Full wwPDB EM Validation Report ⓘ

Aug 10, 2023 – 07:58 pm BST

PDB ID	:	8BGE
EMDB ID	:	EMD-16029
Title	:	Elongating E. coli 70S ribosome containing acylated tRNA(iMet) in the P-site and AAm6A mRNA codon in the A-site after uncompleted di-peptide formation
Authors	:	Koziej, L.; Glatt, S.
Deposited on	:	2022-10-27
Resolution	:	2.11 Å(reported)

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:

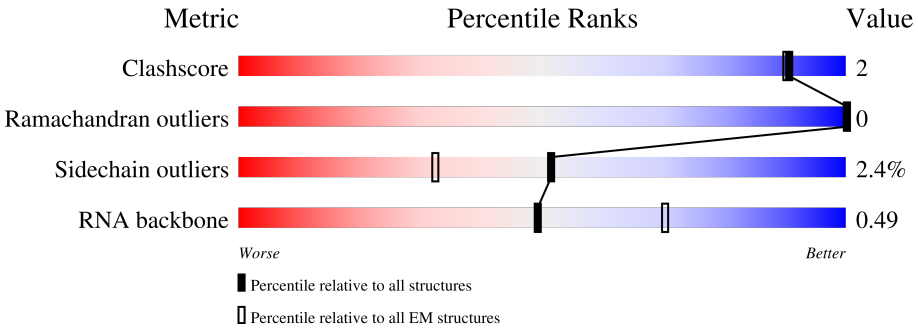
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance

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

The reported resolution of this entry is 2.11 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)
Clashscore	158937	4297
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	273	96%
2	B	209	98%
3	C	201	97%
4	D	179	89% 9%
5	E	177	88% 10%
6	F	149	36% 82% 17%
7	G	142	98%

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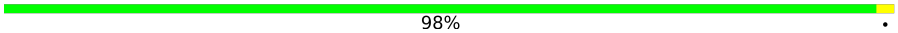
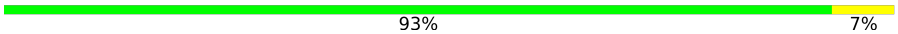
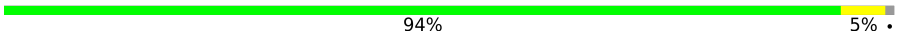
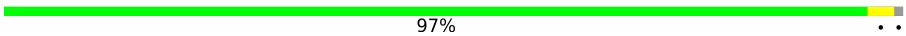
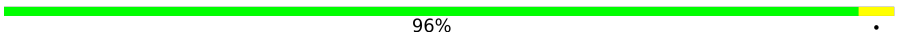
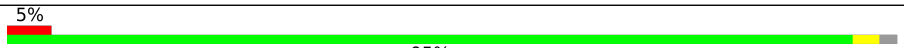
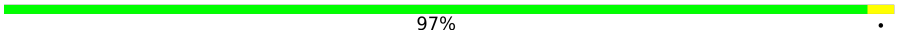
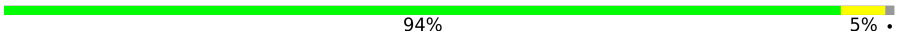
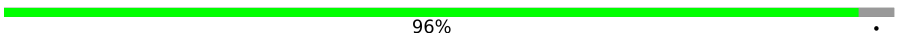
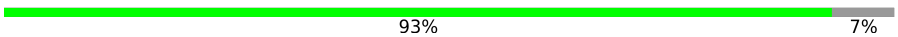
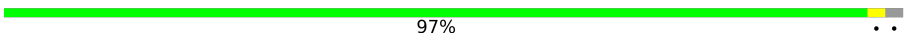
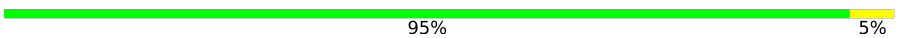
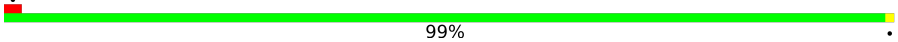
Mol	Chain	Length	Quality of chain
8	H	123	
9	I	144	
10	J	136	
11	K	127	
12	L	117	
13	M	115	
14	N	118	
15	O	103	
16	P	110	
17	Q	100	
18	R	104	
19	S	94	
20	T	85	
21	U	78	
22	V	63	
23	W	59	
24	a	57	
25	b	55	
26	c	46	
27	d	65	
28	e	38	
29	f	241	
30	g	233	
31	h	206	
32	i	167	

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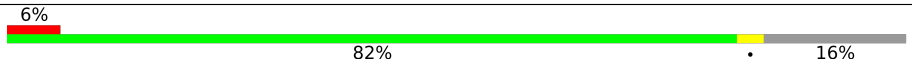
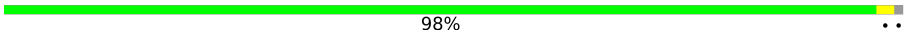
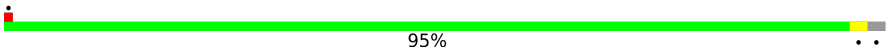
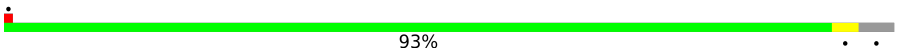
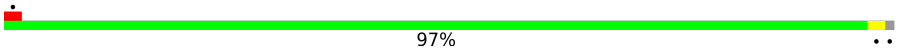
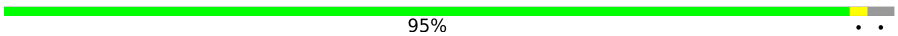
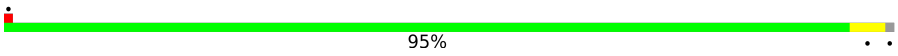
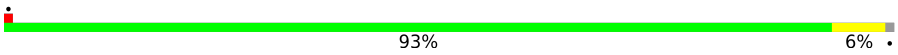
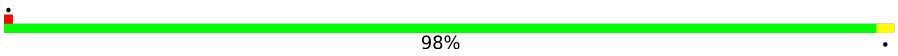
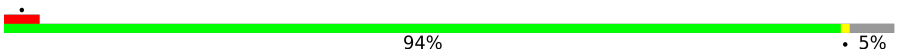
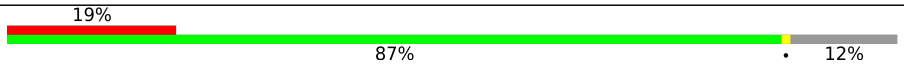
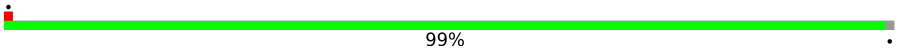
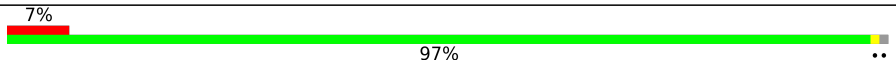
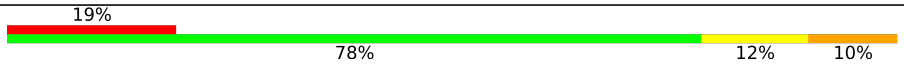
Mol	Chain	Length	Quality of chain
33	j	131	
34	k	179	
35	l	130	
36	m	130	
37	n	103	
38	o	129	
39	p	124	
40	q	118	
41	r	101	
42	s	89	
43	t	82	
44	u	84	
45	v	75	
46	w	92	
47	x	87	
48	y	71	
49	0	2904	
50	1	120	
51	2	1542	
52	3	30	
53	4	77	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 235268 atoms, of which 94708 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 L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	271	4237	1288	2155	423	364	7	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	208	3170	976	1611	287	292	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	201	3171	974	1619	283	290	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	177	2855	899	1445	249	256	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	173	2628	814	1333	237	242	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	149	2259	699	1148	197	214	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	123	Total	C	H	N	O	S	0	0
			1970	593	1023	181	167	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 10 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	118	Total	C	H	N	O	S	0	0
			1934	585	989	194	161	5		

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	116	Total	C	H	N	O	0	0
			1816	552	924	178	162		

- Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	114	Total	C	H	N	O	S	0	0
			1880	574	963	179	163	1		

- Molecule 14 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	117	Total	C	H	N	O	0	0
			1967	604	1020	192	151		

- Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	93	Total	C	H	N	O	S	0	0
			1545	466	807	139	131	2		

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	H	N	O	0	0
			1611	492	832	146	141		

- Molecule 19 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	75	Total	C	H	N	O	S	0	0
			1166	355	594	116	100	1		

- Molecule 21 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	77	Total	C	H	N	O	S	0	0
			1278	388	653	129	106	2		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	60	Total	C	H	N	O	S	0	0
			1015	303	524	96	91	1		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	57	Total	C	H	N	O	S	0	0
			922	276	483	86	75	2		

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	a	55	Total	C	H	N	O	S	0	0
			880	263	446	92	78	1		

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	51	Total	C	H	N	O	0	0
			869	269	452	76	72		

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	c	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	d	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	e	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 29 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	f	224	Total	C	H	N	O	S	0	0
			3534	1109	1781	315	321	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	g	206	Total	C	H	N	O	S	0	0
			3321	1028	1697	305	288	3		

- Molecule 31 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	h	205	Total	C	H	N	O	S	0	0
			3351	1026	1708	315	298	4		

- Molecule 32 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	i	155	Total	C	H	N	O	S	0	0
			2330	711	1186	216	211	6		

- Molecule 33 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	j	106	Total	C	H	N	O	S	0	0
			1726	545	864	156	154	7		

- Molecule 34 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	k	151	Total	C	H	N	O	S	0	0
			2419	735	1238	227	215	4		

- Molecule 35 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	l	129	Total	C	H	N	O	S	0	0
			2011	616	1032	173	184	6		

- Molecule 36 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	m	127	Total	C	H	N	O	S	0	0
			2093	634	1071	206	179	3		

- Molecule 37 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	n	99	Total	C	H	N	O	S	0	0
			1632	498	837	152	144	1		

- Molecule 38 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	o	117	Total	C	H	N	O	S	0	0
			1765	540	888	174	160	3		

- Molecule 39 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	p	123	Total	C	H	N	O	S	0	0
			1972	590	1017	196	165	4		

- Molecule 40 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	q	114	Total	C	H	N	O	S	0	0
			1825	546	942	178	156	3		

- Molecule 41 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	r	100	Total	C	H	N	O	S	0	0
			1650	499	845	164	139	3		

- Molecule 42 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	s	88	Total	C	H	N	O	S	0	0
			1449	439	735	144	130	1		

- Molecule 43 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	t	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 44 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	u	80	Total	C	H	N	O	S	0	0
			1340	411	692	121	113	3		

- Molecule 45 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	v	66	Total	C	H	N	O	S	0	0
			1110	345	566	102	96	1		

- Molecule 46 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	w	79	Total	C	H	N	O	S	0	0
			1303	408	666	120	107	2		

- Molecule 47 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	x	86	Total	C	H	N	O	S	0	0
			1390	414	720	138	115	3		

- Molecule 48 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	y	70	Total	C	H	N	O	S	0	0
			1219	366	629	125	98	1		

- Molecule 49 is a RNA chain called 23S rRNA RRLG-RRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	0	2758	Total	C	H	N	O	P	0	0
			88984	26417	29765	10911	19134	2757		

- Molecule 50 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	1	120	Total	C	H	N	O	P	0	0
			3868	1144	1302	468	835	119		

- Molecule 51 is a RNA chain called 16S rRNA RRSB-RRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	2	1534	Total	C	H	N	O	P	0	0
			49478	14681	16564	6041	10659	1533		

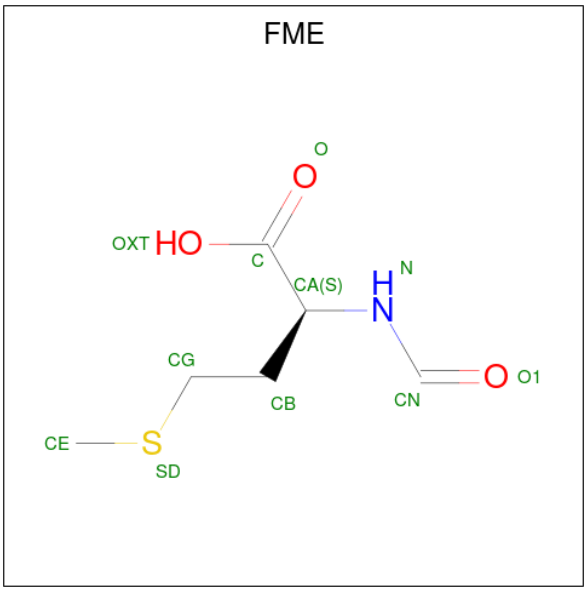
- Molecule 52 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	3	10	Total	C	H	N	O	P	0	0
			325	98	109	41	67	10		

- Molecule 53 is a RNA chain called Acylated P-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
53	4	77	Total	C	H	N	O	P	0	0
			2478	732	835	297	537	77		

- Molecule 54 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$) (labeled as "Ligand of Interest" by depositor).



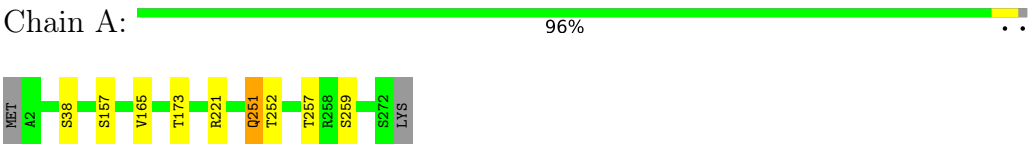
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
54	4	1	20	6	10	1	2	1	0

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.

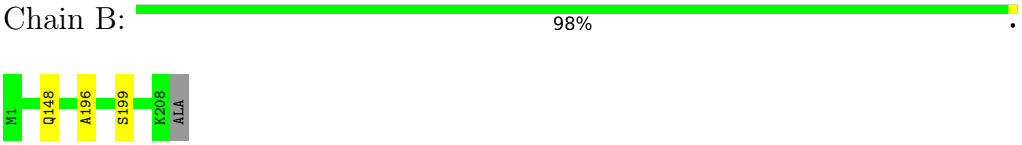
• Molecule 1: 50S ribosomal protein L2

Chain A:



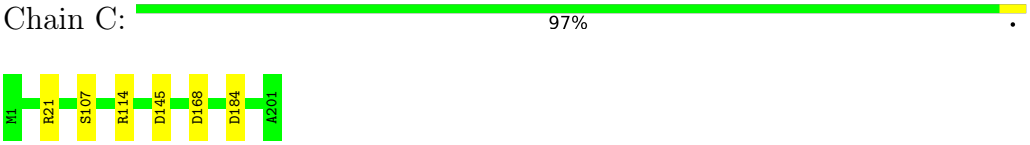
• Molecule 2: 50S ribosomal protein L3

Chain B:



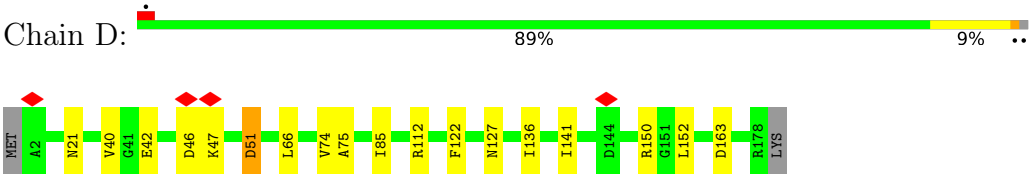
• Molecule 3: 50S ribosomal protein L4

Chain C:



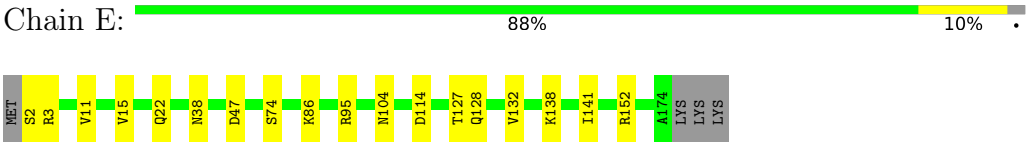
• Molecule 4: 50S ribosomal protein L5

Chain D:



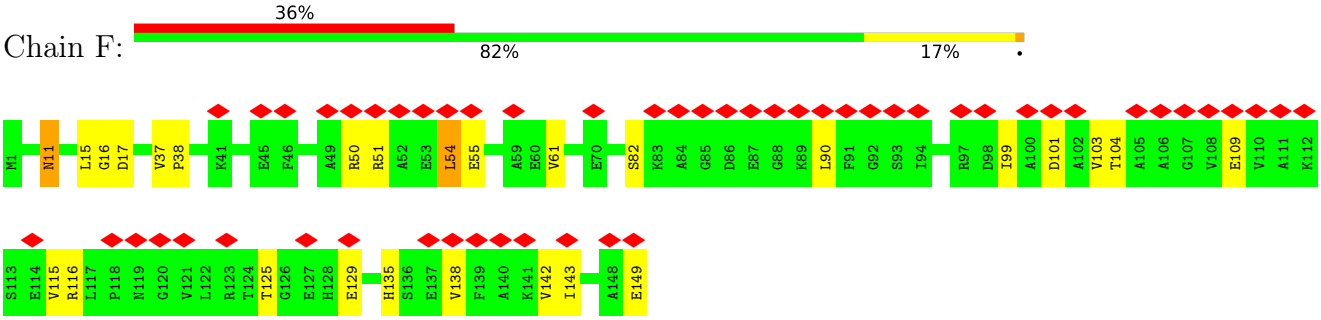
• Molecule 5: 50S ribosomal protein L6

Chain E:



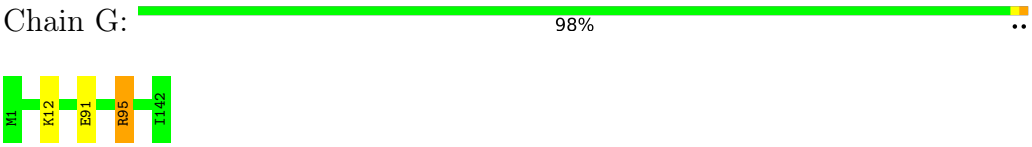
• Molecule 6: 50S ribosomal protein L9

Chain F:



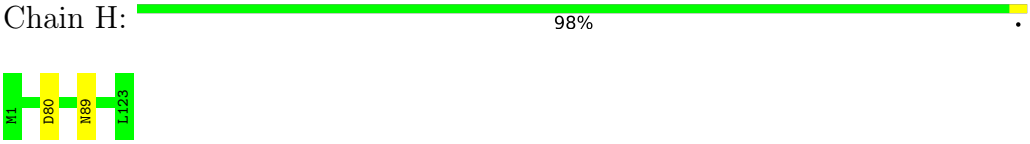
• Molecule 7: 50S ribosomal protein L13

Chain G:



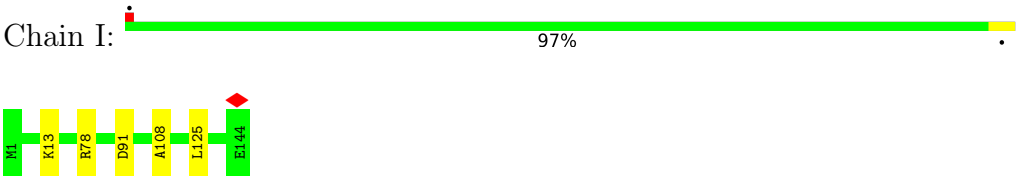
• Molecule 8: 50S ribosomal protein L14

Chain H:



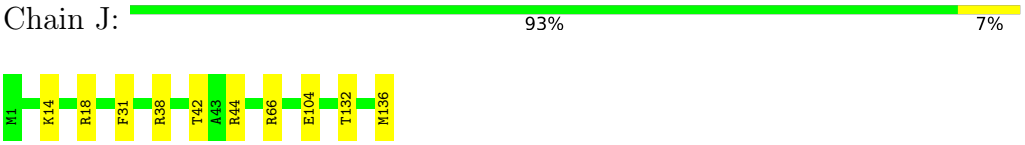
• Molecule 9: 50S ribosomal protein L15

Chain I:



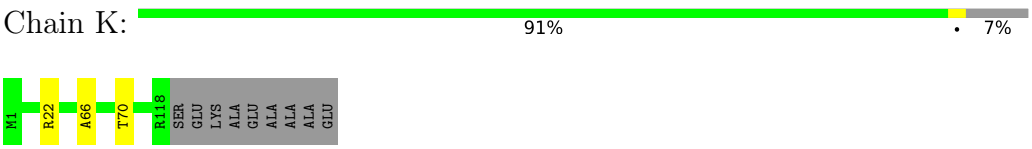
• Molecule 10: 50S ribosomal protein L16

Chain J:



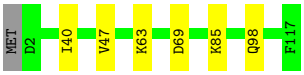
• Molecule 11: 50S ribosomal protein L17

Chain K:



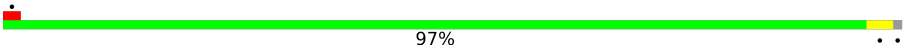
• Molecule 12: 50S ribosomal protein L18

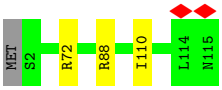
Chain L:



• Molecule 13: 50S ribosomal protein L19

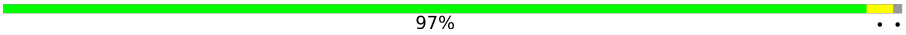
Chain M:

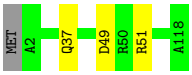




• Molecule 14: 50S ribosomal protein L20

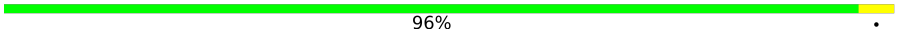
Chain N:

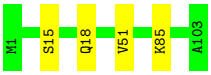




• Molecule 15: 50S ribosomal protein L21

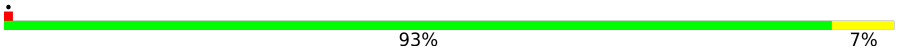
Chain O:





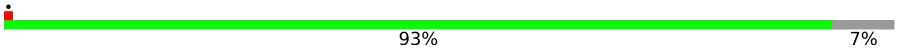
• Molecule 16: 50S ribosomal protein L22

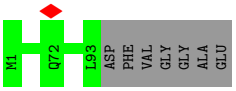
Chain P:



• Molecule 17: 50S ribosomal protein L23

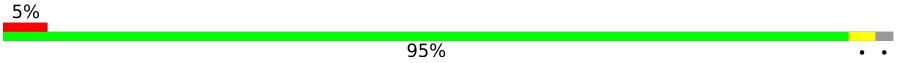
Chain Q:

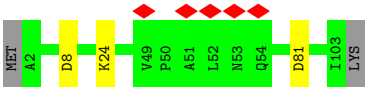




• Molecule 18: 50S ribosomal protein L24

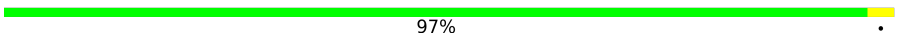
Chain R:

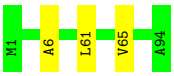




• Molecule 19: 50S ribosomal protein L25

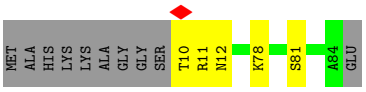
Chain S:





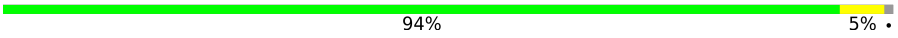
• Molecule 20: 50S ribosomal protein L27

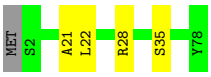
Chain T:



• Molecule 21: 50S ribosomal protein L28

Chain U:



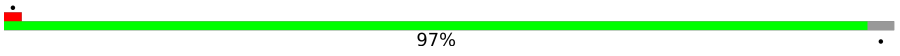


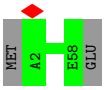
• Molecule 22: 50S ribosomal protein L29

Chain V:

• Molecule 23: 50S ribosomal protein L30

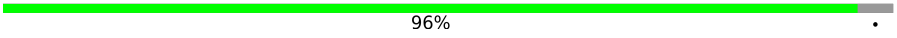
Chain W:





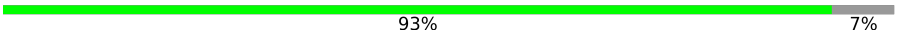
• Molecule 24: 50S ribosomal protein L32

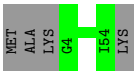
Chain a:



• Molecule 25: 50S ribosomal protein L33

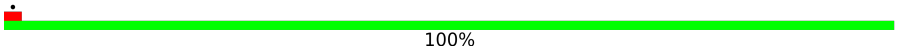
Chain b:





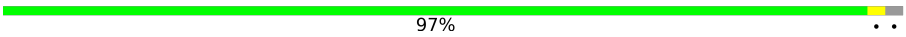
• Molecule 26: 50S ribosomal protein L34

Chain c:



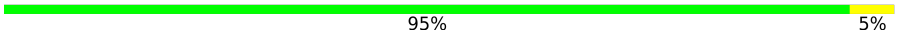
• Molecule 27: 50S ribosomal protein L35

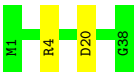
Chain d:



• Molecule 28: 50S ribosomal protein L36

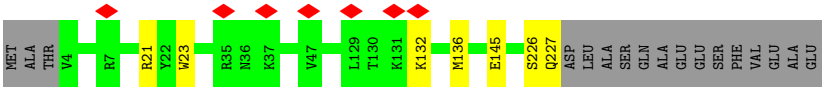
Chain e:





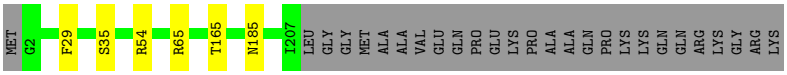
• Molecule 29: 30S ribosomal protein S2

Chain f:



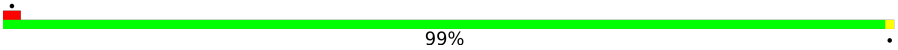
• Molecule 30: 30S ribosomal protein S3

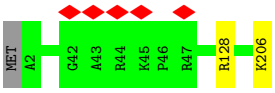
Chain g:



• Molecule 31: 30S ribosomal protein S4

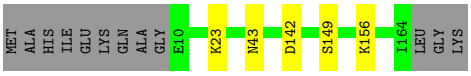
Chain h:





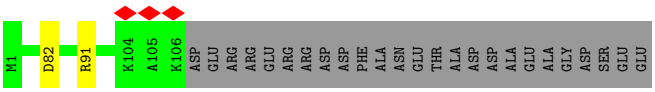
• Molecule 32: 30S ribosomal protein S5

Chain i:



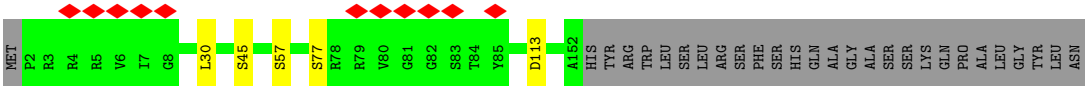
• Molecule 33: 30S ribosomal protein S6

Chain j:



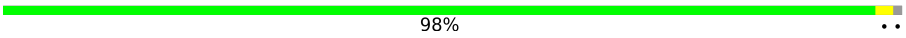
• Molecule 34: 30S ribosomal protein S7

Chain k:



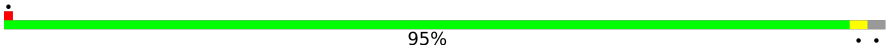
• Molecule 35: 30S ribosomal protein S8

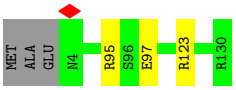
Chain l:



• Molecule 36: 30S ribosomal protein S9

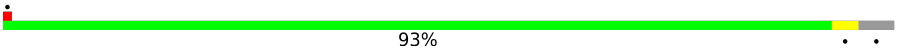
Chain m:

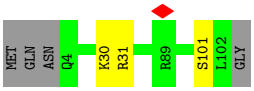




• Molecule 37: 30S ribosomal protein S10

Chain n:



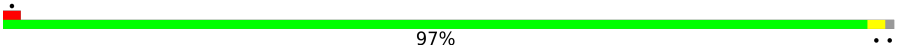


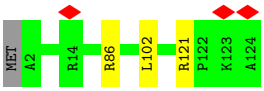
• Molecule 38: 30S ribosomal protein S11

Chain o:

• Molecule 39: 30S ribosomal protein S12

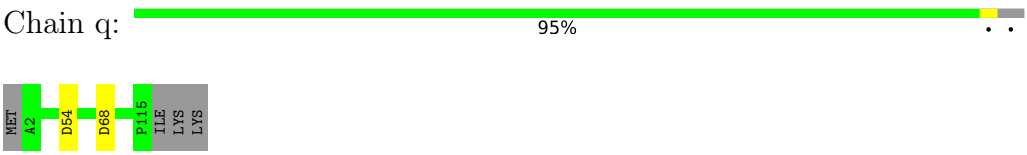
Chain p:





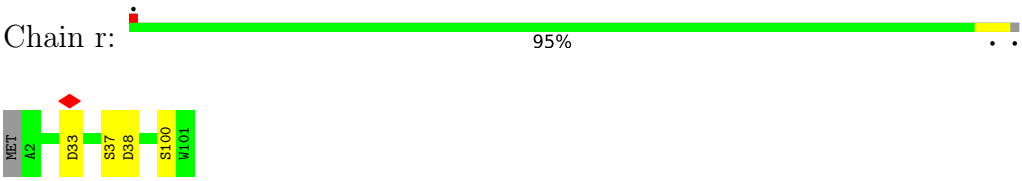
• Molecule 40: 30S ribosomal protein S13

Chain q:



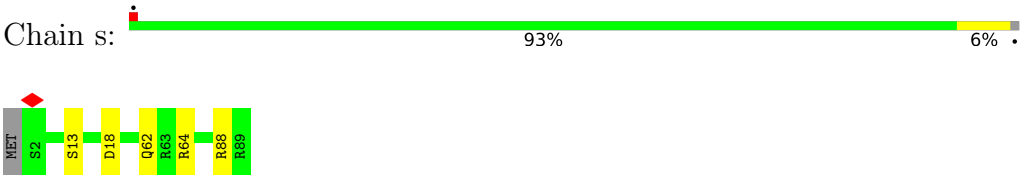
• Molecule 41: 30S ribosomal protein S14

Chain r:



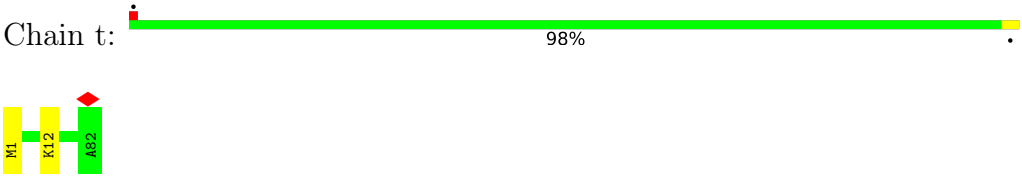
• Molecule 42: 30S ribosomal protein S15

Chain s:



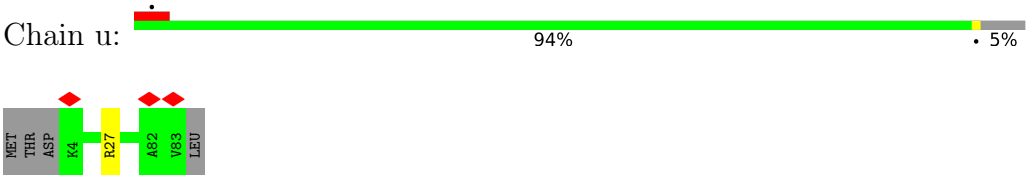
• Molecule 43: 30S ribosomal protein S16

Chain t:



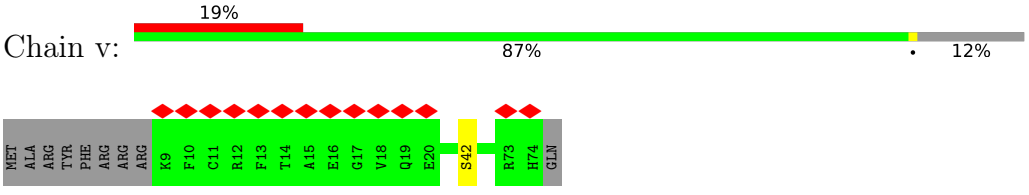
• Molecule 44: 30S ribosomal protein S17

Chain u:



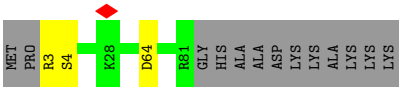
• Molecule 45: 30S ribosomal protein S18

Chain v:



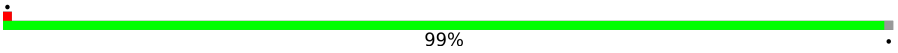
• Molecule 46: 30S ribosomal protein S19

Chain w:



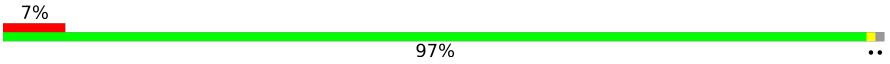
• Molecule 47: 30S ribosomal protein S20

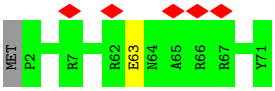
Chain x:



• Molecule 48: 30S ribosomal protein S21

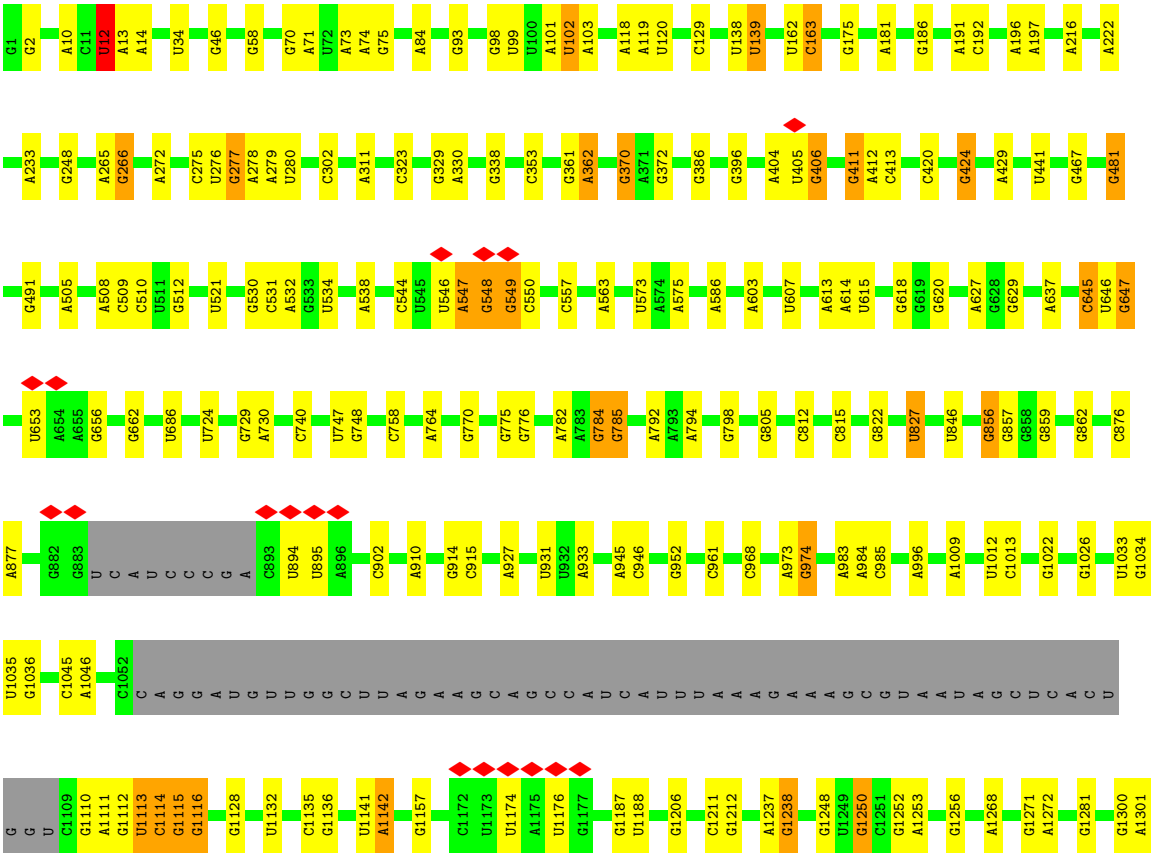
Chain y:

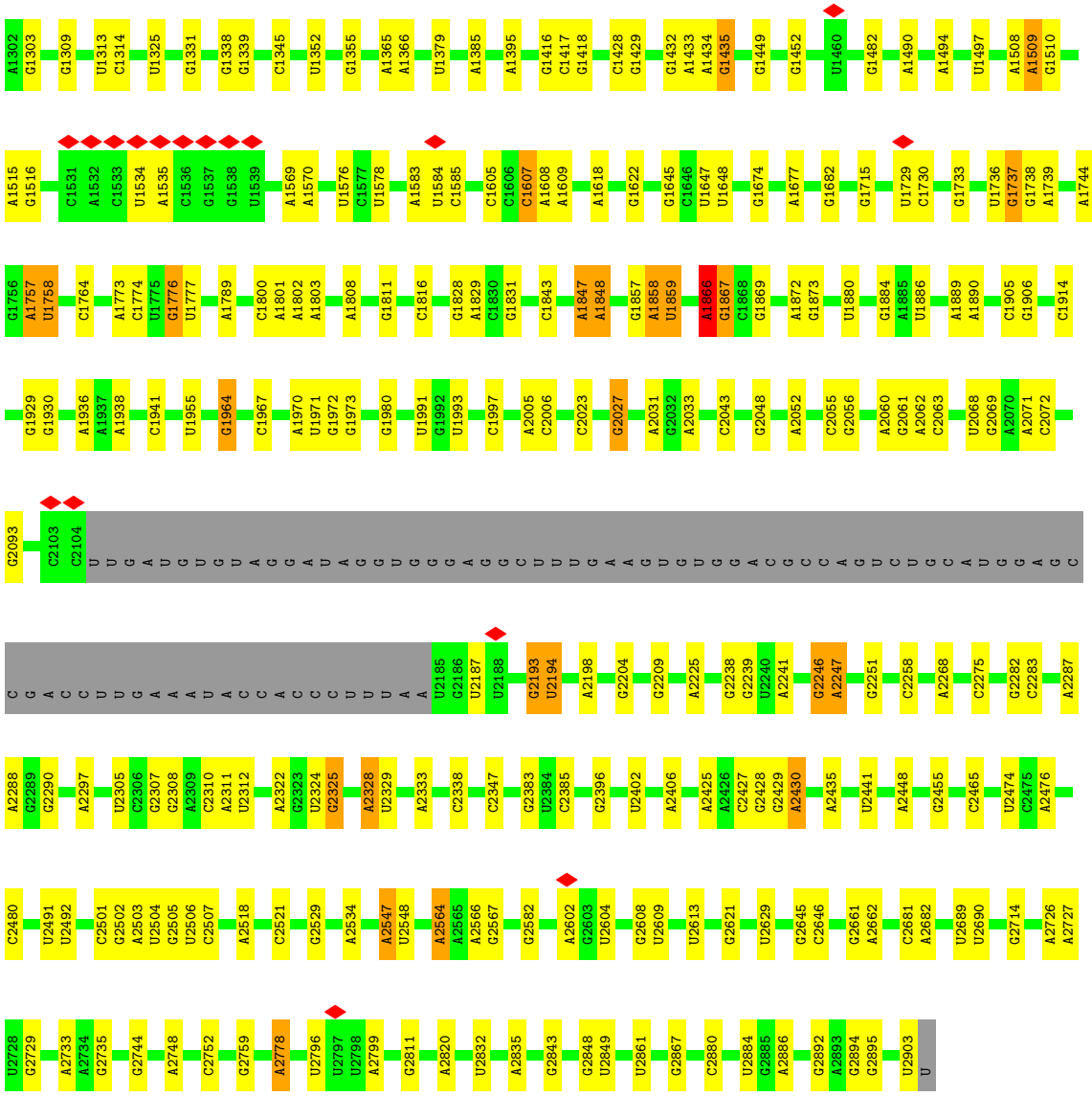




• Molecule 49: 23S rRNA RRLG-RRNA

Chain 0:



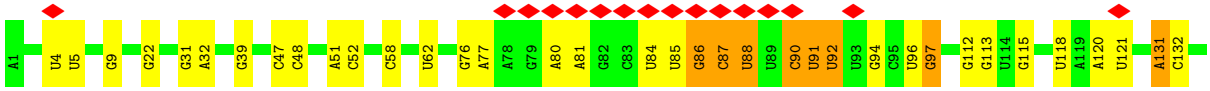


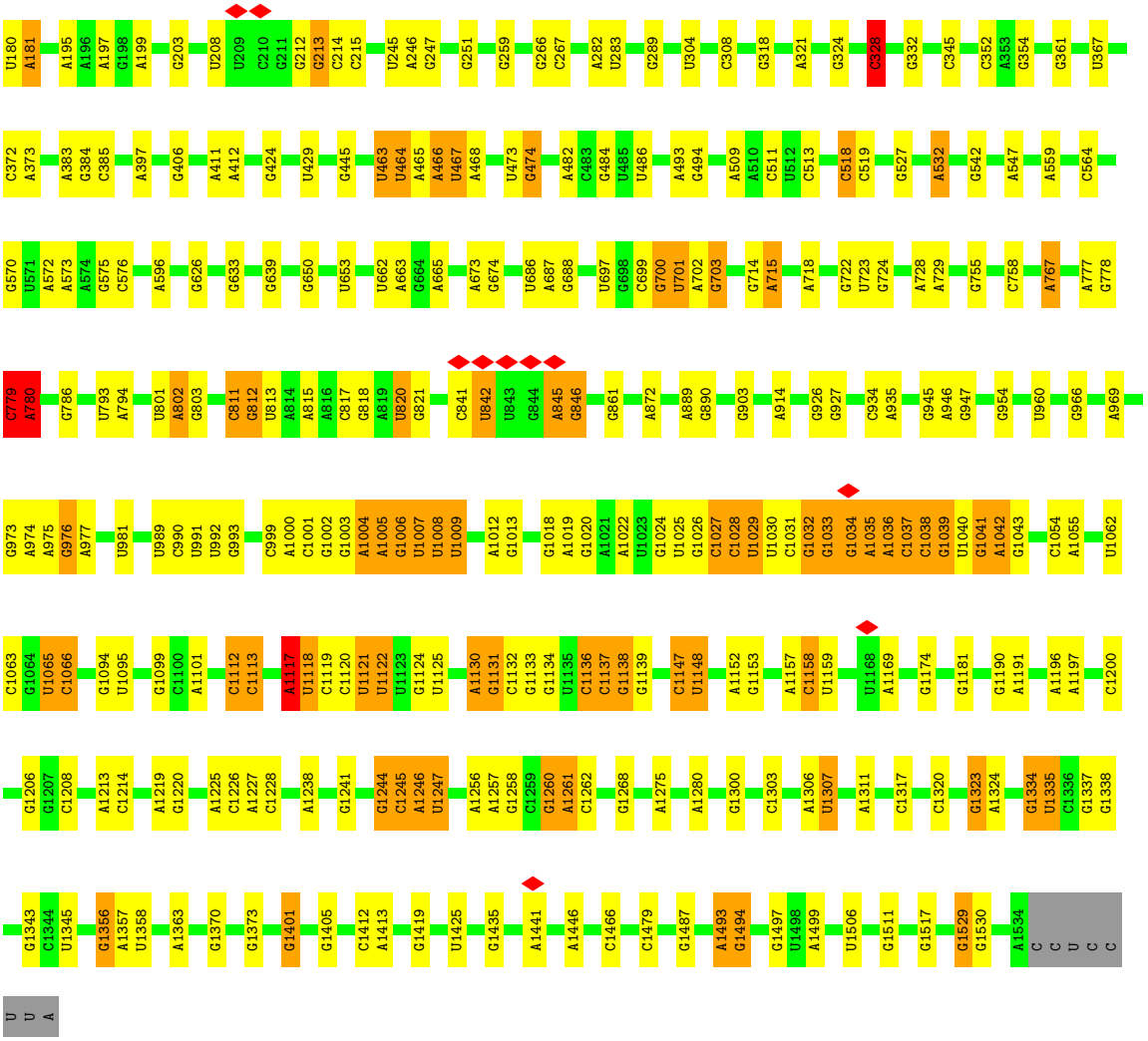
• Molecule 50: 5S rRNA

Chain 1:

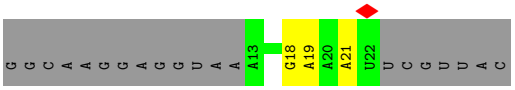
• Molecule 51: 16S rRNA RRSB-RRNA

Chain 2:

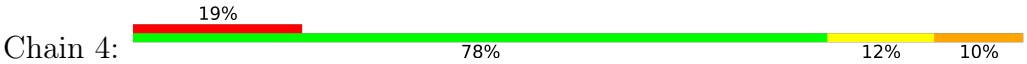


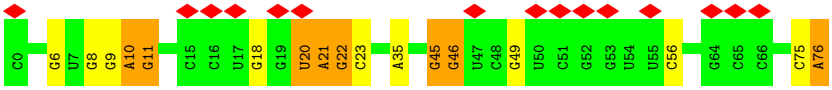


• Molecule 52: mRNA



• Molecule 53: Acylated P-site tRNA(fMet)





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	271987	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	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.461	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.0647	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, 6MZ

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	0.40	0/2121	0.64	0/2852
2	B	0.36	0/1580	0.58	0/2127
3	C	0.38	0/1571	0.57	0/2113
4	D	0.39	0/1434	0.57	0/1926
5	E	0.36	0/1315	0.54	0/1783
6	F	0.27	0/1122	0.50	0/1515
7	G	0.39	0/1152	0.58	0/1551
8	H	0.35	0/956	0.64	0/1279
9	I	0.36	0/1062	0.63	0/1413
10	J	0.39	0/1093	0.62	0/1460
11	K	0.38	0/958	0.66	0/1281
12	L	0.38	0/902	0.59	0/1209
13	M	0.40	0/929	0.61	0/1242
14	N	0.43	0/960	0.62	0/1278
15	O	0.41	0/829	0.60	0/1107
16	P	0.34	0/864	0.60	0/1156
17	Q	0.35	0/744	0.57	0/994
18	R	0.39	0/787	0.54	0/1051
19	S	0.37	0/766	0.56	0/1025
20	T	0.36	0/579	0.57	0/767
21	U	0.33	0/635	0.64	0/848
22	V	0.35	0/492	0.55	0/655
23	W	0.34	0/443	0.59	0/593
24	a	0.35	0/440	0.65	0/588
25	b	0.36	0/424	0.55	0/565
26	c	0.34	0/380	0.72	0/498
27	d	0.35	0/513	0.61	0/676
28	e	0.37	0/303	0.62	0/397
29	f	0.34	0/1784	0.54	0/2403
30	g	0.43	0/1651	0.59	0/2225
31	h	0.42	0/1665	0.57	0/2227
32	i	0.41	0/1157	0.57	0/1557

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	j	0.38	0/881	0.56	0/1189
34	k	0.34	0/1195	0.57	0/1602
35	l	0.41	0/989	0.57	0/1326
36	m	0.41	0/1034	0.63	0/1375
37	n	0.40	0/805	0.60	0/1089
38	o	0.37	0/893	0.60	0/1205
39	p	0.37	0/969	0.63	0/1300
40	q	0.38	0/892	0.62	0/1193
41	r	0.43	0/817	0.62	0/1088
42	s	0.36	0/722	0.60	0/964
43	t	0.40	0/659	0.63	0/884
44	u	0.37	0/657	0.57	0/881
45	v	0.40	0/553	0.62	0/742
46	w	0.40	0/652	0.57	0/877
47	x	0.38	0/676	0.53	0/895
48	y	0.36	0/598	0.61	0/792
49	0	0.82	0/66326	1.05	72/103471 (0.1%)
50	1	0.77	0/2869	0.96	1/4474 (0.0%)
51	2	0.85	0/36856	1.02	32/57497 (0.1%)
52	3	0.77	0/215	0.95	1/330 (0.3%)
53	4	0.56	0/1835	0.87	0/2859
All	All	0.72	0/152704	0.94	106/228394 (0.0%)

There are no bond length outliers.

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	0	2501	C	C6-N1-C2	-7.61	117.26	120.30
49	0	1980	G	N3-C4-C5	-7.34	124.93	128.60
51	2	1323	G	N3-C4-C5	-6.68	125.26	128.60
51	2	92	U	C2-N1-C1'	6.61	125.63	117.70
49	0	2275	C	C6-N1-C2	-6.49	117.71	120.30
49	0	12	U	C2-N1-C1'	6.45	125.44	117.70
51	2	780	A	O4'-C1'-N9	6.35	113.28	108.20
49	0	2455	G	N3-C4-C5	-6.34	125.43	128.60
49	0	2282	G	N3-C4-C5	-6.28	125.46	128.60
49	0	512	G	O4'-C1'-N9	6.25	113.20	108.20
51	2	779	C	N3-C2-O2	-6.21	117.55	121.90
49	0	323	C	C2-N1-C1'	6.08	125.48	118.80
51	2	1153	G	O4'-C1'-N9	6.03	113.03	108.20
49	0	2681	C	C6-N1-C2	-6.00	117.90	120.30
49	0	1980	G	N3-C4-N9	5.96	129.57	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	0	1776	G	N3-C4-N9	5.95	129.57	126.00
51	2	1401	G	N3-C4-C5	-5.93	125.64	128.60
51	2	767	A	O4'-C1'-N9	5.91	112.93	108.20
49	0	729	G	O4'-C1'-N9	5.86	112.89	108.20
49	0	1605	C	N1-C2-O2	5.86	122.41	118.90
49	0	411	G	N3-C4-C5	-5.84	125.68	128.60
49	0	1429	G	N3-C4-N9	5.80	129.48	126.00
49	0	2427	C	C6-N1-C2	-5.77	117.99	120.30
49	0	481	G	O4'-C1'-N9	5.73	112.79	108.20
49	0	629	G	N3-C4-C5	-5.72	125.74	128.60
51	2	1356	G	N3-C4-C5	-5.71	125.74	128.60
49	0	1831	G	N3-C4-C5	-5.71	125.75	128.60
51	2	115	G	N3-C4-C5	-5.70	125.75	128.60
51	2	1000	A	O4'-C1'-N9	5.67	112.73	108.20
51	2	974	A	O4'-C1'-N9	5.66	112.73	108.20
51	2	1466	C	N3-C2-O2	-5.65	117.94	121.90
49	0	1605	C	N3-C2-O2	-5.64	117.95	121.90
49	0	2275	C	N3-C2-O2	-5.64	117.95	121.90
51	2	1405	G	N3-C4-C5	-5.61	125.79	128.60
51	2	328	C	C2-N1-C1'	5.60	124.96	118.80
49	0	481	G	N3-C4-C5	-5.57	125.81	128.60
49	0	2258	C	C6-N1-C2	-5.57	118.07	120.30
49	0	58	G	N1-C6-O6	-5.57	116.56	119.90
51	2	626	G	N3-C4-C5	-5.56	125.82	128.60
51	2	361	G	N3-C4-C5	-5.53	125.83	128.60
51	2	903	G	N3-C4-C5	-5.53	125.83	128.60
51	2	1401	G	N3-C4-N9	5.51	129.31	126.00
49	0	2209	G	N3-C4-C5	-5.48	125.86	128.60
49	0	1313	U	C2-N1-C1'	5.48	124.27	117.70
49	0	98	G	O4'-C1'-N9	5.47	112.58	108.20
49	0	656	G	N3-C4-C5	-5.47	125.86	128.60
49	0	2892	G	N3-C4-C5	-5.45	125.88	128.60
49	0	323	C	C6-N1-C2	-5.44	118.12	120.30
49	0	370	G	N3-C4-C5	-5.44	125.88	128.60
49	0	1281	G	N3-C4-C5	-5.44	125.88	128.60
49	0	2428	G	N3-C4-C5	-5.44	125.88	128.60
49	0	2778	A	C8-N9-C4	-5.42	103.63	105.80
49	0	1645	G	N3-C4-C5	-5.40	125.90	128.60
49	0	856	G	N3-C4-C5	-5.40	125.90	128.60
51	2	686	U	O4'-C1'-N1	5.38	112.50	108.20
49	0	1973	G	N3-C4-C5	-5.38	125.91	128.60
49	0	2564	A	N7-C8-N9	5.37	116.49	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	2	1435	G	N3-C4-N9	5.37	129.22	126.00
49	0	1429	G	N3-C4-C5	-5.36	125.92	128.60
52	3	18	G	N3-C4-C5	-5.35	125.92	128.60
51	2	1529	G	N3-C4-C5	-5.34	125.93	128.60
49	0	1035	U	O4'-C1'-N1	5.32	112.45	108.20
49	0	1187	G	C4-N9-C1'	5.31	133.40	126.50
49	0	1682	G	N3-C4-C5	-5.28	125.96	128.60
51	2	821	G	N3-C4-C5	-5.28	125.96	128.60
50	1	83	G	N3-C4-C5	-5.28	125.96	128.60
51	2	1529	G	N3-C4-N9	5.27	129.16	126.00
49	0	984	A	O4'-C1'-N9	5.27	112.41	108.20
49	0	1250	G	N3-C4-C5	-5.27	125.97	128.60
51	2	1405	G	N3-C4-N9	5.26	129.16	126.00
49	0	2290	G	N3-C4-C5	-5.25	125.98	128.60
49	0	2621	G	N3-C4-C5	-5.25	125.98	128.60
49	0	1964	G	N3-C4-C5	-5.24	125.98	128.60
49	0	1331	G	N1-C6-O6	-5.24	116.76	119.90
49	0	2027	G	N3-C4-C5	-5.24	125.98	128.60
51	2	318	G	N3-C4-C5	-5.23	125.99	128.60
49	0	1682	G	N3-C4-N9	5.22	129.13	126.00
49	0	2455	G	N3-C4-N9	5.22	129.13	126.00
51	2	872	A	O4'-C1'-N9	5.21	112.37	108.20
49	0	2275	C	N1-C2-O2	5.21	122.03	118.90
49	0	1157	G	N3-C4-N9	5.21	129.12	126.00
51	2	973	G	N3-C4-N9	5.19	129.12	126.00
49	0	822	G	N3-C4-N9	5.19	129.11	126.00
49	0	2328	A	C8-N9-C4	-5.16	103.74	105.80
49	0	102	U	C2-N1-C1'	5.15	123.88	117.70
49	0	1776	G	C4-N9-C1'	5.14	133.18	126.50
49	0	1303	G	N3-C4-C5	-5.14	126.03	128.60
49	0	2729	G	N3-C4-N9	5.12	129.07	126.00
51	2	1117	A	C8-N9-C4	-5.12	103.75	105.80
49	0	1314	C	C2-N1-C1'	5.10	124.41	118.80
49	0	974	G	O4'-C1'-N9	5.08	112.26	108.20
49	0	952	G	N3-C4-C5	-5.07	126.06	128.60
49	0	70	G	N3-C4-C5	-5.07	126.07	128.60
49	0	2645	G	O4'-C1'-N9	5.07	112.25	108.20
51	2	570	G	C4-N9-C1'	5.07	133.09	126.50
49	0	2848	G	O4'-C1'-N9	5.06	112.25	108.20
51	2	113	G	N3-C4-C5	-5.05	126.08	128.60
49	0	2048	G	N3-C4-C5	-5.05	126.08	128.60
49	0	1309	G	N3-C4-N9	5.04	129.03	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	0	1866	A	O4'-C1'-N9	5.04	112.23	108.20
51	2	1343	G	N3-C4-C5	-5.03	126.08	128.60
49	0	729	G	C4-N9-C1'	5.02	133.03	126.50
51	2	1306	A	O4'-C1'-N9	5.02	112.21	108.20
49	0	748	G	O4'-C1'-N9	5.01	112.21	108.20
49	0	862	G	N3-C4-N9	5.01	129.00	126.00
49	0	2246	G	N3-C4-C5	-5.00	126.10	128.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2082	2155	2154	7	0
2	B	1559	1611	1611	2	0
3	C	1552	1619	1619	2	0
4	D	1410	1445	1444	10	0
5	E	1295	1333	1332	9	0
6	F	1111	1148	1148	14	0
7	G	1129	1162	1162	1	0
8	H	947	1023	1023	0	0
9	I	1053	1129	1129	2	0
10	J	1074	1157	1157	4	0
11	K	945	989	989	1	0
12	L	892	924	923	2	0
13	M	917	963	962	1	0
14	N	947	1020	1019	2	0
15	O	816	839	839	2	0
16	P	857	922	922	3	0
17	Q	738	807	807	0	0
18	R	779	832	831	1	0
19	S	753	780	780	1	0
20	T	572	594	593	1	0
21	U	625	653	652	1	0
22	V	491	524	523	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	W	439	483	482	0	0
24	a	434	446	445	0	0
25	b	417	452	451	0	0
26	c	377	418	418	0	0
27	d	504	572	572	0	0
28	e	302	343	343	0	0
29	f	1753	1781	1780	0	0
30	g	1624	1697	1696	0	0
31	h	1643	1708	1707	0	0
32	i	1144	1186	1185	0	0
33	j	862	864	864	0	0
34	k	1181	1238	1238	0	0
35	l	979	1032	1031	0	0
36	m	1022	1071	1070	0	0
37	n	795	837	836	0	0
38	o	877	888	887	0	0
39	p	955	1017	1016	0	0
40	q	883	942	941	0	0
41	r	805	845	844	0	0
42	s	714	735	734	0	0
43	t	649	666	666	0	0
44	u	648	692	691	0	0
45	v	544	566	565	0	0
46	w	637	666	665	0	0
47	x	670	720	719	0	0
48	y	590	629	629	0	0
49	0	59219	29765	29790	81	0
50	1	2566	1302	1302	3	0
51	2	32914	16564	16565	129	0
52	3	216	109	110	0	0
53	4	1643	835	835	11	0
54	4	10	10	10	2	0
All	All	140560	94708	94706	278	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (278) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2:1007:U:O2'	51:2:1008:U:O5'	1.88	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2:811:C:O2'	51:2:812:G:OP1	1.89	0.90
16:P:4:ILE:HD13	16:P:106:VAL:HG22	1.55	0.87
49:0:544:C:N4	49:0:549:G:O6	2.07	0.86
51:2:1493:A:O2'	51:2:1494:G:OP1	1.95	0.84
14:N:49:ASP:OD2	49:0:534:U:O2'	1.96	0.83
51:2:1036:A:O2'	51:2:1037:C:OP1	1.97	0.83
51:2:845:A:O2'	51:2:846:G:O5'	1.96	0.83
51:2:1028:C:O2'	51:2:1030:U:O4	1.96	0.82
49:0:138:U:O2'	49:0:139:U:OP2	1.97	0.81
51:2:1334:G:O2'	51:2:1335:U:OP1	1.96	0.81
51:2:779:C:O2'	51:2:780:A:N3	2.13	0.81
51:2:779:C:O2'	51:2:780:A:O5'	1.98	0.81
51:2:463:U:O2'	51:2:464:U:OP1	2.03	0.77
51:2:1005:A:H2'	51:2:1006:G:H21	1.50	0.76
51:2:1037:C:O2'	51:2:1038:C:OP2	2.03	0.76
49:0:2193:G:O2'	49:0:2194:U:OP1	2.06	0.74
53:4:21:A:O2'	53:4:22:G:O5'	2.06	0.73
6:F:82:SER:O	6:F:149:GLU:N	2.23	0.72
15:O:85:LYS:NZ	49:0:815:C:OP2	2.22	0.72
51:2:1335:U:OP1	51:2:1337:G:N2	2.22	0.71
7:G:91:GLU:O	7:G:95:ARG:NE	2.24	0.71
51:2:999:C:N3	51:2:1042:A:N6	2.39	0.71
51:2:1334:G:HO2'	51:2:1335:U:P	2.11	0.71
51:2:976:G:OP2	51:2:1358:U:O2'	2.09	0.70
49:0:1508:A:O2'	49:0:1509:A:O4'	2.10	0.69
51:2:767:A:H8	51:2:1511:G:H21	1.40	0.69
51:2:1004:A:O2'	51:2:1005:A:OP1	2.09	0.68
49:0:1857:G:O2'	49:0:1884:G:N2	2.26	0.68
49:0:2796:U:H3	49:0:2799:A:H61	1.42	0.68
49:0:547:A:H4'	49:0:548:G:O5'	1.94	0.67
53:4:45:G:O2'	53:4:46:G:OP1	2.13	0.66
51:2:1008:U:O2'	51:2:1009:U:OP2	2.15	0.64
51:2:801:U:O2'	51:2:802:A:OP2	2.13	0.64
10:J:18:ARG:O	10:J:38:ARG:NH1	2.31	0.64
50:1:66:A:OP2	50:1:108:A:N6	2.31	0.64
51:2:1005:A:C2'	51:2:1006:G:H21	2.11	0.64
51:2:811:C:HO2'	51:2:812:G:P	2.19	0.63
49:0:1858:A:O2'	49:0:1859:U:O4'	2.15	0.63
49:0:2521:C:HO2'	49:0:2564:A:H8	1.44	0.63
53:4:76:A:H4'	54:4:101:FME:O	1.97	0.63
5:E:95:ARG:NH2	5:E:128:GLN:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2:466:A:O2'	51:2:467:U:O5'	2.16	0.62
49:0:1113:U:O2'	49:0:1114:C:O5'	2.14	0.62
51:2:1013:G:H21	51:2:1219:A:H1'	1.64	0.62
49:0:547:A:H5"	49:0:548:G:C4	2.35	0.61
53:4:21:A:HO2'	53:4:22:G:P	2.24	0.61
51:2:778:G:H2'	51:2:779:C:H5'	1.83	0.60
6:F:37:VAL:HG22	6:F:38:PRO:HD2	1.83	0.60
5:E:2:SER:OG	5:E:3:ARG:N	2.35	0.60
1:A:221:ARG:NH1	49:0:1789:A:OP2	2.34	0.60
49:0:2193:G:HO2'	49:0:2194:U:P	2.26	0.59
51:2:1065:U:O2'	51:2:1066:C:OP2	2.18	0.59
49:0:1757:A:O2'	49:0:1758:U:OP1	2.13	0.59
9:I:78:ARG:NH2	49:0:627:A:OP1	2.35	0.58
49:0:2324:U:H3'	49:0:2325:G:H5"	1.85	0.58
51:2:463:U:HO2'	51:2:464:U:P	2.26	0.57
51:2:1137:C:H1'	51:2:1138:G:OP2	2.04	0.57
10:J:66:ARG:NH1	10:J:104:GLU:OE1	2.38	0.57
6:F:61:VAL:HG12	6:F:61:VAL:O	2.06	0.55
51:2:1041:G:HO2'	51:2:1042:A:H8	1.54	0.55
49:0:277:G:N2	49:0:277:G:OP2	2.36	0.55
49:0:370:G:O2'	49:0:424:G:OP1	2.23	0.55
4:D:66:LEU:HD11	50:1:41:G:C2	2.42	0.54
49:0:1858:A:O2'	49:0:1859:U:O5'	2.25	0.54
49:0:2324:U:H3'	49:0:2325:G:C5'	2.37	0.54
51:2:1027:C:O2	51:2:1033:G:N1	2.37	0.54
49:0:2063:C:O2'	53:4:76:A:O2'	2.25	0.54
12:L:63:LYS:NZ	50:1:51:G:OP1	2.40	0.54
51:2:1036:A:HO2'	51:2:1037:C:P	2.24	0.54
51:2:1007:U:H3	51:2:1020:G:H22	1.56	0.54
51:2:673:A:H2'	51:2:674:G:C8	2.44	0.53
51:2:779:C:H5	51:2:803:G:H22	1.57	0.53
49:0:784:G:H5'	49:0:785:G:OP1	2.08	0.53
49:0:2430:A:N3	49:0:2430:A:H2'	2.24	0.53
51:2:1003:G:O2'	51:2:1004:A:O5'	2.27	0.53
49:0:405:U:O2'	49:0:406:G:OP1	2.26	0.53
49:0:1847:A:O2'	49:0:1848:A:P	2.67	0.52
10:J:42:THR:HG22	10:J:44:ARG:H	1.75	0.52
49:0:1141:U:H4'	49:0:1142:A:O4'	2.09	0.52
51:2:1033:G:O2'	51:2:1035:A:N6	2.42	0.52
49:0:1802:A:H2'	49:0:1803:A:C8	2.45	0.52
51:2:1005:A:O2'	51:2:1006:G:P	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:8:ASP:OD1	18:R:24:LYS:NZ	2.42	0.51
53:4:76:A:C4'	54:4:101:FME:O	2.58	0.51
6:F:115:VAL:O	6:F:116:ARG:NH1	2.43	0.51
22:V:42:LEU:O	22:V:46:VAL:HG23	2.11	0.51
49:0:1115:G:O2'	49:0:1116:G:OP1	2.25	0.51
51:2:1112:C:O2'	51:2:1113:C:OP1	2.19	0.51
49:0:1866:A:O2'	49:0:1867:G:P	2.68	0.50
6:F:135:HIS:HB3	6:F:138:VAL:HG22	1.94	0.50
49:0:1607:C:N4	49:0:1622:G:OP2	2.44	0.50
51:2:714:G:O2'	51:2:715:A:C8	2.64	0.50
51:2:1035:A:N3	51:2:1035:A:H2'	2.27	0.50
51:2:180:U:H2'	51:2:181:A:H5'	1.93	0.50
51:2:1033:G:O2'	51:2:1035:A:N7	2.45	0.50
51:2:1033:G:N2	51:2:1035:A:H61	2.10	0.50
53:4:20:U:H4'	53:4:21:A:OP1	2.11	0.50
49:0:2071:A:H2'	49:0:2072:C:C6	2.47	0.50
51:2:1004:A:HO2'	51:2:1005:A:P	2.30	0.50
2:B:148:GLN:O	49:0:2052:A:H4'	2.10	0.50
49:0:1433:A:O2'	49:0:1434:A:H5'	2.12	0.50
51:2:532:A:N6	51:2:1206:G:O2'	2.44	0.50
1:A:257:THR:CG2	49:0:1803:A:O3'	2.60	0.49
51:2:518:C:H5"	51:2:519:C:C6	2.48	0.49
49:0:827:U:O2'	49:0:2068:U:C2	2.65	0.49
49:0:265:A:H4'	49:0:266:G:OP1	2.13	0.49
51:2:1120:C:HO2'	51:2:1121:U:H6	1.57	0.48
4:D:47:LYS:NZ	4:D:51:ASP:OD2	2.41	0.48
49:0:1115:G:HO2'	49:0:1116:G:P	2.35	0.48
51:2:700:G:O2'	51:2:701:U:O5'	2.23	0.48
4:D:122:PHE:HB3	4:D:163:ASP:OD1	2.13	0.48
1:A:251:GLN:OE1	1:A:252:THR:O	2.32	0.48
49:0:2328:A:H2'	49:0:2329:U:C6	2.48	0.48
51:2:203:G:N2	51:2:215:C:C2	2.81	0.48
51:2:1303:C:O2	51:2:1303:C:O4'	2.31	0.48
49:0:12:U:H2'	49:0:12:U:O2	2.13	0.47
49:0:1869:G:H21	49:0:1872:A:H2	1.62	0.47
49:0:2504:U:O2	49:0:2504:U:O5'	2.32	0.47
51:2:818:G:O2'	51:2:820:U:O2	2.32	0.47
51:2:1035:A:H3'	51:2:1036:A:H5"	1.96	0.47
51:2:92:U:H2'	51:2:92:U:O2	2.13	0.47
51:2:1356:G:H2'	51:2:1357:A:H8	1.79	0.47
49:0:1434:A:HO2'	49:0:1435:G:H8	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2:212:G:C2	51:2:213:G:C8	3.02	0.47
5:E:22:GLN:NE2	5:E:38:ASN:O	2.48	0.47
49:0:2547:A:H2'	49:0:2548:U:C6	2.50	0.47
51:2:981:U:O2	51:2:981:U:O5'	2.33	0.47
5:E:127:THR:HG22	5:E:128:GLN:N	2.29	0.47
51:2:778:G:C2'	51:2:779:C:H5'	2.45	0.47
51:2:1307:U:O2	51:2:1307:U:O5'	2.33	0.47
16:P:66:ILE:HD12	16:P:66:ILE:H	1.80	0.47
51:2:86:G:N3	51:2:87:C:N4	2.61	0.47
49:0:1237:A:H4'	49:0:1238:G:OP1	2.14	0.47
51:2:990:C:O5'	51:2:990:C:O2	2.33	0.47
13:M:88:ARG:NH2	13:M:110:ILE:O	2.44	0.47
5:E:138:LYS:O	5:E:141:ILE:HG22	2.15	0.46
51:2:90:C:O2'	51:2:91:U:O5'	2.33	0.46
51:2:945:G:C2	51:2:946:A:C8	3.03	0.46
49:0:2521:C:O2'	49:0:2564:A:H8	1.97	0.46
5:E:47:ASP:N	5:E:47:ASP:OD1	2.46	0.46
51:2:1120:C:O2'	51:2:1121:U:H6	1.98	0.46
51:2:1136:C:OP1	51:2:1136:C:O4'	2.34	0.46
51:2:1356:G:H2'	51:2:1357:A:C8	2.50	0.46
51:2:131:A:H2'	51:2:132:C:C6	2.51	0.46
51:2:1005:A:O2'	51:2:1006:G:O5'	2.33	0.46
6:F:129:GLU:OE1	6:F:129:GLU:N	2.49	0.46
49:0:102:U:H2'	49:0:102:U:O2	2.15	0.46
51:2:699:C:O2	51:2:699:C:O5'	2.34	0.46
51:2:1130:A:O2'	51:2:1131:G:H8	1.99	0.46
51:2:1121:U:HO2'	51:2:1122:U:P	2.39	0.45
51:2:702:A:H3'	51:2:703:G:H5'	1.98	0.45
51:2:1130:A:O2'	51:2:1131:G:P	2.74	0.45
51:2:1262:C:O2	51:2:1262:C:O4'	2.34	0.45
1:A:257:THR:HG21	49:0:1803:A:O3'	2.17	0.45
51:2:1039:G:C2	51:2:1040:U:C4	3.05	0.45
1:A:259:SER:O	1:A:259:SER:OG	2.32	0.45
51:2:1018:G:C2'	51:2:1019:A:H5'	2.47	0.45
5:E:104:ASN:ND2	5:E:114:ASP:OD2	2.49	0.45
51:2:1117:A:O2'	51:2:1118:U:OP1	2.35	0.45
6:F:11:ASN:OD1	6:F:11:ASN:N	2.50	0.45
6:F:50:ARG:NH2	6:F:55:GLU:OE2	2.44	0.45
51:2:62:U:OP1	51:2:385:C:O2'	2.33	0.45
51:2:328:C:H2'	51:2:328:C:O2	2.17	0.45
51:2:1065:U:H1'	51:2:1066:C:OP2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2:493:A:H2'	51:2:494:G:C8	2.52	0.44
20:T:10:THR:OG1	20:T:11:ARG:N	2.50	0.44
51:2:1147:C:HO2'	51:2:1148:U:P	2.41	0.44
51:2:1307:U:O2	51:2:1307:U:O4'	2.35	0.44
12:L:40:ILE:HD13	12:L:47:VAL:HG22	1.98	0.44
15:O:51:VAL:HG23	15:O:51:VAL:O	2.18	0.44
49:0:607:U:C5	49:0:620:G:C5	3.06	0.44
51:2:1260:G:O2'	51:2:1261:A:P	2.75	0.44
49:0:1736:U:C2'	49:0:1737:G:O5'	2.66	0.44
6:F:15:LEU:HD23	6:F:16:GLY:N	2.32	0.44
51:2:946:A:H2'	51:2:947:G:C8	2.53	0.44
51:2:1244:G:HO2'	51:2:1245:C:P	2.40	0.44
2:B:196:ALA:O	2:B:199:SER:OG	2.35	0.44
49:0:2193:G:O2'	49:0:2194:U:P	2.73	0.44
49:0:645:C:H2'	49:0:647:G:C8	2.52	0.43
51:2:801:U:O2'	51:2:802:A:H8	2.01	0.43
51:2:801:U:O2'	51:2:802:A:P	2.76	0.43
1:A:165:VAL:HG22	1:A:173:THR:O	2.18	0.43
49:0:138:U:HO2'	49:0:139:U:P	2.31	0.43
4:D:51:ASP:OD1	4:D:51:ASP:N	2.51	0.43
49:0:973:A:H5'	49:0:1188:U:H1'	1.99	0.43
22:V:2:LYS:O	22:V:3:ALA:HB3	2.18	0.43
49:0:876:C:H2'	49:0:877:A:O4'	2.18	0.43
51:2:80:A:N6	51:2:81:A:N3	2.66	0.43
51:2:96:U:HO2'	51:2:97:G:H8	1.65	0.43
51:2:1225:A:H2'	51:2:1226:C:C5	2.53	0.43
11:K:66:ALA:O	11:K:70:THR:OG1	2.32	0.43
49:0:197:A:N6	49:0:2430:A:O2'	2.52	0.43
49:0:549:G:H2'	49:0:550:C:O4'	2.19	0.43
49:0:1858:A:H2'	49:0:1859:U:C6	2.53	0.43
51:2:714:G:O2'	51:2:715:A:H8	2.02	0.43
51:2:841:C:H3'	51:2:842:U:C5'	2.49	0.43
51:2:1008:U:O2'	51:2:1009:U:P	2.76	0.43
51:2:1029:U:O2	51:2:1032:G:N1	2.51	0.43
5:E:86:LYS:HG2	5:E:132:VAL:HG22	1.99	0.43
53:4:6:G:O2'	53:4:49:G:OP2	2.25	0.43
5:E:11:VAL:HG12	5:E:15:VAL:CG2	2.49	0.43
49:0:279:A:H2'	49:0:280:U:O4'	2.19	0.43
51:2:473:U:O2'	51:2:474:G:P	2.76	0.43
49:0:1889:A:H2'	49:0:1890:A:C8	2.54	0.43
51:2:812:G:O3'	51:2:813:U:O2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2:1002:G:H2'	51:2:1003:G:O4'	2.18	0.43
9:I:108:ALA:HB3	9:I:125:LEU:HD22	2.01	0.42
51:2:889:A:H4'	51:2:890:G:OP1	2.19	0.42
51:2:1038:C:N3	51:2:1039:G:N7	2.67	0.42
49:0:162:U:H4'	49:0:163:C:OP1	2.19	0.42
51:2:688:G:H1	51:2:699:C:H5	1.67	0.42
49:0:1774:C:O2	49:0:1774:C:H2'	2.18	0.42
3:C:21:ARG:O	3:C:114:ARG:NH2	2.48	0.42
51:2:1033:G:H21	51:2:1035:A:H61	1.66	0.42
51:2:1121:U:O2'	51:2:1122:U:P	2.76	0.42
51:2:1132:C:O2'	51:2:1133:G:H5'	2.20	0.42
10:J:31:PHE:HD1	10:J:132:THR:HG22	1.85	0.42
49:0:856:G:H2'	49:0:857:G:C8	2.54	0.42
49:0:1113:U:O2'	49:0:1114:C:P	2.77	0.42
51:2:1007:U:O2'	51:2:1008:U:C5'	2.66	0.42
19:S:6:ALA:HB3	19:S:65:VAL:HG22	2.00	0.42
51:2:779:C:O2	51:2:779:C:H2'	2.18	0.42
51:2:1006:G:C6	51:2:1007:U:C5	3.08	0.42
4:D:75:ALA:HB2	53:4:56:C:O2'	2.20	0.42
51:2:87:C:O2'	51:2:88:U:OP1	2.27	0.42
14:N:37:GLN:HE21	49:0:1252:G:H1	1.67	0.42
51:2:662:U:H2'	51:2:663:A:C8	2.55	0.42
51:2:989:U:O2	51:2:989:U:O4'	2.38	0.42
49:0:1847:A:O2'	49:0:1848:A:H8	2.02	0.42
51:2:181:A:N6	51:2:195:A:C8	2.87	0.42
4:D:40:VAL:HG12	4:D:42:GLU:H	1.85	0.41
51:2:1018:G:H2'	51:2:1019:A:H5'	2.00	0.41
53:4:10:A:O2'	53:4:11:G:P	2.78	0.41
51:2:1024:G:H4'	51:2:1025:U:H5'	2.02	0.41
1:A:251:GLN:NE2	49:0:1843:C:H4'	2.35	0.41
16:P:37:THR:O	16:P:37:THR:HG22	2.21	0.41
49:0:191:A:H2'	49:0:192:C:C6	2.55	0.41
51:2:466:A:O2'	51:2:467:U:P	2.78	0.41
51:2:1157:A:H4'	51:2:1158:C:O5'	2.21	0.41
49:0:277:G:C2'	49:0:278:A:OP2	2.68	0.41
49:0:646:U:H3'	49:0:647:G:C5'	2.49	0.41
51:2:246:A:C2	51:2:282:A:C6	3.08	0.41
51:2:246:A:C2	51:2:282:A:C5	3.09	0.41
3:C:145:ASP:HB3	3:C:184:ASP:HB2	2.02	0.41
49:0:1858:A:O2'	49:0:1859:U:C5'	2.68	0.41
51:2:1005:A:N6	51:2:1022:A:H2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2:1038:C:C2	51:2:1039:G:C8	3.09	0.41
53:4:10:A:HO2'	53:4:11:G:P	2.43	0.41
6:F:104:THR:OG1	6:F:109:GLU:OE1	2.39	0.41
49:0:1115:G:O2'	49:0:1116:G:P	2.79	0.41
21:U:21:ALA:O	21:U:22:LEU:HB2	2.21	0.41
51:2:780:A:H8	51:2:802:A:H62	1.69	0.41
51:2:1412:C:H2'	51:2:1413:A:C8	2.56	0.41
6:F:90:LEU:HD21	6:F:125:THR:HG23	2.02	0.41
49:0:1432:G:H2'	49:0:1433:A:C8	2.56	0.41
49:0:2246:G:H2'	49:0:2247:A:H8	1.86	0.41
49:0:2504:U:O2	49:0:2504:U:O4'	2.38	0.41
51:2:714:G:O2'	51:2:715:A:OP2	2.38	0.41
51:2:1323:G:H2'	51:2:1324:A:C8	2.56	0.41
4:D:85:ILE:HD12	49:0:2311:A:O2'	2.20	0.41
4:D:136:ILE:HG22	4:D:141:ILE:HD11	2.03	0.41
4:D:74:VAL:O	4:D:74:VAL:HG23	2.20	0.40
49:0:278:A:N6	49:0:362:A:C8	2.89	0.40
51:2:1121:U:O2'	51:2:1122:U:H6	2.04	0.40
6:F:99:ILE:O	6:F:103:VAL:HG23	2.22	0.40
6:F:142:VAL:HG12	6:F:143:ILE:N	2.37	0.40
51:2:728:A:H2'	51:2:729:A:C8	2.56	0.40
51:2:1062:U:H2'	51:2:1063:C:C6	2.57	0.40
4:D:46:ASP:OD1	4:D:47:LYS:N	2.52	0.40
49:0:278:A:N6	49:0:362:A:N7	2.69	0.40
49:0:607:U:C5	49:0:620:G:C4	3.09	0.40
49:0:1847:A:O2'	49:0:1848:A:OP2	2.39	0.40
51:2:1002:G:C2'	51:2:1003:G:O5'	2.69	0.40
6:F:50:ARG:HA	6:F:54:LEU:HD21	2.04	0.40
51:2:1029:U:O2	51:2:1032:G:C2	2.74	0.40
51:2:1034:G:H4'	51:2:1035:A:O5'	2.22	0.40
51:2:1246:A:O2'	51:2:1247:U:C5	2.71	0.40

There are no symmetry-related clashes.

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	A	269/273 (98%)	254 (94%)	15 (6%)	0	100	100
2	B	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
3	C	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
4	D	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
5	E	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
6	F	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
7	G	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
8	H	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
9	I	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
10	J	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
11	K	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
12	L	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
13	M	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
14	N	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
15	O	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
16	P	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
17	Q	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
18	R	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
19	S	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
20	T	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
21	U	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
22	V	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
23	W	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
24	a	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
25	b	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
26	c	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
27	d	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
28	e	36/38 (95%)	36 (100%)	0	0	100	100
29	f	222/241 (92%)	205 (92%)	17 (8%)	0	100	100
30	g	204/233 (88%)	195 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	h	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
32	i	153/167 (92%)	145 (95%)	8 (5%)	0	100	100
33	j	104/131 (79%)	101 (97%)	3 (3%)	0	100	100
34	k	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
35	l	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
36	m	125/130 (96%)	113 (90%)	12 (10%)	0	100	100
37	n	97/103 (94%)	86 (89%)	11 (11%)	0	100	100
38	o	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
39	p	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
40	q	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
41	r	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
42	s	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
43	t	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
44	u	78/84 (93%)	72 (92%)	6 (8%)	0	100	100
45	v	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
46	w	77/92 (84%)	74 (96%)	3 (4%)	0	100	100
47	x	84/87 (97%)	84 (100%)	0	0	100	100
48	y	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	5525/5839 (95%)	5261 (95%)	264 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	A	216/218 (99%)	213 (99%)	3 (1%)	67	72
2	B	164/164 (100%)	164 (100%)	0	100	100
3	C	165/165 (100%)	163 (99%)	2 (1%)	71	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	148/150 (99%)	142 (96%)	6 (4%)	30	30
5	E	134/138 (97%)	132 (98%)	2 (2%)	65	70
6	F	114/114 (100%)	109 (96%)	5 (4%)	28	27
7	G	116/116 (100%)	114 (98%)	2 (2%)	60	66
8	H	104/104 (100%)	102 (98%)	2 (2%)	57	61
9	I	103/103 (100%)	101 (98%)	2 (2%)	57	61
10	J	109/109 (100%)	107 (98%)	2 (2%)	59	63
11	K	98/103 (95%)	97 (99%)	1 (1%)	76	81
12	L	86/87 (99%)	83 (96%)	3 (4%)	36	37
13	M	99/100 (99%)	98 (99%)	1 (1%)	76	81
14	N	89/90 (99%)	88 (99%)	1 (1%)	73	79
15	O	84/84 (100%)	82 (98%)	2 (2%)	49	52
16	P	93/93 (100%)	89 (96%)	4 (4%)	29	28
17	Q	80/84 (95%)	80 (100%)	0	100	100
18	R	83/85 (98%)	82 (99%)	1 (1%)	71	77
19	S	78/78 (100%)	77 (99%)	1 (1%)	69	74
20	T	57/63 (90%)	54 (95%)	3 (5%)	22	20
21	U	67/68 (98%)	65 (97%)	2 (3%)	41	43
22	V	54/55 (98%)	51 (94%)	3 (6%)	21	18
23	W	47/49 (96%)	47 (100%)	0	100	100
24	a	46/48 (96%)	46 (100%)	0	100	100
25	b	46/49 (94%)	46 (100%)	0	100	100
26	c	38/38 (100%)	38 (100%)	0	100	100
27	d	51/52 (98%)	50 (98%)	1 (2%)	55	59
28	e	34/34 (100%)	32 (94%)	2 (6%)	19	16
29	f	186/199 (94%)	179 (96%)	7 (4%)	33	33
30	g	170/190 (90%)	164 (96%)	6 (4%)	36	37
31	h	172/173 (99%)	170 (99%)	2 (1%)	71	77
32	i	118/126 (94%)	113 (96%)	5 (4%)	30	29
33	j	92/112 (82%)	90 (98%)	2 (2%)	52	55
34	k	124/147 (84%)	119 (96%)	5 (4%)	31	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	l	104/105 (99%)	102 (98%)	2 (2%)	57 61
36	m	105/107 (98%)	102 (97%)	3 (3%)	42 44
37	n	87/90 (97%)	84 (97%)	3 (3%)	37 38
38	o	90/99 (91%)	89 (99%)	1 (1%)	73 79
39	p	103/104 (99%)	100 (97%)	3 (3%)	42 44
40	q	92/96 (96%)	90 (98%)	2 (2%)	52 55
41	r	83/84 (99%)	79 (95%)	4 (5%)	25 23
42	s	76/77 (99%)	71 (93%)	5 (7%)	16 13
43	t	65/65 (100%)	63 (97%)	2 (3%)	40 42
44	u	74/78 (95%)	73 (99%)	1 (1%)	67 72
45	v	57/65 (88%)	56 (98%)	1 (2%)	59 63
46	w	70/79 (89%)	67 (96%)	3 (4%)	29 28
47	x	65/66 (98%)	65 (100%)	0	100 100
48	y	60/61 (98%)	59 (98%)	1 (2%)	60 66
All	All	4596/4764 (96%)	4487 (98%)	109 (2%)	51 52

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	157	SER
1	A	251	GLN
3	C	107	SER
3	C	168	ASP
4	D	21	ASN
4	D	51	ASP
4	D	112	ARG
4	D	127	ASN
4	D	150	ARG
4	D	152	LEU
5	E	74	SER
5	E	152	ARG
6	F	11	ASN
6	F	17	ASP
6	F	51	ARG
6	F	54	LEU
6	F	101	ASP

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Mol	Chain	Res	Type
7	G	12	LYS
7	G	95	ARG
8	H	80	ASP
8	H	89	ASN
9	I	13	LYS
9	I	91	ASP
10	J	14	LYS
10	J	136	MET
11	K	22	ARG
12	L	69	ASP
12	L	85	LYS
12	L	98	GLN
13	M	72	ARG
14	N	51	ARG
15	O	15	SER
15	O	18	GLN
16	P	7	HIS
16	P	11	ARG
16	P	67	ASP
16	P	95	ARG
18	R	81	ASP
19	S	61	LEU
20	T	12	ASN
20	T	78	LYS
20	T	81	SER
21	U	28	ARG
21	U	35	SER
22	V	4	LYS
22	V	58	ASN
22	V	60	LYS
27	d	31	HIS
28	e	4	ARG
28	e	20	ASP
29	f	21	ARG
29	f	23	TRP
29	f	132	LYS
29	f	136	MET
29	f	145	GLU
29	f	226	SER
29	f	227	GLN
30	g	29	PHE
30	g	35	SER

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Mol	Chain	Res	Type
30	g	54	ARG
30	g	65	ARG
30	g	165	THR
30	g	185	ASN
31	h	128	ARG
31	h	206	LYS
32	i	23	LYS
32	i	43	ASN
32	i	142	ASP
32	i	149	SER
32	i	156	LYS
33	j	82	ASP
33	j	91	ARG
34	k	30	LEU
34	k	45	SER
34	k	57	SER
34	k	77	SER
34	k	113	ASP
35	l	38	ASN
35	l	107	SER
36	m	95	ARG
36	m	97	GLU
36	m	123	ARG
37	n	30	LYS
37	n	31	ARG
37	n	101	SER
38	o	53	ARG
39	p	86	ARG
39	p	102	LEU
39	p	121	ARG
40	q	54	ASP
40	q	68	ASP
41	r	33	ASP
41	r	37	SER
41	r	38	ASP
41	r	100	SER
42	s	13	SER
42	s	18	ASP
42	s	62	GLN
42	s	64	ARG
42	s	88	ARG
43	t	1	MET

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Mol	Chain	Res	Type
43	t	12	LYS
44	u	27	ARG
45	v	42	SER
46	w	3	ARG
46	w	4	SER
46	w	64	ASP
48	y	63	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
34	k	68	ASN
38	o	22	HIS
41	r	35	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	0	2754/2904 (94%)	350 (12%)	12 (0%)
50	1	119/120 (99%)	14 (11%)	0
51	2	1533/1542 (99%)	233 (15%)	18 (1%)
52	3	8/30 (26%)	1 (12%)	0
53	4	76/77 (98%)	12 (15%)	4 (5%)
All	All	4490/4673 (96%)	610 (13%)	34 (0%)

All (610) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
49	0	2	G
49	0	10	A
49	0	12	U
49	0	13	A
49	0	14	A
49	0	34	U
49	0	46	G
49	0	71	A
49	0	73	A
49	0	74	A
49	0	75	G
49	0	84	A

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Mol	Chain	Res	Type
49	0	93	G
49	0	99	U
49	0	101	A
49	0	103	A
49	0	118	A
49	0	119	A
49	0	120	U
49	0	129	C
49	0	139	U
49	0	163	C
49	0	175	G
49	0	181	A
49	0	186	G
49	0	196	A
49	0	216	A
49	0	222	A
49	0	233	A
49	0	248	G
49	0	266	G
49	0	272	A
49	0	275	C
49	0	276	U
49	0	277	G
49	0	302	C
49	0	311	A
49	0	329	G
49	0	330	A
49	0	338	G
49	0	353	C
49	0	361	G
49	0	362	A
49	0	372	G
49	0	386	G
49	0	396	G
49	0	404	A
49	0	406	G
49	0	411	G
49	0	412	A
49	0	413	C
49	0	420	C
49	0	424	G
49	0	429	A

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Mol	Chain	Res	Type
49	0	441	U
49	0	467	G
49	0	481	G
49	0	491	G
49	0	505	A
49	0	508	A
49	0	509	C
49	0	510	C
49	0	521	U
49	0	530	G
49	0	531	C
49	0	532	A
49	0	538	A
49	0	546	U
49	0	547	A
49	0	548	G
49	0	549	G
49	0	557	C
49	0	563	A
49	0	573	U
49	0	575	A
49	0	586	A
49	0	603	A
49	0	613	A
49	0	614	A
49	0	615	U
49	0	618	G
49	0	637	A
49	0	645	C
49	0	647	G
49	0	653	U
49	0	662	G
49	0	686	U
49	0	724	U
49	0	730	A
49	0	740	C
49	0	747	U
49	0	758	C
49	0	764	A
49	0	770	G
49	0	775	G
49	0	776	G

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Mol	Chain	Res	Type
49	0	782	A
49	0	784	G
49	0	785	G
49	0	792	A
49	0	794	A
49	0	798	G
49	0	805	G
49	0	812	C
49	0	827	U
49	0	846	U
49	0	859	G
49	0	894	U
49	0	895	U
49	0	902	C
49	0	910	A
49	0	914	G
49	0	915	C
49	0	927	A
49	0	931	U
49	0	933	A
49	0	945	A
49	0	946	C
49	0	961	C
49	0	968	C
49	0	974	G
49	0	983	A
49	0	985	C
49	0	996	A
49	0	1009	A
49	0	1012	U
49	0	1013	C
49	0	1022	G
49	0	1026	G
49	0	1033	U
49	0	1034	G
49	0	1036	G
49	0	1046	A
49	0	1110	G
49	0	1111	A
49	0	1112	G
49	0	1114	C
49	0	1116	G

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Mol	Chain	Res	Type
49	0	1128	G
49	0	1132	U
49	0	1135	C
49	0	1136	G
49	0	1142	A
49	0	1174	U
49	0	1176	U
49	0	1206	G
49	0	1211	C
49	0	1212	G
49	0	1238	G
49	0	1248	G
49	0	1250	G
49	0	1253	A
49	0	1256	G
49	0	1268	A
49	0	1271	G
49	0	1272	A
49	0	1300	G
49	0	1301	A
49	0	1325	U
49	0	1338	G
49	0	1339	G
49	0	1345	C
49	0	1352	U
49	0	1355	G
49	0	1365	A
49	0	1366	A
49	0	1379	U
49	0	1385	A
49	0	1395	A
49	0	1416	G
49	0	1417	C
49	0	1418	G
49	0	1428	C
49	0	1435	G
49	0	1449	G
49	0	1452	G
49	0	1482	G
49	0	1490	A
49	0	1494	A
49	0	1497	U

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Mol	Chain	Res	Type
49	0	1509	A
49	0	1510	G
49	0	1515	A
49	0	1516	G
49	0	1534	U
49	0	1535	A
49	0	1569	A
49	0	1570	A
49	0	1576	U
49	0	1578	U
49	0	1583	A
49	0	1584	U
49	0	1585	C
49	0	1607	C
49	0	1608	A
49	0	1609	A
49	0	1618	A
49	0	1647	U
49	0	1648	U
49	0	1674	G
49	0	1677	A
49	0	1715	G
49	0	1729	U
49	0	1730	C
49	0	1733	G
49	0	1737	G
49	0	1738	G
49	0	1739	A
49	0	1744	A
49	0	1755	A
49	0	1758	U
49	0	1764	C
49	0	1773	A
49	0	1776	G
49	0	1777	U
49	0	1800	C
49	0	1801	A
49	0	1808	A
49	0	1811	G
49	0	1816	C
49	0	1828	G
49	0	1829	A

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Mol	Chain	Res	Type
49	0	1848	A
49	0	1858	A
49	0	1859	U
49	0	1866	A
49	0	1867	G
49	0	1873	G
49	0	1880	U
49	0	1886	U
49	0	1905	C
49	0	1906	G
49	0	1914	C
49	0	1929	G
49	0	1930	G
49	0	1936	A
49	0	1938	A
49	0	1941	C
49	0	1955	U
49	0	1964	G
49	0	1967	C
49	0	1970	A
49	0	1971	U
49	0	1972	G
49	0	1991	U
49	0	1993	U
49	0	1997	C
49	0	2005	A
49	0	2006	C
49	0	2023	C
49	0	2027	G
49	0	2031	A
49	0	2033	A
49	0	2043	C
49	0	2055	C
49	0	2056	G
49	0	2060	A
49	0	2061	G
49	0	2062	A
49	0	2069	G
49	0	2093	G
49	0	2187	U
49	0	2194	U
49	0	2198	A

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Mol	Chain	Res	Type
49	0	2204	G
49	0	2225	A
49	0	2238	G
49	0	2239	G
49	0	2241	A
49	0	2247	A
49	0	2251	G
49	0	2268	A
49	0	2283	C
49	0	2287	A
49	0	2288	A
49	0	2297	A
49	0	2305	U
49	0	2308	G
49	0	2310	C
49	0	2312	U
49	0	2322	A
49	0	2325	G
49	0	2333	A
49	0	2338	C
49	0	2347	C
49	0	2383	G
49	0	2385	C
49	0	2396	G
49	0	2402	U
49	0	2406	A
49	0	2425	A
49	0	2429	G
49	0	2430	A
49	0	2435	A
49	0	2441	U
49	0	2448	A
49	0	2465	C
49	0	2474	U
49	0	2476	A
49	0	2480	C
49	0	2491	U
49	0	2492	U
49	0	2502	G
49	0	2503	A
49	0	2505	G
49	0	2506	U

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Mol	Chain	Res	Type
49	0	2507	C
49	0	2518	A
49	0	2529	G
49	0	2534	A
49	0	2547	A
49	0	2566	A
49	0	2567	G
49	0	2582	G
49	0	2602	A
49	0	2604	U
49	0	2608	G
49	0	2609	U
49	0	2613	U
49	0	2629	U
49	0	2646	C
49	0	2661	G
49	0	2662	A
49	0	2682	A
49	0	2689	U
49	0	2690	U
49	0	2714	G
49	0	2726	A
49	0	2727	A
49	0	2733	A
49	0	2735	G
49	0	2744	G
49	0	2748	A
49	0	2752	C
49	0	2759	G
49	0	2778	A
49	0	2811	G
49	0	2820	A
49	0	2832	U
49	0	2835	A
49	0	2843	G
49	0	2849	U
49	0	2861	U
49	0	2867	G
49	0	2880	C
49	0	2884	U
49	0	2886	A
49	0	2894	G

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Mol	Chain	Res	Type
49	0	2895	G
49	0	2903	U
50	1	25	U
50	1	35	C
50	1	42	C
50	1	44	G
50	1	45	A
50	1	56	G
50	1	57	A
50	1	89	U
50	1	90	C
50	1	103	U
50	1	105	G
50	1	108	A
50	1	109	A
50	1	119	A
51	2	4	U
51	2	5	U
51	2	9	G
51	2	22	G
51	2	31	G
51	2	32	A
51	2	39	G
51	2	47	C
51	2	48	C
51	2	51	A
51	2	52	C
51	2	58	C
51	2	76	G
51	2	77	A
51	2	84	U
51	2	85	U
51	2	86	G
51	2	88	U
51	2	90	C
51	2	91	U
51	2	94	G
51	2	97	G
51	2	112	G
51	2	118	U
51	2	120	A
51	2	121	U

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Mol	Chain	Res	Type
51	2	131	A
51	2	181	A
51	2	197	A
51	2	199	A
51	2	208	U
51	2	214	C
51	2	245	U
51	2	247	G
51	2	251	G
51	2	259	G
51	2	266	G
51	2	267	C
51	2	283	U
51	2	289	G
51	2	304	U
51	2	308	C
51	2	321	A
51	2	324	G
51	2	328	C
51	2	332	G
51	2	345	C
51	2	352	C
51	2	354	G
51	2	367	U
51	2	372	C
51	2	373	A
51	2	383	A
51	2	384	G
51	2	397	A
51	2	406	G
51	2	411	A
51	2	412	A
51	2	424	G
51	2	429	U
51	2	445	G
51	2	464	U
51	2	465	A
51	2	467	U
51	2	468	A
51	2	474	G
51	2	482	A
51	2	484	G

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Mol	Chain	Res	Type
51	2	486	U
51	2	509	A
51	2	511	C
51	2	513	C
51	2	518	C
51	2	527	G
51	2	532	A
51	2	542	G
51	2	547	A
51	2	559	A
51	2	564	C
51	2	572	A
51	2	573	A
51	2	575	G
51	2	576	C
51	2	596	A
51	2	633	G
51	2	639	G
51	2	650	G
51	2	653	U
51	2	665	A
51	2	687	A
51	2	697	U
51	2	701	U
51	2	703	G
51	2	715	A
51	2	718	A
51	2	722	G
51	2	723	U
51	2	724	G
51	2	755	G
51	2	758	C
51	2	777	A
51	2	779	C
51	2	780	A
51	2	786	G
51	2	793	U
51	2	794	A
51	2	802	A
51	2	812	G
51	2	815	A
51	2	817	C

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Mol	Chain	Res	Type
51	2	820	U
51	2	842	U
51	2	845	A
51	2	846	G
51	2	861	G
51	2	914	A
51	2	926	G
51	2	927	G
51	2	934	C
51	2	935	A
51	2	954	G
51	2	960	U
51	2	966	G
51	2	969	A
51	2	975	A
51	2	976	G
51	2	977	A
51	2	991	U
51	2	992	U
51	2	993	G
51	2	1001	C
51	2	1004	A
51	2	1005	A
51	2	1006	G
51	2	1007	U
51	2	1008	U
51	2	1009	U
51	2	1012	A
51	2	1026	G
51	2	1027	C
51	2	1028	C
51	2	1029	U
51	2	1031	C
51	2	1032	G
51	2	1033	G
51	2	1034	G
51	2	1035	A
51	2	1036	A
51	2	1037	C
51	2	1038	C
51	2	1039	G
51	2	1041	G

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Mol	Chain	Res	Type
51	2	1042	A
51	2	1043	G
51	2	1054	C
51	2	1055	A
51	2	1065	U
51	2	1066	C
51	2	1094	G
51	2	1095	U
51	2	1099	G
51	2	1101	A
51	2	1113	C
51	2	1117	A
51	2	1118	U
51	2	1119	C
51	2	1121	U
51	2	1122	U
51	2	1124	G
51	2	1125	U
51	2	1130	A
51	2	1131	G
51	2	1134	G
51	2	1136	C
51	2	1137	C
51	2	1138	G
51	2	1139	G
51	2	1148	U
51	2	1152	A
51	2	1158	C
51	2	1159	U
51	2	1169	A
51	2	1174	G
51	2	1181	G
51	2	1191	A
51	2	1196	A
51	2	1197	A
51	2	1200	C
51	2	1208	C
51	2	1213	A
51	2	1214	C
51	2	1220	G
51	2	1227	A
51	2	1228	C

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Mol	Chain	Res	Type
51	2	1238	A
51	2	1241	G
51	2	1245	C
51	2	1246	A
51	2	1247	U
51	2	1256	A
51	2	1257	A
51	2	1258	G
51	2	1260	G
51	2	1261	A
51	2	1268	G
51	2	1275	A
51	2	1280	A
51	2	1300	G
51	2	1307	U
51	2	1311	A
51	2	1317	C
51	2	1320	C
51	2	1335	U
51	2	1338	G
51	2	1345	U
51	2	1363	A
51	2	1370	G
51	2	1373	G
51	2	1401	G
51	2	1419	G
51	2	1425	U
51	2	1441	A
51	2	1446	A
51	2	1479	C
51	2	1487	G
51	2	1493	A
51	2	1494	G
51	2	1497	G
51	2	1499	A
51	2	1506	U
51	2	1517	G
51	2	1529	G
51	2	1530	G
52	3	19	A
53	4	8	G
53	4	9	G

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Mol	Chain	Res	Type
53	4	11	G
53	4	18	G
53	4	20	U
53	4	21	A
53	4	22	G
53	4	23	C
53	4	35	A
53	4	46	G
53	4	75	C
53	4	76	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
49	0	546	U
49	0	547	A
49	0	784	G
49	0	1045	C
49	0	1113	U
49	0	1115	G
49	0	1738	G
49	0	1757	A
49	0	1847	A
49	0	2193	G
49	0	2307	G
49	0	2406	A
51	2	87	C
51	2	213	G
51	2	463	U
51	2	466	A
51	2	700	G
51	2	779	C
51	2	811	C
51	2	1004	A
51	2	1034	G
51	2	1036	A
51	2	1065	U
51	2	1112	C
51	2	1117	A
51	2	1137	C
51	2	1147	C
51	2	1190	G

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Mol	Chain	Res	Type
51	2	1244	G
51	2	1334	G
53	4	10	A
53	4	20	U
53	4	21	A
53	4	45	G

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
52	6MZ	3	21	52	18,25,26	1.73	4 (22%)	16,36,39	1.96	4 (25%)

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
52	6MZ	3	21	52	-	2/5/27/28	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	3	21	6MZ	C6-N6	5.19	1.43	1.35
52	3	21	6MZ	C5-C4	-2.49	1.34	1.40
52	3	21	6MZ	C2-N3	2.04	1.35	1.32
52	3	21	6MZ	C9-N6	-2.02	1.41	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	3	21	6MZ	N3-C2-N1	-5.40	120.23	128.68
52	3	21	6MZ	C2-N1-C6	3.61	119.68	116.59
52	3	21	6MZ	C9-N6-C6	-2.90	120.38	122.87
52	3	21	6MZ	C1'-N9-C4	-2.82	121.69	126.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	3	21	6MZ	O4'-C4'-C5'-O5'
52	3	21	6MZ	C3'-C4'-C5'-O5'

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)

1 ligand is 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	$\#\|Z\| > 2$
54	FME	4	101	53	8,9,10	0.91	0	7,9,11	1.14	1 (14%)

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
54	FME	4	101	53	-	3/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	4	101	FME	O-C-CA	-2.40	118.49	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	4	101	FME	O1-CN-N-CA
54	4	101	FME	O-C-CA-CB
54	4	101	FME	N-CA-CB-CG

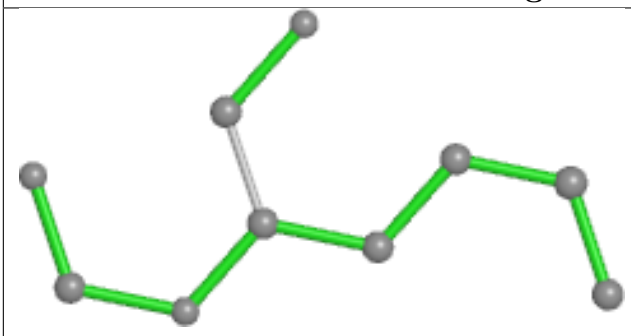
There are no ring outliers.

1 monomer is involved in 2 short contacts:

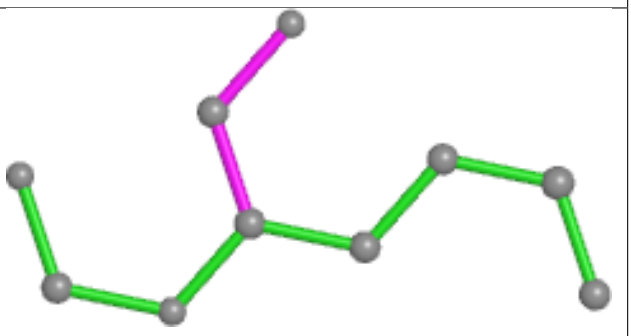
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	4	101	FME	2	0

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.

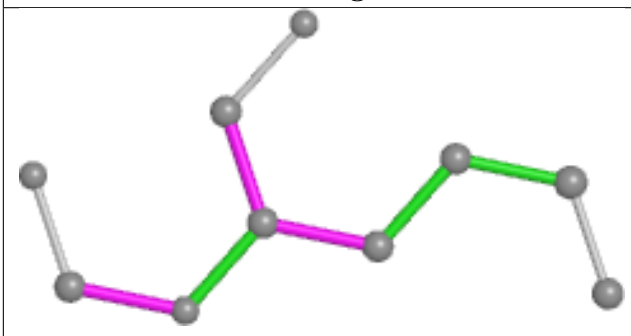
Ligand FME 4 101



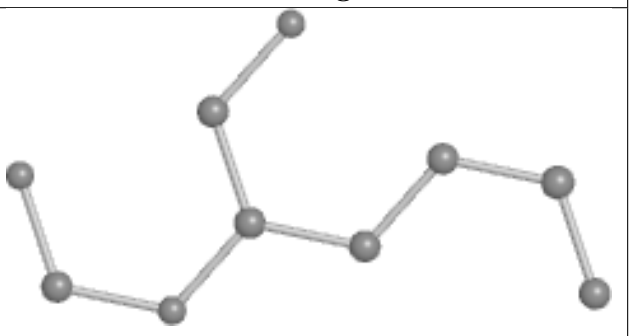
Bond lengths



Bond angles



Torsions



Rings

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.

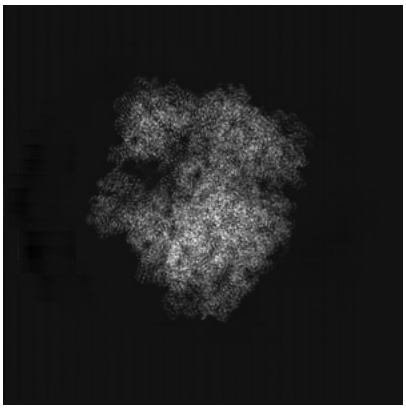
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16029. These allow visual inspection of the internal detail of the map and identification of artifacts.

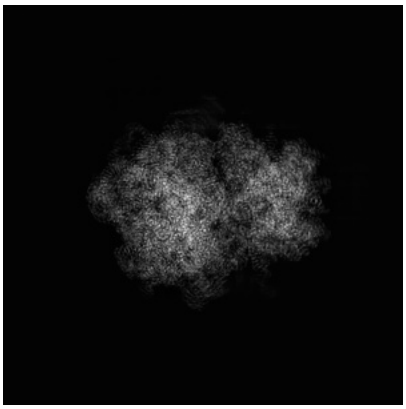
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

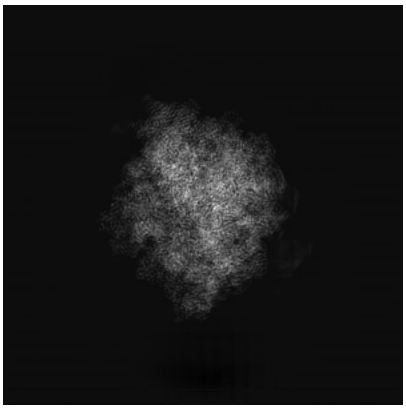
6.1.1 Primary map



X

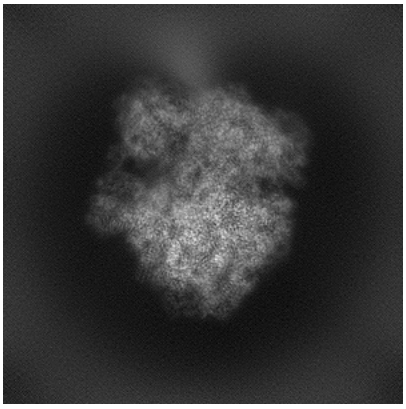


Y

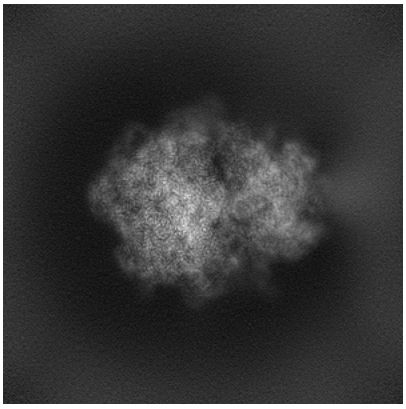


Z

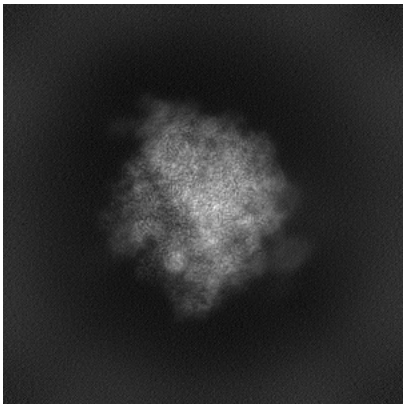
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

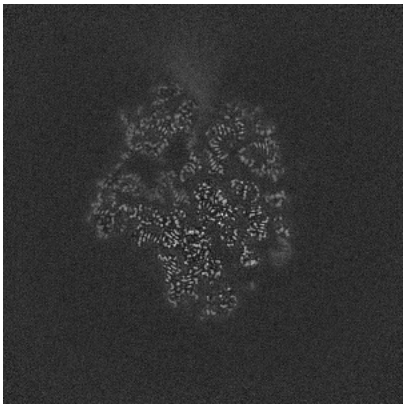
6.2.1 Primary map

X Index: 256

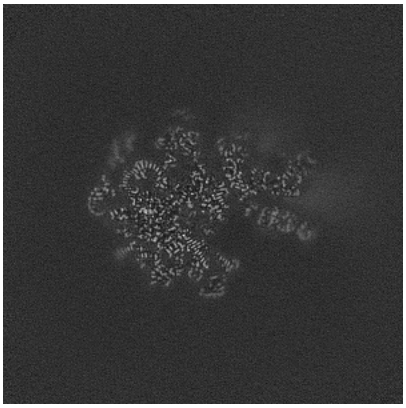
Y Index: 256

Z Index: 256

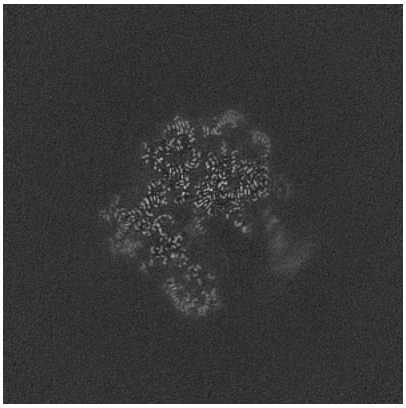
6.2.2 Raw map



X Index: 256



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)

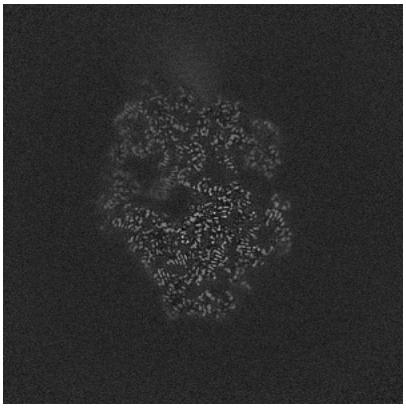
6.3.1 Primary map

X Index: 270

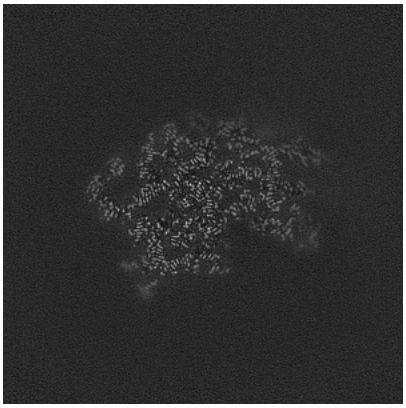
Y Index: 277

Z Index: 213

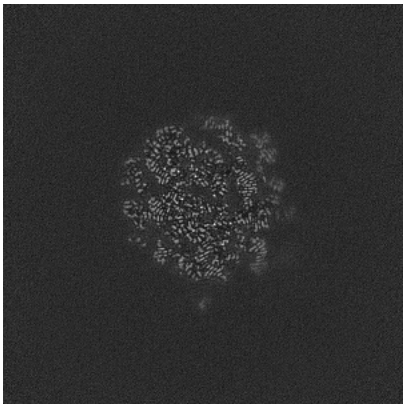
6.3.2 Raw map



X Index: 270



Y Index: 278

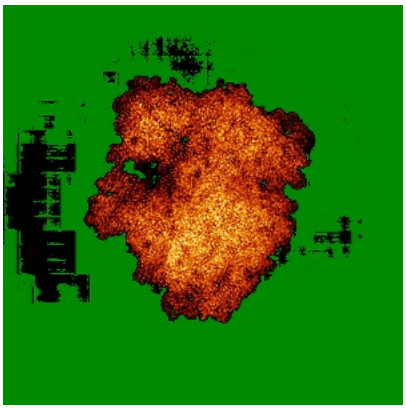


Z Index: 213

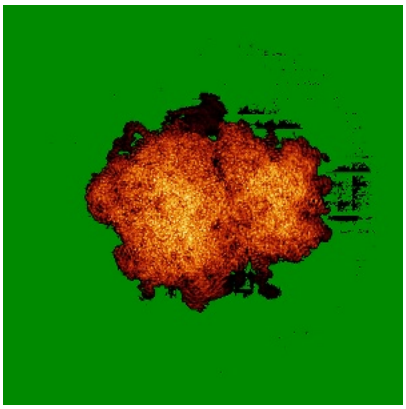
The images above show the largest variance slices of the map in three orthogonal directions.

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

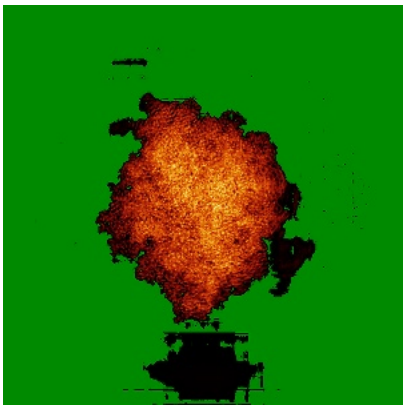
6.4.1 Primary map



X

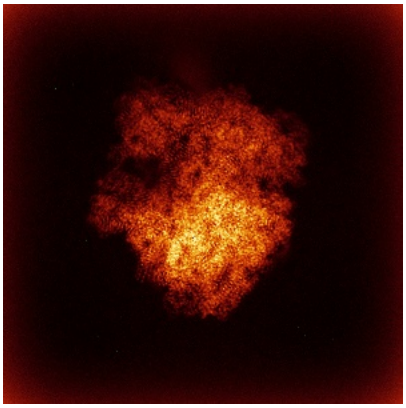


Y

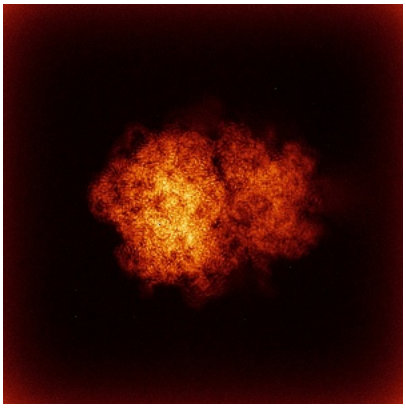


Z

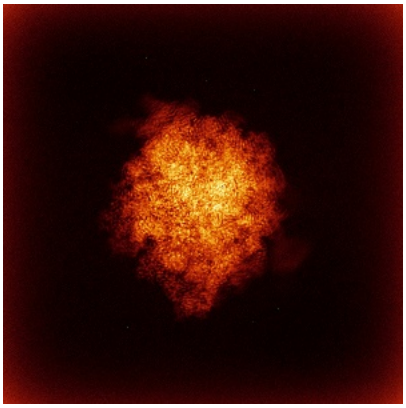
6.4.2 Raw map



X



Y

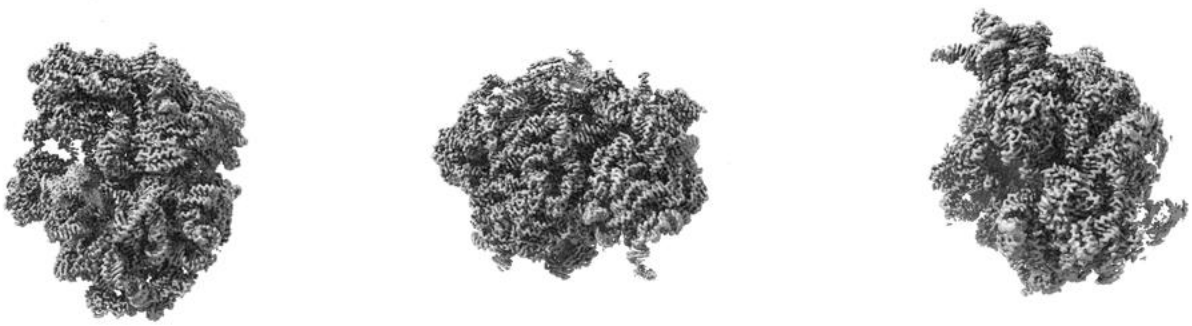


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0647. 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.

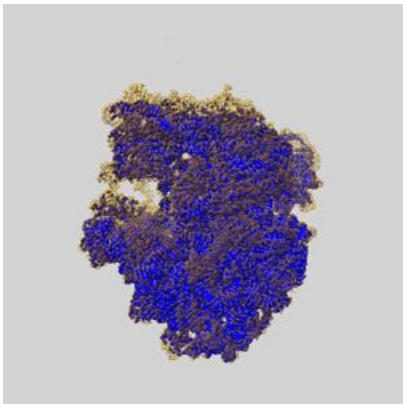
6.6 Mask visualisation (i)

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

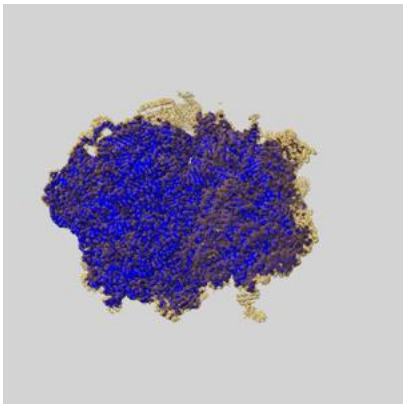
A mask typically either:

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

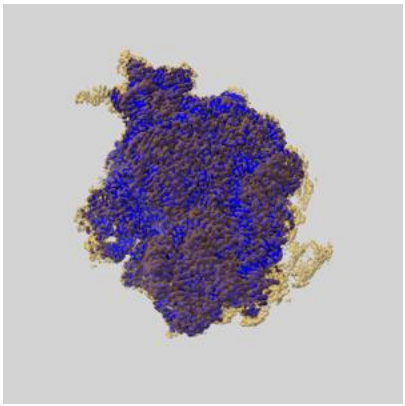
6.6.1 emd_16029_msk_1.map (i)



X



Y

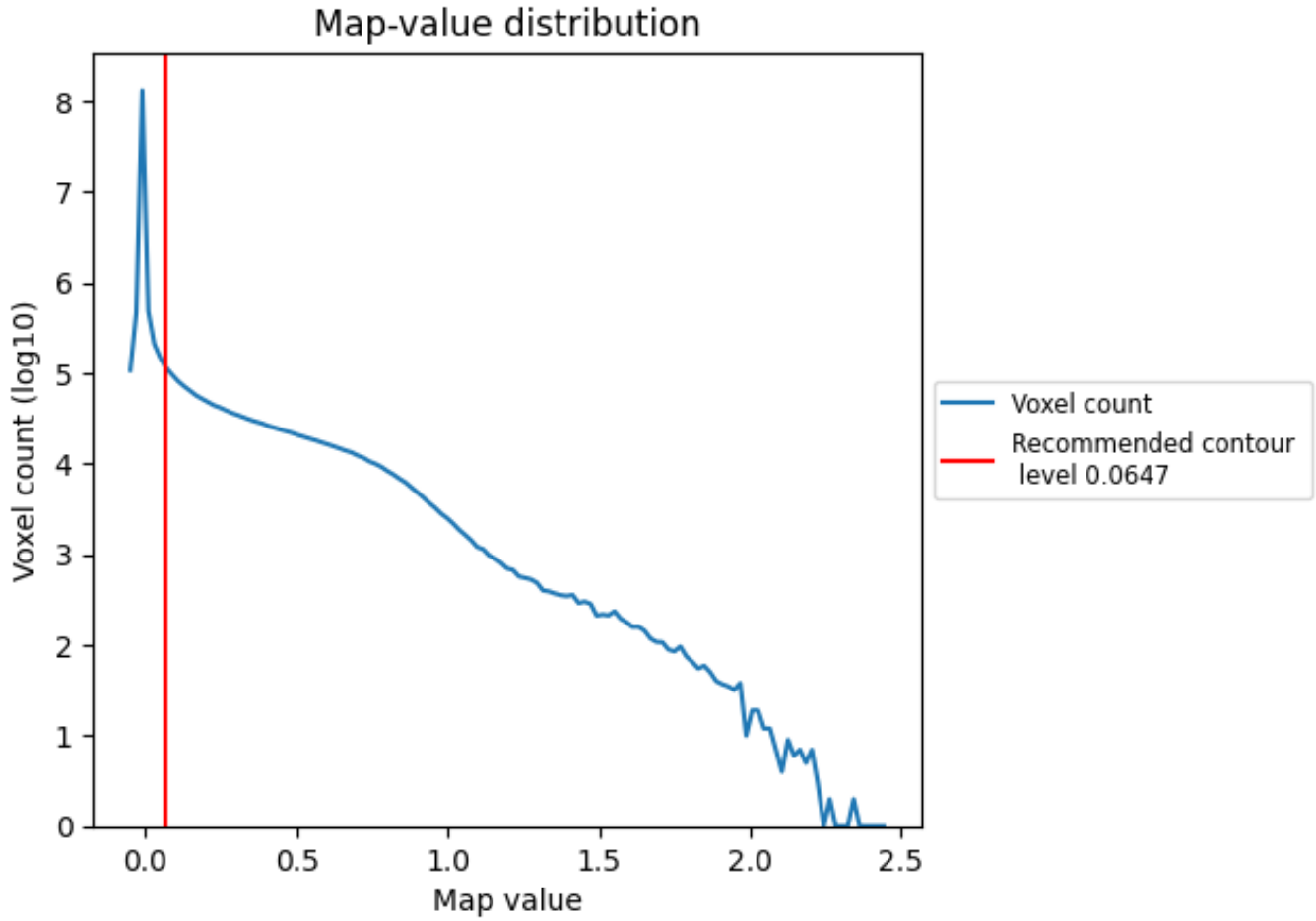


Z

7 Map analysis

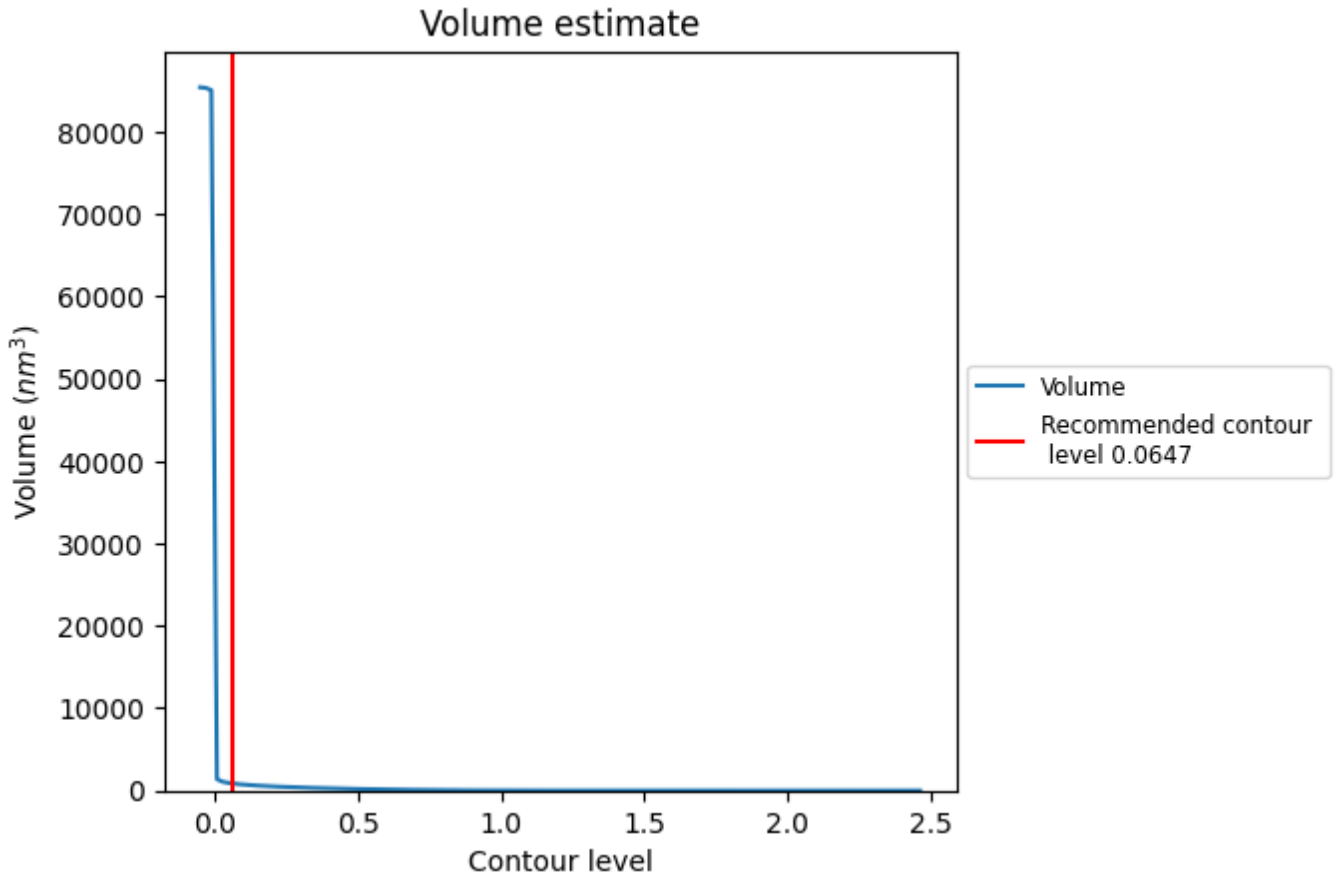
This section contains the results of statistical analysis of the map.

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.

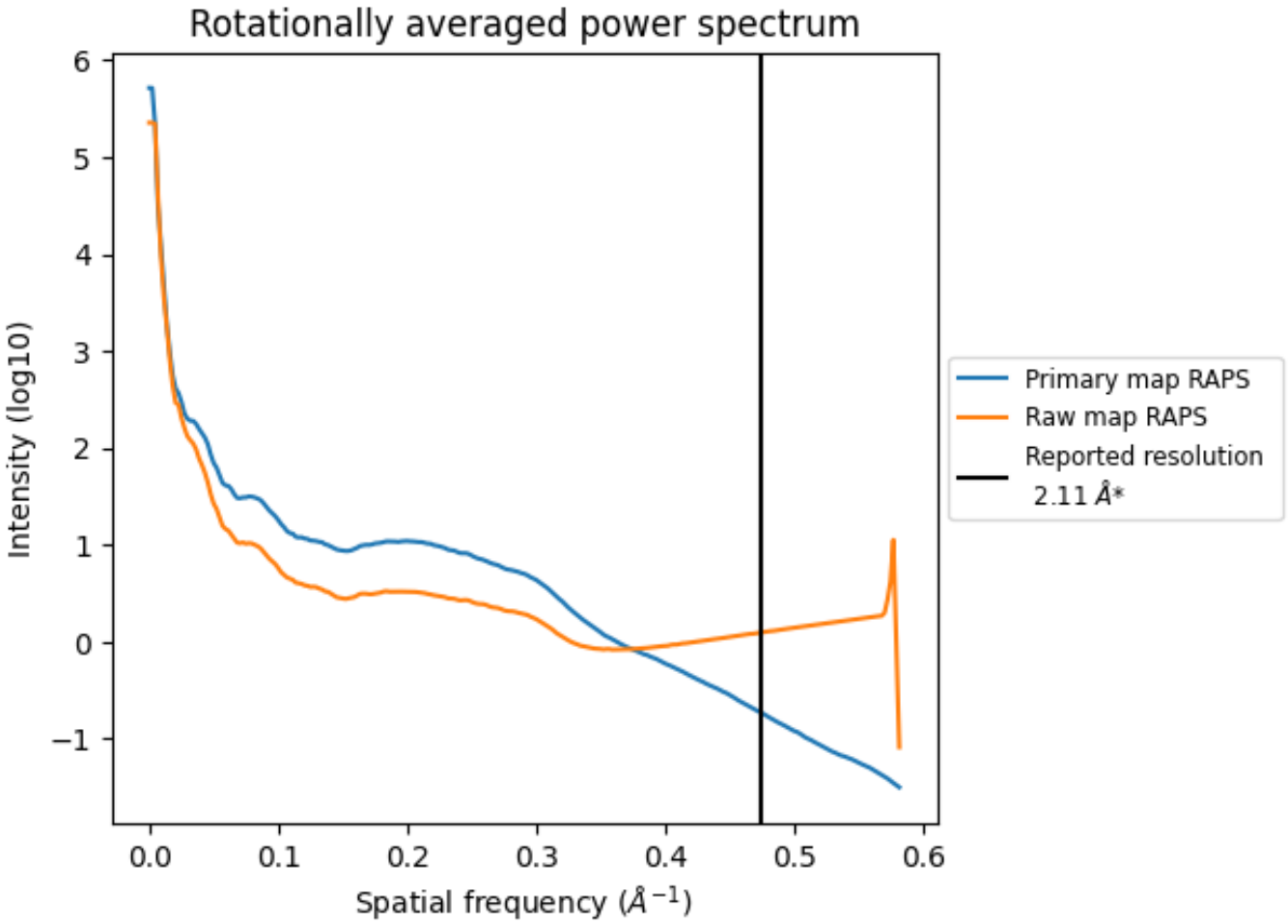
7.2 Volume estimate



The volume at the recommended contour level is 854 nm^3; this corresponds to an approximate mass of 771 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)

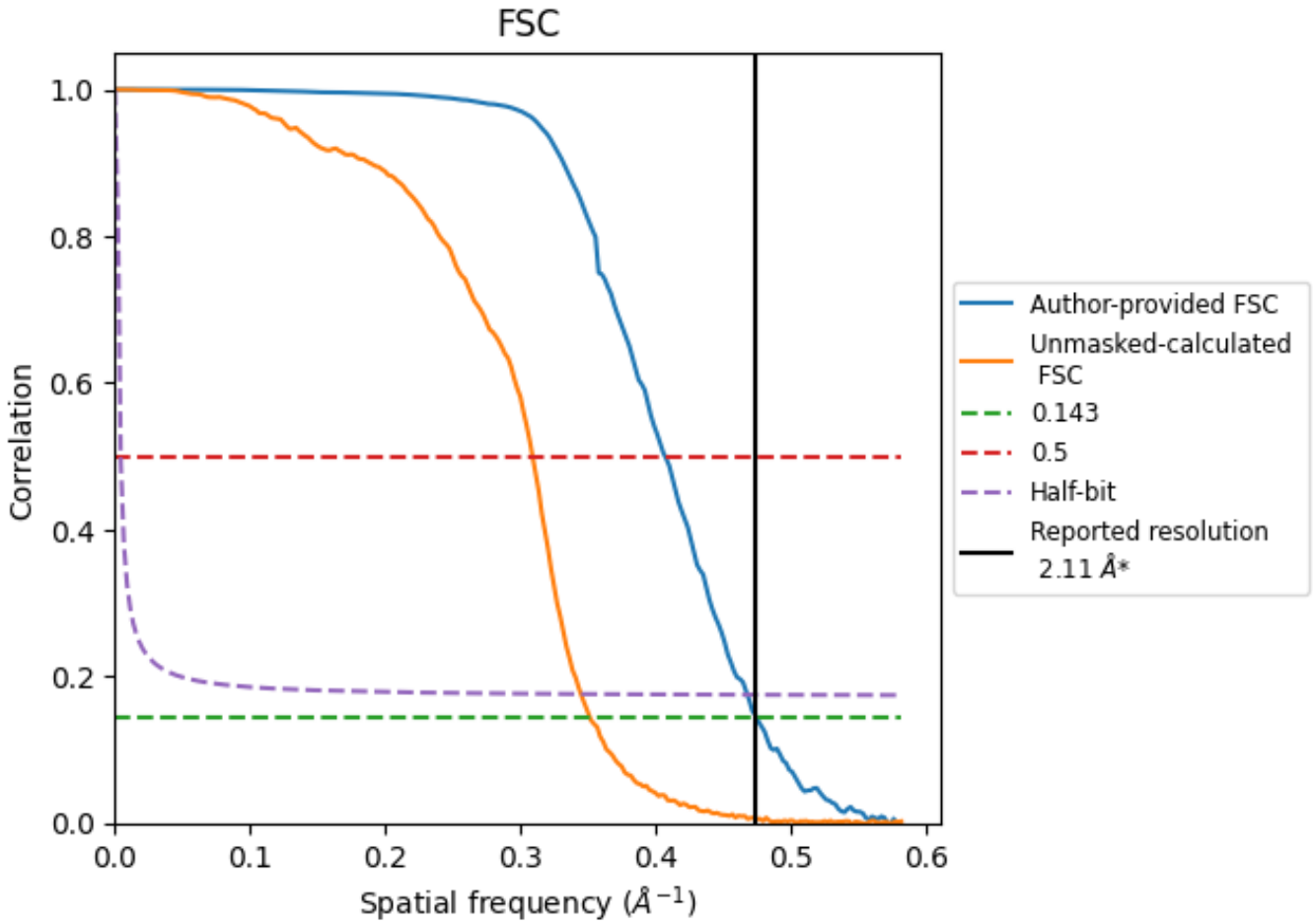


*Reported resolution corresponds to spatial frequency of 0.474 Å^{-1}

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 0.474 $Å^{-1}$

8.2 Resolution estimates (i)

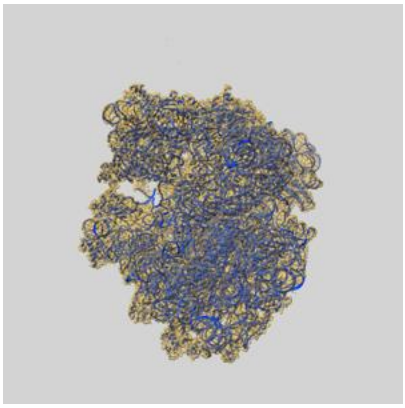
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.11	-	-
Author-provided FSC curve	2.11	2.46	2.14
Unmasked-calculated*	2.85	3.24	2.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.85 differs from the reported value 2.11 by more than 10 %

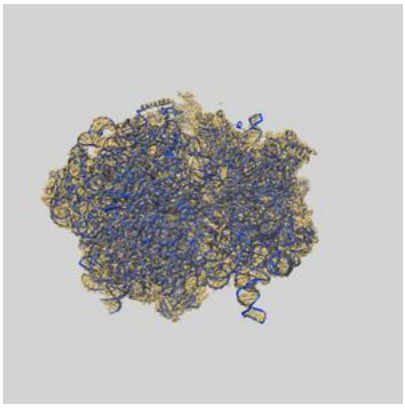
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16029 and PDB model 8BGE. Per-residue inclusion information can be found in section 3 on page 14.

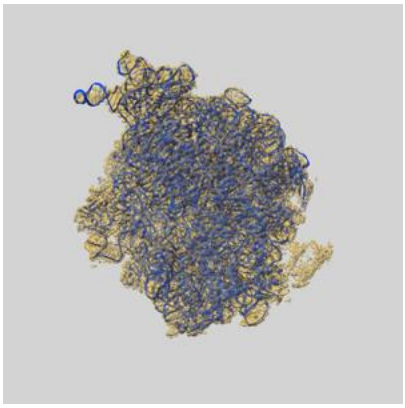
9.1 Map-model overlay



X



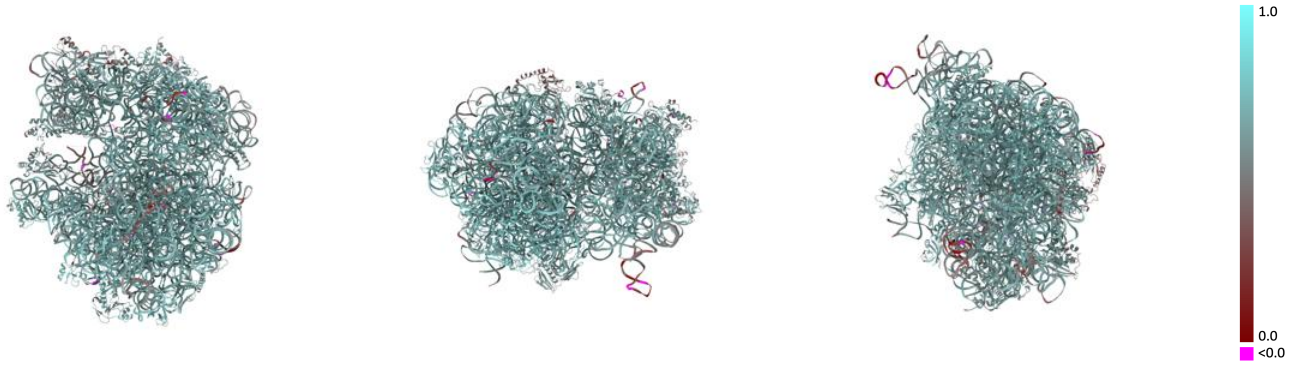
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0647 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

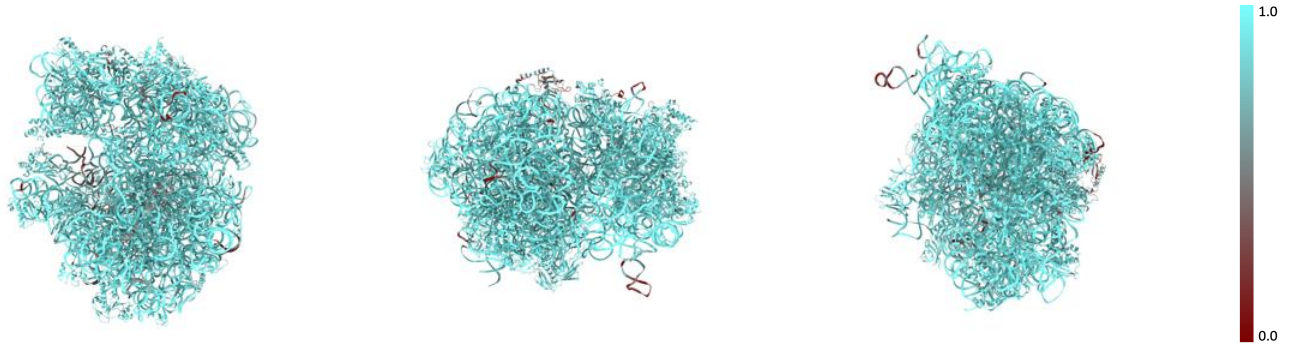
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

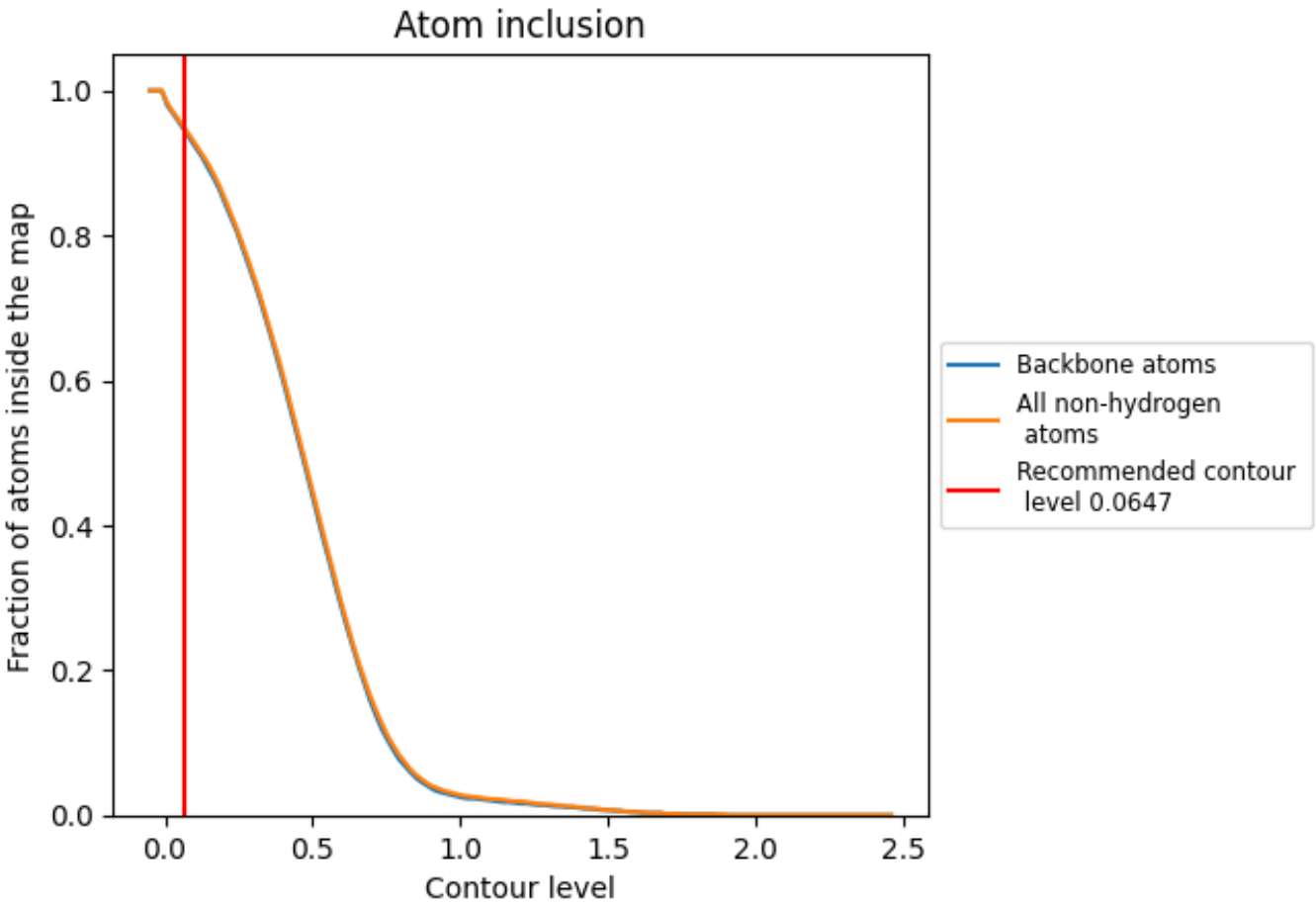
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0647).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0647) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9490	0.6490
0	0.9710	0.6700
1	0.9700	0.6430
2	0.9620	0.6290
3	0.8520	0.6020
4	0.7320	0.5240
A	0.9700	0.7080
B	0.9580	0.6970
C	0.9470	0.6730
D	0.8490	0.5560
E	0.9110	0.6130
F	0.5440	0.4290
G	0.9640	0.6950
H	0.9630	0.6990
I	0.9610	0.6930
J	0.9600	0.6850
K	0.9840	0.7210
L	0.9430	0.6490
M	0.9370	0.6780
N	0.9780	0.7180
O	0.9470	0.6850
P	0.9490	0.6820
Q	0.9140	0.6500
R	0.9020	0.6550
S	0.9310	0.6550
T	0.9500	0.6900
U	0.9630	0.6970
V	0.9140	0.6400
W	0.9460	0.6860
a	0.9500	0.7050
b	0.8970	0.6510
c	0.9720	0.7090
d	0.9720	0.7090
e	0.9560	0.6860
f	0.8680	0.5650

Continued on next page...

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Chain	Atom inclusion	Q-score
g	0.9330	0.6300
h	0.8880	0.6060
i	0.9570	0.6710
j	0.8970	0.6020
k	0.8220	0.5420
l	0.9530	0.6680
m	0.9020	0.5950
n	0.8830	0.5490
o	0.9350	0.6390
p	0.9150	0.6420
q	0.8970	0.5950
r	0.9260	0.6270
s	0.9160	0.6350
t	0.9360	0.6420
u	0.8940	0.6170
v	0.7610	0.5230
w	0.9020	0.5740
x	0.9420	0.6550
y	0.7710	0.5180