Full wwPDB EM Validation Report ⓘ

Apr 27, 2024 – 01:58 PM EDT

PDB ID	:	8UU7
EMDB ID	:	EMD-42566
Title	:	Cryo-EM structure of the Listeria innocua 70S ribosome in complex with HflXr, HPF, and E-site tRNA (structure II-B)
Authors	:	Seely, S.M.; Basu, R.S.; Gagnon, M.G.
Deposited on	:	2023-10-31
Resolution	:	3.20 Å(reported)
Based on initial model	:	7NHN

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

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

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

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

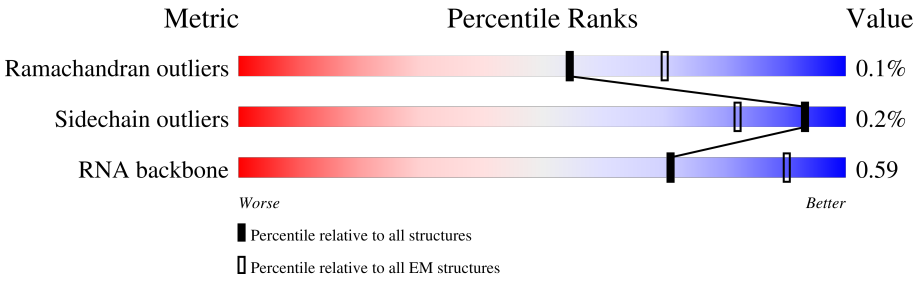
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	a	1550	82% 16%
2	b	249	22% 88% 10%
3	c	218	93% 6%
4	d	200	98%
5	e	167	94% 6%
6	f	97	9% 96%
7	g	156	5% 96%
8	h	132	99%

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Mol	Chain	Length	Quality of chain
9	i	130	97%
10	j	102	95% 5%
11	k	129	10% 88% 12%
12	l	137	99%
13	m	121	14% 94% 6%
14	n	61	98%
15	o	89	6% 98%
16	p	90	97%
17	q	87	93% 7%
18	r	79	81% 19%
19	s	92	88% 12%
20	t	84	96%
21	y	76	87% 67% 25% 5%
22	v	418	7% 99%
23	w	187	16% 53% 47%
24	A	2932	6% 83% 16%
25	B	116	90% 9%
26	C	277	98%
27	D	209	99%
28	E	207	99%
29	F	179	29% 98%
30	G	178	15% 99%
31	L	145	99%
32	M	122	100%
33	N	146	99%

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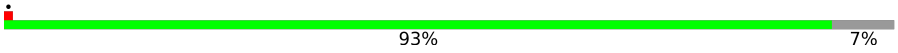
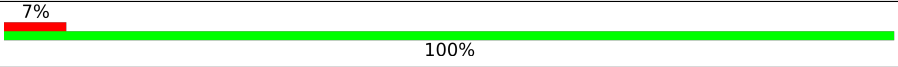
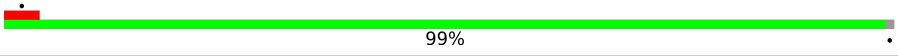
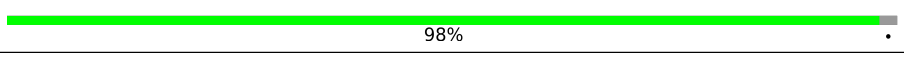
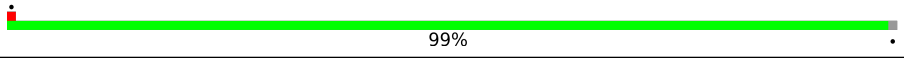
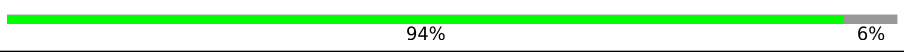
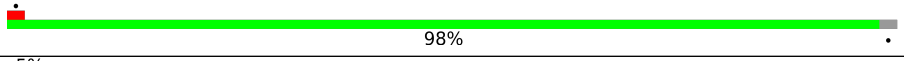
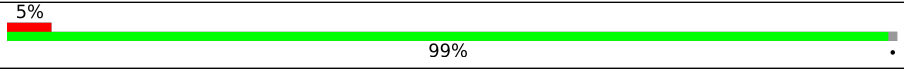
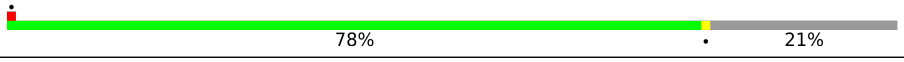
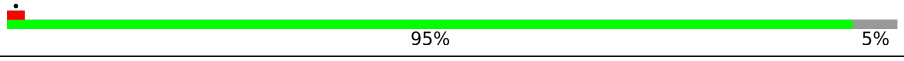
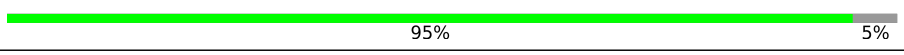
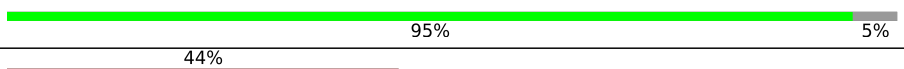
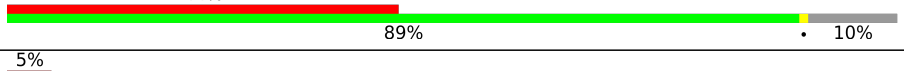
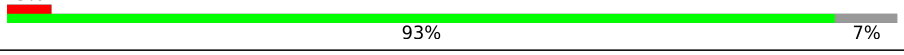
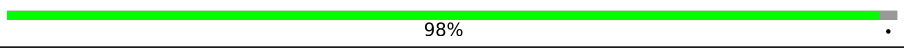
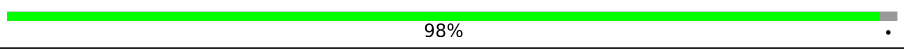
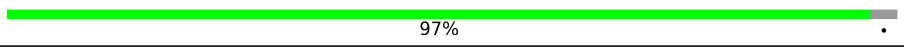
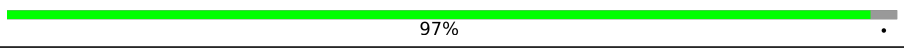
Mol	Chain	Length	Quality of chain
34	O	144	
35	P	135	
36	Q	119	
37	R	114	
38	S	119	
39	T	102	
40	U	118	
41	V	94	
42	W	103	
43	Y	96	
44	Z	62	
45	1	63	
46	2	59	
47	3	81	
48	4	57	
49	5	49	
50	6	44	
51	7	66	
52	8	37	

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 145251 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 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1516	32515	14504	5960	10535	1516	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	224	1806	1153	318	328	7	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	204	1624	1013	311	297	3	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	199	1592	996	299	295	2	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	157	1154	725	211	216	2	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	93	781	494	136	149	2	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1186	740	224	214	8		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	131	Total	C	N	O	S	0	0
			1022	651	180	189	2		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	126	Total	C	N	O	S	0	0
			984	618	194	171	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	97	Total	C	N	O	S	0	0
			776	488	142	144	2		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	114	Total	C	N	O	S	0	0
			837	516	161	157	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			1049	651	211	185	2		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			906	557	180	168	1		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			490	313	97	75	5		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	87	Total	C	N	O	S	0	0
			727	451	146	128	2		

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	88	Total	C	N	O	S	0	0
			711	450	132	126	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	81	Total	C	N	O	S	0	0
			657	411	124	121	1		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	64	Total	C	N	O	S	0	0
			518	334	95	87	2		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	81	Total	C	N	O	S	0	0
			655	418	120	115	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	81	Total	C	N	O	S	0	0
			619	375	126	117	1		

- Molecule 21 is a RNA chain called E-site Phenylalanine tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		

- Molecule 22 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	v	416	Total	C	N	O	S	0	0
			3254	2047	563	634	10		

- Molecule 23 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	w	100	Total	C	N	O	S	0	0
			828	526	145	156	1		

- Molecule 24 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	2909	Total	C	N	O	P	0	0
			62493	27889	11561	20134	2909		

- Molecule 25 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	114	Total	C	N	O	P	0	0
			2428	1082	428	804	114		

- Molecule 26 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C	273	Total	C	N	O	S	0	0
			2108	1307	415	379	7		

- Molecule 27 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D	206	Total	C	N	O	S	0	0
			1583	995	291	293	4		

- Molecule 28 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	E	205	Total	C	N	O	0	0
			1579	998	289	292		

- Molecule 29 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	175	Total	C	N	O	S	0	0
			1356	861	233	256	6		

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	G	176	Total	C	N	O	S	0	0
			1347	847	247	252	1		

- Molecule 31 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	143	Total	C	N	O	S	0	0
			1128	715	205	205	3		

- Molecule 32 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	122	Total	C	N	O	S	0	0
			925	573	175	172	5		

- Molecule 33 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	N	145	Total	C	N	O	0	0
			1104	682	215	207		

- Molecule 34 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	O	134	Total	C	N	O	S	0	0
			1063	680	206	171	6		

- Molecule 35 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	P	122	Total 982	C 616	N 193	O 172	S 1	0	0

- Molecule 36 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Q	119	Total 921	C 568	N 177	O 175	S 1	0	0

- Molecule 37 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	R	113	Total 909	C 573	N 181	O 154	S 1	0	0

- Molecule 38 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	S	117	Total 944	C 599	N 186	O 155	S 4	0	0

- Molecule 39 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	T	101	Total 785	C 506	N 134	O 144	S 1	0	0

- Molecule 40 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	U	111	Total 855	C 539	N 161	O 155	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	V	92	Total 751	C 477	N 131	O 140	S 3	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	W	102	Total	C	N	O	S	0	0
			775	491	142	139	3		

- Molecule 43 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Y	76	Total	C	N	O	S	0	0
			585	357	114	113	1		

- Molecule 44 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Z	59	Total	C	N	O	S	0	0
			462	286	97	77	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	60	Total	C	N	O	S	0	0
			495	304	95	95	1		

- Molecule 46 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	56	Total	C	N	O	S	0	0
			433	272	82	78	1		

- Molecule 47 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	73	Total	C	N	O	S	0	0
			511	322	89	99	1		

- Molecule 48 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	53	Total	C	N	O	S	0	0
			425	259	87	74	5		

- Molecule 49 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5	48	Total 408	C 248	N 82	O 74	S 4	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	6	43	Total 365	C 222	N 88	O 53	S 2	0	0

- Molecule 51 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	7	64	Total 520	C 322	N 114	O 79	S 5	0	0

- Molecule 52 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	8	36	Total 292	C 183	N 59	O 44	S 6	0	0

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	a	169	Total 169	Mg 169	0
53	i	2	Total 2	Mg 2	0
53	j	1	Total 1	Mg 1	0
53	m	1	Total 1	Mg 1	0
53	n	1	Total 1	Mg 1	0
53	v	1	Total 1	Mg 1	0
53	A	212	Total 212	Mg 212	0
53	B	1	Total 1	Mg 1	0
53	D	1	Total 1	Mg 1	0

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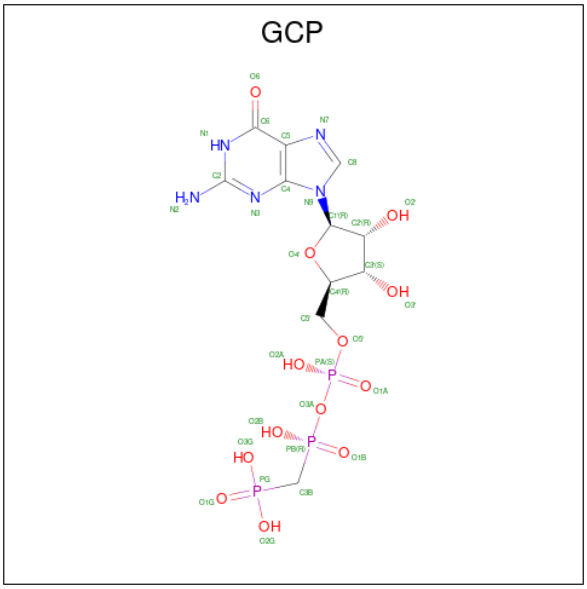
Mol	Chain	Residues	Atoms	AltConf
53	L	1	Total Mg 1 1	0
53	N	1	Total Mg 1 1	0
53	Y	1	Total Mg 1 1	0

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
54	n	1	Total Zn 1 1	0
54	4	1	Total Zn 1 1	0
54	5	1	Total Zn 1 1	0
54	8	1	Total Zn 1 1	0

- Molecule 55 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
55	v	1	Total C N O P 32 11 5 13 3	0

- Molecule 56 is water.

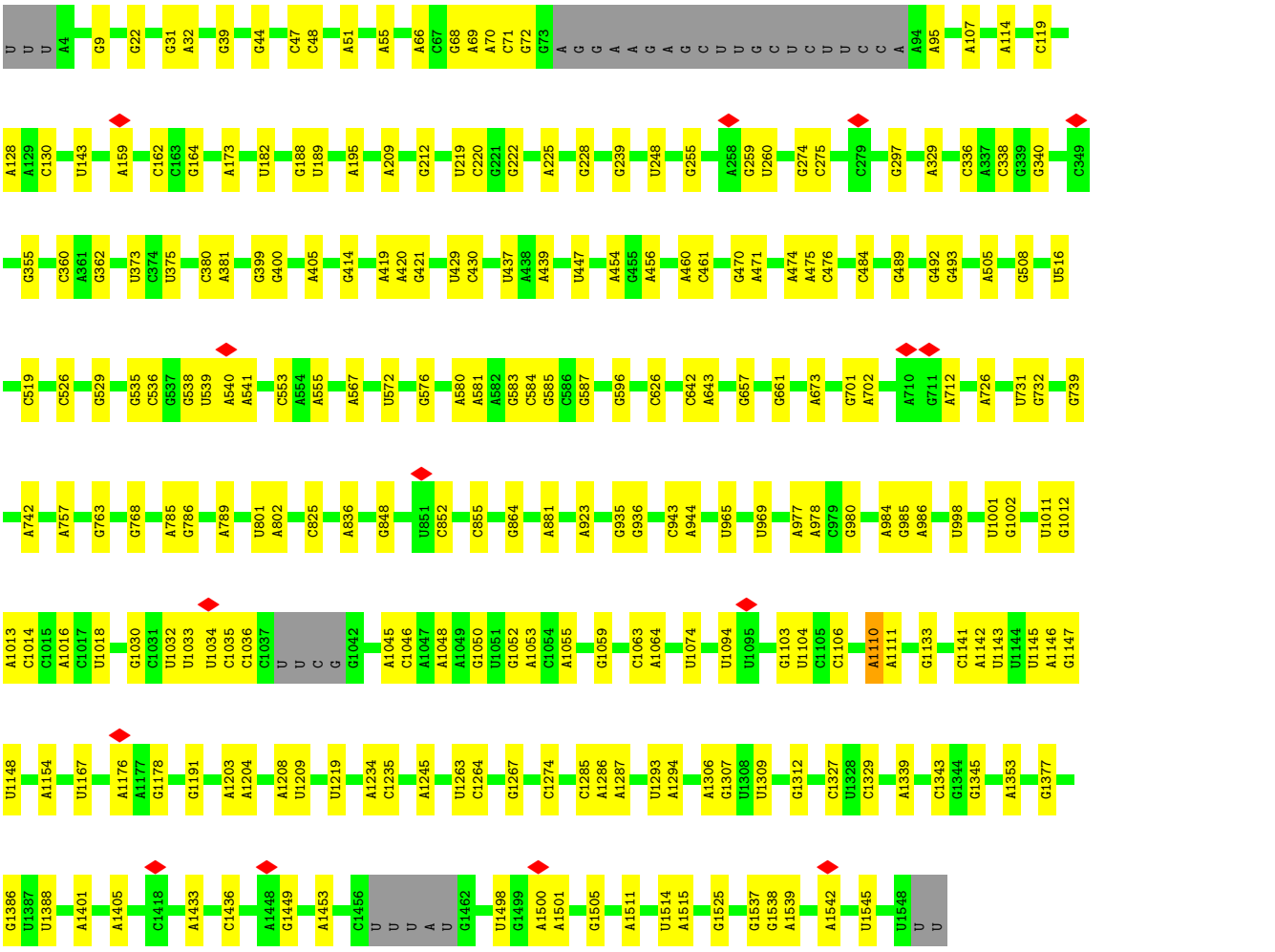
Mol	Chain	Residues	Atoms	AltConf
56	a	7	Total O 7 7	0
56	n	1	Total O 1 1	0
56	A	7	Total O 7 7	0

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.

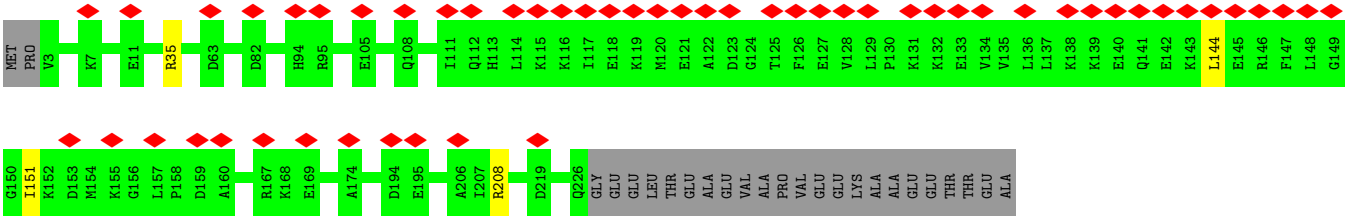
• Molecule 1: 16S Ribosomal RNA

Chain a:

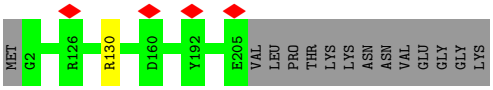


• Molecule 2: Small ribosomal subunit protein uS2

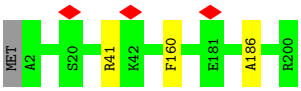
Chain b:



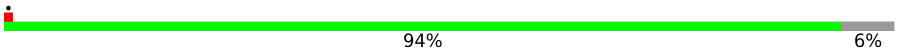
• Molecule 3: Small ribosomal subunit protein uS3

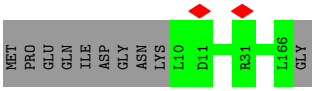


• Molecule 4: Small ribosomal subunit protein uS4

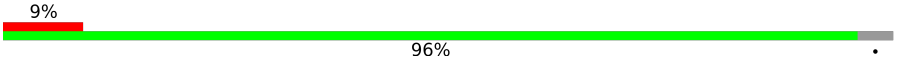


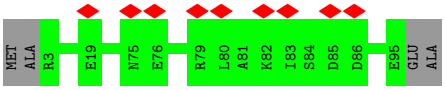
• Molecule 5: Small ribosomal subunit protein uS5



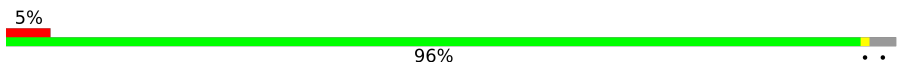


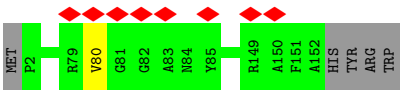
• Molecule 6: Small ribosomal subunit protein bS6



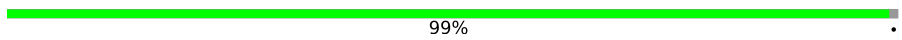


• Molecule 7: Small ribosomal subunit protein uS7



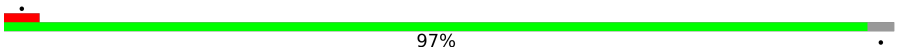


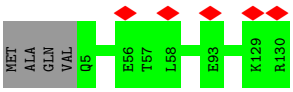
• Molecule 8: Small ribosomal subunit protein uS8



• Molecule 9: Small ribosomal subunit protein uS9

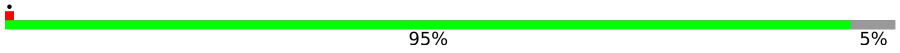
Chain i:

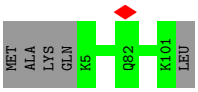




• Molecule 10: Small ribosomal subunit protein uS10

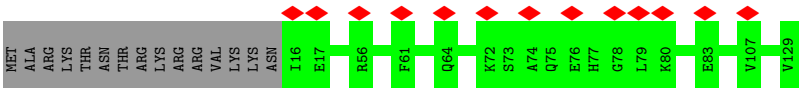
Chain j:





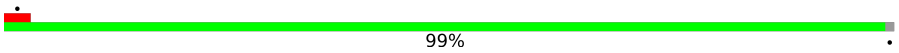
• Molecule 11: Small ribosomal subunit protein uS11

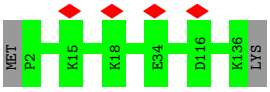
Chain k:



• Molecule 12: Small ribosomal subunit protein uS12

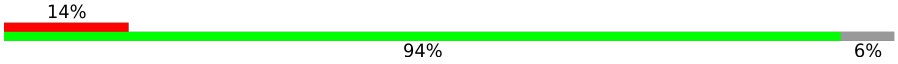
Chain l:

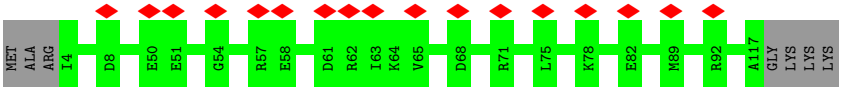




• Molecule 13: Small ribosomal subunit protein uS13

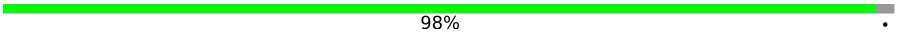
Chain m:





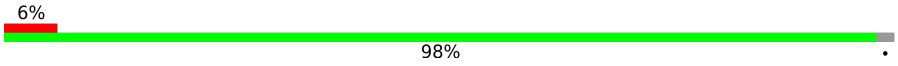
• Molecule 14: Small ribosomal subunit protein uS14

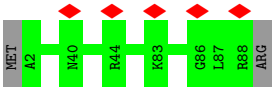
Chain n:



• Molecule 15: Small ribosomal subunit protein uS15

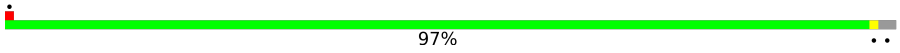
Chain o:

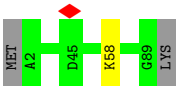




• Molecule 16: Small ribosomal subunit protein bS16

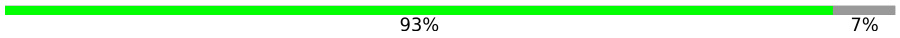
Chain p:

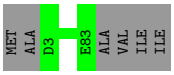




• Molecule 17: Small ribosomal subunit protein uS17

Chain q:



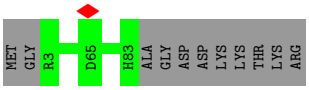


• Molecule 18: Small ribosomal subunit protein bS18

Chain r:

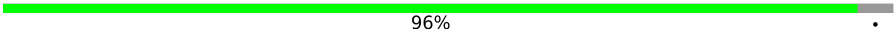
• Molecule 19: Small ribosomal subunit protein uS19

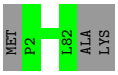
Chain s:



• Molecule 20: Small ribosomal subunit protein bS20

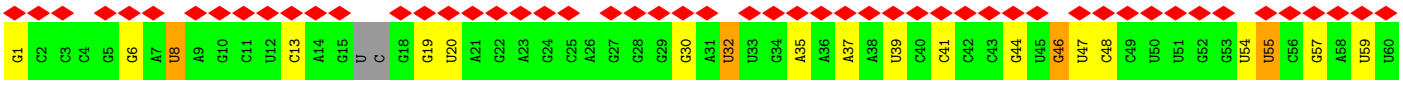
Chain t:

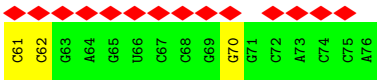




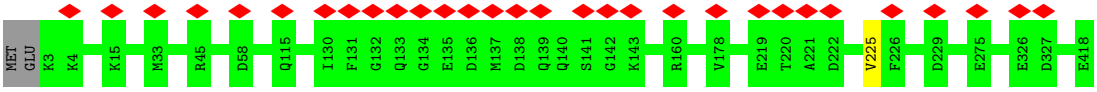
• Molecule 21: E-site Phenylalanine tRNA

Chain y:

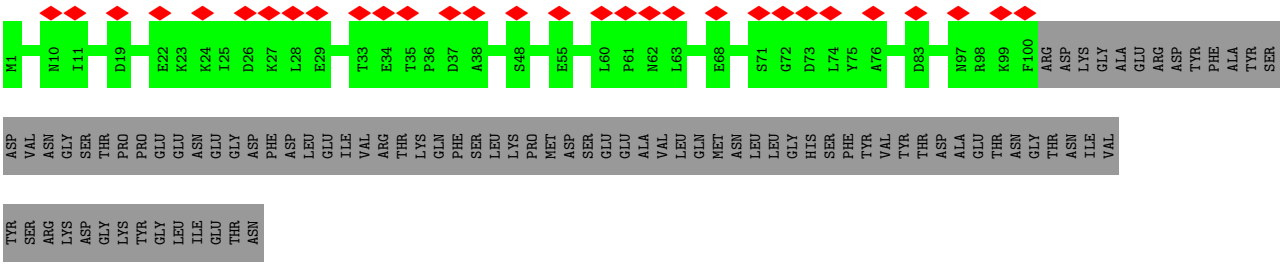




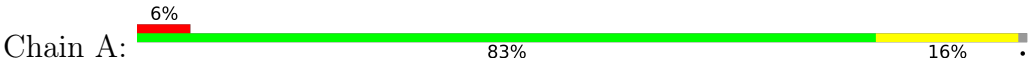
• Molecule 22: GTPase HflX

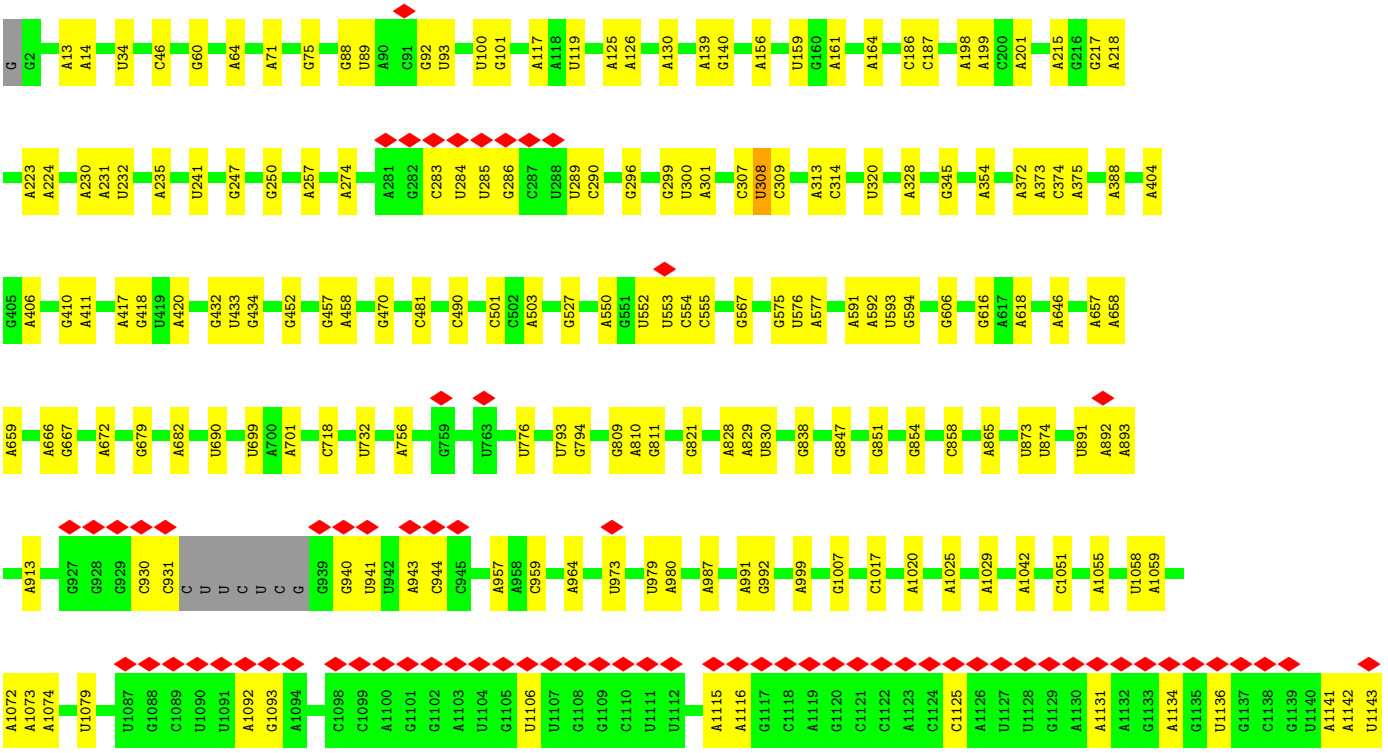


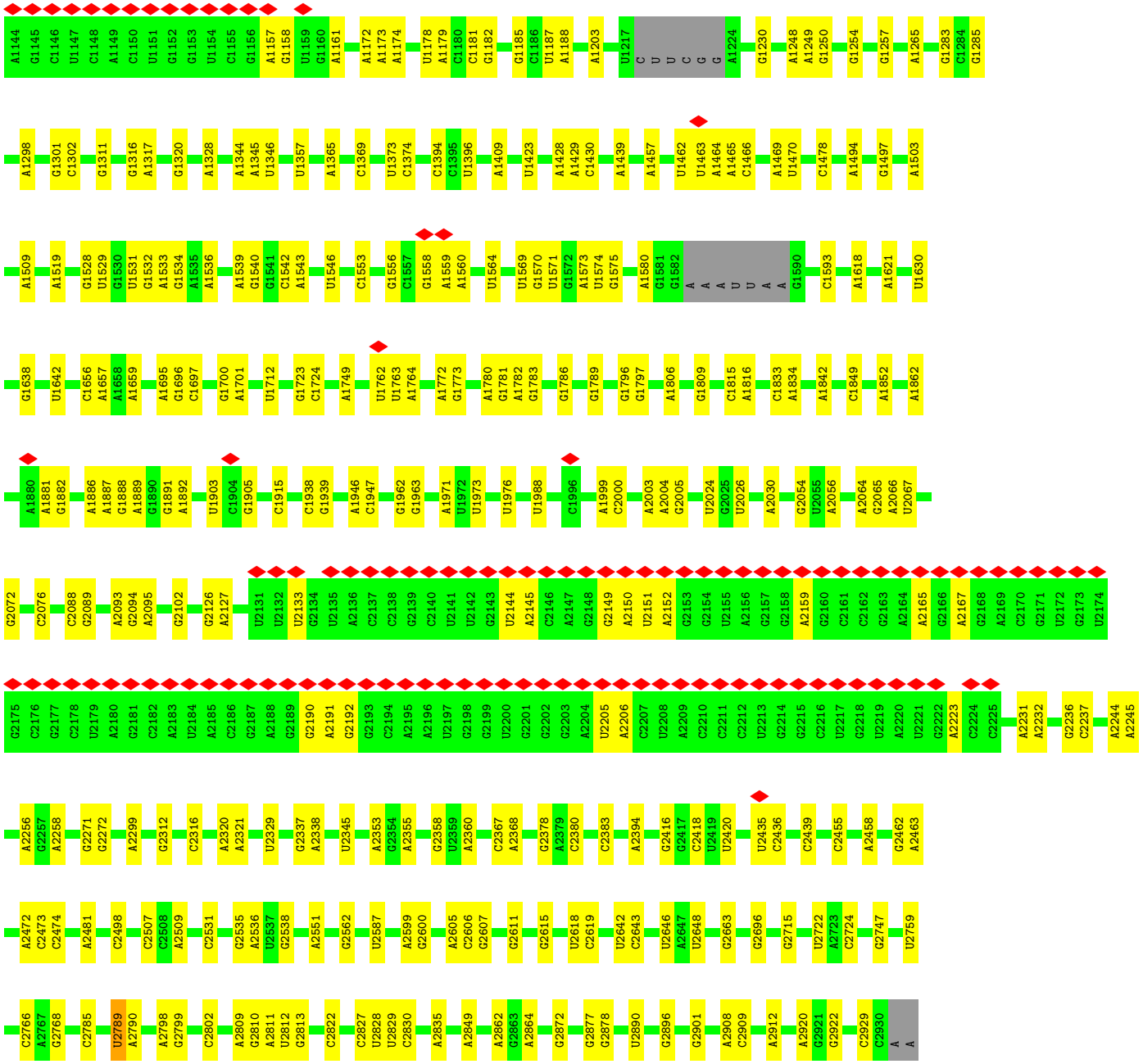
• Molecule 23: Ribosome hibernation promoting factor



• Molecule 24: 23S Ribosomal RNA

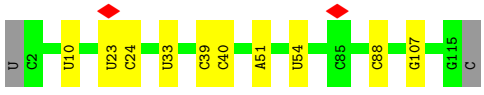






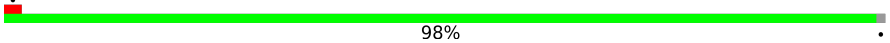
• Molecule 25: 5S Ribosomal RNA

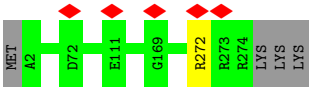
Chain B:



• Molecule 26: Large ribosomal subunit protein uL2

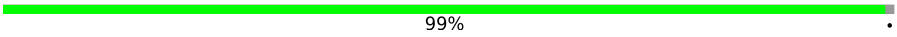
Chain C:

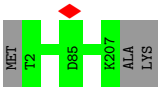




• Molecule 27: Large ribosomal subunit protein uL3

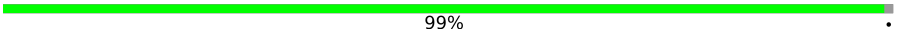
Chain D:

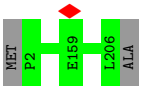




• Molecule 28: Large ribosomal subunit protein uL4

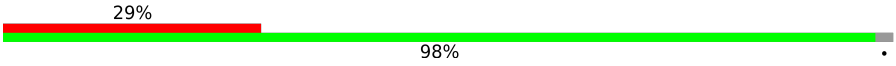
Chain E:

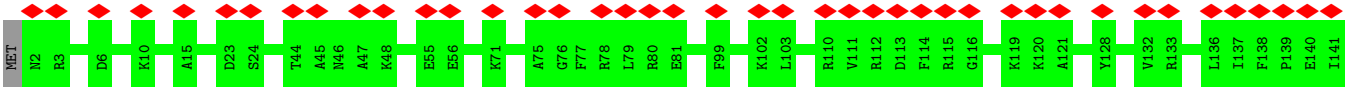


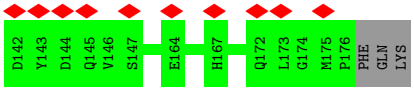


• Molecule 29: Large ribosomal subunit protein uL5

Chain F:

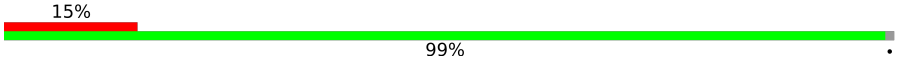


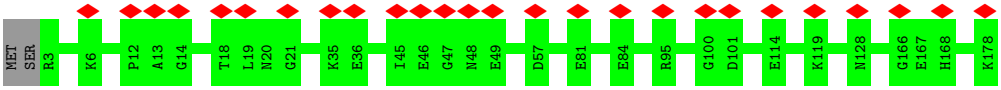




• Molecule 30: Large ribosomal subunit protein uL6

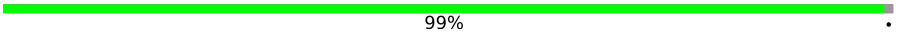
Chain G:





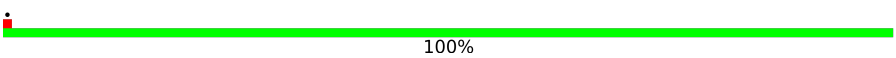
• Molecule 31: Large ribosomal subunit protein uL13

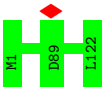
Chain L:



• Molecule 32: Large ribosomal subunit protein uL14

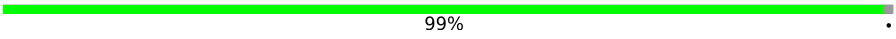
Chain M:





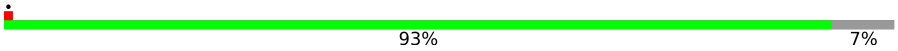
• Molecule 33: Large ribosomal subunit protein uL15

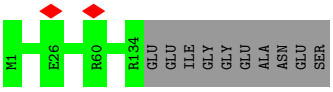
Chain N:



• Molecule 34: Large ribosomal subunit protein uL16

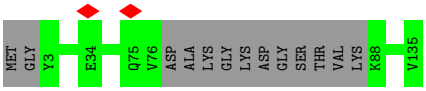
Chain O:





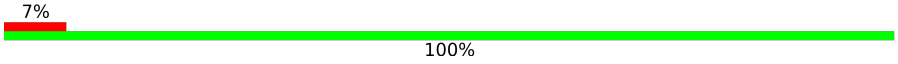
• Molecule 35: Large ribosomal subunit protein bL17

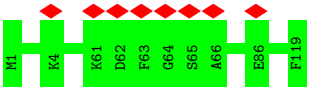
Chain P:



• Molecule 36: Large ribosomal subunit protein uL18

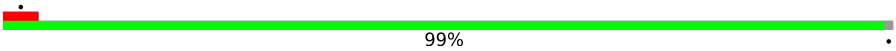
Chain Q:

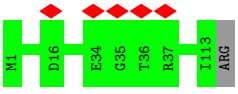




• Molecule 37: Large ribosomal subunit protein bL19

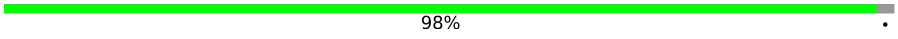
Chain R:





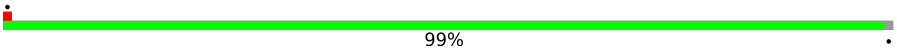
• Molecule 38: Large ribosomal subunit protein bL20

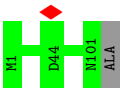
Chain S:



• Molecule 39: Large ribosomal subunit protein bL21

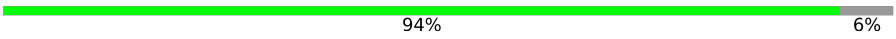
Chain T:

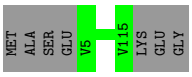




• Molecule 40: Large ribosomal subunit protein uL22

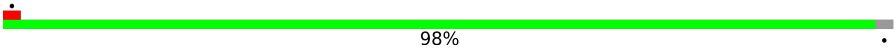
Chain U:

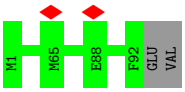




• Molecule 41: Large ribosomal subunit protein uL23

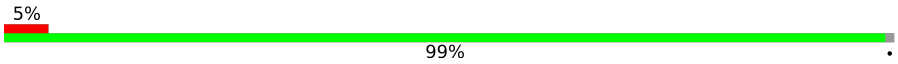
Chain V:

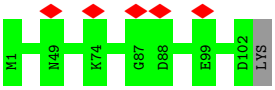




• Molecule 42: Large ribosomal subunit protein uL24

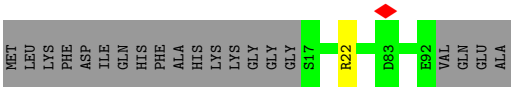
Chain W:





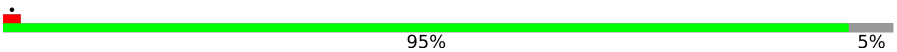
• Molecule 43: Large ribosomal subunit protein bL27

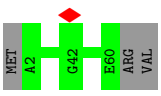
Chain Y:



• Molecule 44: Large ribosomal subunit protein bL28

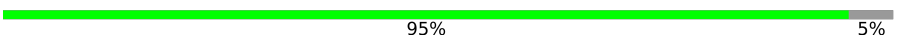
Chain Z:

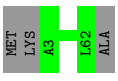




• Molecule 45: Large ribosomal subunit protein uL29

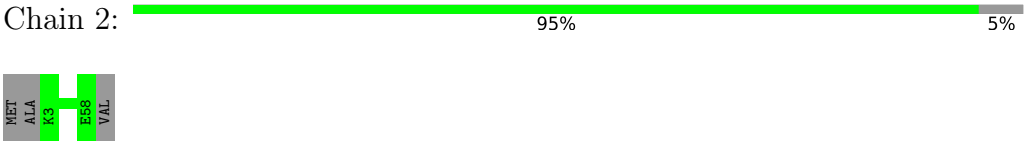
Chain 1:





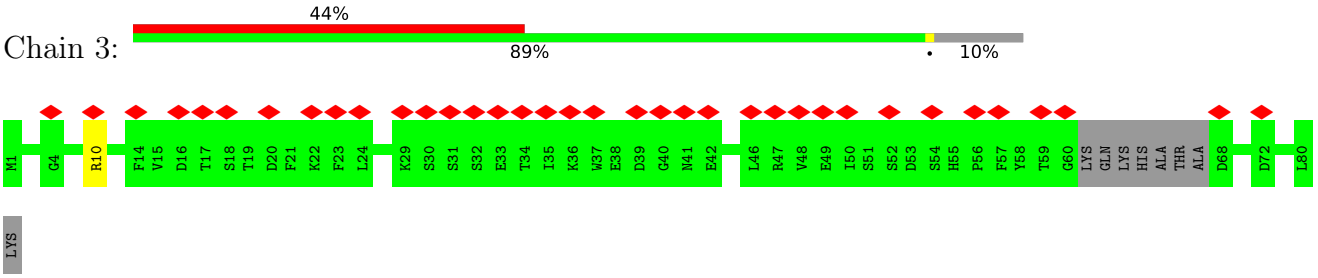
• Molecule 46: Large ribosomal subunit protein uL30

Chain 2:



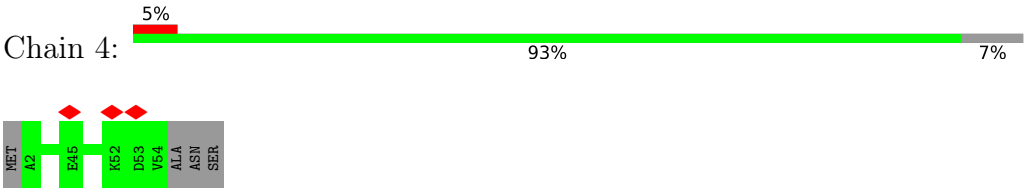
• Molecule 47: Large ribosomal subunit protein bL31B

Chain 3:



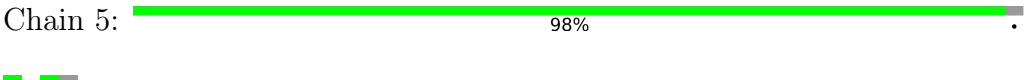
• Molecule 48: Large ribosomal subunit protein bL32

Chain 4:



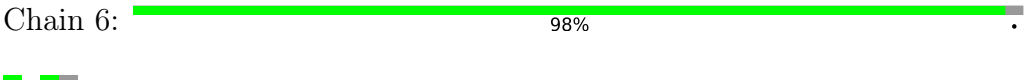
• Molecule 49: Large ribosomal subunit protein bL33

Chain 5:



• Molecule 50: Large ribosomal subunit protein bL34

Chain 6:

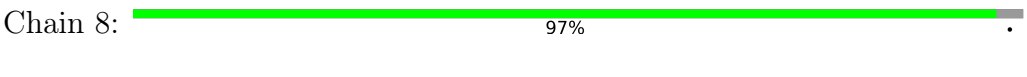


• Molecule 51: Large ribosomal subunit protein bL35

Chain 7:

• Molecule 52: Large ribosomal subunit protein bL36

Chain 8:




M1
Q56
GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27543	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	31.720	Depositor
Minimum map value	-16.412	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	1.092	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: GCP, 5MU, MG, MIA, 4SU, ZN, 7MG, PSU

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	a	0.42	0/36403	0.79	5/56778 (0.0%)
2	b	0.26	0/1835	0.52	1/2466 (0.0%)
3	c	0.30	0/1649	0.56	0/2218
4	d	0.29	0/1620	0.55	0/2176
5	e	0.28	0/1167	0.54	0/1576
6	f	0.27	0/793	0.53	0/1062
7	g	0.29	0/1202	0.59	0/1613
8	h	0.30	0/1035	0.54	0/1392
9	i	0.29	0/1002	0.59	0/1348
10	j	0.32	0/788	0.56	0/1063
11	k	0.25	0/851	0.54	0/1148
12	l	0.31	0/1065	0.58	0/1429
13	m	0.28	0/912	0.60	0/1220
14	n	0.36	0/500	0.60	0/664
15	o	0.28	0/737	0.56	0/987
16	p	0.30	0/724	0.58	0/970
17	q	0.28	0/665	0.56	0/889
18	r	0.29	0/526	0.51	0/704
19	s	0.31	0/671	0.51	0/902
20	t	0.25	0/622	0.52	0/828
21	y	0.37	1/1606 (0.1%)	0.94	3/2497 (0.1%)
22	v	0.28	0/3295	0.54	0/4447
23	w	0.26	0/840	0.50	0/1132
24	A	0.37	0/70015	0.78	3/109224 (0.0%)
25	B	0.26	0/2711	0.75	0/4224
26	C	0.28	0/2144	0.54	0/2875
27	D	0.30	0/1605	0.53	0/2156
28	E	0.27	0/1600	0.50	0/2155
29	F	0.26	0/1374	0.50	0/1852
30	G	0.26	0/1369	0.51	0/1847
31	L	0.27	0/1151	0.47	0/1546
32	M	0.28	0/932	0.55	0/1248

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	N	0.27	0/1115	0.54	0/1482
34	O	0.28	0/1085	0.53	0/1449
35	P	0.27	0/993	0.57	0/1328
36	Q	0.25	0/930	0.52	0/1241
37	R	0.29	0/921	0.59	0/1234
38	S	0.29	0/957	0.49	0/1273
39	T	0.30	0/798	0.49	0/1071
40	U	0.28	0/865	0.55	0/1170
41	V	0.29	0/760	0.51	0/1017
42	W	0.26	0/785	0.49	0/1049
43	Y	0.29	0/592	0.59	0/788
44	Z	0.26	0/467	0.58	0/619
45	1	0.25	0/496	0.53	0/662
46	2	0.25	0/436	0.52	0/585
47	3	0.25	0/521	0.46	0/707
48	4	0.29	0/433	0.63	0/577
49	5	0.27	0/412	0.59	0/551
50	6	0.27	0/368	0.63	0/479
51	7	0.27	0/527	0.58	0/685
52	8	0.27	0/295	0.53	0/387
All	All	0.35	1/157165 (0.0%)	0.73	12/234990 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	y	1	G	OP3-P	-10.70	1.48	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	y	62	C	N3-C2-O2	-8.42	116.00	121.90
1	a	1106	C	N3-C2-O2	-7.00	117.00	121.90
21	y	62	C	N1-C2-O2	6.89	123.03	118.90
24	A	1357	U	C2-N1-C1'	6.64	125.67	117.70
21	y	41	C	N3-C2-O2	-6.62	117.26	121.90
1	a	260	U	C2-N1-C1'	6.28	125.23	117.70
2	b	144	LEU	CA-CB-CG	5.87	128.81	115.30
24	A	308	U	C2-N1-C1'	5.61	124.43	117.70
24	A	2789	U	P-O3'-C3'	5.44	126.23	119.70
1	a	1208	A	P-O3'-C3'	5.08	125.79	119.70
1	a	536	C	N1-C2-O2	5.07	121.94	118.90
1	a	1110	A	P-O3'-C3'	5.04	125.74	119.70

There are no chirality outliers.

There are no planarity outliers.

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	
2	b	222/249 (89%)	202 (91%)	19 (9%)	1 (0%)	29	67
3	c	202/218 (93%)	187 (93%)	15 (7%)	0	100	100
4	d	197/200 (98%)	182 (92%)	13 (7%)	2 (1%)	15	54
5	e	155/167 (93%)	145 (94%)	10 (6%)	0	100	100
6	f	91/97 (94%)	84 (92%)	7 (8%)	0	100	100
7	g	149/156 (96%)	137 (92%)	11 (7%)	1 (1%)	22	61
8	h	129/132 (98%)	122 (95%)	7 (5%)	0	100	100
9	i	124/130 (95%)	119 (96%)	5 (4%)	0	100	100
10	j	95/102 (93%)	91 (96%)	4 (4%)	0	100	100
11	k	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
12	l	133/137 (97%)	123 (92%)	10 (8%)	0	100	100
13	m	112/121 (93%)	100 (89%)	12 (11%)	0	100	100
14	n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	o	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
16	p	86/90 (96%)	82 (95%)	4 (5%)	0	100	100
17	q	79/87 (91%)	76 (96%)	3 (4%)	0	100	100
18	r	62/79 (78%)	59 (95%)	3 (5%)	0	100	100
19	s	79/92 (86%)	74 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	t	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
22	v	414/418 (99%)	385 (93%)	28 (7%)	1 (0%)	47	79
23	w	98/187 (52%)	92 (94%)	6 (6%)	0	100	100
26	C	271/277 (98%)	260 (96%)	11 (4%)	0	100	100
27	D	204/209 (98%)	193 (95%)	11 (5%)	0	100	100
28	E	203/207 (98%)	188 (93%)	15 (7%)	0	100	100
29	F	173/179 (97%)	166 (96%)	7 (4%)	0	100	100
30	G	174/178 (98%)	167 (96%)	7 (4%)	0	100	100
31	L	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
32	M	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
33	N	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
34	O	132/144 (92%)	130 (98%)	2 (2%)	0	100	100
35	P	118/135 (87%)	113 (96%)	5 (4%)	0	100	100
36	Q	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
37	R	111/114 (97%)	106 (96%)	5 (4%)	0	100	100
38	S	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
39	T	99/102 (97%)	95 (96%)	4 (4%)	0	100	100
40	U	109/118 (92%)	106 (97%)	3 (3%)	0	100	100
41	V	90/94 (96%)	86 (96%)	4 (4%)	0	100	100
42	W	100/103 (97%)	96 (96%)	4 (4%)	0	100	100
43	Y	74/96 (77%)	73 (99%)	1 (1%)	0	100	100
44	Z	57/62 (92%)	50 (88%)	7 (12%)	0	100	100
45	1	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
46	2	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
47	3	69/81 (85%)	57 (83%)	12 (17%)	0	100	100
48	4	51/57 (90%)	51 (100%)	0	0	100	100
49	5	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
50	6	41/44 (93%)	41 (100%)	0	0	100	100
51	7	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
52	8	34/37 (92%)	34 (100%)	0	0	100	100
All	All	5727/6150 (93%)	5418 (95%)	304 (5%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	151	ILE
22	v	225	VAL
4	d	160	PHE
4	d	186	ALA
7	g	80	VAL

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
2	b	195/214 (91%)	193 (99%)	2 (1%)	76 90
3	c	165/177 (93%)	164 (99%)	1 (1%)	86 94
4	d	169/170 (99%)	168 (99%)	1 (1%)	86 94
5	e	123/131 (94%)	123 (100%)	0	100 100
6	f	83/85 (98%)	83 (100%)	0	100 100
7	g	124/130 (95%)	124 (100%)	0	100 100
8	h	109/110 (99%)	109 (100%)	0	100 100
9	i	98/102 (96%)	98 (100%)	0	100 100
10	j	88/93 (95%)	88 (100%)	0	100 100
11	k	86/100 (86%)	86 (100%)	0	100 100
12	l	116/118 (98%)	116 (100%)	0	100 100
13	m	97/102 (95%)	97 (100%)	0	100 100
14	n	51/52 (98%)	51 (100%)	0	100 100
15	o	79/81 (98%)	79 (100%)	0	100 100
16	p	78/80 (98%)	77 (99%)	1 (1%)	69 87
17	q	73/78 (94%)	73 (100%)	0	100 100
18	r	57/67 (85%)	57 (100%)	0	100 100
19	s	70/78 (90%)	70 (100%)	0	100 100
20	t	64/66 (97%)	64 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	v	344/365 (94%)	344 (100%)	0	100 100
23	w	94/170 (55%)	94 (100%)	0	100 100
26	C	221/225 (98%)	220 (100%)	1 (0%)	88 95
27	D	169/171 (99%)	169 (100%)	0	100 100
28	E	173/174 (99%)	173 (100%)	0	100 100
29	F	149/155 (96%)	149 (100%)	0	100 100
30	G	144/147 (98%)	144 (100%)	0	100 100
31	L	120/121 (99%)	120 (100%)	0	100 100
32	M	101/101 (100%)	101 (100%)	0	100 100
33	N	114/115 (99%)	114 (100%)	0	100 100
34	O	106/113 (94%)	106 (100%)	0	100 100
35	P	102/111 (92%)	102 (100%)	0	100 100
36	Q	97/97 (100%)	97 (100%)	0	100 100
37	R	98/99 (99%)	98 (100%)	0	100 100
38	S	95/97 (98%)	95 (100%)	0	100 100
39	T	82/82 (100%)	82 (100%)	0	100 100
40	U	92/97 (95%)	92 (100%)	0	100 100
41	V	82/84 (98%)	82 (100%)	0	100 100
42	W	87/88 (99%)	87 (100%)	0	100 100
43	Y	61/76 (80%)	60 (98%)	1 (2%)	62 84
44	Z	50/53 (94%)	50 (100%)	0	100 100
45	1	53/55 (96%)	53 (100%)	0	100 100
46	2	50/52 (96%)	50 (100%)	0	100 100
47	3	45/73 (62%)	44 (98%)	1 (2%)	52 79
48	4	47/50 (94%)	47 (100%)	0	100 100
49	5	47/48 (98%)	47 (100%)	0	100 100
50	6	39/39 (100%)	39 (100%)	0	100 100
51	7	54/56 (96%)	54 (100%)	0	100 100
52	8	35/35 (100%)	35 (100%)	0	100 100
All	All	4876/5183 (94%)	4868 (100%)	8 (0%)	93 98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	35	ARG
2	b	208	ARG
3	c	130	ARG
4	d	41	ARG
16	p	58	LYS
26	C	272	ARG
43	Y	22	ARG
47	3	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	77	GLN
2	b	113	HIS
2	b	203	ASN
3	c	133	GLN
3	c	175	HIS
4	d	85	ASN
4	d	112	GLN
4	d	116	HIS
4	d	118	HIS
4	d	137	GLN
5	e	44	ASN
6	f	14	ASN
6	f	34	ASN
6	f	90	HIS
7	g	68	ASN
7	g	130	ASN
9	i	50	GLN
11	k	38	HIS
11	k	40	ASN
12	l	5	ASN
12	l	29	ASN
12	l	59	ASN
12	l	86	ASN
12	l	109	HIS
13	m	76	ASN
13	m	91	HIS
15	o	18	HIS
15	o	28	GLN
15	o	40	ASN
15	o	51	HIS
16	p	61	HIS

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Mol	Chain	Res	Type
16	p	86	GLN
20	t	74	ASN
22	v	12	GLN
22	v	31	ASN
22	v	67	GLN
22	v	115	GLN
22	v	139	GLN
22	v	165	HIS
22	v	169	HIS
22	v	247	ASN
22	v	382	ASN
22	v	398	GLN
23	w	41	HIS
23	w	92	HIS
23	w	97	ASN
26	C	53	HIS
26	C	153	GLN
26	C	163	GLN
27	D	50	GLN
27	D	152	ASN
28	E	162	ASN
29	F	37	ASN
29	F	63	GLN
30	G	20	ASN
30	G	38	ASN
30	G	99	GLN
30	G	130	GLN
31	L	41	ASN
32	M	110	ASN
33	N	83	ASN
35	P	61	GLN
35	P	89	ASN
36	Q	43	GLN
36	Q	49	ASN
37	R	41	GLN
39	T	90	GLN
40	U	107	HIS
42	W	2	HIS
47	3	6	HIS
47	3	75	ASN
51	7	35	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1512/1550 (97%)	238 (15%)	0
21	y	71/76 (93%)	17 (23%)	0
24	A	2905/2932 (99%)	459 (15%)	23 (0%)
25	B	113/116 (97%)	10 (8%)	0
All	All	4601/4674 (98%)	724 (15%)	23 (0%)

All (724) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	22	G
1	a	31	G
1	a	32	A
1	a	39	G
1	a	44	G
1	a	47	C
1	a	48	C
1	a	51	A
1	a	55	A
1	a	66	A
1	a	68	G
1	a	69	A
1	a	70	A
1	a	71	C
1	a	72	G
1	a	95	A
1	a	107	A
1	a	114	A
1	a	119	C
1	a	128	A
1	a	130	C
1	a	143	U
1	a	159	A
1	a	162	C
1	a	164	G
1	a	173	A
1	a	182	U
1	a	188	G
1	a	189	U
1	a	195	A
1	a	209	A

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Mol	Chain	Res	Type
1	a	212	G
1	a	219	U
1	a	220	C
1	a	222	G
1	a	225	A
1	a	228	G
1	a	239	G
1	a	248	U
1	a	255	G
1	a	259	G
1	a	274	G
1	a	275	C
1	a	297	G
1	a	329	A
1	a	336	C
1	a	338	C
1	a	340	G
1	a	355	G
1	a	360	C
1	a	362	G
1	a	373	U
1	a	375	U
1	a	380	C
1	a	381	A
1	a	399	G
1	a	400	G
1	a	405	A
1	a	414	G
1	a	419	A
1	a	420	A
1	a	421	G
1	a	429	U
1	a	430	C
1	a	437	U
1	a	439	A
1	a	447	U
1	a	454	A
1	a	456	A
1	a	460	A
1	a	461	C
1	a	470	G
1	a	471	A

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Mol	Chain	Res	Type
1	a	474	A
1	a	475	A
1	a	476	C
1	a	484	C
1	a	489	G
1	a	492	G
1	a	493	G
1	a	505	A
1	a	508	G
1	a	516	U
1	a	519	C
1	a	526	C
1	a	529	G
1	a	535	G
1	a	538	G
1	a	539	U
1	a	540	A
1	a	541	A
1	a	553	C
1	a	555	A
1	a	567	A
1	a	572	U
1	a	576	G
1	a	580	A
1	a	581	A
1	a	583	G
1	a	584	C
1	a	585	G
1	a	587	G
1	a	596	G
1	a	626	C
1	a	642	C
1	a	643	A
1	a	657	G
1	a	661	G
1	a	673	A
1	a	701	G
1	a	702	A
1	a	712	A
1	a	726	A
1	a	731	U
1	a	732	G

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Mol	Chain	Res	Type
1	a	739	G
1	a	742	A
1	a	757	A
1	a	763	G
1	a	768	G
1	a	785	A
1	a	786	G
1	a	789	A
1	a	801	U
1	a	802	A
1	a	825	C
1	a	836	A
1	a	848	G
1	a	852	C
1	a	855	C
1	a	864	G
1	a	881	A
1	a	923	A
1	a	935	G
1	a	936	G
1	a	943	C
1	a	944	A
1	a	965	U
1	a	969	U
1	a	977	A
1	a	978	A
1	a	980	G
1	a	984	A
1	a	985	G
1	a	986	A
1	a	998	U
1	a	1001	U
1	a	1002	G
1	a	1011	U
1	a	1012	G
1	a	1013	A
1	a	1014	C
1	a	1016	A
1	a	1018	U
1	a	1030	G
1	a	1032	U
1	a	1033	U

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Mol	Chain	Res	Type
1	a	1034	U
1	a	1035	C
1	a	1036	C
1	a	1045	A
1	a	1046	C
1	a	1048	A
1	a	1050	G
1	a	1052	G
1	a	1053	A
1	a	1055	A
1	a	1059	G
1	a	1063	C
1	a	1064	A
1	a	1074	U
1	a	1094	U
1	a	1103	G
1	a	1104	U
1	a	1110	A
1	a	1111	A
1	a	1133	G
1	a	1141	C
1	a	1142	A
1	a	1143	U
1	a	1145	U
1	a	1146	A
1	a	1147	G
1	a	1148	U
1	a	1154	A
1	a	1167	U
1	a	1176	A
1	a	1178	G
1	a	1191	G
1	a	1203	A
1	a	1204	A
1	a	1209	U
1	a	1219	U
1	a	1234	A
1	a	1235	C
1	a	1245	A
1	a	1263	U
1	a	1264	C
1	a	1267	G

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Mol	Chain	Res	Type
1	a	1274	C
1	a	1285	C
1	a	1286	A
1	a	1287	A
1	a	1293	U
1	a	1294	A
1	a	1306	A
1	a	1307	G
1	a	1309	U
1	a	1312	G
1	a	1327	C
1	a	1329	C
1	a	1339	A
1	a	1343	C
1	a	1345	G
1	a	1353	A
1	a	1377	G
1	a	1386	G
1	a	1388	U
1	a	1401	A
1	a	1405	A
1	a	1433	A
1	a	1436	C
1	a	1449	G
1	a	1453	A
1	a	1498	U
1	a	1500	A
1	a	1501	A
1	a	1505	G
1	a	1511	A
1	a	1514	U
1	a	1515	A
1	a	1525	G
1	a	1537	G
1	a	1538	G
1	a	1539	A
1	a	1542	A
1	a	1545	U
21	y	6	G
21	y	8	4SU
21	y	13	C
21	y	19	G

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Mol	Chain	Res	Type
21	y	20	U
21	y	30	G
21	y	32	PSU
21	y	35	A
21	y	44	G
21	y	46	7MG
21	y	47	U
21	y	48	C
21	y	55	PSU
21	y	57	G
21	y	59	U
21	y	61	C
21	y	70	G
24	A	13	A
24	A	14	A
24	A	34	U
24	A	46	C
24	A	60	G
24	A	64	A
24	A	71	A
24	A	75	G
24	A	89	U
24	A	93	U
24	A	100	U
24	A	101	G
24	A	117	A
24	A	119	U
24	A	125	A
24	A	126	A
24	A	130	A
24	A	140	G
24	A	156	A
24	A	159	U
24	A	161	A
24	A	164	A
24	A	186	C
24	A	187	C
24	A	198	A
24	A	199	A
24	A	201	A
24	A	215	A
24	A	217	G

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Mol	Chain	Res	Type
24	A	218	A
24	A	223	A
24	A	224	A
24	A	230	A
24	A	231	A
24	A	232	U
24	A	235	A
24	A	241	U
24	A	247	G
24	A	250	G
24	A	257	A
24	A	274	A
24	A	283	C
24	A	284	U
24	A	285	U
24	A	286	G
24	A	289	U
24	A	290	C
24	A	296	G
24	A	299	G
24	A	300	U
24	A	301	A
24	A	307	C
24	A	308	U
24	A	309	C
24	A	313	A
24	A	314	C
24	A	320	U
24	A	328	A
24	A	345	G
24	A	354	A
24	A	372	A
24	A	373	A
24	A	374	C
24	A	375	A
24	A	388	A
24	A	404	A
24	A	406	A
24	A	410	G
24	A	411	A
24	A	417	A
24	A	418	G

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Mol	Chain	Res	Type
24	A	420	A
24	A	432	G
24	A	433	U
24	A	434	G
24	A	452	G
24	A	457	G
24	A	458	A
24	A	470	G
24	A	481	C
24	A	490	C
24	A	501	C
24	A	503	A
24	A	527	G
24	A	550	A
24	A	552	U
24	A	553	U
24	A	554	C
24	A	555	C
24	A	567	G
24	A	575	G
24	A	576	U
24	A	577	A
24	A	591	A
24	A	592	A
24	A	593	U
24	A	594	G
24	A	606	G
24	A	616	G
24	A	618	A
24	A	646	A
24	A	657	A
24	A	658	A
24	A	659	A
24	A	666	A
24	A	667	G
24	A	672	A
24	A	679	G
24	A	682	A
24	A	690	U
24	A	699	U
24	A	701	A
24	A	718	C

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Mol	Chain	Res	Type
24	A	732	U
24	A	776	U
24	A	793	U
24	A	794	G
24	A	810	A
24	A	811	G
24	A	821	G
24	A	828	A
24	A	829	A
24	A	830	U
24	A	838	G
24	A	851	G
24	A	858	C
24	A	865	A
24	A	873	U
24	A	874	U
24	A	891	U
24	A	892	A
24	A	893	A
24	A	913	A
24	A	930	C
24	A	931	C
24	A	940	G
24	A	941	U
24	A	943	A
24	A	944	C
24	A	957	A
24	A	959	C
24	A	964	A
24	A	973	U
24	A	979	U
24	A	980	A
24	A	987	A
24	A	991	A
24	A	992	G
24	A	999	A
24	A	1007	G
24	A	1020	A
24	A	1025	A
24	A	1029	A
24	A	1042	A
24	A	1051	C

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Mol	Chain	Res	Type
24	A	1055	A
24	A	1058	U
24	A	1059	A
24	A	1072	A
24	A	1073	A
24	A	1074	A
24	A	1079	U
24	A	1092	A
24	A	1093	G
24	A	1106	U
24	A	1115	A
24	A	1116	A
24	A	1125	C
24	A	1131	A
24	A	1134	A
24	A	1136	U
24	A	1141	A
24	A	1142	A
24	A	1143	U
24	A	1157	A
24	A	1158	G
24	A	1161	A
24	A	1173	A
24	A	1174	A
24	A	1178	U
24	A	1179	A
24	A	1181	C
24	A	1182	G
24	A	1185	G
24	A	1187	U
24	A	1188	A
24	A	1203	A
24	A	1230	G
24	A	1249	A
24	A	1250	G
24	A	1254	G
24	A	1257	G
24	A	1265	A
24	A	1283	G
24	A	1285	G
24	A	1298	A
24	A	1301	G

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Mol	Chain	Res	Type
24	A	1302	C
24	A	1311	G
24	A	1316	G
24	A	1317	A
24	A	1320	G
24	A	1328	A
24	A	1344	A
24	A	1345	A
24	A	1346	U
24	A	1365	A
24	A	1369	C
24	A	1373	U
24	A	1374	C
24	A	1394	C
24	A	1396	U
24	A	1409	A
24	A	1423	U
24	A	1428	A
24	A	1429	A
24	A	1430	C
24	A	1439	A
24	A	1457	A
24	A	1462	U
24	A	1463	U
24	A	1464	A
24	A	1465	A
24	A	1466	C
24	A	1469	A
24	A	1470	U
24	A	1478	C
24	A	1494	A
24	A	1503	A
24	A	1509	A
24	A	1519	A
24	A	1528	G
24	A	1529	U
24	A	1531	U
24	A	1532	G
24	A	1533	A
24	A	1534	G
24	A	1536	A
24	A	1539	A

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Mol	Chain	Res	Type
24	A	1540	G
24	A	1542	C
24	A	1543	A
24	A	1546	U
24	A	1553	C
24	A	1556	G
24	A	1558	G
24	A	1559	A
24	A	1560	A
24	A	1564	U
24	A	1570	G
24	A	1571	U
24	A	1573	A
24	A	1574	U
24	A	1575	G
24	A	1580	A
24	A	1593	C
24	A	1618	A
24	A	1621	A
24	A	1630	U
24	A	1638	G
24	A	1642	U
24	A	1656	C
24	A	1657	A
24	A	1659	A
24	A	1695	A
24	A	1696	G
24	A	1697	C
24	A	1700	G
24	A	1701	A
24	A	1712	U
24	A	1723	G
24	A	1724	C
24	A	1749	A
24	A	1762	U
24	A	1763	U
24	A	1764	A
24	A	1772	A
24	A	1773	G
24	A	1780	A
24	A	1781	G
24	A	1782	A

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Mol	Chain	Res	Type
24	A	1783	G
24	A	1786	G
24	A	1789	G
24	A	1796	G
24	A	1797	G
24	A	1806	A
24	A	1809	G
24	A	1815	C
24	A	1816	A
24	A	1833	C
24	A	1834	A
24	A	1842	A
24	A	1849	C
24	A	1852	A
24	A	1862	A
24	A	1881	A
24	A	1882	G
24	A	1886	A
24	A	1887	A
24	A	1889	A
24	A	1891	G
24	A	1892	A
24	A	1903	U
24	A	1905	G
24	A	1915	C
24	A	1938	C
24	A	1939	G
24	A	1946	A
24	A	1947	C
24	A	1962	G
24	A	1963	G
24	A	1971	A
24	A	1973	U
24	A	1976	U
24	A	1988	U
24	A	1999	A
24	A	2000	C
24	A	2003	A
24	A	2004	A
24	A	2005	G
24	A	2024	U
24	A	2026	U

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Mol	Chain	Res	Type
24	A	2030	A
24	A	2054	G
24	A	2056	A
24	A	2064	A
24	A	2065	G
24	A	2066	A
24	A	2067	U
24	A	2072	G
24	A	2076	C
24	A	2088	C
24	A	2089	G
24	A	2093	A
24	A	2094	G
24	A	2095	A
24	A	2102	G
24	A	2126	G
24	A	2127	A
24	A	2133	U
24	A	2144	U
24	A	2145	A
24	A	2149	G
24	A	2150	A
24	A	2151	U
24	A	2152	A
24	A	2159	A
24	A	2165	A
24	A	2167	A
24	A	2190	G
24	A	2191	A
24	A	2192	G
24	A	2205	U
24	A	2206	A
24	A	2223	A
24	A	2231	A
24	A	2232	A
24	A	2236	G
24	A	2237	C
24	A	2244	A
24	A	2245	A
24	A	2256	A
24	A	2258	A
24	A	2271	G

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Mol	Chain	Res	Type
24	A	2272	G
24	A	2299	A
24	A	2312	G
24	A	2316	C
24	A	2320	A
24	A	2321	A
24	A	2329	U
24	A	2337	G
24	A	2338	A
24	A	2345	U
24	A	2353	A
24	A	2355	A
24	A	2358	G
24	A	2360	A
24	A	2367	C
24	A	2368	A
24	A	2378	G
24	A	2380	C
24	A	2383	C
24	A	2394	A
24	A	2416	G
24	A	2418	C
24	A	2420	U
24	A	2435	U
24	A	2436	C
24	A	2439	C
24	A	2455	C
24	A	2458	A
24	A	2462	G
24	A	2463	A
24	A	2473	C
24	A	2474	C
24	A	2481	A
24	A	2498	C
24	A	2507	C
24	A	2509	A
24	A	2531	C
24	A	2535	G
24	A	2536	A
24	A	2538	G
24	A	2551	A
24	A	2562	G

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Mol	Chain	Res	Type
24	A	2587	U
24	A	2599	A
24	A	2600	G
24	A	2605	A
24	A	2606	C
24	A	2607	G
24	A	2611	G
24	A	2615	G
24	A	2618	U
24	A	2619	C
24	A	2642	U
24	A	2643	C
24	A	2646	U
24	A	2648	U
24	A	2663	G
24	A	2696	G
24	A	2715	G
24	A	2722	U
24	A	2724	C
24	A	2747	G
24	A	2759	U
24	A	2766	C
24	A	2768	G
24	A	2785	C
24	A	2790	A
24	A	2798	A
24	A	2799	G
24	A	2802	C
24	A	2810	G
24	A	2811	A
24	A	2812	U
24	A	2813	G
24	A	2822	C
24	A	2827	C
24	A	2828	U
24	A	2829	U
24	A	2830	C
24	A	2835	A
24	A	2849	A
24	A	2862	A
24	A	2864	A
24	A	2872	G

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Mol	Chain	Res	Type
24	A	2877	G
24	A	2878	G
24	A	2890	U
24	A	2896	G
24	A	2901	G
24	A	2909	C
24	A	2912	A
24	A	2920	A
24	A	2922	G
24	A	2929	C
25	B	10	U
25	B	23	U
25	B	24	C
25	B	33	U
25	B	39	C
25	B	40	C
25	B	51	A
25	B	54	U
25	B	88	C
25	B	107	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	88	G
24	A	92	G
24	A	139	A
24	A	553	U
24	A	756	A
24	A	809	G
24	A	847	G
24	A	854	G
24	A	1017	C
24	A	1172	A
24	A	1248	A
24	A	1249	A
24	A	1497	G
24	A	1528	G
24	A	1532	G
24	A	1533	A
24	A	1569	U
24	A	1886	A

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Mol	Chain	Res	Type
24	A	1888	G
24	A	2472	A
24	A	2789	U
24	A	2809	A
24	A	2908	A

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

7 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	$\#\|Z\| > 2$
21	MIA	y	37	21	18,24,32	1.05	2 (11%)	18,35,47	1.23	2 (11%)
21	5MU	y	54	21	19,22,23	1.39	4 (21%)	28,32,35	2.13	6 (21%)
21	4SU	y	8	21	18,21,22	1.78	5 (27%)	26,30,33	2.21	5 (19%)
21	7MG	y	46	21	22,26,27	1.31	3 (13%)	29,39,42	2.59	7 (24%)
21	PSU	y	39	21	18,21,22	1.31	2 (11%)	22,30,33	1.94	4 (18%)
21	PSU	y	55	21	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
21	PSU	y	32	21	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	MIA	y	37	21	-	2/3/25/34	0/3/3/3
21	5MU	y	54	21	-	0/7/25/26	0/2/2/2
21	4SU	y	8	21	-	3/7/25/26	0/2/2/2
21	7MG	y	46	21	-	5/7/37/38	0/3/3/3
21	PSU	y	39	21	-	0/7/25/26	0/2/2/2
21	PSU	y	55	21	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	PSU	y	32	21	-	2/7/25/26	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	y	8	4SU	C4-S4	-4.58	1.59	1.68
21	y	55	PSU	C6-C5	3.38	1.39	1.35
21	y	8	4SU	C4-N3	-3.28	1.34	1.37
21	y	32	PSU	C6-C5	3.24	1.39	1.35
21	y	39	PSU	C6-C5	3.10	1.38	1.35
21	y	46	7MG	C5-C4	3.02	1.47	1.38
21	y	54	5MU	C6-C5	2.78	1.39	1.34
21	y	39	PSU	C4-N3	-2.65	1.33	1.38
21	y	55	PSU	C4-N3	-2.62	1.34	1.38
21	y	54	5MU	C4-N3	-2.62	1.34	1.38
21	y	8	4SU	C5-C4	-2.60	1.39	1.42
21	y	32	PSU	C4-N3	-2.57	1.34	1.38
21	y	37	MIA	C5-C4	2.51	1.47	1.40
21	y	37	MIA	C2-N3	2.51	1.36	1.32
21	y	46	7MG	C6-N1	-2.46	1.34	1.38
21	y	54	5MU	C4-C5	2.46	1.48	1.44
21	y	8	4SU	C2-N1	2.30	1.42	1.38
21	y	54	5MU	C6-N1	-2.25	1.34	1.38
21	y	46	7MG	C4-N9	-2.21	1.35	1.37
21	y	8	4SU	C2-N3	-2.10	1.34	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	y	46	7MG	N9-C4-N3	9.30	139.38	125.47
21	y	8	4SU	C4-N3-C2	-6.61	120.92	127.34
21	y	39	PSU	N1-C2-N3	6.02	121.95	115.13
21	y	8	4SU	C5-C4-N3	6.00	120.25	114.69
21	y	55	PSU	N1-C2-N3	5.98	121.91	115.13
21	y	32	PSU	N1-C2-N3	5.92	121.84	115.13
21	y	46	7MG	C5-C4-N3	-5.80	117.07	128.13
21	y	54	5MU	C4-N3-C2	-5.37	120.40	127.35
21	y	54	5MU	N3-C2-N1	5.14	121.72	114.89
21	y	46	7MG	N9-C8-N7	-4.82	96.49	103.38
21	y	46	7MG	C2-N3-C4	4.50	120.32	112.30
21	y	54	5MU	C5-C4-N3	4.36	119.03	115.31
21	y	39	PSU	C4-N3-C2	-4.15	120.36	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	y	8	4SU	N3-C2-N1	3.92	120.10	114.89
21	y	32	PSU	C4-N3-C2	-3.87	120.76	126.34
21	y	55	PSU	C4-N3-C2	-3.86	120.77	126.34
21	y	54	5MU	C5-C6-N1	-3.83	119.40	123.34
21	y	54	5MU	O4-C4-C5	-3.78	120.52	124.90
21	y	8	4SU	C5-C4-S4	-3.68	119.73	124.47
21	y	39	PSU	O2-C2-N1	-3.59	118.84	122.79
21	y	37	MIA	N3-C2-N1	-3.36	123.42	128.68
21	y	32	PSU	O2-C2-N1	-3.34	119.11	122.79
21	y	55	PSU	O2-C2-N1	-3.33	119.12	122.79
21	y	54	5MU	O2-C2-N1	-3.22	118.50	122.79
21	y	37	MIA	C4-C5-N7	-2.82	106.45	109.40
21	y	46	7MG	C5-C6-N1	2.80	115.92	110.99
21	y	8	4SU	C1'-N1-C2	2.69	122.45	117.57
21	y	39	PSU	C5-C6-N1	-2.19	118.83	122.11
21	y	46	7MG	C5-C4-N9	-2.17	103.53	106.35
21	y	46	7MG	O6-C6-C5	-2.14	122.29	127.54

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	y	8	4SU	O4'-C4'-C5'-O5'
21	y	37	MIA	O4'-C4'-C5'-O5'
21	y	37	MIA	C3'-C4'-C5'-O5'
21	y	46	7MG	O4'-C4'-C5'-O5'
21	y	46	7MG	C3'-C4'-C5'-O5'
21	y	8	4SU	C3'-C4'-C5'-O5'
21	y	46	7MG	O4'-C1'-N9-C4
21	y	46	7MG	C2'-C1'-N9-C8
21	y	32	PSU	C4'-C5'-O5'-P
21	y	55	PSU	C4'-C5'-O5'-P
21	y	32	PSU	O4'-C1'-C5-C4
21	y	46	7MG	O4'-C1'-N9-C8
21	y	55	PSU	O4'-C1'-C5-C6
21	y	8	4SU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 397 ligands modelled in this entry, 396 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	$\#\|Z\| > 2$
55	GCP	v	501	-	27,34,34	1.46	6 (22%)	34,54,54	1.96	8 (23%)

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
55	GCP	v	501	-	-	6/15/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	501	GCP	C5-C6	3.84	1.48	1.41
55	v	501	GCP	PG-O2G	2.80	1.61	1.54
55	v	501	GCP	PG-O3G	2.74	1.61	1.54
55	v	501	GCP	PB-O3A	2.63	1.61	1.58
55	v	501	GCP	C5-C4	2.33	1.47	1.40
55	v	501	GCP	PB-O2B	2.14	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	v	501	GCP	C2-N3-C4	4.70	120.72	115.36
55	v	501	GCP	C5-C6-N1	-3.98	117.99	123.43
55	v	501	GCP	C2-N1-C6	3.90	122.13	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	v	501	GCP	PB-O3A-PA	-3.86	120.32	132.56
55	v	501	GCP	C4-C5-C6	-3.55	117.41	120.80
55	v	501	GCP	C3'-C2'-C1'	3.39	106.09	100.98
55	v	501	GCP	N3-C2-N1	-3.11	123.07	127.22
55	v	501	GCP	C4-C5-N7	-2.46	106.83	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

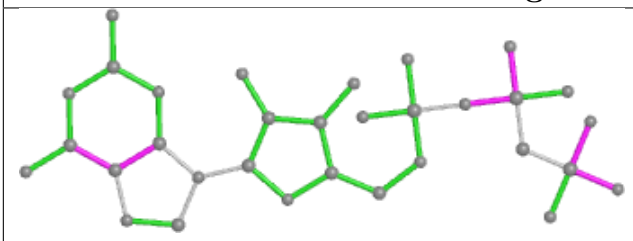
Mol	Chain	Res	Type	Atoms
55	v	501	GCP	PG-C3B-PB-O1B
55	v	501	GCP	PG-C3B-PB-O2B
55	v	501	GCP	PG-C3B-PB-O3A
55	v	501	GCP	C5'-O5'-PA-O3A
55	v	501	GCP	C5'-O5'-PA-O2A
55	v	501	GCP	O4'-C4'-C5'-O5'

There are no ring outliers.

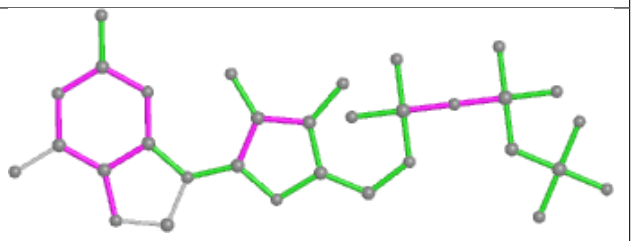
No monomer is involved in short contacts.

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

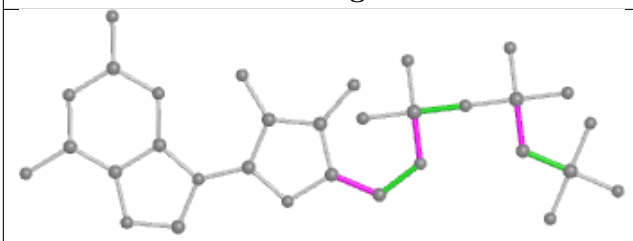
Ligand GCP v 501



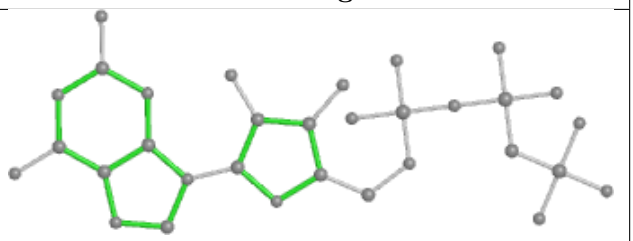
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

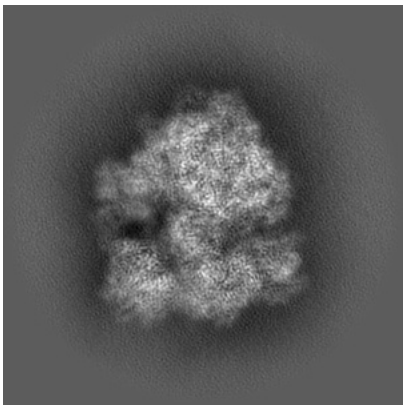
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42566. These allow visual inspection of the internal detail of the map and identification of artifacts.

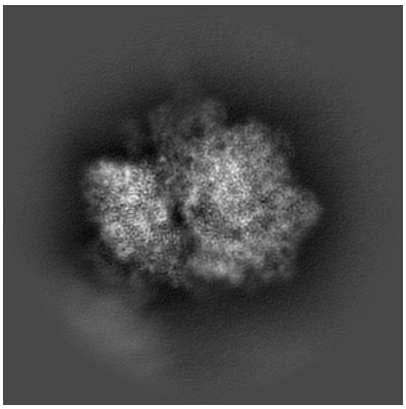
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

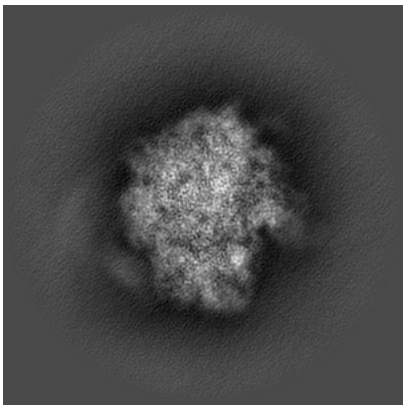
6.1.1 Primary map



X

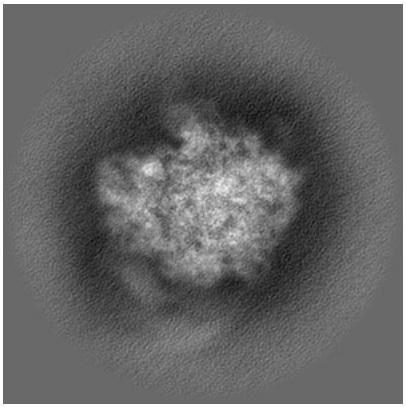


Y

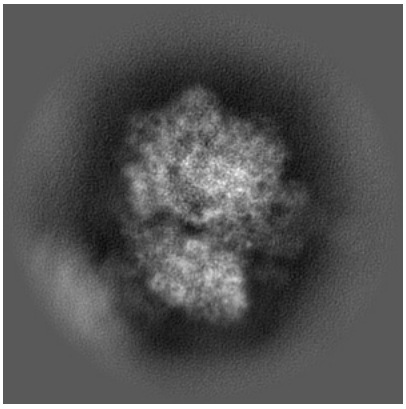


Z

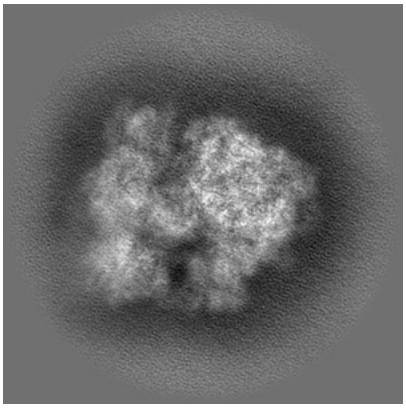
6.1.2 Raw map



X



Y

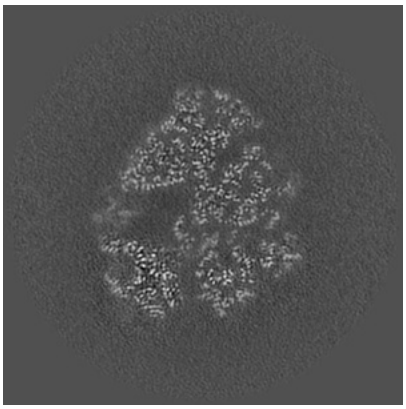


Z

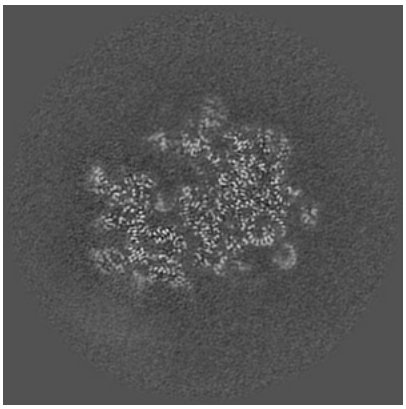
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 256



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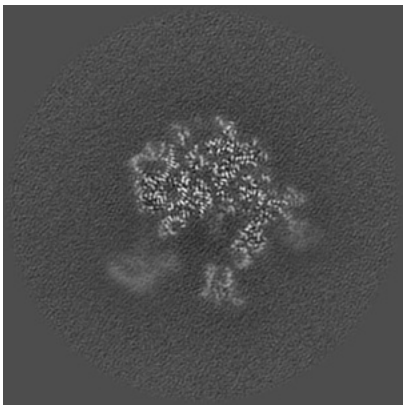
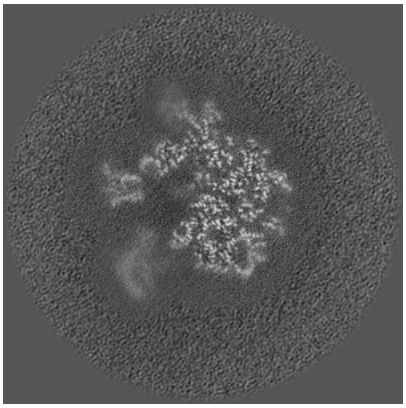


Z Index: 256

6.2.2 Raw map



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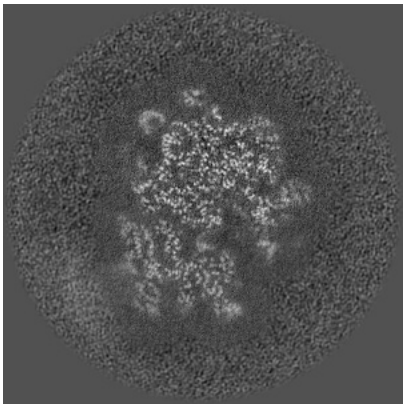
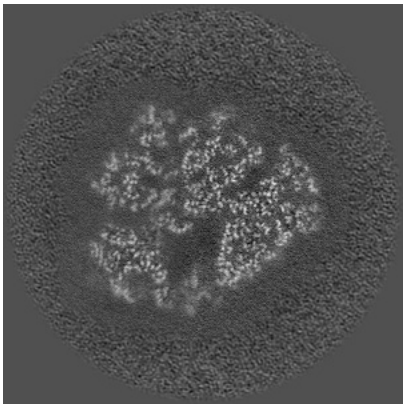


Y Index: 256

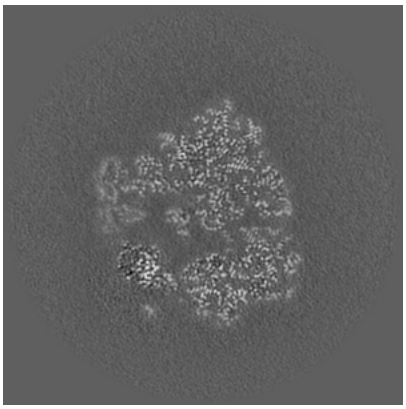


Z Index: 256

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

6.3 Largest variance slices (i)

6.3.1 Primary map



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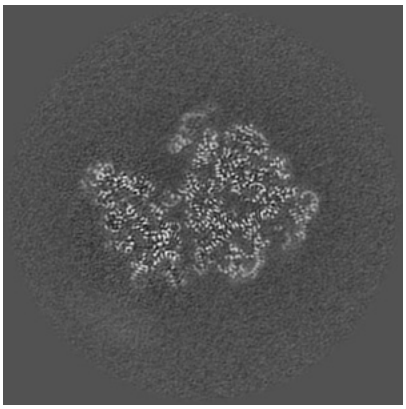

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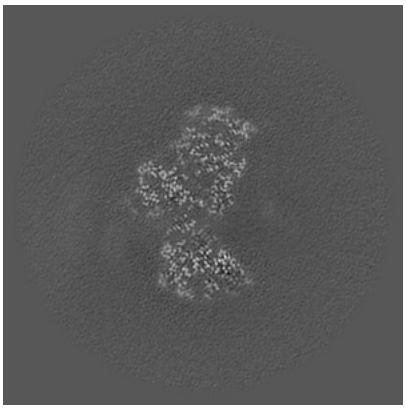
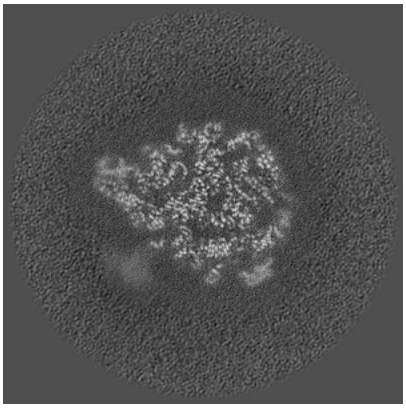
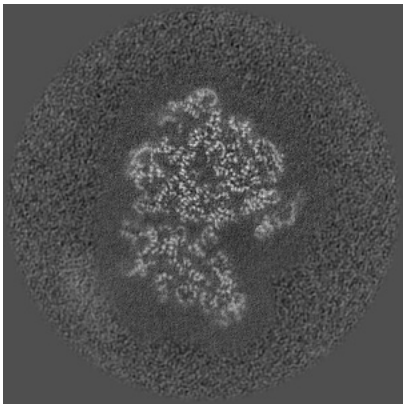


Z Index: 182

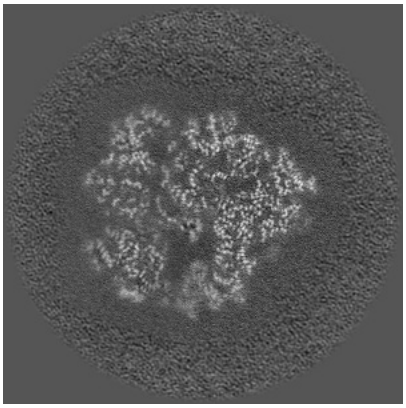
6.3.2 Raw map



X Index: 298



Y Index: 273

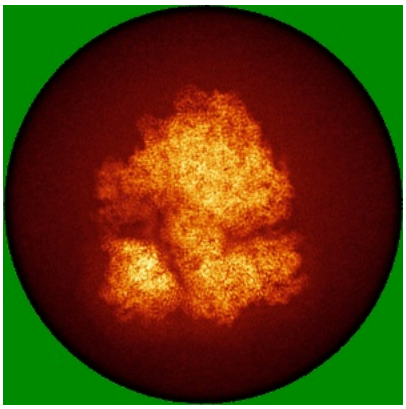


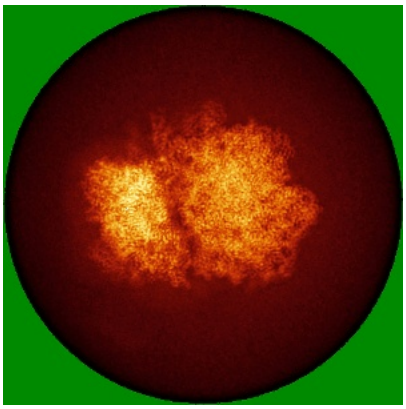
Z Index: 266

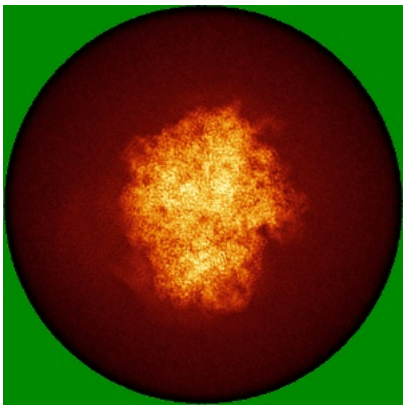
The images above show the largest variance slices of the map in three orthogonal directions.

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

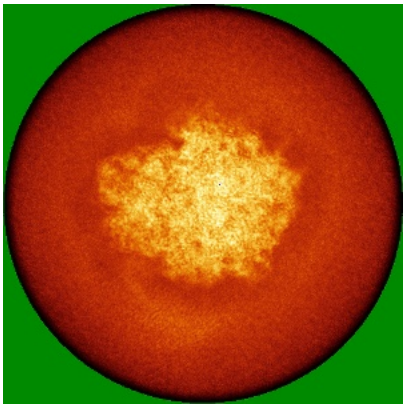
6.4.1 Primary map

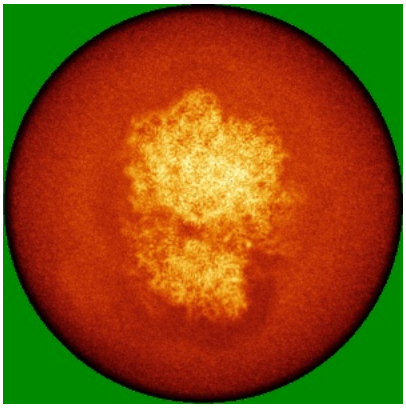

X

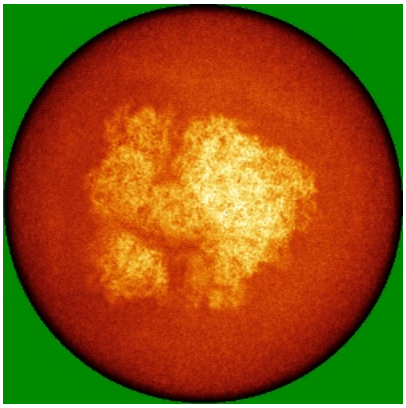

Y


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.

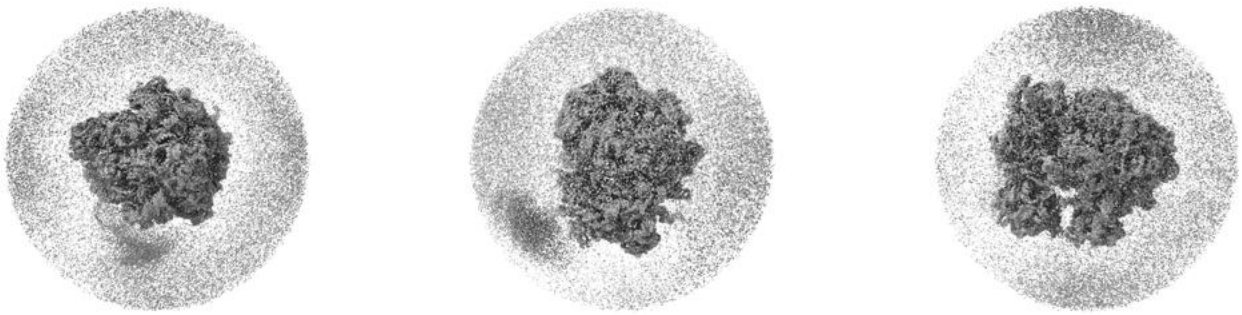
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

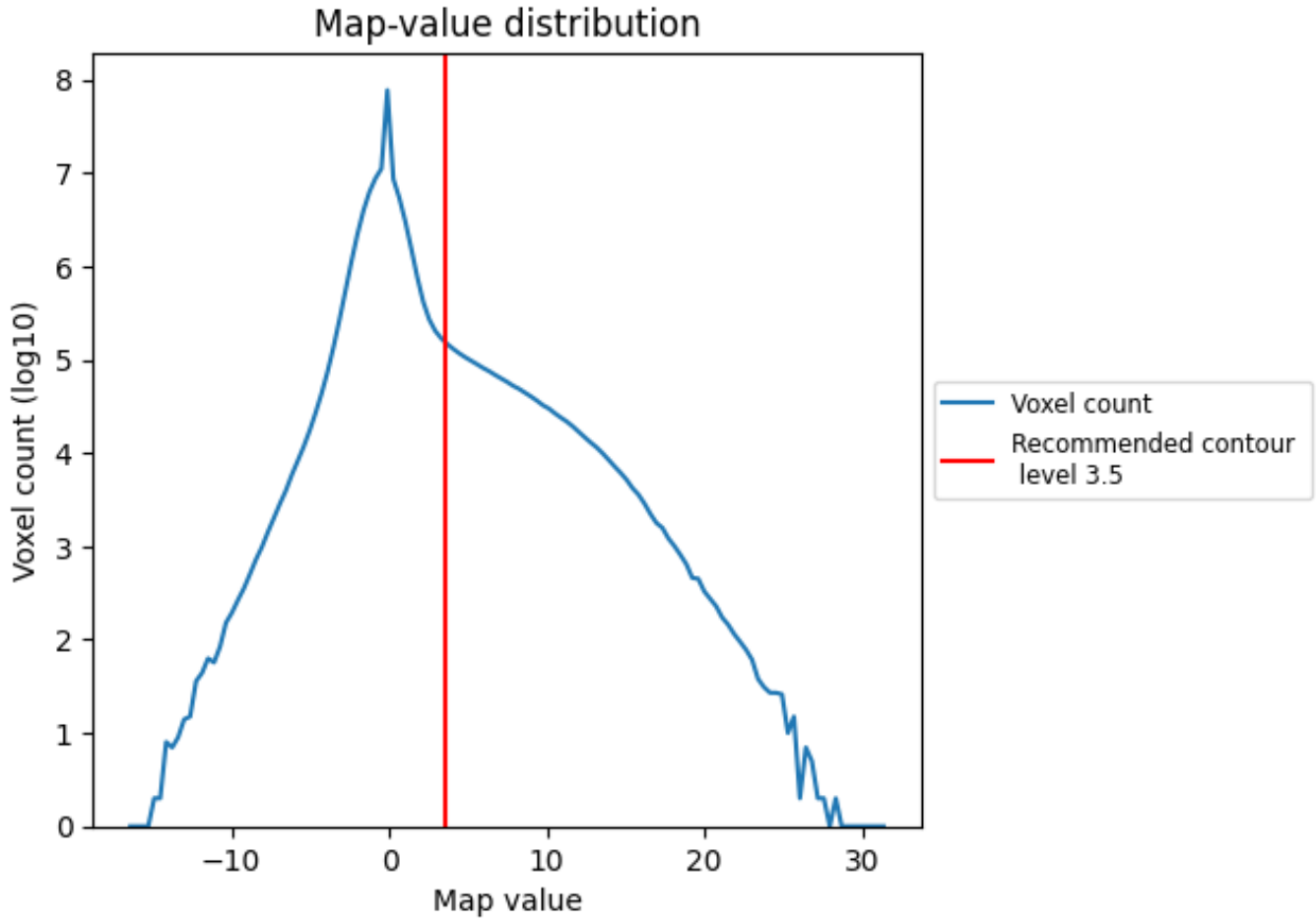
6.6 Mask visualisation (i)

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

7 Map analysis

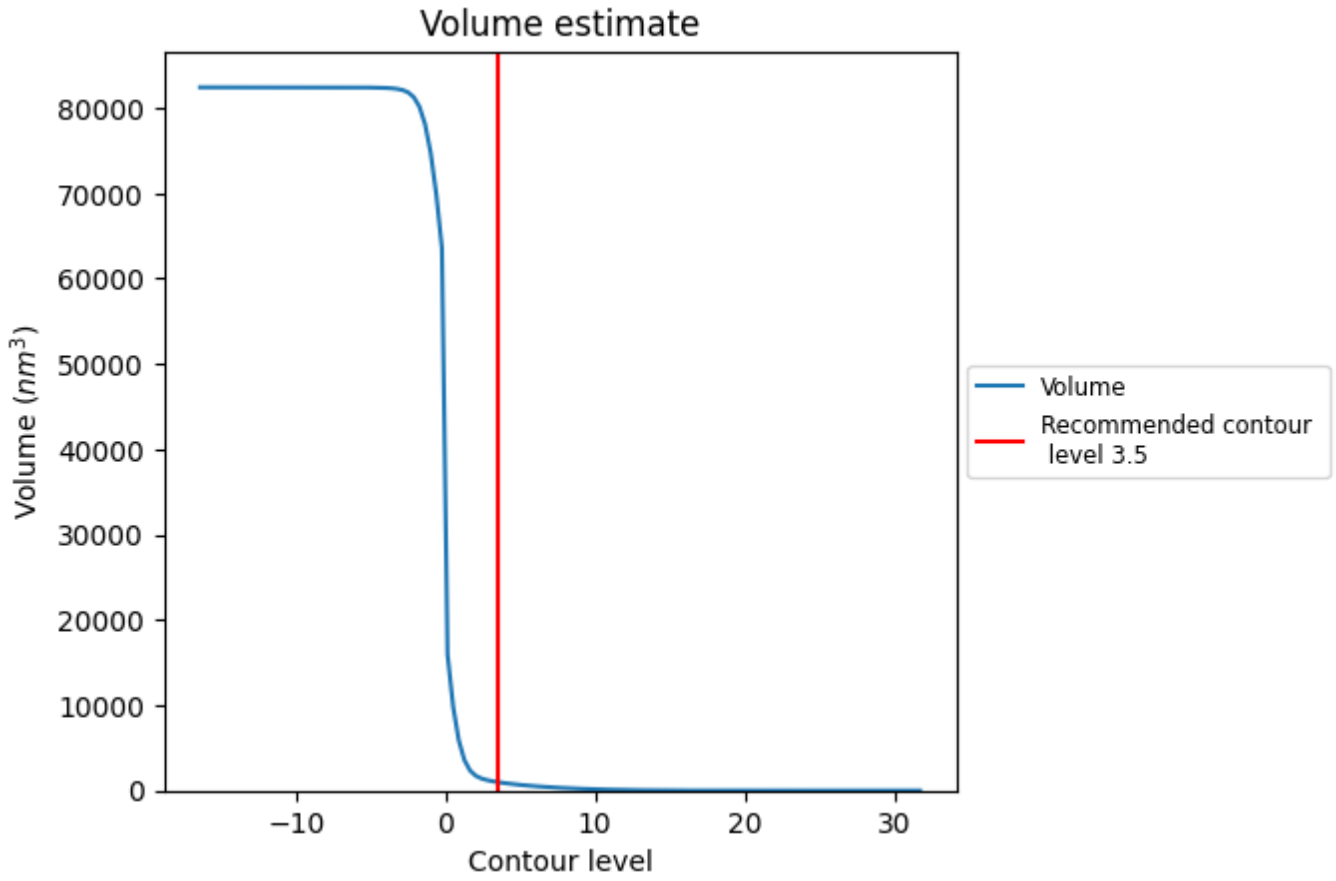
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

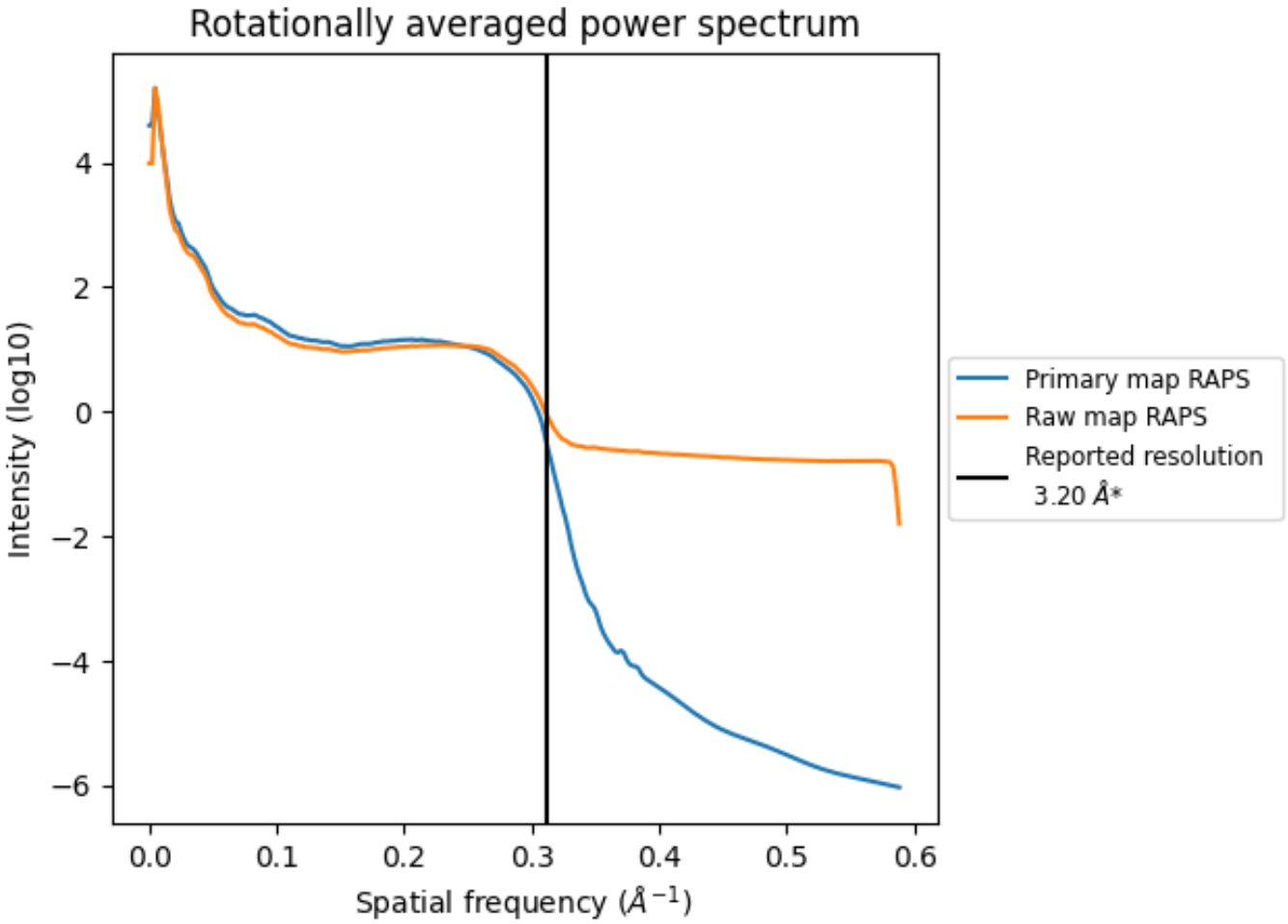
7.2 Volume estimate



The volume at the recommended contour level is 986 nm^3; this corresponds to an approximate mass of 891 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)

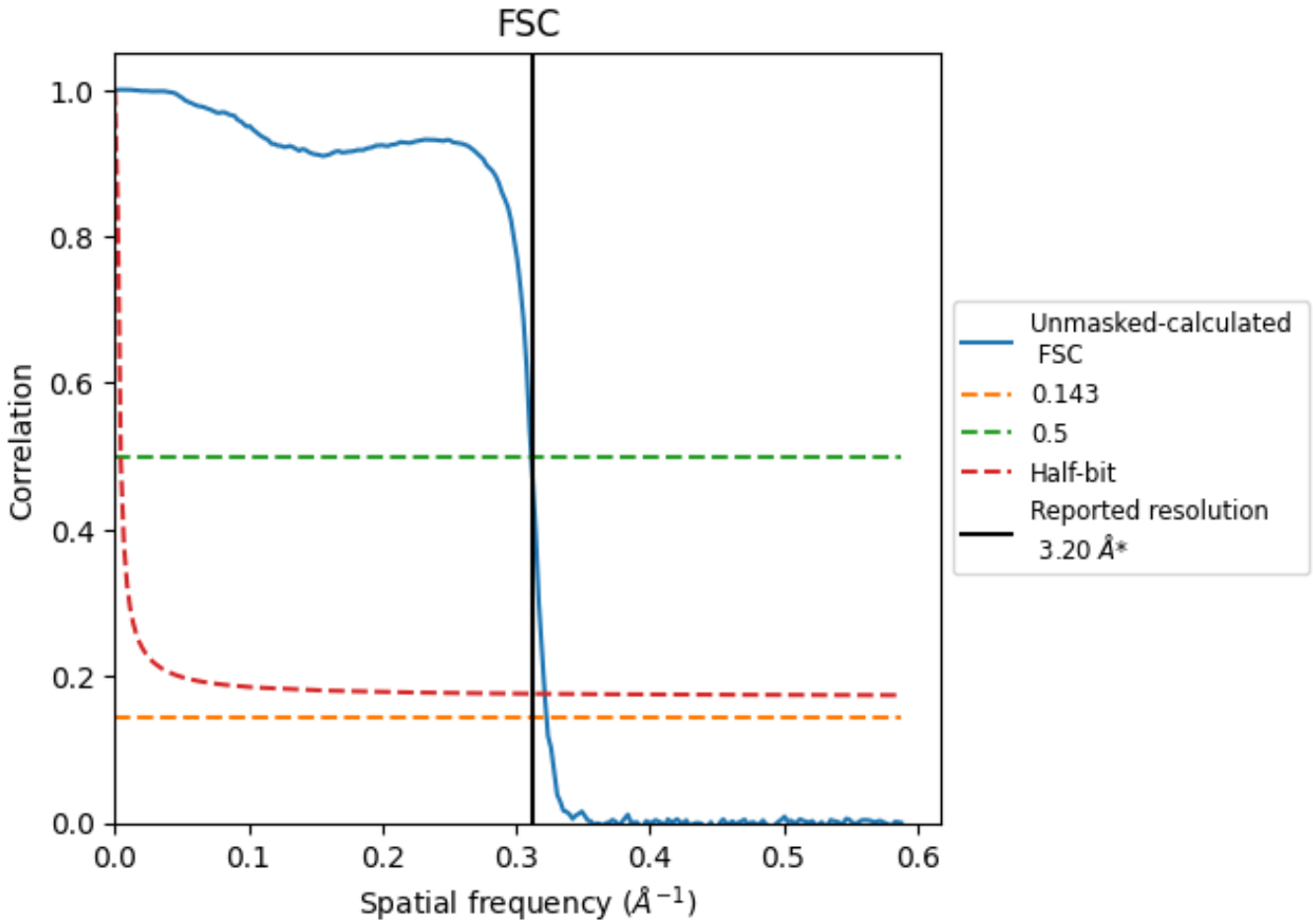


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

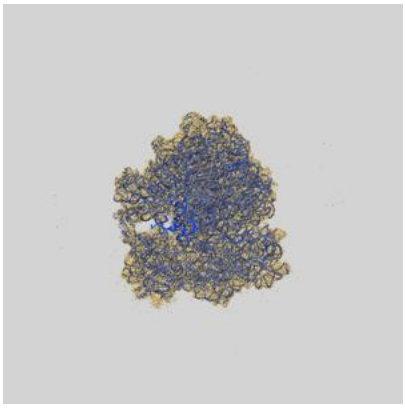
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.10	3.21	3.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

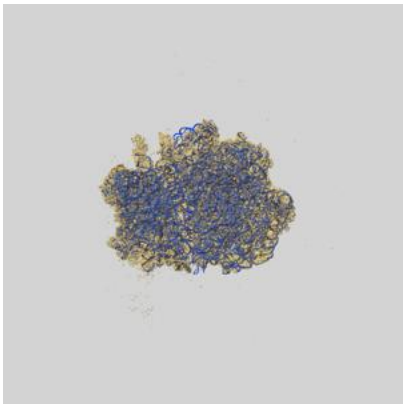
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42566 and PDB model 8UU7. Per-residue inclusion information can be found in section 3 on page 15.

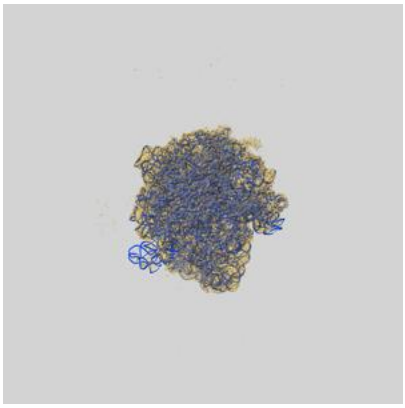
9.1 Map-model overlay



X



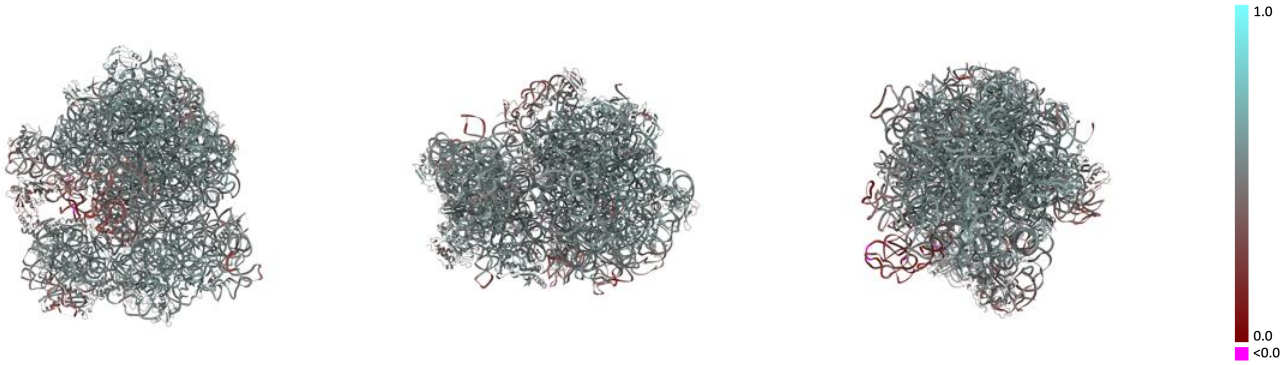
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

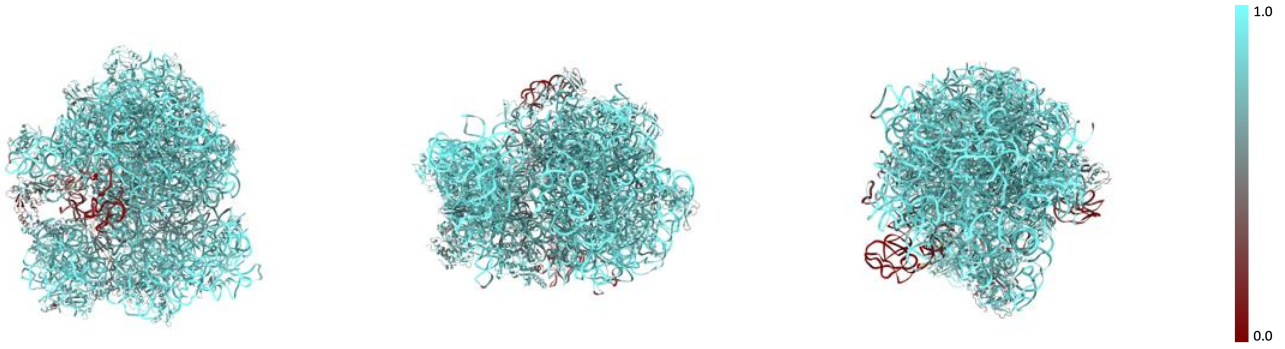
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

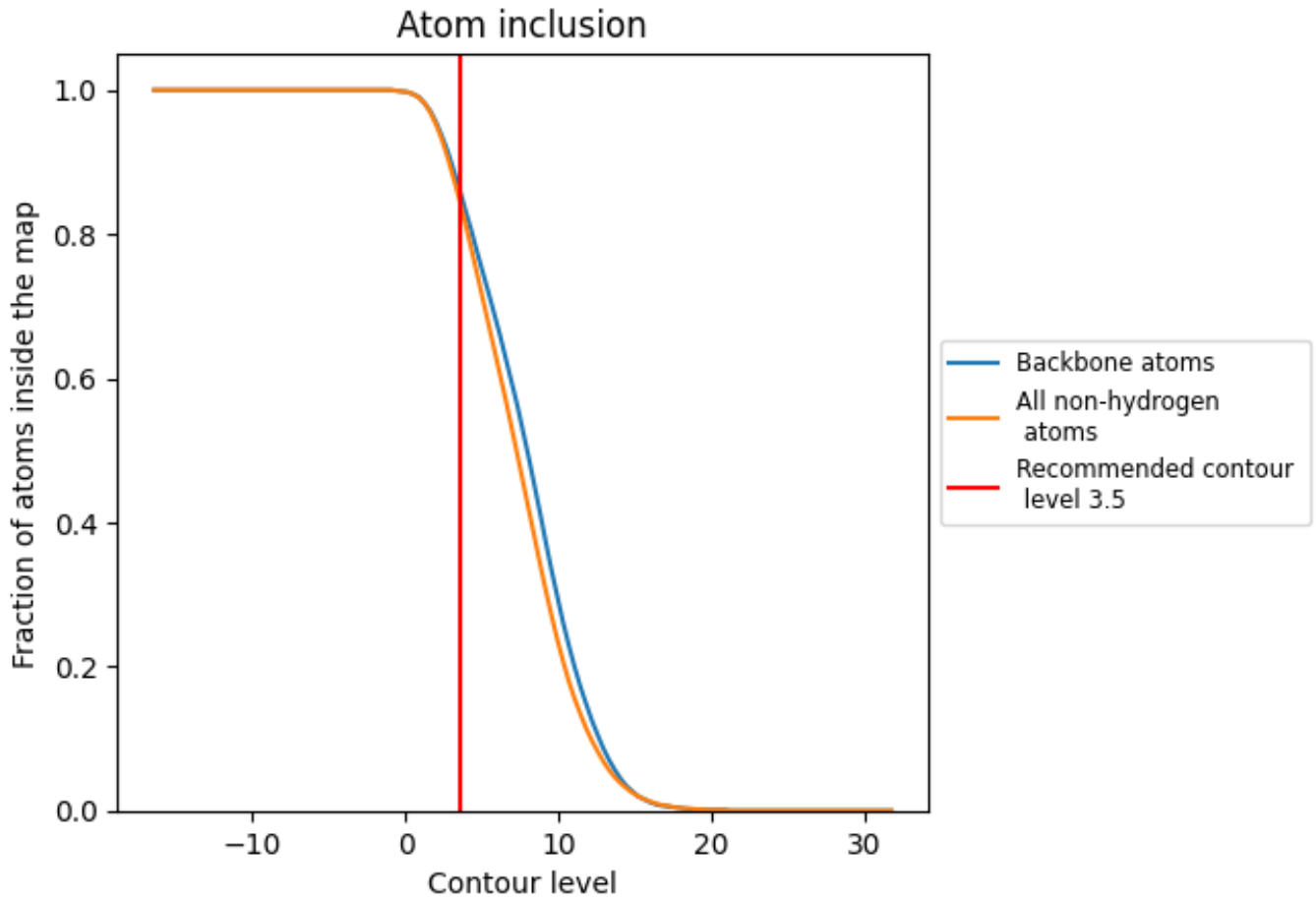
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8500	0.5120
1	0.7890	0.5040
2	0.8210	0.5410
3	0.4220	0.3940
4	0.8370	0.5230
5	0.8390	0.5470
6	0.8860	0.5880
7	0.8840	0.5740
8	0.7940	0.5530
A	0.8830	0.5140
B	0.8940	0.4570
C	0.8190	0.5700
D	0.8520	0.5580
E	0.8270	0.5520
F	0.5150	0.4010
G	0.6390	0.4450
L	0.8800	0.5670
M	0.7530	0.5510
N	0.8120	0.5420
O	0.8150	0.5540
P	0.8530	0.5510
Q	0.7080	0.4670
R	0.7830	0.5460
S	0.9110	0.5690
T	0.8720	0.5550
U	0.8480	0.5620
V	0.7900	0.5340
W	0.7410	0.5100
Y	0.8510	0.5560
Z	0.8120	0.5500
a	0.9140	0.5200
b	0.5780	0.4740
c	0.8490	0.5150
d	0.8540	0.5260
e	0.8160	0.5410

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Chain	Atom inclusion	Q-score
f	0.7350	0.4970
g	0.8250	0.4800
h	0.8570	0.5430
i	0.8420	0.4850
j	0.8530	0.4940
k	0.6960	0.4900
l	0.8250	0.5410
m	0.7200	0.4830
n	0.9450	0.5600
o	0.7520	0.5320
p	0.8900	0.5390
q	0.8560	0.5340
r	0.8550	0.5270
s	0.8170	0.5290
t	0.8310	0.5200
v	0.7310	0.4360
w	0.5250	0.4900
y	0.1730	0.2160