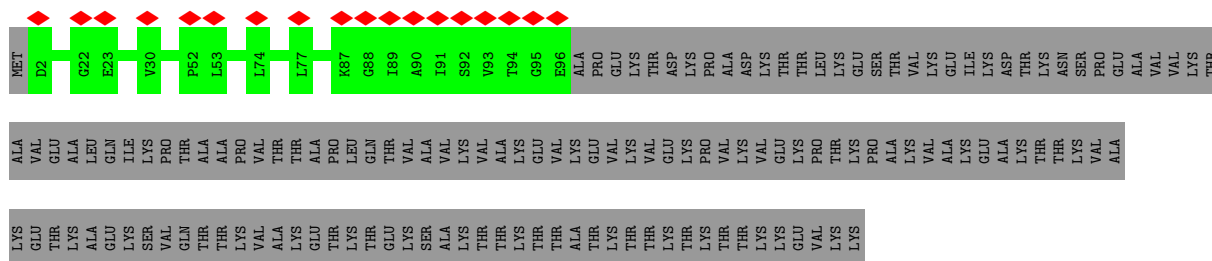


- Molecule 49: 50S ribosomal protein L22

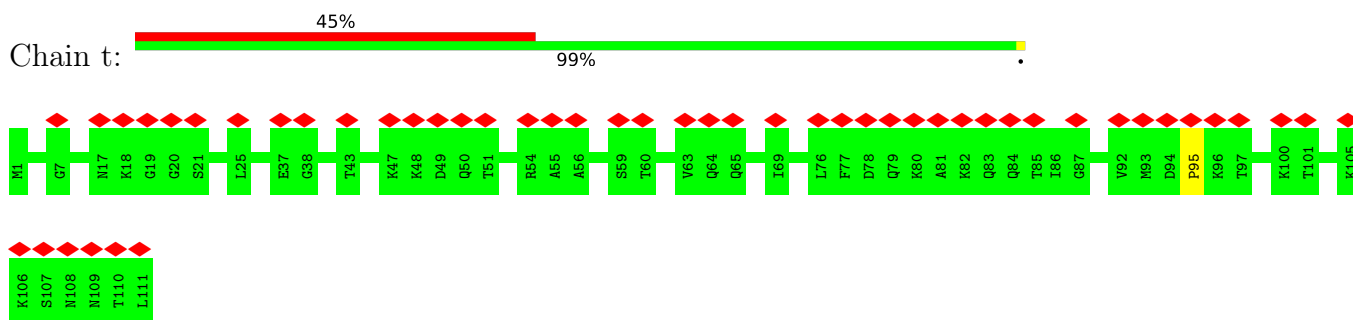


- Molecule 50: 50S ribosomal protein L23

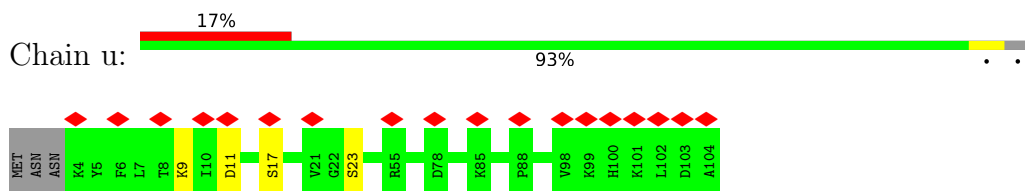




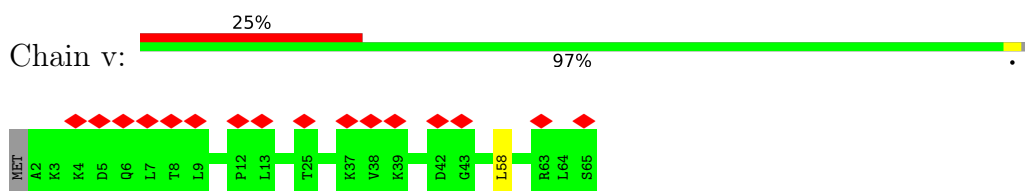
• Molecule 51: 50S ribosomal protein L24



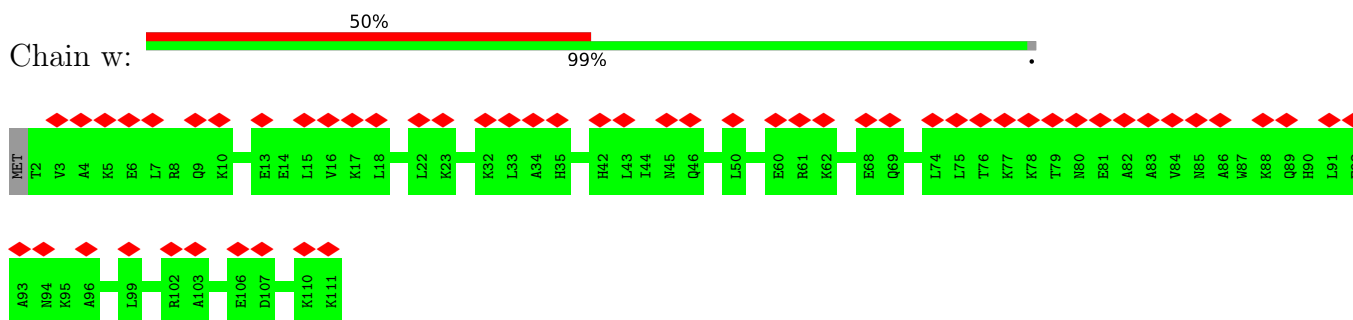
• Molecule 52: 50S ribosomal protein L27



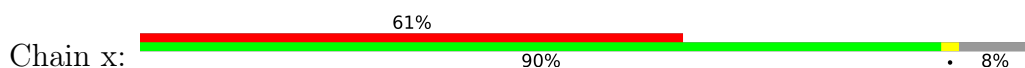
• Molecule 53: 50S ribosomal protein L28

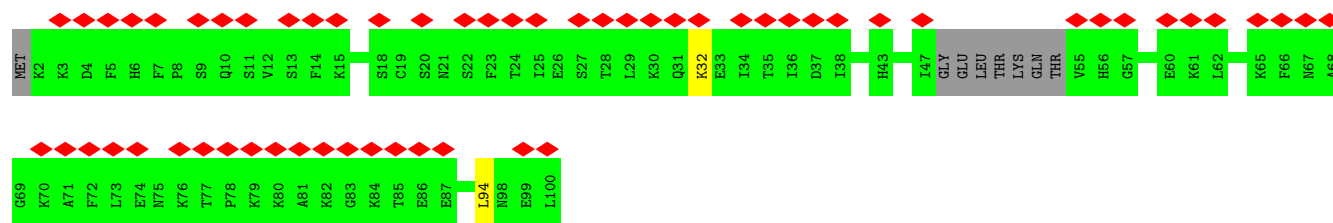


• Molecule 54: 50S ribosomal protein L29

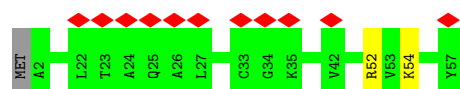
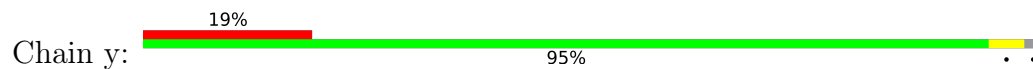


• Molecule 55: 50S ribosomal protein L31

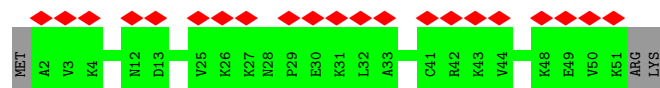
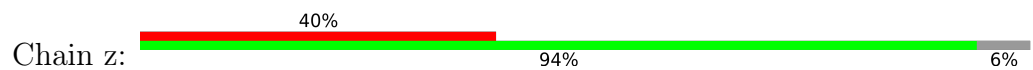




- Molecule 56: 50S ribosomal protein L32



- Molecule 57: 50S ribosomal protein L33 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	963	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.477	Depositor
Minimum map value	-2.425	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.237	Depositor
Recommended contour level	1.2	Depositor
Map size ( $\text{\AA}$ )	793.6, 793.6, 793.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	3.1, 3.1, 3.1	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 7MG, K, B8T, OMG, MG, 5MC, CLM, 2MA, MA6, 1MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.25	0/383	0.61	0/504
2	1	0.25	0/484	0.53	0/637
3	2	0.27	0/306	0.68	0/401
4	3	0.18	0/69363	0.73	9/108161 (0.0%)
5	4	0.15	0/2578	0.72	0/4016
6	5	0.18	0/35992	0.72	5/56111 (0.0%)
7	6	0.34	1/1810 (0.1%)	0.86	3/2817 (0.1%)
8	7	0.40	2/1785 (0.1%)	0.77	0/2779
9	A	0.31	0/2186	0.67	4/2952 (0.1%)
10	B	0.28	0/1800	0.62	1/2433 (0.0%)
11	C	0.34	0/1700	0.72	0/2278
11	U	0.34	0/1700	0.78	0/2278
12	D	0.30	0/1365	0.66	0/1827
13	E	0.28	0/1384	0.71	2/1867 (0.1%)
14	F	0.29	0/1274	0.66	0/1710
15	G	0.31	0/1134	0.69	1/1527 (0.1%)
16	H	0.28	0/1056	0.65	0/1409
17	I	0.30	0/843	0.69	2/1132 (0.2%)
18	J	0.27	0/844	0.57	0/1136
19	K	0.26	0/1089	0.63	0/1461
20	L	0.28	0/986	0.67	0/1321
21	M	0.35	0/483	0.69	0/643
22	N	0.24	0/703	0.61	0/936
23	O	0.32	0/718	0.76	0/962
24	P	0.25	0/702	0.62	0/934
25	Q	0.27	0/663	0.69	0/883
26	R	0.30	0/716	0.61	1/958 (0.1%)
27	S	0.26	0/645	0.55	0/857
28	T	0.30	0/524	0.79	1/685 (0.1%)
29	X	0.28	0/245	0.72	0/325
30	Y	0.29	0/699	0.90	0/1087
31	Z	0.74	0/26	1.33	0/33

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	a	0.26	0/2267	0.61	1/3044 (0.0%)
33	b	0.29	0/1812	0.63	1/2436 (0.0%)
34	c	0.27	0/1681	0.57	0/2257
35	d	0.27	0/1437	0.61	0/1931
36	e	0.30	0/1420	0.60	0/1912
37	f	0.27	0/1233	0.59	0/1653
38	g	0.28	0/960	0.56	0/1284
39	h	0.25	0/968	0.54	0/1298
40	i	0.26	0/1186	0.58	0/1592
41	j	0.29	0/953	0.68	0/1275
42	k	0.26	0/1187	0.62	1/1581 (0.1%)
43	l	0.30	0/1104	0.61	0/1481
44	m	0.27	0/973	0.58	0/1309
45	n	0.25	0/927	0.61	0/1239
46	o	0.29	0/976	0.65	0/1296
47	p	0.25	0/996	0.55	0/1325
48	q	0.30	0/828	0.64	0/1111
49	r	0.27	0/1100	0.67	3/1471 (0.2%)
50	s	0.26	0/752	0.53	0/1015
51	t	0.30	0/878	0.69	1/1165 (0.1%)
52	u	0.25	0/798	0.58	0/1063
53	v	0.30	0/526	0.82	1/703 (0.1%)
54	w	0.23	0/916	0.50	0/1222
55	x	0.30	0/722	0.71	2/959 (0.2%)
56	y	0.27	0/457	0.74	1/601 (0.2%)
57	z	0.26	0/412	0.59	0/547
All	All	0.22	3/163655 (0.0%)	0.71	40/243830 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	U	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	6	1	G	OP3-P	-10.58	1.48	1.61
8	7	1	G	OP3-P	-10.54	1.48	1.61
8	7	72	G	O3'-P	-8.01	1.51	1.61



All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	2109	A	O5'-P-OP2	-10.18	96.54	105.70
6	5	1434	C	P-O3'-C3'	-9.93	107.79	119.70
53	v	58	LEU	CA-CB-CG	8.88	135.72	115.30
55	x	94	LEU	CA-CB-CG	7.74	133.10	115.30
4	3	393	C	C6-N1-C2	-7.29	117.38	120.30
4	3	1486	U	C2-N1-C1'	7.18	126.32	117.70
49	r	69	LEU	CA-CB-CG	6.66	130.62	115.30
4	3	1486	U	N1-C2-O2	6.58	127.41	122.80
42	k	90	LEU	CA-CB-CG	6.56	130.40	115.30
7	6	46	G	P-O3'-C3'	6.23	127.17	119.70
49	r	137	MET	CA-CB-CG	6.18	123.81	113.30
13	E	13	LEU	CA-CB-CG	6.07	129.26	115.30
51	t	95	PRO	CA-N-CD	-6.03	103.05	111.50
4	3	1486	U	N3-C2-O2	-6.03	117.98	122.20
9	A	32	MET	CB-CG-SD	-5.88	94.78	112.40
26	R	76	PRO	CA-N-CD	-5.86	103.30	111.50
4	3	1341	U	C2-N1-C1'	5.67	124.51	117.70
9	A	17	LEU	CA-CB-CG	5.65	128.30	115.30
32	a	128	ILE	CG1-CB-CG2	-5.62	99.03	111.40
7	6	33	U	P-O3'-C3'	5.54	126.34	119.70
4	3	1303	U	C2-N1-C1'	5.50	124.30	117.70
55	x	94	LEU	C-N-CA	5.47	135.37	121.70
7	6	75	C	O5'-P-OP1	-5.45	100.80	105.70
13	E	163	MET	CA-CB-CG	5.40	122.49	113.30
28	T	36	LEU	CA-CB-CG	5.40	127.72	115.30
4	3	1921	C	P-O3'-C3'	5.39	126.17	119.70
9	A	26	MET	CA-CB-CG	5.37	122.42	113.30
17	I	106	PHE	CB-CG-CD2	-5.34	117.06	120.80
10	B	224	HIS	C-N-CD	-5.29	108.96	120.60
56	y	52	ARG	CA-CB-CG	5.29	125.05	113.40
6	5	994	C	N1-C2-O2	5.29	122.07	118.90
33	b	45	ASP	CB-CG-OD1	5.25	123.03	118.30
9	A	245	MET	CG-SD-CE	-5.19	91.89	100.20
15	G	52	GLY	N-CA-C	5.18	126.04	113.10
4	3	393	C	P-O3'-C3'	5.17	125.91	119.70
6	5	1375	5MC	P-O3'-C3'	-5.16	113.50	119.70
17	I	106	PHE	CB-CG-CD1	5.08	124.36	120.80
49	r	1	MET	CA-CB-CG	5.07	121.92	113.30
6	5	1134	C	C2-N1-C1'	5.05	124.35	118.80
6	5	1119	C	N1-C2-O2	5.01	121.91	118.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	U	121	HIS	Peptide
11	U	153	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	
1	0	45/48 (94%)	45 (100%)	0	0	100	100
2	1	57/59 (97%)	57 (100%)	0	0	100	100
3	2	35/37 (95%)	35 (100%)	0	0	100	100
9	A	264/294 (90%)	233 (88%)	25 (10%)	6 (2%)	5	28
10	B	223/273 (82%)	197 (88%)	24 (11%)	2 (1%)	14	52
11	C	202/205 (98%)	166 (82%)	33 (16%)	3 (2%)	8	40
11	U	202/205 (98%)	148 (73%)	41 (20%)	13 (6%)	1	13
12	D	171/219 (78%)	141 (82%)	25 (15%)	5 (3%)	3	23
13	E	165/215 (77%)	142 (86%)	18 (11%)	5 (3%)	3	23
14	F	153/155 (99%)	132 (86%)	15 (10%)	6 (4%)	2	19
15	G	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
16	H	127/132 (96%)	115 (91%)	12 (9%)	0	100	100
17	I	102/108 (94%)	88 (86%)	13 (13%)	1 (1%)	13	49
18	J	112/121 (93%)	105 (94%)	7 (6%)	0	100	100
19	K	133/139 (96%)	113 (85%)	15 (11%)	5 (4%)	2	19
20	L	119/124 (96%)	112 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	M	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
22	N	84/86 (98%)	77 (92%)	6 (7%)	1 (1%)	11	44
23	O	85/94 (90%)	78 (92%)	5 (6%)	2 (2%)	5	27
24	P	83/85 (98%)	71 (86%)	11 (13%)	1 (1%)	11	44
25	Q	76/104 (73%)	65 (86%)	9 (12%)	2 (3%)	4	26
26	R	84/87 (97%)	79 (94%)	5 (6%)	0	100	100
27	S	77/87 (88%)	74 (96%)	2 (3%)	1 (1%)	10	43
28	T	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	X	28/444 (6%)	24 (86%)	4 (14%)	0	100	100
31	Z	3/36 (8%)	3 (100%)	0	0	100	100
32	a	283/287 (99%)	267 (94%)	15 (5%)	1 (0%)	30	68
33	b	229/287 (80%)	219 (96%)	9 (4%)	1 (0%)	30	68
34	c	209/212 (99%)	198 (95%)	11 (5%)	0	100	100
35	d	177/180 (98%)	169 (96%)	8 (4%)	0	100	100
36	e	174/184 (95%)	162 (93%)	12 (7%)	0	100	100
37	f	147/149 (99%)	131 (89%)	15 (10%)	1 (1%)	19	57
38	g	123/161 (76%)	117 (95%)	6 (5%)	0	100	100
39	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
40	i	142/146 (97%)	133 (94%)	9 (6%)	0	100	100
41	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
42	k	148/151 (98%)	138 (93%)	10 (7%)	0	100	100
43	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
44	m	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
45	n	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
46	o	116/119 (98%)	108 (93%)	8 (7%)	0	100	100
47	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
48	q	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
49	r	140/159 (88%)	137 (98%)	3 (2%)	0	100	100
50	s	93/237 (39%)	89 (96%)	4 (4%)	0	100	100
51	t	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
52	u	99/104 (95%)	86 (87%)	9 (9%)	4 (4%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	v	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
54	w	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
55	x	85/97 (88%)	64 (75%)	21 (25%)	0	100	100
56	y	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
57	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	6255/7355 (85%)	5717 (91%)	478 (8%)	60 (1%)	16	49

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	D	67	GLU
12	D	69	ARG
12	D	212	ARG
12	D	216	LEU
13	E	81	GLN
13	E	143	LEU
14	F	151	ALA
24	P	54	LEU
11	U	39	GLY
11	U	126	ASP
11	U	163	VAL
52	u	9	LYS
52	u	11	ASP
52	u	17	SER
52	u	23	SER
11	C	81	GLN
11	C	182	PRO
14	F	9	ARG
14	F	15	PRO
14	F	79	ILE
22	N	4	ASP
27	S	37	LYS
11	U	3	TYR
11	U	24	GLU
11	U	81	GLN
11	U	154	VAL
11	U	155	LYS
9	A	49	ARG
9	A	219	ASN
13	E	163	MET

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Mol	Chain	Res	Type
14	F	12	LEU
19	K	56	LYS
11	U	27	LYS
11	U	30	LYS
37	f	12	LEU
9	A	54	ASP
10	B	216	ASN
13	E	55	ALA
14	F	153	MET
19	K	70	LEU
23	O	47	LYS
23	O	49	LYS
25	Q	37	SER
32	a	128	ILE
9	A	16	GLU
9	A	17	LEU
11	C	188	PRO
12	D	62	PHE
17	I	100	VAL
19	K	72	ASN
25	Q	35	LYS
11	U	157	ALA
11	U	181	PHE
13	E	82	VAL
11	U	50	TYR
33	b	230	PRO
9	A	198	VAL
10	B	46	VAL
19	K	57	LYS
19	K	55	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	40/41 (98%)	40 (100%)	0	100   100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	51/51 (100%)	51 (100%)	0	100	100
3	2	35/35 (100%)	35 (100%)	0	100	100
9	A	239/262 (91%)	238 (100%)	1 (0%)	89	91
10	B	188/232 (81%)	187 (100%)	1 (0%)	86	89
11	C	182/183 (100%)	178 (98%)	4 (2%)	47	65
11	U	182/183 (100%)	180 (99%)	2 (1%)	70	80
12	D	141/178 (79%)	139 (99%)	2 (1%)	62	75
13	E	150/196 (76%)	150 (100%)	0	100	100
14	F	132/132 (100%)	131 (99%)	1 (1%)	79	85
15	G	124/124 (100%)	122 (98%)	2 (2%)	58	73
16	H	112/115 (97%)	111 (99%)	1 (1%)	75	83
17	I	97/99 (98%)	96 (99%)	1 (1%)	73	82
18	J	91/97 (94%)	91 (100%)	0	100	100
19	K	117/120 (98%)	116 (99%)	1 (1%)	75	83
20	L	102/105 (97%)	101 (99%)	1 (1%)	73	82
21	M	47/48 (98%)	47 (100%)	0	100	100
22	N	78/78 (100%)	78 (100%)	0	100	100
23	O	76/82 (93%)	76 (100%)	0	100	100
24	P	75/75 (100%)	75 (100%)	0	100	100
25	Q	69/94 (73%)	69 (100%)	0	100	100
26	R	76/77 (99%)	76 (100%)	0	100	100
27	S	71/77 (92%)	71 (100%)	0	100	100
28	T	55/56 (98%)	55 (100%)	0	100	100
29	X	27/406 (7%)	26 (96%)	1 (4%)	29	49
31	Z	2/2 (100%)	2 (100%)	0	100	100
32	a	241/243 (99%)	240 (100%)	1 (0%)	89	91
33	b	188/233 (81%)	187 (100%)	1 (0%)	86	89
34	c	183/184 (100%)	183 (100%)	0	100	100
35	d	153/154 (99%)	152 (99%)	1 (1%)	81	87
36	e	153/159 (96%)	152 (99%)	1 (1%)	81	87
37	f	134/134 (100%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	g	100/129 (78%)	98 (98%)	2 (2%)	50	68
39	h	102/110 (93%)	102 (100%)	0	100	100
40	i	126/128 (98%)	125 (99%)	1 (1%)	79	85
41	j	103/103 (100%)	101 (98%)	2 (2%)	52	69
42	k	125/126 (99%)	125 (100%)	0	100	100
43	l	113/115 (98%)	112 (99%)	1 (1%)	75	83
44	m	105/109 (96%)	104 (99%)	1 (1%)	73	82
45	n	99/99 (100%)	99 (100%)	0	100	100
46	o	104/105 (99%)	104 (100%)	0	100	100
47	p	104/108 (96%)	104 (100%)	0	100	100
48	q	90/91 (99%)	90 (100%)	0	100	100
49	r	118/132 (89%)	118 (100%)	0	100	100
50	s	84/208 (40%)	84 (100%)	0	100	100
51	t	96/96 (100%)	96 (100%)	0	100	100
52	u	82/85 (96%)	82 (100%)	0	100	100
53	v	59/60 (98%)	59 (100%)	0	100	100
54	w	97/98 (99%)	97 (100%)	0	100	100
55	x	79/86 (92%)	78 (99%)	1 (1%)	65	77
56	y	48/49 (98%)	47 (98%)	1 (2%)	48	66
57	z	47/50 (94%)	47 (100%)	0	100	100
All	All	5492/6342 (87%)	5461 (99%)	31 (1%)	82	88

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	A	286	ARG
10	B	93	LYS
11	C	55	GLN
11	C	76	ARG
11	C	143	ARG
11	C	184	ARG
12	D	72	LYS
12	D	133	LYS
14	F	154	ARG
15	G	67	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	G	132	LYS
16	H	70	LYS
17	I	59	ARG
19	K	124	ARG
20	L	78	LYS
11	U	31	ARG
11	U	202	ARG
29	X	36	LYS
32	a	84	LYS
33	b	151	ARG
35	d	45	ARG
36	e	174	ARG
38	g	50	LYS
38	g	125	LYS
40	i	132	LYS
41	j	7	ARG
41	j	91	LYS
43	l	60	LYS
44	m	30	LYS
55	x	32	LYS
56	y	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	A	221	GLN
10	B	6	ASN
10	B	91	GLN
11	C	81	GLN
11	C	88	ASN
12	D	193	HIS
13	E	20	GLN
13	E	79	ASN
14	F	19	ASN
14	F	67	ASN
14	F	83	ASN
14	F	85	GLN
15	G	11	HIS
15	G	85	ASN
16	H	62	ASN
19	K	29	ASN
20	L	36	GLN

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Mol	Chain	Res	Type
20	L	100	GLN
22	N	13	GLN
24	P	49	ASN
27	S	63	ASN
11	U	37	GLN
11	U	53	GLN
11	U	88	ASN
11	U	171	ASN
33	b	34	ASN
33	b	144	GLN
33	b	188	ASN
35	d	63	GLN
36	e	33	GLN
37	f	96	GLN
40	i	80	HIS
41	j	18	GLN
41	j	69	GLN
42	k	24	HIS
43	l	99	GLN
43	l	113	GLN
45	n	49	ASN
45	n	66	ASN
45	n	69	ASN
46	o	17	GLN
48	q	2	HIS
52	u	100	HIS
53	v	34	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	Y	28/29 (96%)	16 (57%)	4 (14%)
4	3	2891/2907 (99%)	537 (18%)	18 (0%)
5	4	107/108 (99%)	29 (27%)	0
6	5	1503/1520 (98%)	257 (17%)	10 (0%)
7	6	76/76 (100%)	23 (30%)	5 (6%)
8	7	74/75 (98%)	20 (27%)	2 (2%)
All	All	4679/4715 (99%)	882 (18%)	39 (0%)

All (882) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	3	11	U
4	3	12	A
4	3	13	C
4	3	14	U
4	3	28	G
4	3	37	G
4	3	48	G
4	3	64	U
4	3	65	A
4	3	73	A
4	3	76	A
4	3	77	G
4	3	102	A
4	3	103	G
4	3	119	A
4	3	121	U
4	3	126	C
4	3	132	G
4	3	141	A
4	3	142	A
4	3	163	A
4	3	180	A
4	3	184	A
4	3	187	C
4	3	200	A
4	3	203	A
4	3	219	G
4	3	220	A
4	3	225	A
4	3	226	A
4	3	232	A
4	3	234	G
4	3	237	A
4	3	245	U
4	3	246	G
4	3	252	G
4	3	269	A
4	3	276	A
4	3	284	U
4	3	287	G
4	3	295	U
4	3	296	U
4	3	297	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	298	U
4	3	299	A
4	3	309	A
4	3	310	U
4	3	311	G
4	3	315	A
4	3	316	C
4	3	317	U
4	3	319	G
4	3	325	G
4	3	336	C
4	3	345	A
4	3	363	G
4	3	364	A
4	3	365	U
4	3	402	A
4	3	409	A
4	3	410	G
4	3	411	U
4	3	418	G
4	3	419	A
4	3	424	G
4	3	425	U
4	3	426	U
4	3	432	G
4	3	437	A
4	3	440	C
4	3	460	G
4	3	463	U
4	3	483	A
4	3	517	G
4	3	539	U
4	3	540	A
4	3	548	A
4	3	562	C
4	3	565	C
4	3	566	G
4	3	567	U
4	3	573	A
4	3	581	A
4	3	583	U
4	3	596	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	598	G
4	3	607	U
4	3	608	A
4	3	610	G
4	3	620	G
4	3	636	U
4	3	637	U
4	3	638	A
4	3	648	G
4	3	649	A
4	3	650	G
4	3	663	A
4	3	670	G
4	3	673	A
4	3	681	A
4	3	682	A
4	3	689	U
4	3	691	G
4	3	705	A
4	3	712	A
4	3	716	G
4	3	721	G
4	3	722	C
4	3	765	A
4	3	775	C
4	3	782	U
4	3	792	G
4	3	797	U
4	3	800	C
4	3	810	G
4	3	811	G
4	3	817	A
4	3	819	U
4	3	820	U
4	3	824	A
4	3	828	A
4	3	829	A
4	3	840	G
4	3	846	U
4	3	847	C
4	3	854	A
4	3	862	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	881	A
4	3	882	C
4	3	883	A
4	3	901	C
4	3	902	U
4	3	904	C
4	3	906	G
4	3	911	U
4	3	912	A
4	3	914	G
4	3	915	A
4	3	925	C
4	3	929	G
4	3	931	G
4	3	932	U
4	3	933	A
4	3	934	C
4	3	941	C
4	3	942	A
4	3	944	U
4	3	947	A
4	3	949	C
4	3	951	C
4	3	952	U
4	3	953	G
4	3	970	U
4	3	981	A
4	3	982	G
4	3	994	U
4	3	997	G
4	3	998	C
4	3	1008	A
4	3	1010	G
4	3	1016	A
4	3	1019	A
4	3	1026	A
4	3	1032	A
4	3	1039	G
4	3	1045	A
4	3	1049	U
4	3	1058	U
4	3	1060	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	1061	A
4	3	1068	U
4	3	1074	A
4	3	1080	A
4	3	1082	A
4	3	1084	C
4	3	1096	U
4	3	1097	G
4	3	1098	G
4	3	1099	C
4	3	1102	A
4	3	1104	A
4	3	1105	A
4	3	1106	G
4	3	1107	C
4	3	1110	C
4	3	1111	C
4	3	1113	U
4	3	1114	C
4	3	1115	G
4	3	1120	A
4	3	1122	G
4	3	1123	A
4	3	1125	U
4	3	1130	A
4	3	1132	C
4	3	1138	A
4	3	1144	C
4	3	1145	G
4	3	1146	A
4	3	1147	G
4	3	1165	U
4	3	1167	U
4	3	1168	A
4	3	1170	C
4	3	1176	U
4	3	1177	A
4	3	1178	A
4	3	1204	A
4	3	1208	A
4	3	1209	U
4	3	1210	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	1212	C
4	3	1215	G
4	3	1234	U
4	3	1235	U
4	3	1236	G
4	3	1242	G
4	3	1246	U
4	3	1250	A
4	3	1251	G
4	3	1253	G
4	3	1256	A
4	3	1257	G
4	3	1266	G
4	3	1268	U
4	3	1280	G
4	3	1281	A
4	3	1283	A
4	3	1285	U
4	3	1286	G
4	3	1292	A
4	3	1301	G
4	3	1304	U
4	3	1313	G
4	3	1325	C
4	3	1328	A
4	3	1329	U
4	3	1330	U
4	3	1369	U
4	3	1378	C
4	3	1380	U
4	3	1388	G
4	3	1393	A
4	3	1406	A
4	3	1407	U
4	3	1412	A
4	3	1423	A
4	3	1424	U
4	3	1431	A
4	3	1444	C
4	3	1445	U
4	3	1446	G
4	3	1448	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	1456	C
4	3	1463	G
4	3	1467	U
4	3	1480	A
4	3	1481	U
4	3	1483	G
4	3	1486	U
4	3	1487	U
4	3	1502	A
4	3	1504	G
4	3	1508	G
4	3	1510	A
4	3	1513	A
4	3	1514	U
4	3	1515	A
4	3	1519	A
4	3	1522	U
4	3	1534	A
4	3	1535	A
4	3	1541	A
4	3	1546	U
4	3	1550	G
4	3	1569	A
4	3	1570	A
4	3	1571	G
4	3	1580	G
4	3	1582	G
4	3	1584	U
4	3	1585	A
4	3	1588	A
4	3	1589	A
4	3	1603	A
4	3	1612	U
4	3	1617	U
4	3	1618	U
4	3	1619	A
4	3	1641	A
4	3	1642	G
4	3	1643	A
4	3	1644	A
4	3	1645	C
4	3	1650	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	1651	C
4	3	1661	A
4	3	1668	G
4	3	1680	A
4	3	1681	G
4	3	1682	C
4	3	1688	A
4	3	1694	A
4	3	1708	G
4	3	1727	U
4	3	1737	G
4	3	1748	U
4	3	1749	A
4	3	1764	U
4	3	1769	A
4	3	1770	A
4	3	1771	C
4	3	1780	A
4	3	1789	C
4	3	1791	A
4	3	1807	C
4	3	1808	C
4	3	1809	A
4	3	1816	A
4	3	1823	U
4	3	1836	A
4	3	1854	A
4	3	1855	A
4	3	1866	G
4	3	1869	G
4	3	1878	A
4	3	1886	C
4	3	1910	G
4	3	1913	G
4	3	1919	A
4	3	1920	A
4	3	1921	C
4	3	1922	U
4	3	1936	G
4	3	1937	G
4	3	1938	U
4	3	1943	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	1944	A
4	3	1962	U
4	3	1974	U
4	3	1977	A
4	3	1978	U
4	3	1979	G
4	3	1998	U
4	3	1999	G
4	3	2000	U
4	3	2004	G
4	3	2028	G
4	3	2030	A
4	3	2038	A
4	3	2040	A
4	3	2041	C
4	3	2042	A
4	3	2050	G
4	3	2057	C
4	3	2062	C
4	3	2063	G
4	3	2067	A
4	3	2068	G
4	3	2069	A
4	3	2076	G
4	3	2084	A
4	3	2099	U
4	3	2100	G
4	3	2103	C
4	3	2106	G
4	3	2107	A
4	3	2108	C
4	3	2109	A
4	3	2111	U
4	3	2112	A
4	3	2113	U
4	3	2114	C
4	3	2118	U
4	3	2119	A
4	3	2123	A
4	3	2124	A
4	3	2125	U
4	3	2126	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	2127	G
4	3	2128	G
4	3	2130	A
4	3	2134	G
4	3	2135	C
4	3	2138	U
4	3	2139	C
4	3	2140	G
4	3	2141	A
4	3	2145	A
4	3	2146	A
4	3	2152	C
4	3	2153	U
4	3	2157	A
4	3	2158	C
4	3	2163	U
4	3	2164	G
4	3	2165	A
4	3	2166	U
4	3	2167	G
4	3	2168	C
4	3	2169	G
4	3	2170	A
4	3	2171	A
4	3	2172	A
4	3	2173	G
4	3	2175	U
4	3	2179	A
4	3	2180	U
4	3	2181	A
4	3	2186	C
4	3	2190	G
4	3	2193	U
4	3	2194	G
4	3	2195	U
4	3	2196	G
4	3	2197	U
4	3	2198	G
4	3	2199	C
4	3	2200	U
4	3	2202	U
4	3	2207	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	2211	G
4	3	2212	U
4	3	2219	U
4	3	2220	A
4	3	2221	U
4	3	2227	U
4	3	2228	U
4	3	2233	A
4	3	2246	G
4	3	2247	G
4	3	2259	OMG
4	3	2274	A
4	3	2276	A
4	3	2287	G
4	3	2291	U
4	3	2295	A
4	3	2298	G
4	3	2305	C
4	3	2311	G
4	3	2313	U
4	3	2316	G
4	3	2319	A
4	3	2327	U
4	3	2329	G
4	3	2333	G
4	3	2335	A
4	3	2336	A
4	3	2342	U
4	3	2343	A
4	3	2344	A
4	3	2353	G
4	3	2355	C
4	3	2358	U
4	3	2366	A
4	3	2391	G
4	3	2393	C
4	3	2397	G
4	3	2410	C
4	3	2411	C
4	3	2414	U
4	3	2422	G
4	3	2431	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	2433	A
4	3	2437	G
4	3	2438	A
4	3	2443	A
4	3	2449	U
4	3	2456	A
4	3	2477	A
4	3	2481	U
4	3	2482	U
4	3	2483	C
4	3	2484	A
4	3	2486	A
4	3	2488	C
4	3	2499	U
4	3	2510	G
4	3	2512	U
4	3	2513	G
4	3	2521	A
4	3	2526	A
4	3	2537	G
4	3	2543	G
4	3	2574	A
4	3	2575	G
4	3	2580	A
4	3	2585	A
4	3	2593	U
4	3	2594	C
4	3	2605	G
4	3	2610	A
4	3	2617	U
4	3	2618	C
4	3	2621	U
4	3	2623	U
4	3	2637	A
4	3	2638	G
4	3	2654	U
4	3	2668	A
4	3	2669	G
4	3	2697	C
4	3	2698	U
4	3	2722	G
4	3	2734	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3	2737	G
4	3	2741	A
4	3	2752	G
4	3	2756	A
4	3	2760	C
4	3	2764	U
4	3	2765	A
4	3	2773	A
4	3	2786	A
4	3	2798	A
4	3	2799	U
4	3	2804	C
4	3	2806	A
4	3	2807	G
4	3	2808	A
4	3	2810	A
4	3	2813	A
4	3	2822	C
4	3	2824	A
4	3	2829	G
4	3	2839	A
4	3	2853	U
4	3	2862	U
4	3	2863	G
4	3	2871	G
4	3	2876	G
4	3	2884	C
4	3	2887	A
4	3	2888	U
4	3	2895	A
4	3	2896	G
4	3	2899	C
5	4	9	C
5	4	10	C
5	4	11	A
5	4	13	G
5	4	14	U
5	4	22	G
5	4	23	A
5	4	28	C
5	4	33	U
5	4	35	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	4	39	U
5	4	41	C
5	4	48	A
5	4	49	G
5	4	54	U
5	4	56	A
5	4	60	C
5	4	64	G
5	4	65	G
5	4	80	G
5	4	82	U
5	4	83	U
5	4	84	C
5	4	85	A
5	4	88	G
5	4	89	A
5	4	99	A
5	4	106	A
5	4	108	C
6	5	6	C
6	5	10	G
6	5	33	A
6	5	40	G
6	5	48	C
6	5	49	C
6	5	52	A
6	5	57	U
6	5	61	A
6	5	106	C
6	5	114	C
6	5	115	A
6	5	117	U
6	5	120	A
6	5	149	G
6	5	154	G
6	5	163	G
6	5	167	A
6	5	171	A
6	5	173	U
6	5	176	G
6	5	180	C
6	5	182	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	5	185	G
6	5	186	A
6	5	189	C
6	5	190	A
6	5	197	A
6	5	198	A
6	5	199	A
6	5	220	U
6	5	223	G
6	5	239	A
6	5	241	C
6	5	243	G
6	5	247	G
6	5	262	G
6	5	263	C
6	5	269	A
6	5	275	A
6	5	285	G
6	5	301	G
6	5	302	A
6	5	324	C
6	5	325	A
6	5	326	C
6	5	328	G
6	5	341	C
6	5	342	G
6	5	344	G
6	5	347	G
6	5	348	C
6	5	350	G
6	5	359	A
6	5	362	U
6	5	363	U
6	5	364	U
6	5	365	U
6	5	368	C
6	5	369	A
6	5	370	A
6	5	374	G
6	5	380	G
6	5	383	U
6	5	388	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	5	394	U
6	5	402	G
6	5	408	U
6	5	416	U
6	5	418	U
6	5	419	A
6	5	422	A
6	5	425	G
6	5	426	U
6	5	447	G
6	5	449	A
6	5	450	U
6	5	452	A
6	5	461	G
6	5	462	G
6	5	464	A
6	5	468	G
6	5	470	U
6	5	475	U
6	5	476	U
6	5	477	U
6	5	480	C
6	5	481	U
6	5	482	G
6	5	488	U
6	5	489	U
6	5	493	A
6	5	494	A
6	5	495	U
6	5	507	A
6	5	509	C
6	5	510	U
6	5	516	C
6	5	517	C
6	5	522	G
6	5	525	7MG
6	5	530	A
6	5	531	A
6	5	545	A
6	5	557	A
6	5	560	U
6	5	562	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	5	570	A
6	5	571	A
6	5	574	C
6	5	575	A
6	5	579	G
6	5	586	G
6	5	594	A
6	5	595	G
6	5	628	A
6	5	650	A
6	5	661	G
6	5	662	G
6	5	683	G
6	5	700	G
6	5	715	A
6	5	719	G
6	5	720	U
6	5	721	G
6	5	728	G
6	5	745	U
6	5	752	G
6	5	768	G
6	5	790	U
6	5	791	A
6	5	811	A
6	5	812	A
6	5	814	C
6	5	818	A
6	5	825	A
6	5	829	G
6	5	836	C
6	5	838	A
6	5	839	U
6	5	867	A
6	5	883	A
6	5	885	U
6	5	908	A
6	5	910	C
6	5	911	G
6	5	921	G
6	5	922	G
6	5	929	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	5	930	A
6	5	955	U
6	5	964	A
6	5	970	A
6	5	971	A
6	5	972	A
6	5	982	A
6	5	987	U
6	5	988	G
6	5	989	A
6	5	994	C
6	5	995	U
6	5	996	U
6	5	997	G
6	5	998	G
6	5	999	C
6	5	1000	A
6	5	1002	A
6	5	1007	U
6	5	1009	G
6	5	1015	U
6	5	1018	U
6	5	1019	G
6	5	1020	G
6	5	1022	G
6	5	1023	G
6	5	1024	U
6	5	1025	U
6	5	1027	A
6	5	1028	C
6	5	1029	C
6	5	1030	G
6	5	1032	G
6	5	1034	G
6	5	1036	C
6	5	1044	G
6	5	1045	C
6	5	1047	U
6	5	1056	U
6	5	1072	G
6	5	1076	U
6	5	1078	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	5	1083	A
6	5	1085	G
6	5	1086	U
6	5	1092	A
6	5	1118	A
6	5	1121	U
6	5	1122	U
6	5	1123	G
6	5	1124	U
6	5	1134	C
6	5	1135	U
6	5	1141	U
6	5	1142	G
6	5	1158	A
6	5	1159	A
6	5	1170	C
6	5	1171	A
6	5	1172	A
6	5	1188	A
6	5	1189	U
6	5	1202	A
6	5	1203	A
6	5	1215	U
6	5	1231	U
6	5	1232	C
6	5	1233	G
6	5	1235	C
6	5	1255	A
6	5	1260	U
6	5	1271	U
6	5	1274	G
6	5	1279	G
6	5	1291	C
6	5	1294	U
6	5	1296	C
6	5	1297	G
6	5	1306	A
6	5	1312	G
6	5	1320	A
6	5	1321	G
6	5	1337	U
6	5	1338	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	5	1339	U
6	5	1343	G
6	5	1345	G
6	5	1372	C
6	5	1373	A
6	5	1397	G
6	5	1417	U
6	5	1426	U
6	5	1427	U
6	5	1428	A
6	5	1429	G
6	5	1462	G
6	5	1467	A
6	5	1468	A
6	5	1472	G
6	5	1478	A
6	5	1480	G
6	5	1481	U
6	5	1482	A
6	5	1492	G
6	5	1504	G
6	5	1505	G
6	5	1510	C
6	5	1511	C
7	6	2	G
7	6	3	G
7	6	13	C
7	6	15	A
7	6	16	C
7	6	17	U
7	6	18	G
7	6	19	A
7	6	20	U
7	6	21	A
7	6	33	U
7	6	34	U
7	6	37	A
7	6	46	G
7	6	47	U
7	6	48	U
7	6	59	G
7	6	65	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	6	70	U
7	6	71	C
7	6	72	C
7	6	73	A
7	6	75	C
8	7	4	U
8	7	11	U
8	7	13	U
8	7	15	G
8	7	16	U
8	7	17	G
8	7	19	A
8	7	20	U
8	7	21	A
8	7	22	A
8	7	34	G
8	7	44	G
8	7	46	U
8	7	47	U
8	7	48	G
8	7	51	G
8	7	57	A
8	7	71	C
8	7	73	C
8	7	75	A
30	Y	29	A
30	Y	31	A
30	Y	32	A
30	Y	34	A
30	Y	35	C
30	Y	36	U
30	Y	37	G
30	Y	40	G
30	Y	47	U
30	Y	49	U
30	Y	50	U
30	Y	51	C
30	Y	52	A
30	Y	53	A
30	Y	54	A
30	Y	56	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	3	315	A
4	3	410	G
4	3	881	A
4	3	901	C
4	3	1124	G
4	3	1209	U
4	3	1583	G
4	3	1618	U
4	3	2107	A
4	3	2110	U
4	3	2124	A
4	3	2152	C
4	3	2164	G
4	3	2169	G
4	3	2180	U
4	3	2199	C
4	3	2410	C
4	3	2764	U
6	5	196	G
6	5	363	U
6	5	364	U
6	5	571	A
6	5	994	C
6	5	995	U
6	5	1024	U
6	5	1123	G
6	5	1158	A
6	5	1338	A
7	6	1	G
7	6	15	A
7	6	33	U
7	6	46	G
7	6	74	C
8	7	10	G
8	7	46	U
30	Y	34	A
30	Y	35	C
30	Y	49	U
30	Y	51	C

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

8 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
4	1MG	3	783	4	18,26,27	0.94	1 (5%)	19,39,42	0.81	0
6	5MC	5	1375	6	18,22,23	0.34	0	26,32,35	0.69	2 (7%)
6	B8T	5	1377	6	19,22,23	4.71	13 (68%)	26,31,34	0.97	1 (3%)
6	MA6	5	1494	6	18,26,27	1.06	2 (11%)	19,38,41	3.37	3 (15%)
4	2MA	3	2511	61,4	17,25,26	6.17	10 (58%)	17,37,40	1.54	3 (17%)
6	7MG	5	525	6	22,26,27	3.89	10 (45%)	29,39,42	2.03	9 (31%)
4	OMG	3	2259	8,4	18,26,27	0.99	2 (11%)	19,38,41	0.71	0
6	MA6	5	1493	6	18,26,27	1.06	2 (11%)	19,38,41	3.31	3 (15%)

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
4	1MG	3	783	4	-	0/3/25/26	0/3/3/3
6	5MC	5	1375	6	-	0/7/25/26	0/2/2/2
6	B8T	5	1377	6	-	0/7/27/28	0/2/2/2
6	MA6	5	1494	6	-	2/7/29/30	0/3/3/3
4	2MA	3	2511	61,4	-	2/3/25/26	0/3/3/3
6	7MG	5	525	6	-	2/7/37/38	0/3/3/3
4	OMG	3	2259	8,4	-	3/5/27/28	0/3/3/3
6	MA6	5	1493	6	-	0/7/29/30	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	2511	2MA	C2'-C1'	-15.49	1.30	1.53
4	3	2511	2MA	O4'-C1'	15.36	1.62	1.41
6	5	525	7MG	C8-N9	9.90	1.51	1.46
6	5	1377	B8T	O4'-C1'	8.89	1.63	1.42
4	3	2511	2MA	C2-N3	7.94	1.48	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	525	7MG	C5-N7	7.90	1.44	1.35
6	5	1377	B8T	O4'-C4'	-7.64	1.27	1.45
6	5	1377	B8T	C2'-C1'	-7.36	1.30	1.53
6	5	1377	B8T	C4-N3	7.33	1.45	1.32
6	5	1377	B8T	C2-N3	6.44	1.49	1.36
4	3	2511	2MA	O4'-C4'	-6.00	1.31	1.45
6	5	525	7MG	C2-N3	5.90	1.47	1.33
6	5	1377	B8T	C6-C5	5.81	1.48	1.35
6	5	525	7MG	C4-N9	5.80	1.44	1.37
6	5	525	7MG	C4-N3	5.59	1.47	1.34
4	3	2511	2MA	C4-N3	5.19	1.50	1.37
6	5	525	7MG	C2-N2	4.78	1.45	1.34
6	5	1377	B8T	C4-N4	4.67	1.45	1.35
6	5	1377	B8T	C2-N1	4.35	1.49	1.40
6	5	525	7MG	C2-N1	3.83	1.47	1.37
6	5	1377	B8T	C5-C4	3.77	1.48	1.40
6	5	1377	B8T	O2'-C2'	3.65	1.51	1.43
6	5	525	7MG	C5-C6	3.63	1.52	1.43
6	5	525	7MG	C6-N1	3.42	1.45	1.38
4	3	2511	2MA	C6-N1	3.14	1.44	1.38
6	5	1377	B8T	C6-N1	3.04	1.45	1.38
6	5	1377	B8T	O3'-C3'	-2.93	1.36	1.43
4	3	2511	2MA	C2-N1	2.72	1.45	1.36
4	3	2511	2MA	O3'-C3'	-2.71	1.36	1.43
4	3	2511	2MA	O2'-C2'	2.68	1.49	1.43
6	5	1493	MA6	C2-N3	2.67	1.36	1.32
6	5	1377	B8T	O2-C2	-2.66	1.18	1.23
4	3	2259	OMG	C5-C6	-2.62	1.42	1.47
6	5	1494	MA6	C2-N3	2.61	1.36	1.32
6	5	525	7MG	O6-C6	-2.44	1.18	1.23
6	5	1494	MA6	C5-C4	-2.31	1.34	1.40
6	5	1493	MA6	C5-C4	-2.23	1.35	1.40
4	3	783	1MG	C5-C4	-2.20	1.37	1.43
4	3	2511	2MA	C5-C4	-2.14	1.37	1.43
4	3	2259	OMG	C8-N7	-2.07	1.31	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1494	MA6	N1-C6-N6	-12.24	104.18	117.06
6	5	1493	MA6	N1-C6-N6	-11.86	104.57	117.06
6	5	1494	MA6	N3-C2-N1	-5.64	119.86	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1493	MA6	C1'-N9-C4	5.54	136.38	126.64
6	5	1493	MA6	N3-C2-N1	-5.54	120.02	128.68
6	5	1494	MA6	C1'-N9-C4	5.25	135.87	126.64
6	5	525	7MG	C5-C6-N1	4.96	119.74	110.99
6	5	525	7MG	C2-N3-C4	4.48	120.28	112.30
6	5	525	7MG	C5-C4-N3	-4.13	120.26	128.13
4	3	2511	2MA	C5-C6-N1	3.32	119.74	114.02
4	3	2511	2MA	C3'-C2'-C1'	3.26	105.88	100.98
6	5	525	7MG	C5-C4-N9	3.13	110.42	106.35
6	5	525	7MG	C4-C5-N7	3.04	109.75	105.53
6	5	525	7MG	C2-N1-C6	-2.85	119.90	125.10
6	5	525	7MG	O6-C6-C5	-2.77	120.75	127.54
6	5	525	7MG	N9-C4-N3	2.58	129.32	125.47
4	3	2511	2MA	C8-N7-C5	2.56	107.87	102.99
6	5	525	7MG	N9-C8-N7	2.27	106.62	103.38
6	5	1377	B8T	C6-C5-C4	2.13	119.57	116.96
6	5	1375	5MC	C5-C6-N1	-2.09	121.19	123.34
6	5	1375	5MC	O3'-C3'-C2'	-2.00	105.35	111.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	3	2259	OMG	C1'-C2'-O2'-CM2
6	5	525	7MG	O4'-C4'-C5'-O5'
6	5	525	7MG	C3'-C4'-C5'-O5'
6	5	1494	MA6	O4'-C4'-C5'-O5'
6	5	1494	MA6	C3'-C4'-C5'-O5'
4	3	2511	2MA	C3'-C4'-C5'-O5'
4	3	2259	OMG	O4'-C4'-C5'-O5'
4	3	2511	2MA	O4'-C4'-C5'-O5'
4	3	2259	OMG	C3'-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 316 ligands modelled in this entry, 315 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
59	CLM	3	3001	-	19,20,20	2.08	2 (10%)	23,27,27	0.84	0

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
59	CLM	3	3001	-	-	2/20/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	3	3001	CLM	C2-N2	7.25	1.50	1.34
59	3	3001	CLM	O9B-N9	-2.65	1.18	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

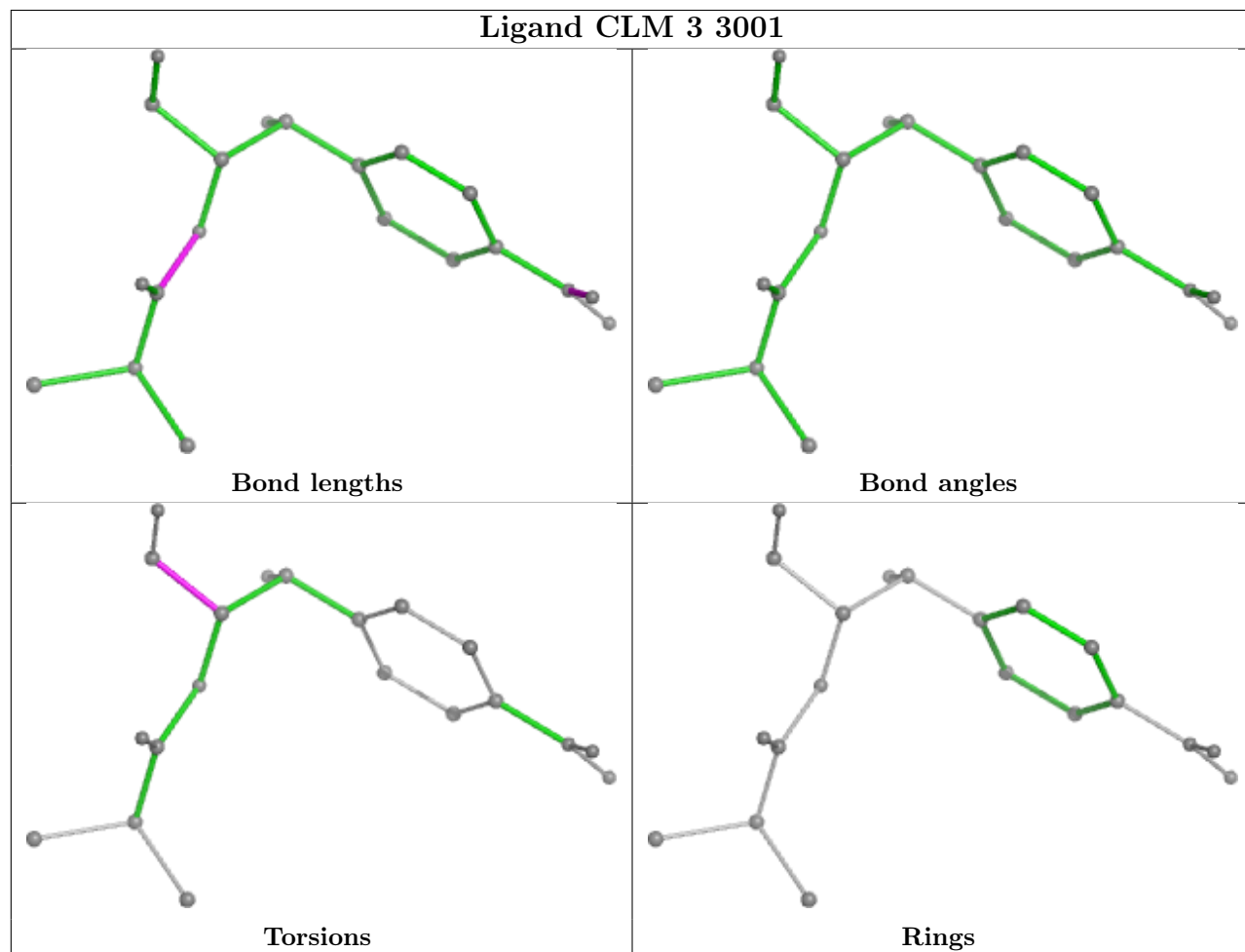
Mol	Chain	Res	Type	Atoms
59	3	3001	CLM	C5-C3-C4-O4
59	3	3001	CLM	N2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

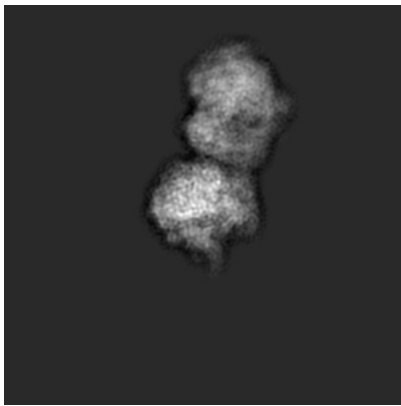
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17145. These allow visual inspection of the internal detail of the map and identification of artifacts.

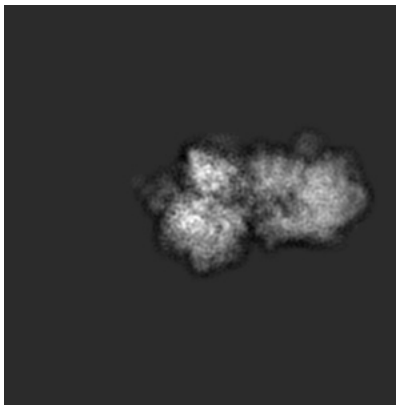
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

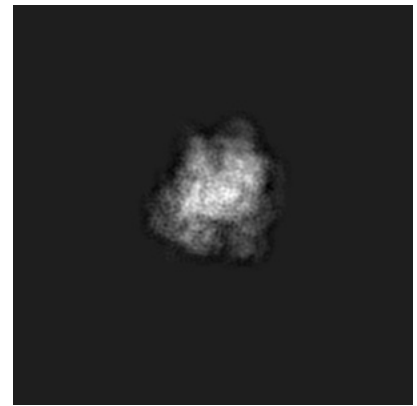
#### 6.1.1 Primary map



X

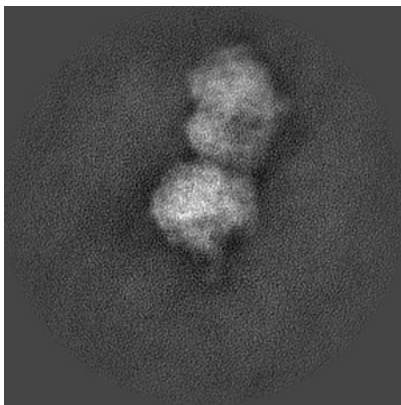


Y

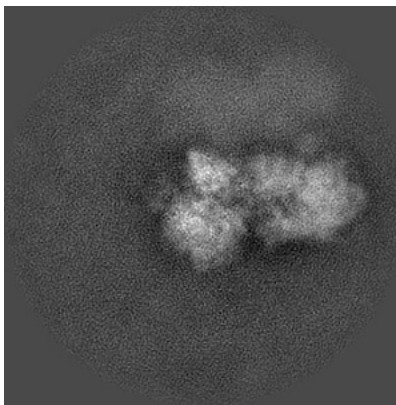


Z

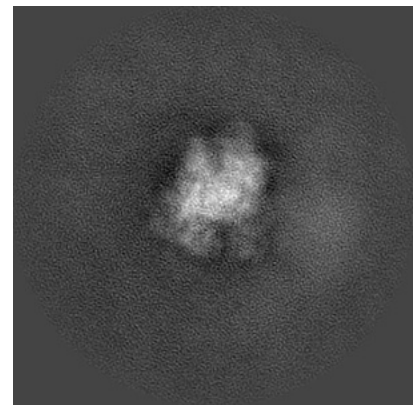
#### 6.1.2 Raw map



X



Y

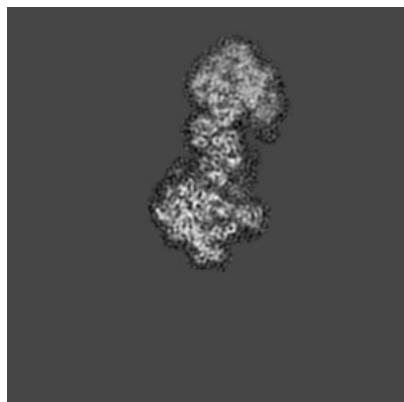


Z

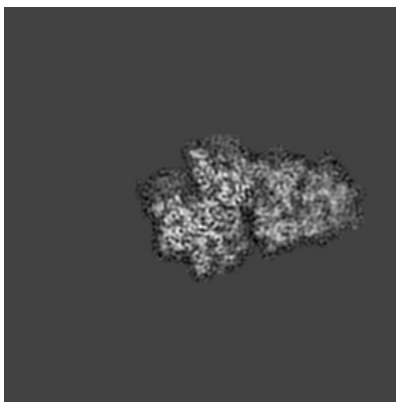
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

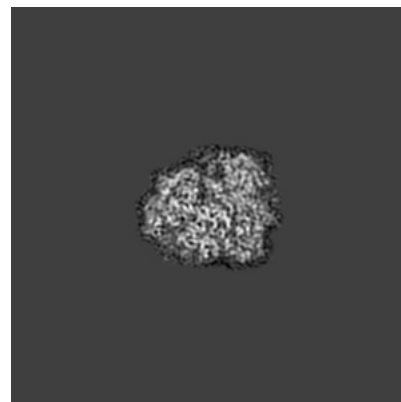
### 6.2.1 Primary map



X Index: 128

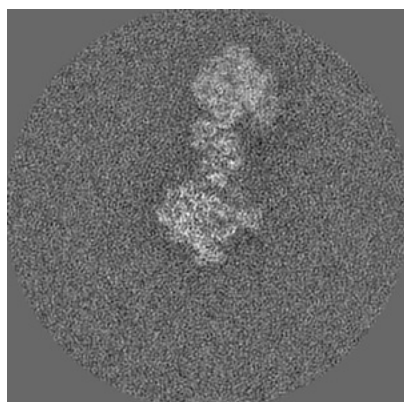


Y Index: 128

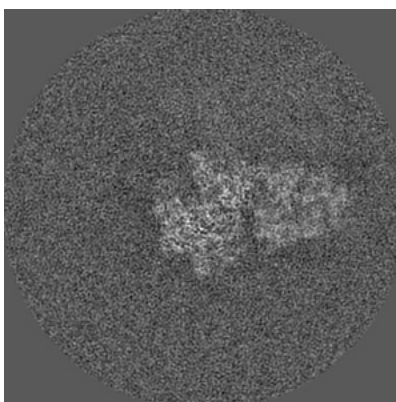


Z Index: 128

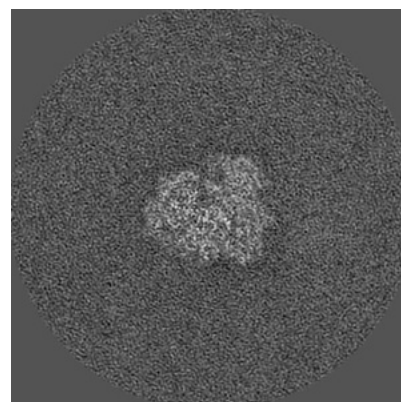
### 6.2.2 Raw map



X Index: 128



Y Index: 128

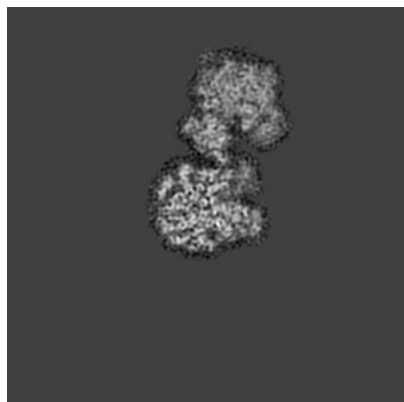


Z Index: 128

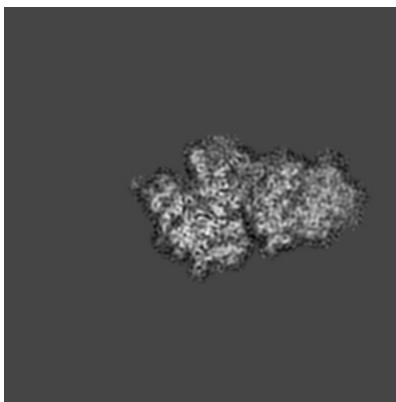
The images above show central slices of the map in three orthogonal directions.

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

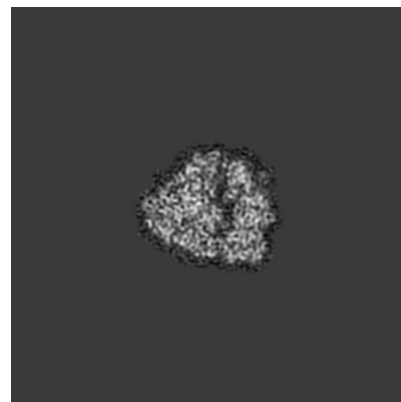
### 6.3.1 Primary map



X Index: 117

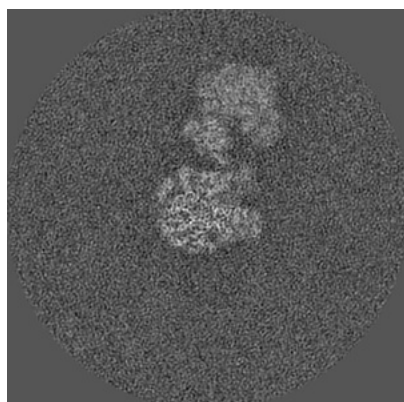


Y Index: 131

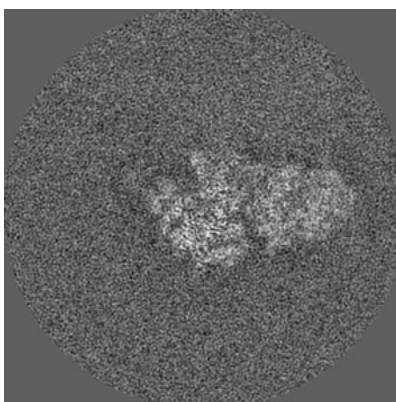


Z Index: 124

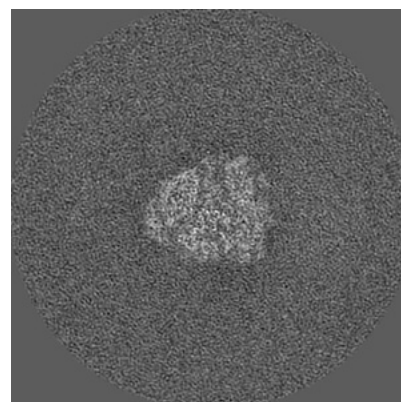
### 6.3.2 Raw map



X Index: 117



Y Index: 131

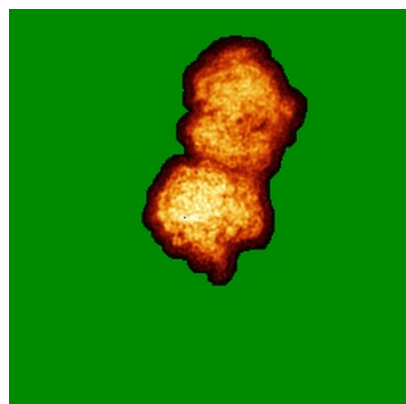


Z Index: 127

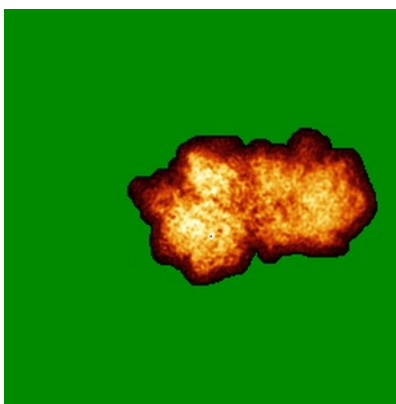
The images above show the largest variance slices of the map in three orthogonal directions.

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

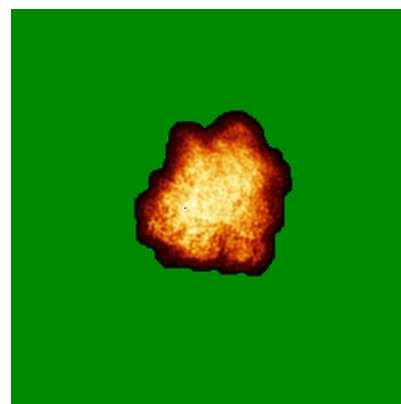
### 6.4.1 Primary map



X

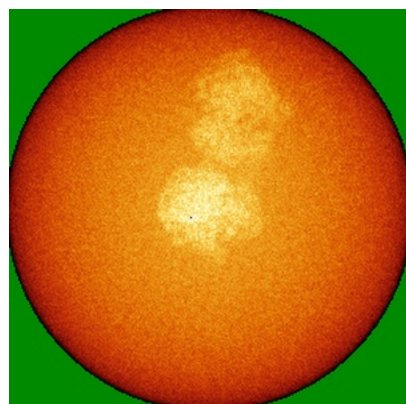


Y

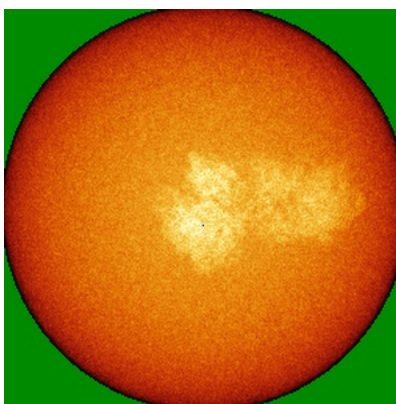


Z

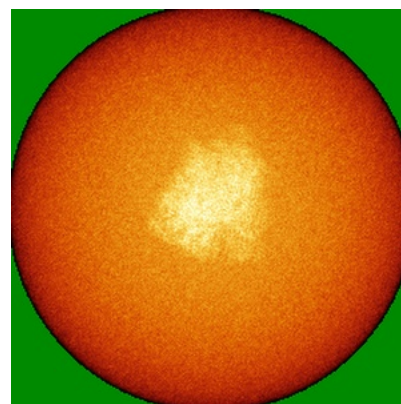
### 6.4.2 Raw map



X



Y



Z

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

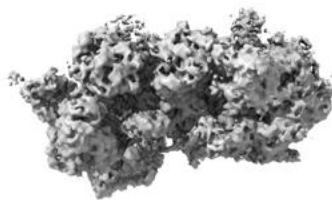


## 6.5 Orthogonal surface views [i](#)

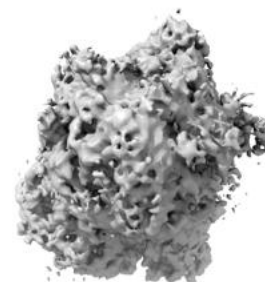
### 6.5.1 Primary map



X



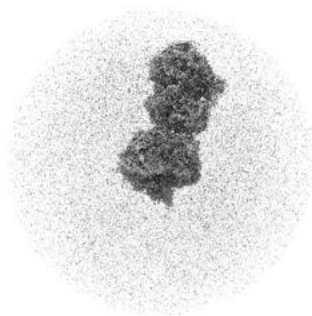
Y



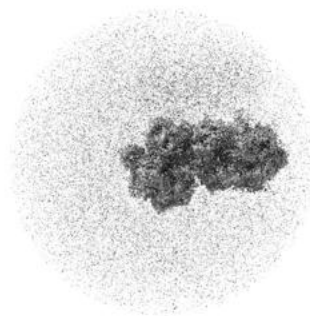
Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

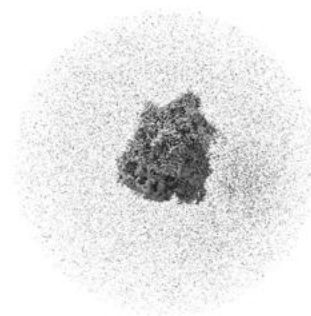
### 6.5.2 Raw map



X



Y



Z

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

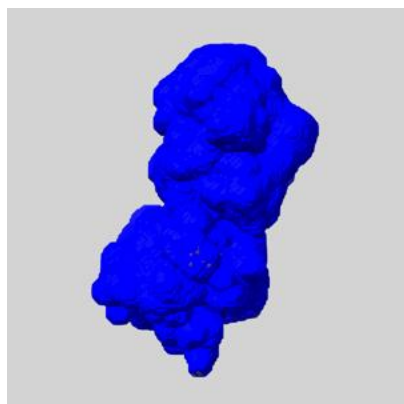
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

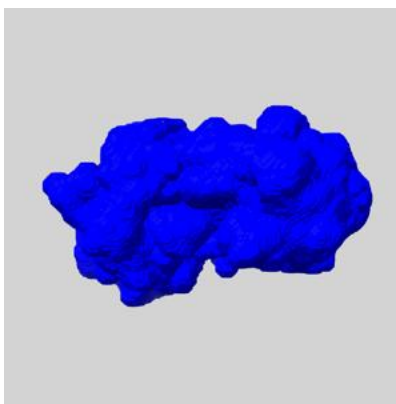
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

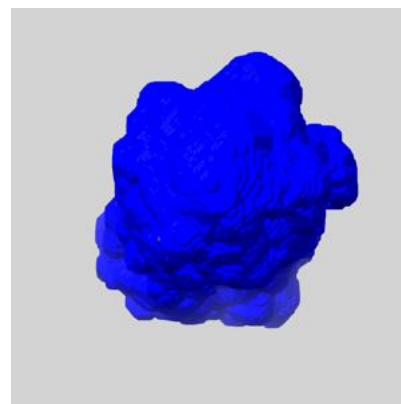
### 6.6.1 emd\_17145\_msk\_1.map [i](#)



X



Y

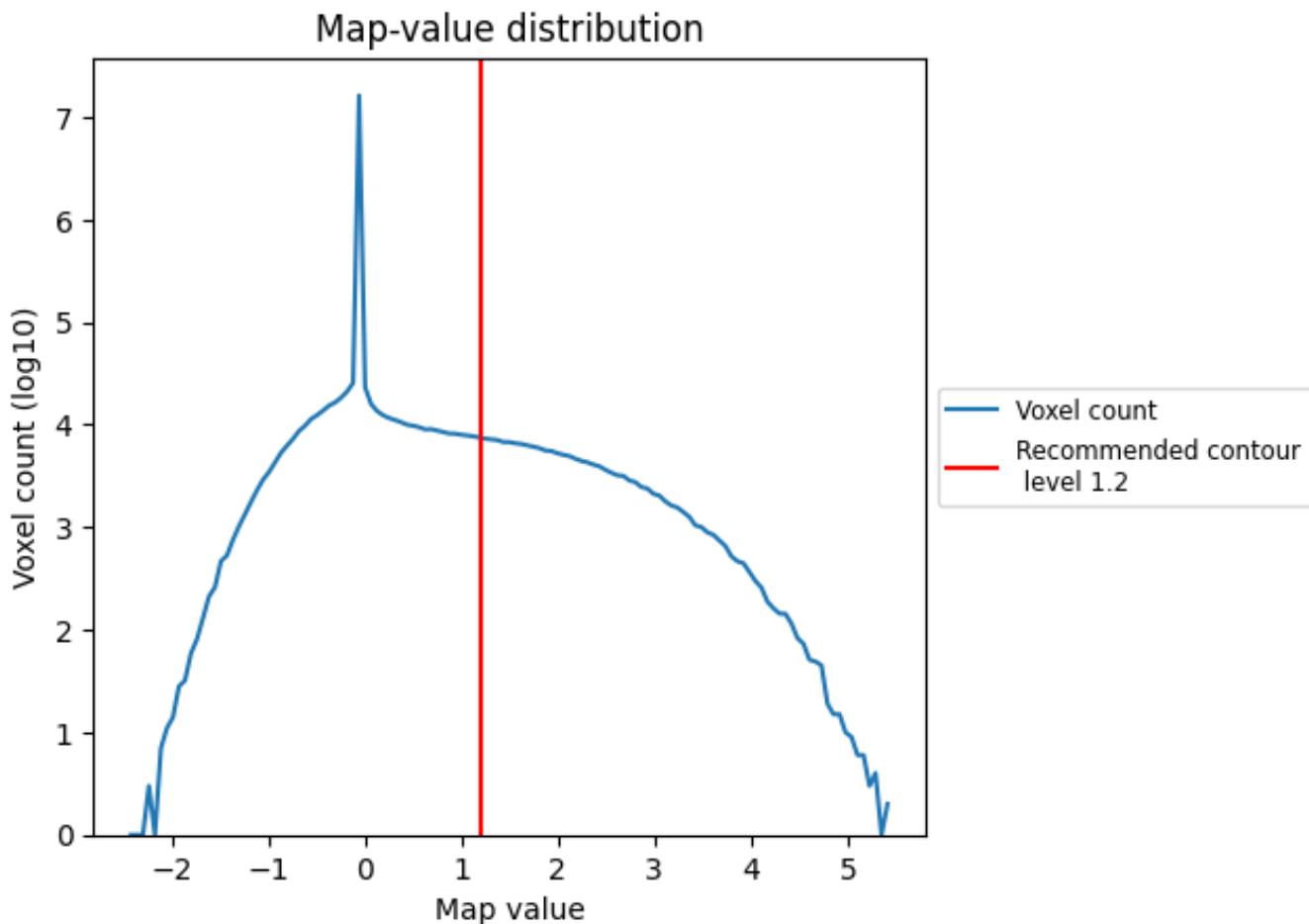


Z

## 7 Map analysis [i](#)

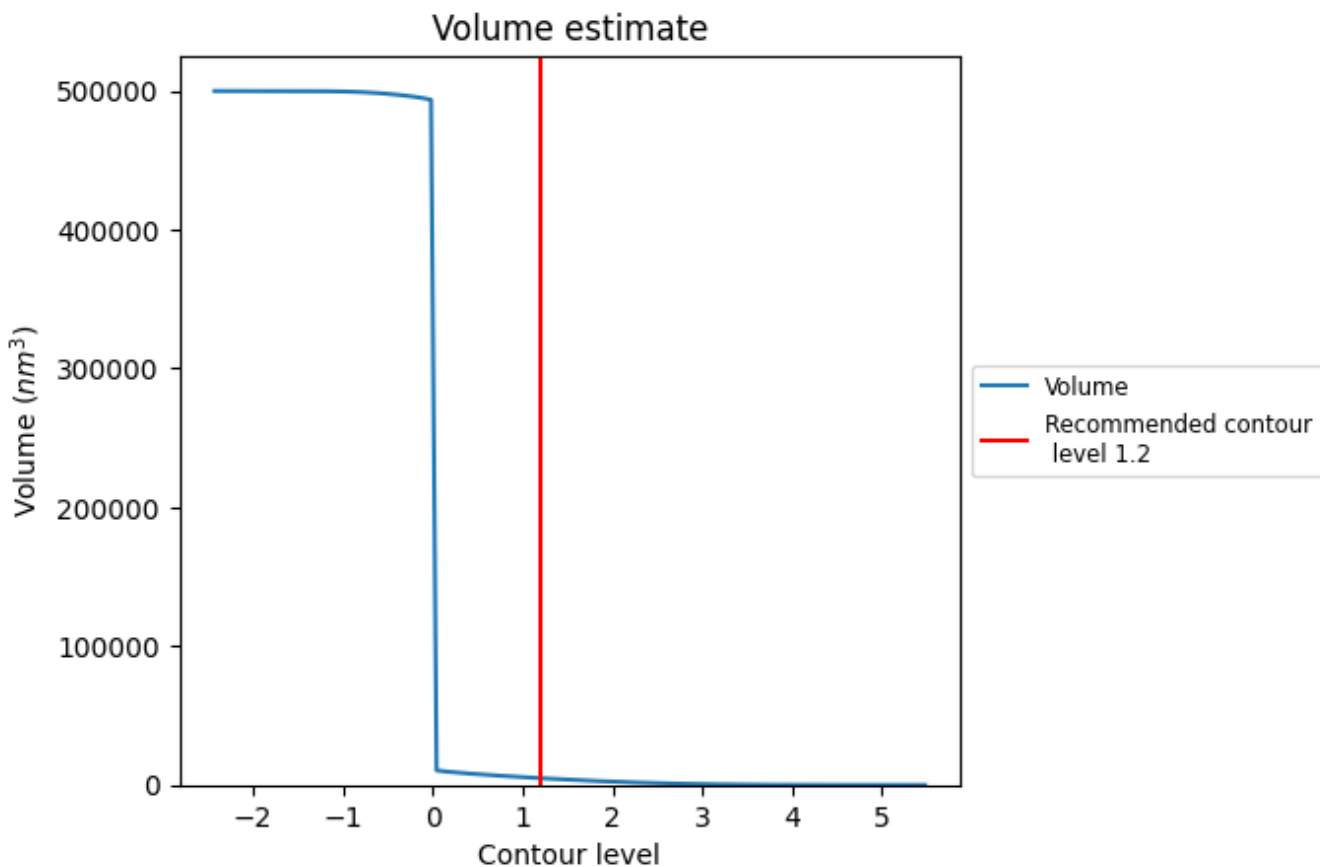
This section contains the results of statistical analysis of the map.

### 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.

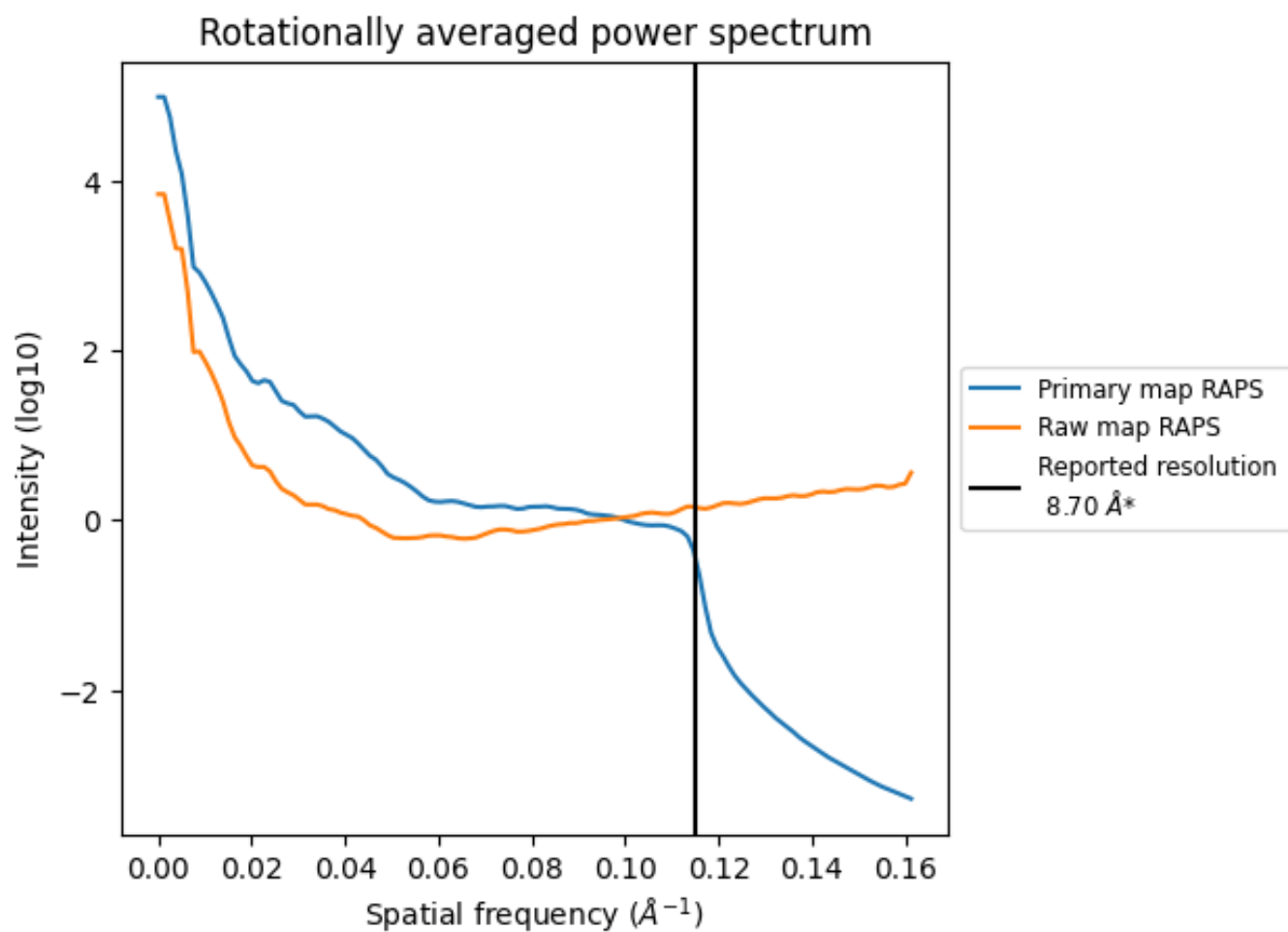
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 4893 nm<sup>3</sup>; this corresponds to an approximate mass of 4420 kDa.

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

### 7.3 Rotationally averaged power spectrum i

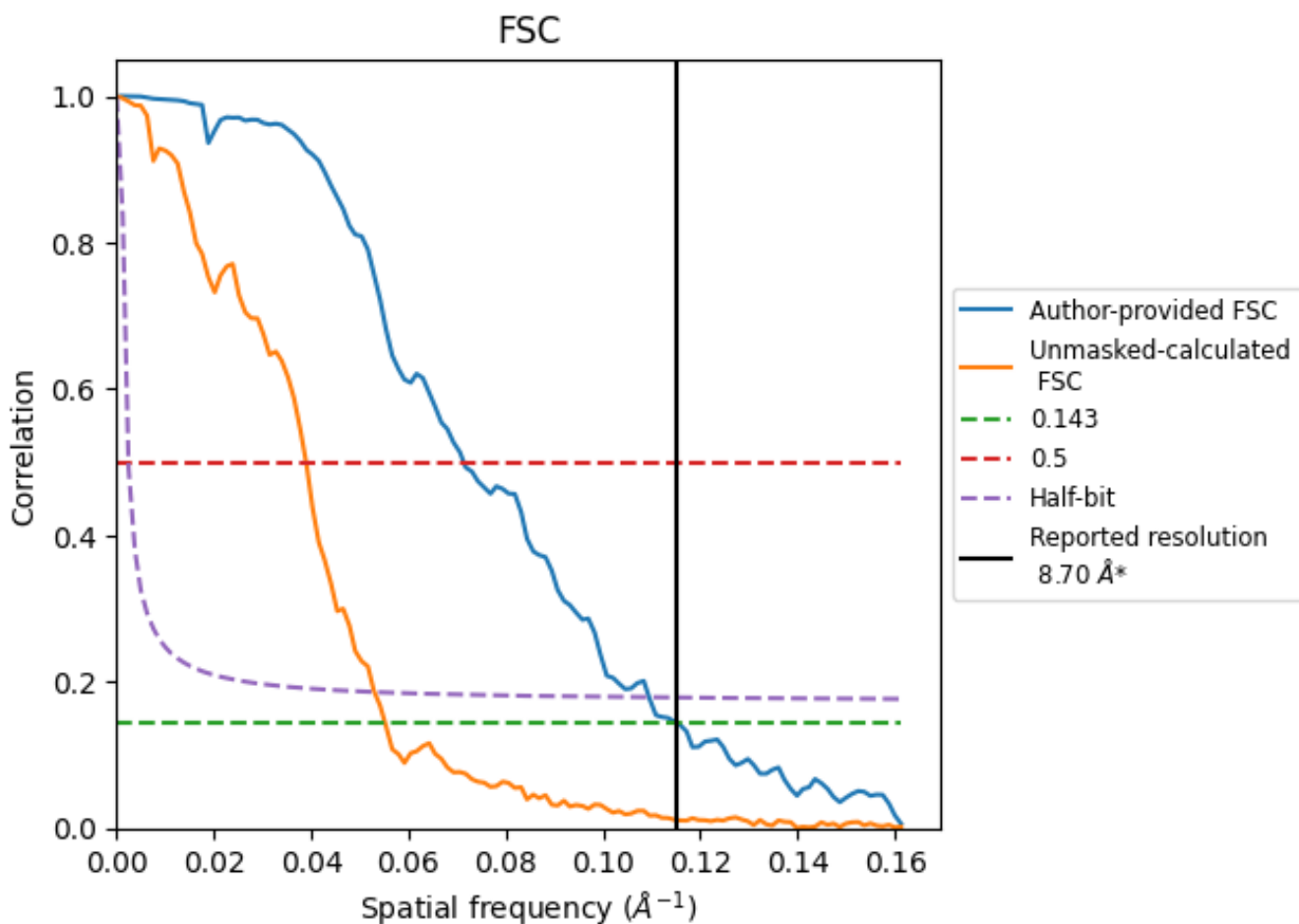


\*Reported resolution corresponds to spatial frequency of 0.115 Å<sup>-1</sup>

## 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 0.115 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

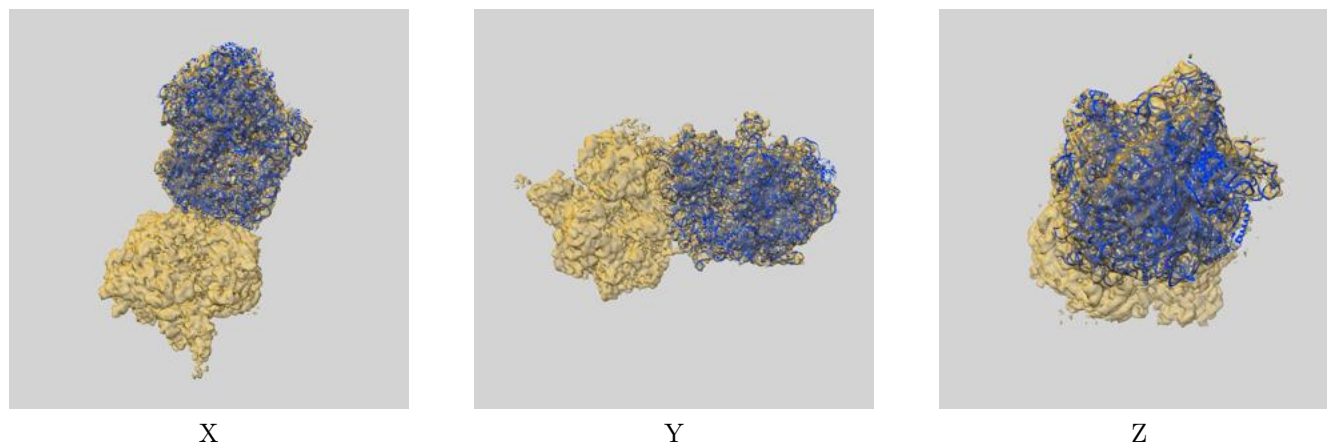
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.70	-	-
Author-provided FSC curve	8.68	14.01	9.13
Unmasked-calculated*	18.08	25.71	18.83

\*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 18.08 differs from the reported value 8.7 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-17145 and PDB model 8P8W. Per-residue inclusion information can be found in section 3 on page 16.

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



The images above show the 3D surface view of the map at the recommended contour level 1.2 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.

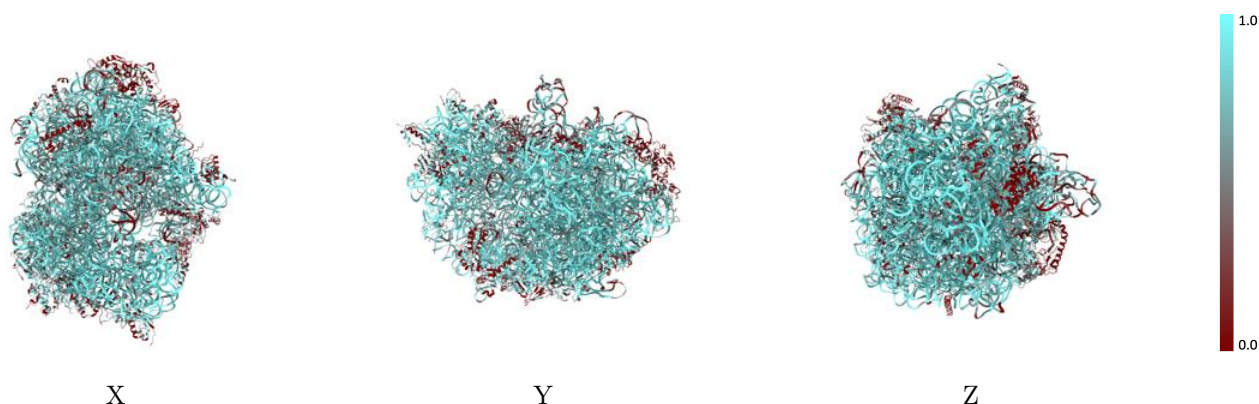


## 9.2 Q-score mapped to coordinate model [i](#)



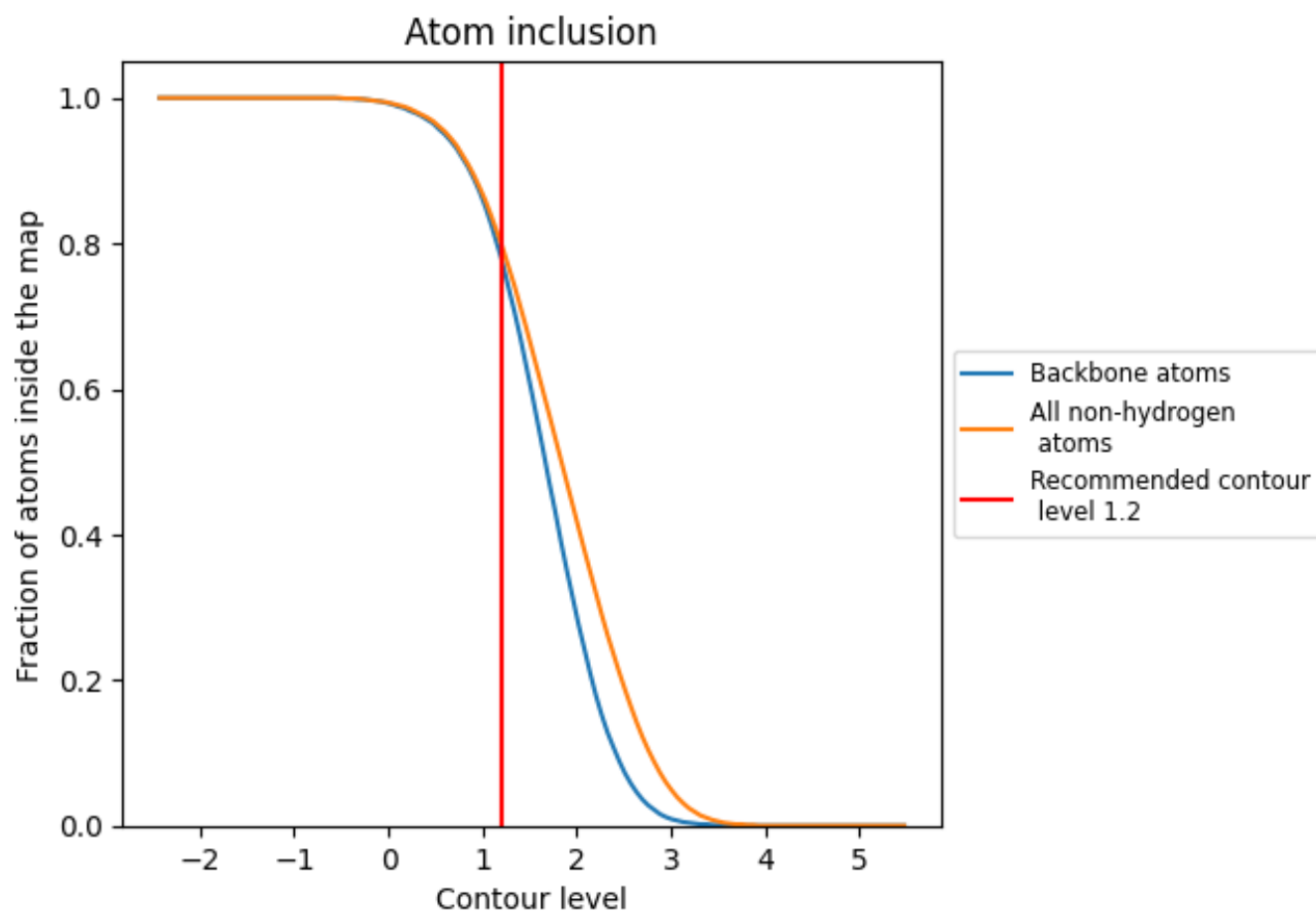
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.2).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 80% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8000	 0.1070
0	 0.7730	 0.0600
1	 0.7720	 0.0250
2	 0.8280	 0.0470
3	 0.9090	 0.1110
4	 0.8440	 0.0940
5	 0.9450	 0.1390
6	 0.3120	 0.0370
7	 0.8440	 0.1400
A	 0.5340	 0.1330
B	 0.5980	 0.1260
C	 0.6970	 0.1340
D	 0.5490	 0.1380
E	 0.5910	 0.1420
F	 0.6460	 0.1170
G	 0.6170	 0.1040
H	 0.6700	 0.0840
I	 0.5560	 0.0880
J	 0.7060	 0.1090
K	 0.6840	 0.1020
L	 0.6610	 0.0890
M	 0.7590	 0.0890
N	 0.7240	 0.1390
O	 0.7320	 0.0820
P	 0.6770	 0.1220
Q	 0.6270	 0.1190
R	 0.6910	 0.0810
S	 0.8540	 0.1100
T	 0.6430	 0.1400
U	 0.0650	 0.0250
X	 0.2090	 0.0830
Y	 0.6830	 0.1210
Z	 0.3740	 0.0170
a	 0.6680	 0.0610
b	 0.6670	 0.0530



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Chain	Atom inclusion	Q-score
c	 0.5230	 0.0460
d	 0.4860	 0.0750
e	 0.5300	 0.0720
f	 0.0820	 0.0390
g	 0.3180	 0.0540
h	 0.1740	 0.0270
i	 0.7780	 0.0780
j	 0.5340	 0.0690
k	 0.5770	 0.0380
l	 0.7390	 0.0670
m	 0.8010	 0.0970
n	 0.4970	 0.0520
o	 0.6210	 0.1010
p	 0.7690	 0.0620
q	 0.5270	 0.0470
r	 0.7510	 0.1020
s	 0.7340	 0.0600
t	 0.5020	 0.0800
u	 0.7590	 0.0310
v	 0.6990	 0.0830
w	 0.3980	 0.0770
x	 0.3170	 0.0920
y	 0.8010	 0.0860
z	 0.5130	 0.0190