wwPDB EM Validation Summary Report

Mar 2, 2024 – 01:35 PM EST

PDB ID	:	5UYP
EMDB ID	:	EMD-8619
Title	:	70S ribosome bound with near-cognate ternary complex base-paired to A site codon, open 30S (Structure II-nc)
Authors	:	Loveland, A.B.; Demo, G.; Grigorieff, N.; Korostelev, A.A.
Deposited on	:	2017-02-24
Resolution	:	3.90 Å(reported)

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

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

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

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

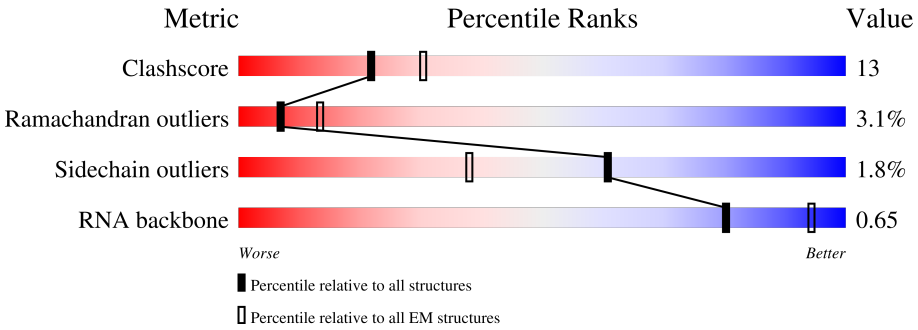
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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	04	271	58% 40%
2	05	209	65% 34%
3	06	201	5% 68% 31%
4	07	177	57% 41%
5	08	176	60% 40%
6	09	149	44% 56% 42%
7	10	131	40% 46% 47% 7%

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Mol	Chain	Length	Quality of chain
8	11	141	35% 44% 52%
9	12	142	66% 33%
10	13	122	11% 47% 51%
11	14	143	64% 34%
12	15	136	6% 65% 33%
13	16	120	67% 31%
14	17	116	64% 34%
15	18	114	55% 45%
16	19	117	64% 35%
17	20	103	51% 48%
18	21	110	68% 30%
19	22	93	61% 37%
20	23	102	52% 45%
21	24	94	65% 34%
22	25	75	5% 65% 33%
23	26	77	51% 49%
24	27	63	5% 60% 40%
25	28	58	5% 48% 50%
26	29	66	8% 70% 29%
27	30	56	54% 46%
28	31	50	62% 38%
29	32	46	67% 33%
30	33	64	61% 38%
31	34	38	76% 21%
32	B	218	8% 50% 46%

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Mol	Chain	Length	Quality of chain
33	C	206	9% 64% 36%
34	D	205	7% 67% 29%
35	E	157	6% 50% 46%
36	F	100	48% 46% 6%
37	G	151	8% 52% 47%
38	H	129	66% 33%
39	I	127	49% 48%
40	J	98	16% 41% 48% 11%
41	K	116	5% 65% 31%
42	L	123	15% 54% 41%
43	M	114	61% 34%
44	N	100	7% 42% 56%
45	O	88	68% 32%
46	P	82	6% 61% 35%
47	Q	80	46% 51%
48	R	65	5% 58% 34% 8%
49	S	79	53% 44%
50	T	85	60% 39%
51	U	65	18% 55% 38% 6%
52	03	223	18% 33% 25% 40%
53	A	1539	56% 38% 6%
54	01	2903	54% 40% 5%
55	02	120	63% 28% 8%
56	W	77	69% 27%
56	X	77	8% 58% 38%

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Mol	Chain	Length	Quality of chain
57	V	19	
58	Y	76	
59	Z	392	

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 153780 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	04	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	05	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	06	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	07	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	08	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	09	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	10	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	11	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	12	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	13	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	14	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	15	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	16	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	17	116	Total 892	C 552	N 178	O 162	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	18	114	Total 917	C 574	N 179	O 163	S 1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	19	117	Total 947	C 604	N 192	O 151	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	20	103	Total 816	C 516	N 153	O 145	S 2	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	21	110	Total 857	C 532	N 166	O 156	S 3	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	22	93	Total 739	C 466	N 139	O 132	S 2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	23	102	Total 780	C 492	N 146	O 142	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	24	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	25	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	26	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	27	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	28	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	29	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	30	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	31	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	32	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	33	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	34	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	C	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	F	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	G	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	J	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	K	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	M	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	R	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S	79	Total 638	C 408	N 120	O 108	S 2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	T	85	Total 665	C 411	N 137	O 114	S 3	0	0

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	U	65	Total 545	C 335	N 117	O 92	S 1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	03	134	Total 1027	C 645	N 186	O 194	S 2	0	0

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A	1539	Total 33012	C 14725	N 6052	O 10697	P 1538	0	0

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	01	2903	Total 62317	C 27801	N 11468	O 20146	P 2902	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
01	747	C	U	conflict	GB 802133627

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	02	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

- Molecule 56 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
56	W	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	V	19	Total	C	N	O	P	0	0
			417	188	89	122	18		

- Molecule 58 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Y	76	Total	C	N	O	P	S	0	0
			1618	723	282	536	76	1		

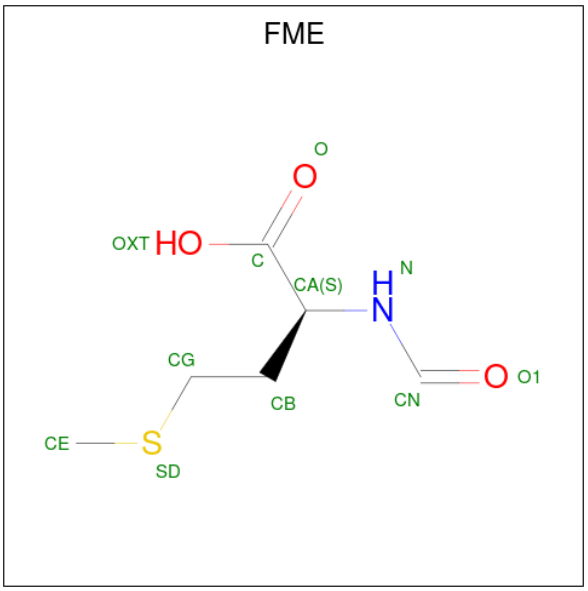
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	34	U8U	-	insertion	GB 558570689

- Molecule 59 is a protein called Elongation factor Tu 2.

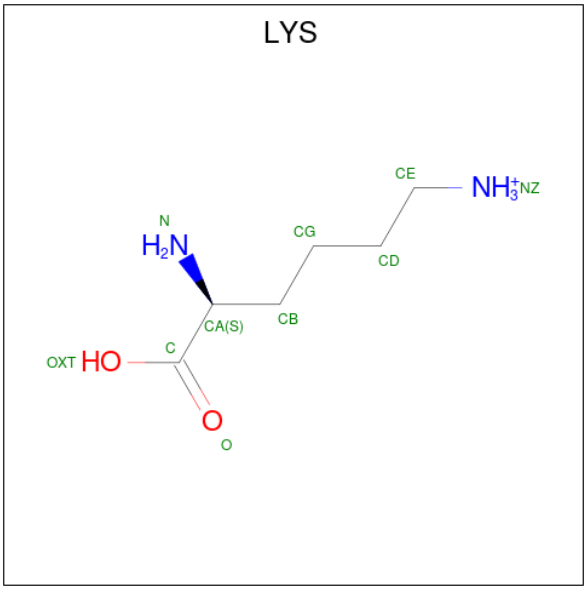
Mol	Chain	Residues	Atoms					AltConf	Trace
59	Z	392	Total	C	N	O	S	0	0
			3029	1915	521	580	13		

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



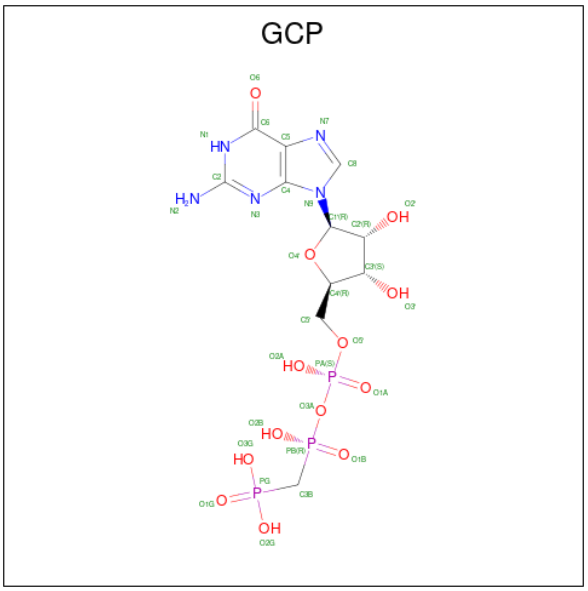
Mol	Chain	Residues	Atoms					AltConf
60	W	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 61 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
61	Y	1	Total	C	N	O	0
			9	6	2	1	

- Molecule 62 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



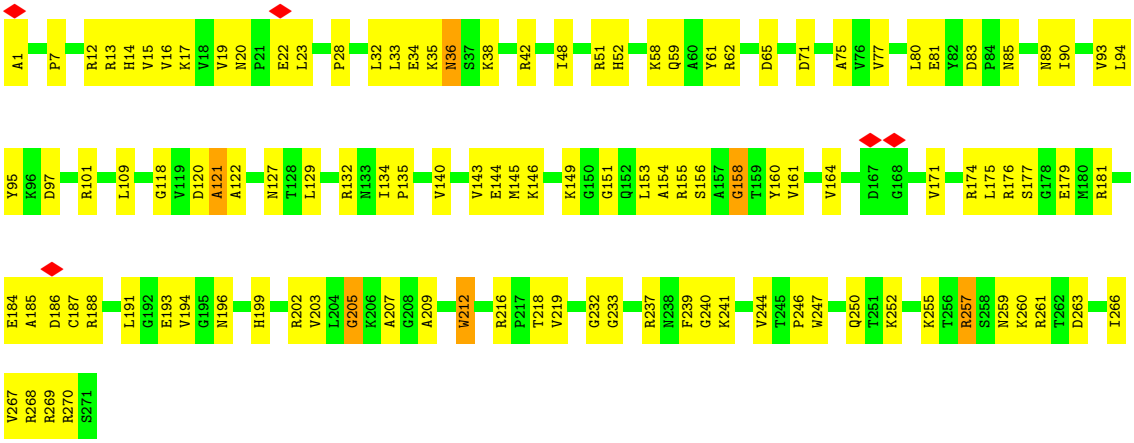
Mol	Chain	Residues	Atoms					AltConf
62	Z	1	Total	C	N	O	P	0
			32	11	5	13	3	

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.

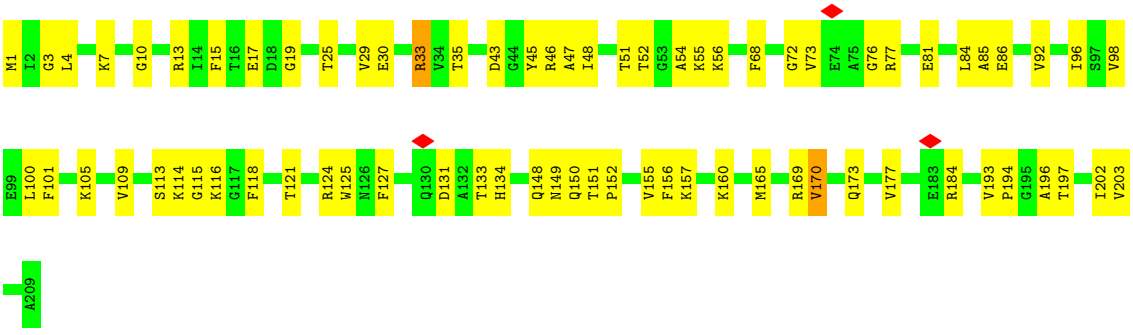
• Molecule 1: 50S ribosomal protein L2

Chain 04:



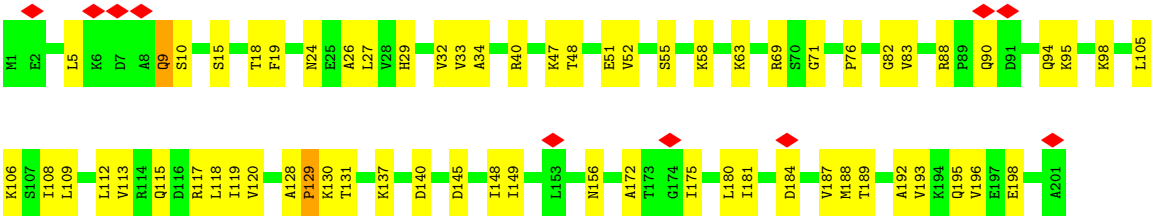
• Molecule 2: 50S ribosomal protein L3

Chain 05:



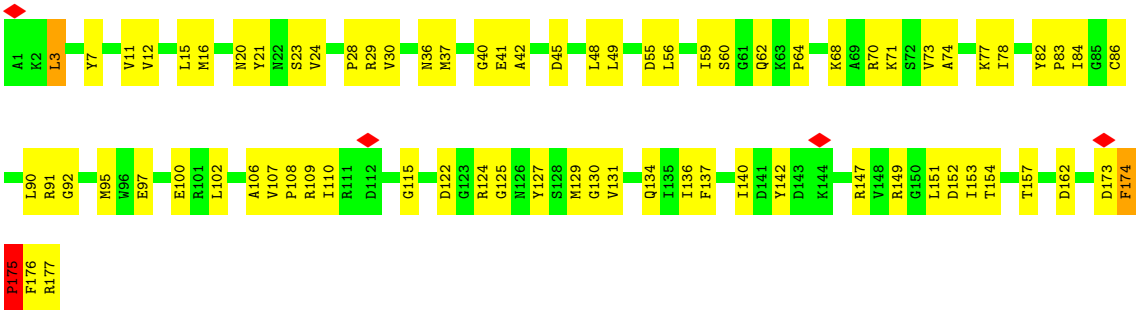
• Molecule 3: 50S ribosomal protein L4

Chain 06:



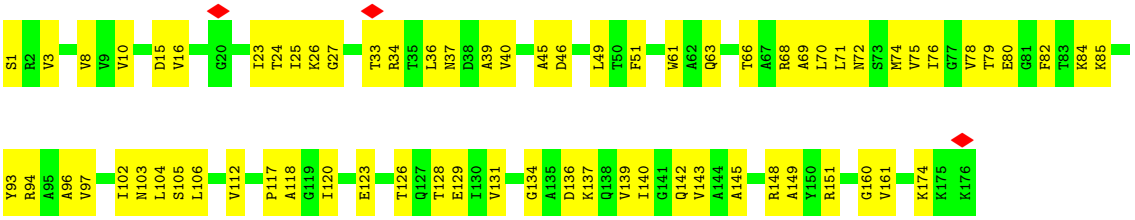
• Molecule 4: 50S ribosomal protein L5

Chain 07:



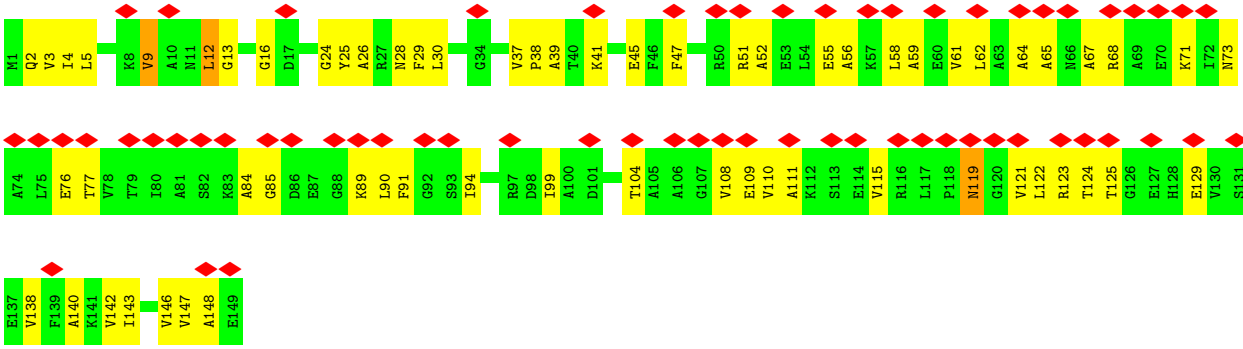
• Molecule 5: 50S ribosomal protein L6

Chain 08:



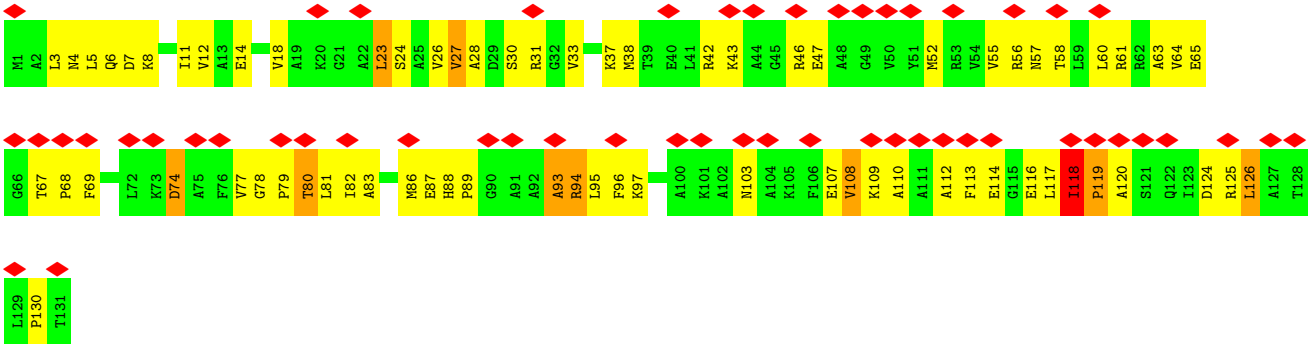
• Molecule 6: 50S ribosomal protein L9

Chain 09:

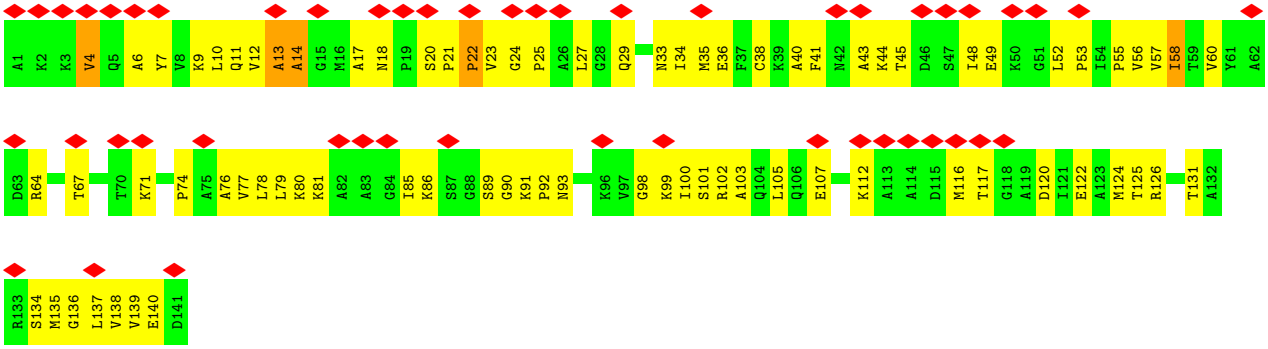


• Molecule 7: 50S ribosomal protein L10

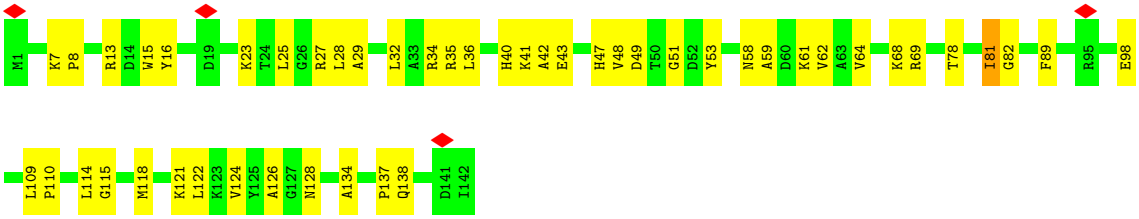
Chain 10:



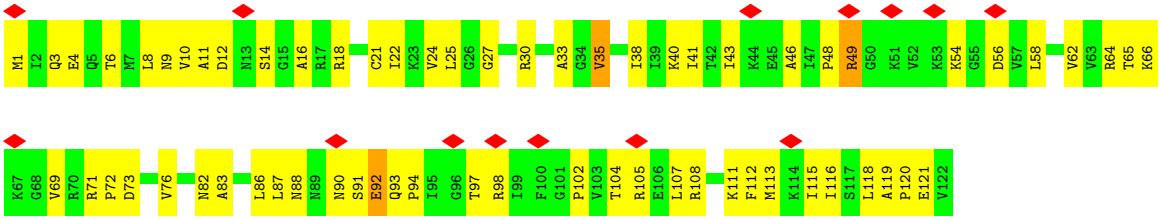
• Molecule 8: 50S ribosomal protein L11



• Molecule 9: 50S ribosomal protein L13

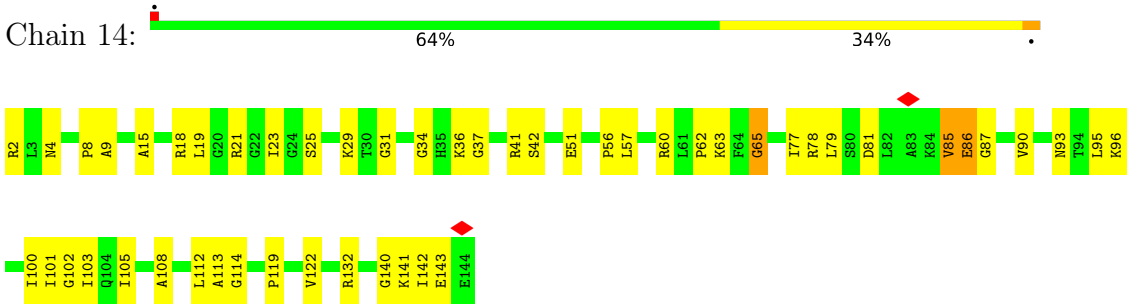


• Molecule 10: 50S ribosomal protein L14



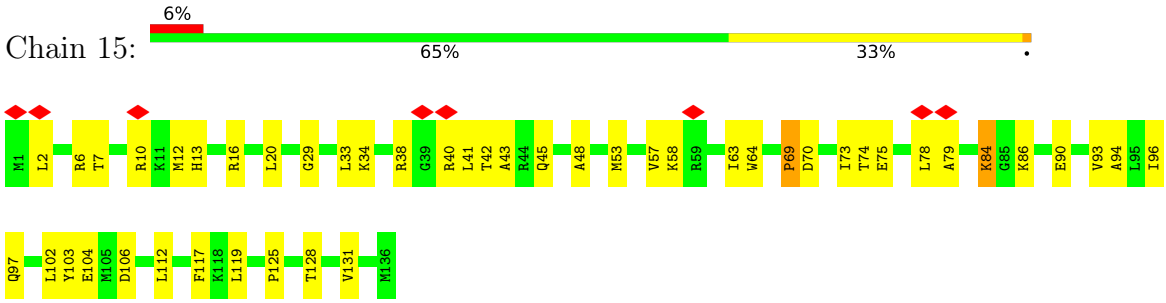
• Molecule 11: 50S ribosomal protein L15

Chain 14:



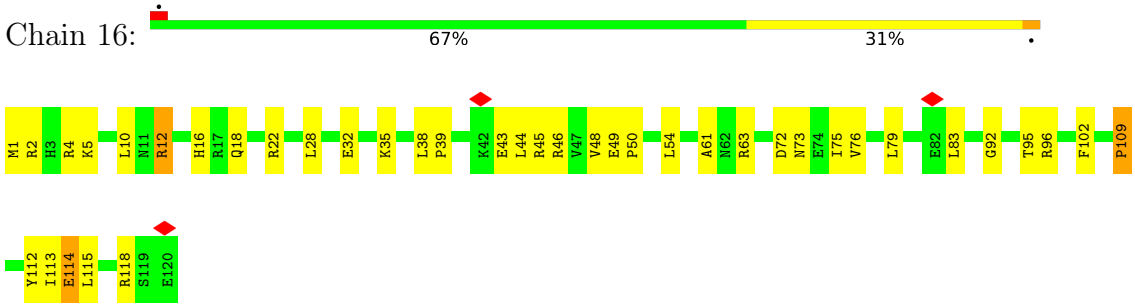
• Molecule 12: 50S ribosomal protein L16

Chain 15:



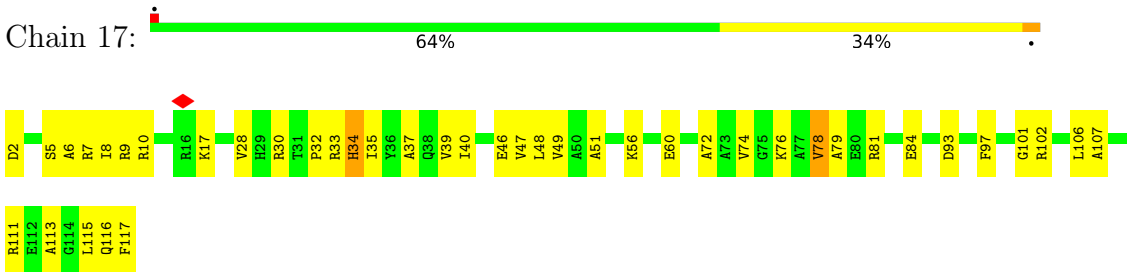
• Molecule 13: 50S ribosomal protein L17

Chain 16:



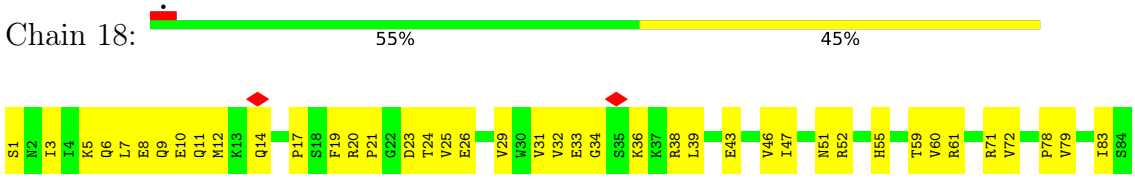
• Molecule 14: 50S ribosomal protein L18

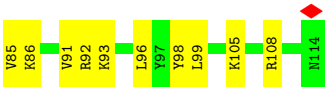
Chain 17:



• Molecule 15: 50S ribosomal protein L19

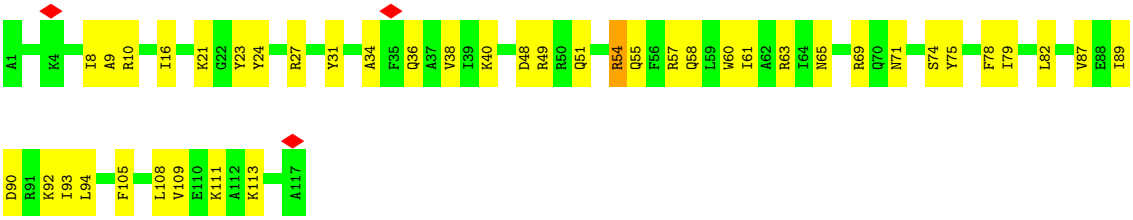
Chain 18:





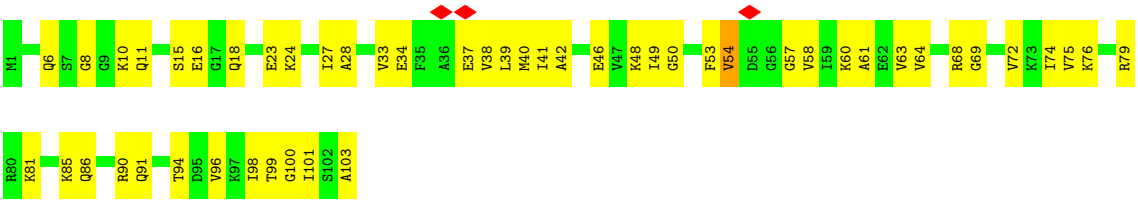
• Molecule 16: 50S ribosomal protein L20

Chain 19:



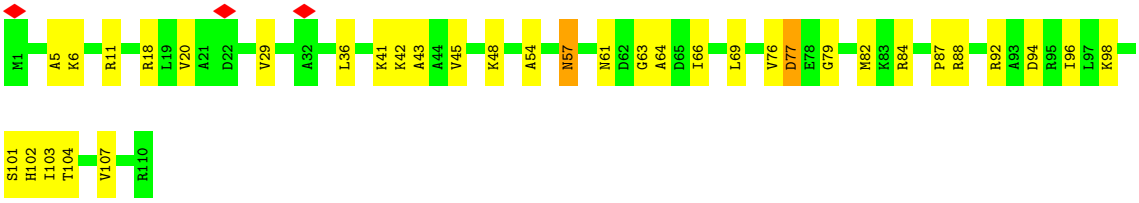
• Molecule 17: 50S ribosomal protein L21

Chain 20:



• Molecule 18: 50S ribosomal protein L22

Chain 21:

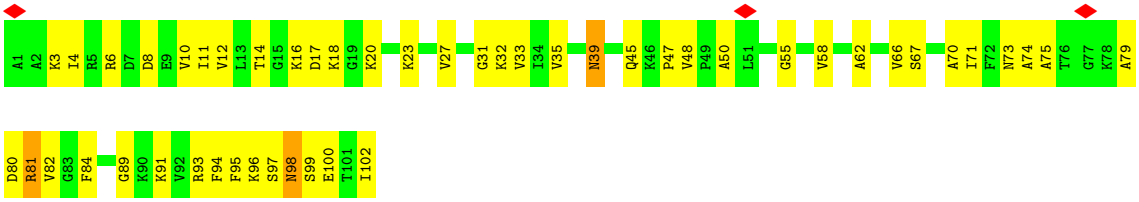


• Molecule 19: 50S ribosomal protein L23

Chain 22:

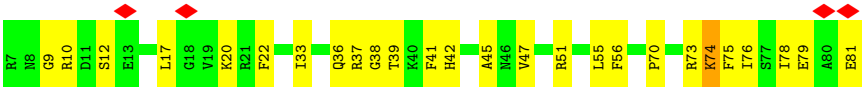
• Molecule 20: 50S ribosomal protein L24

Chain 23:

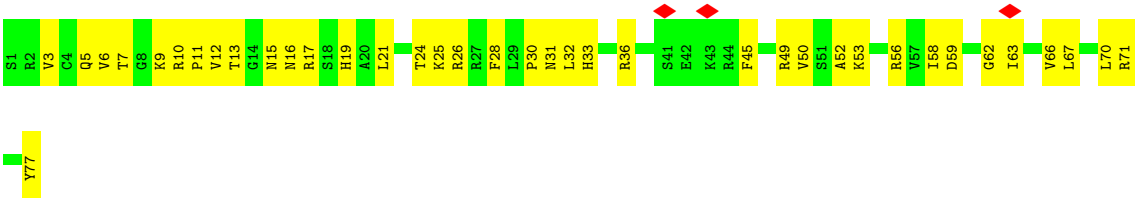


• Molecule 21: 50S ribosomal protein L25

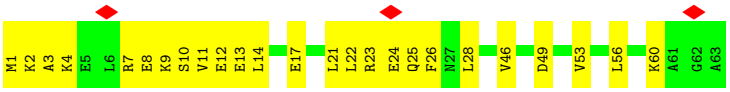
• Molecule 22: 50S ribosomal protein L27



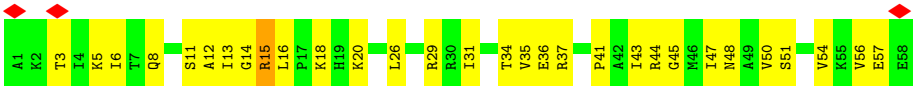
• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29

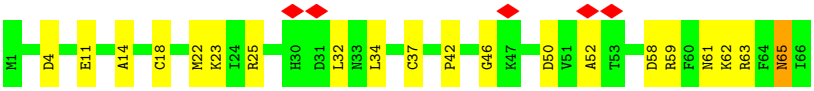


• Molecule 25: 50S ribosomal protein L30



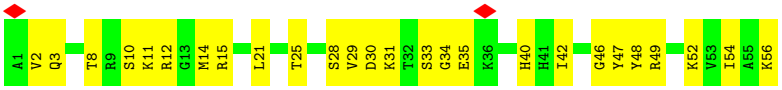
• Molecule 26: 50S ribosomal protein L31

Chain 29:



• Molecule 27: 50S ribosomal protein L32

Chain 30:

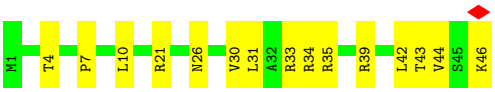


• Molecule 28: 50S ribosomal protein L33

Chain 31:

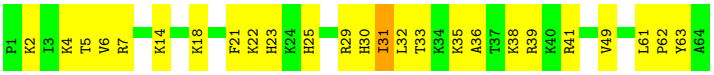
• Molecule 29: 50S ribosomal protein L34

Chain 32:



• Molecule 30: 50S ribosomal protein L35

Chain 33:

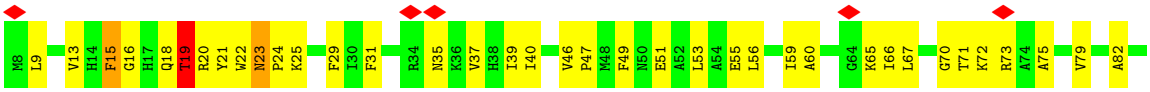


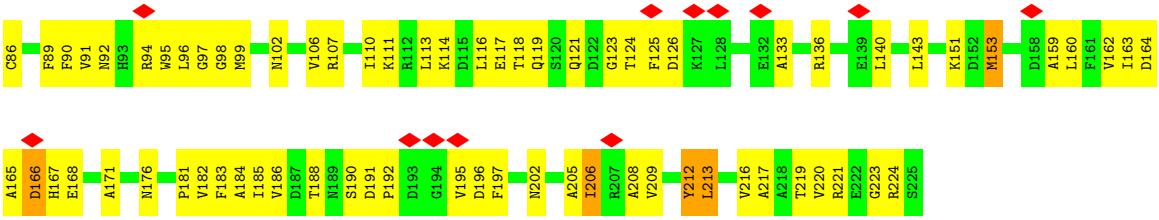
• Molecule 31: 50S ribosomal protein L36

Chain 34:

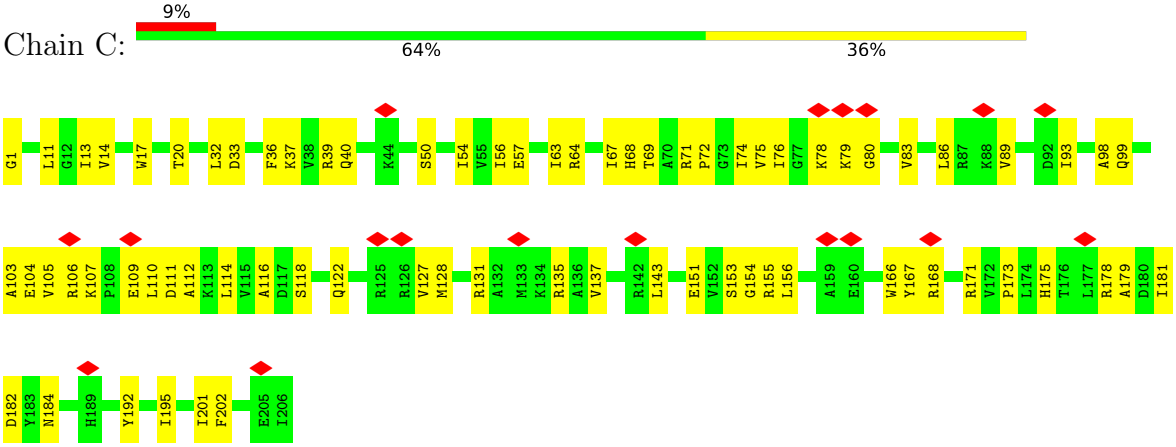
• Molecule 32: 30S ribosomal protein S2

Chain B:

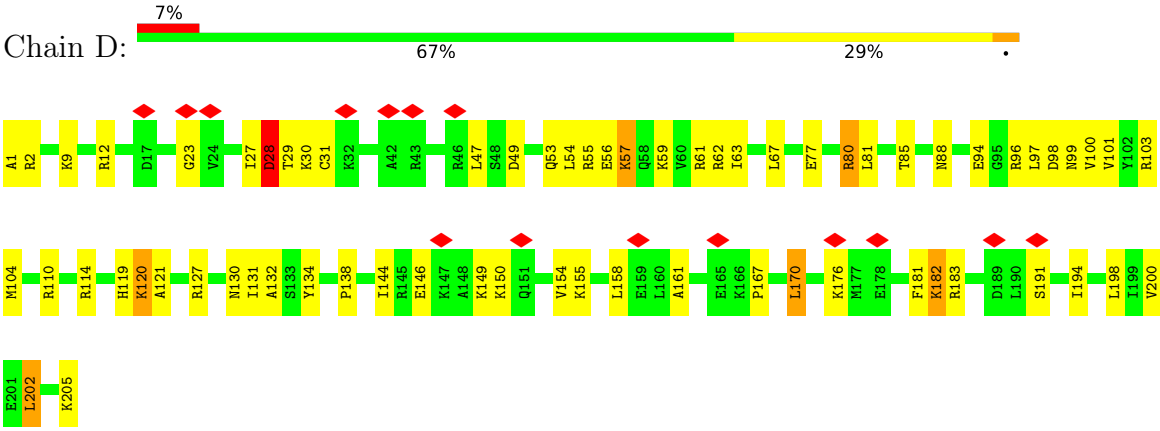




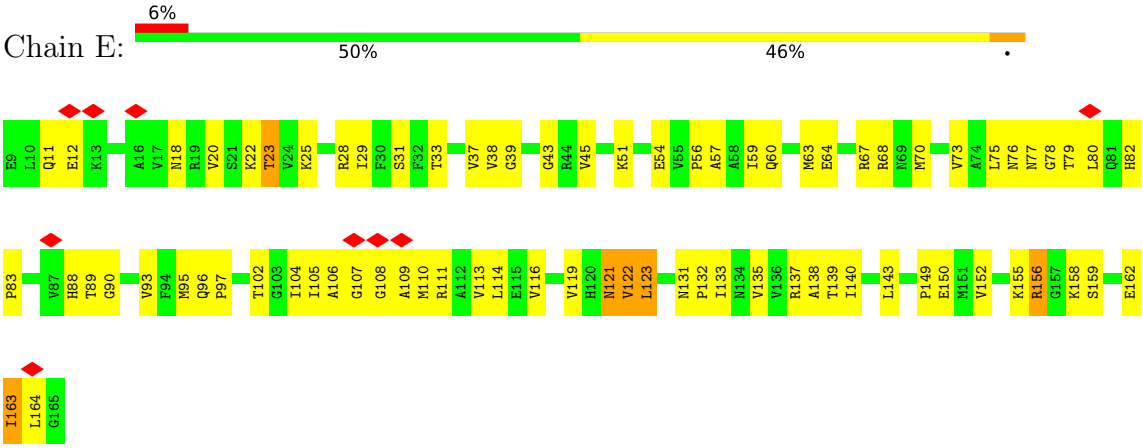
• Molecule 33: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S4

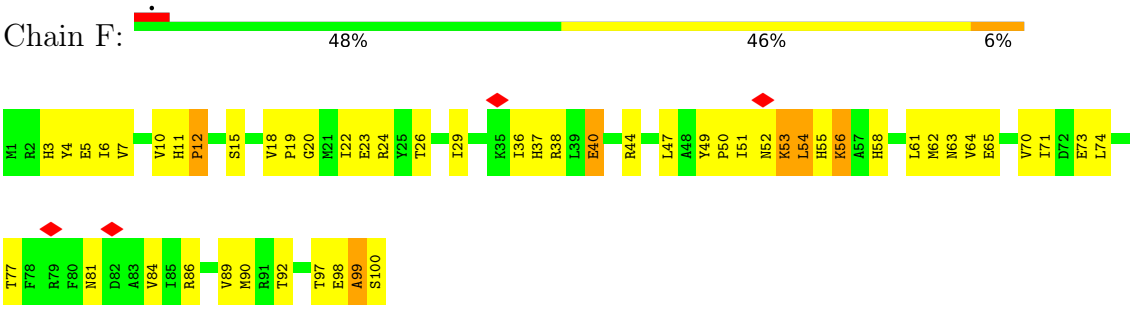


• Molecule 35: 30S ribosomal protein S5



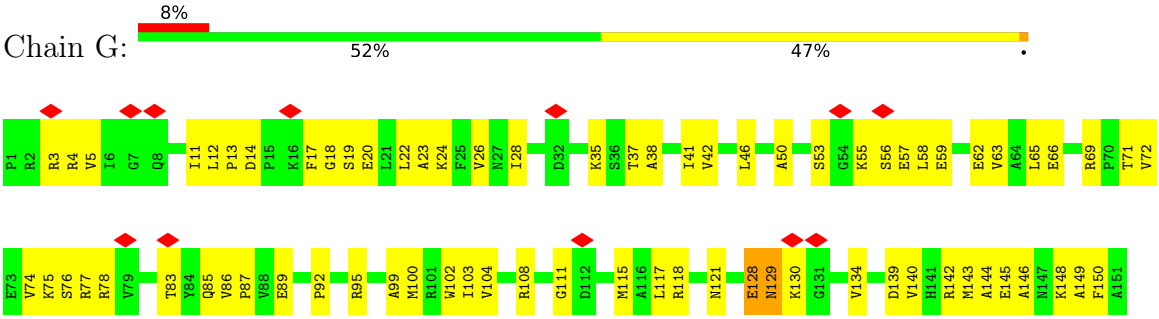
• Molecule 36: 30S ribosomal protein S6

Chain F:



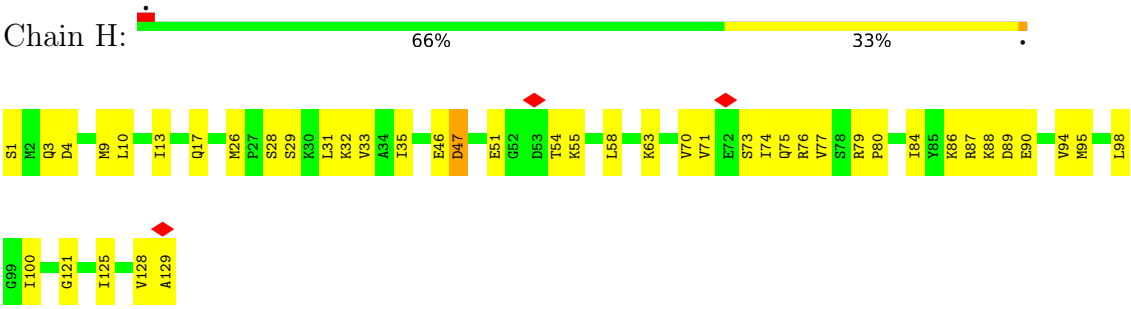
• Molecule 37: 30S ribosomal protein S7

Chain G:



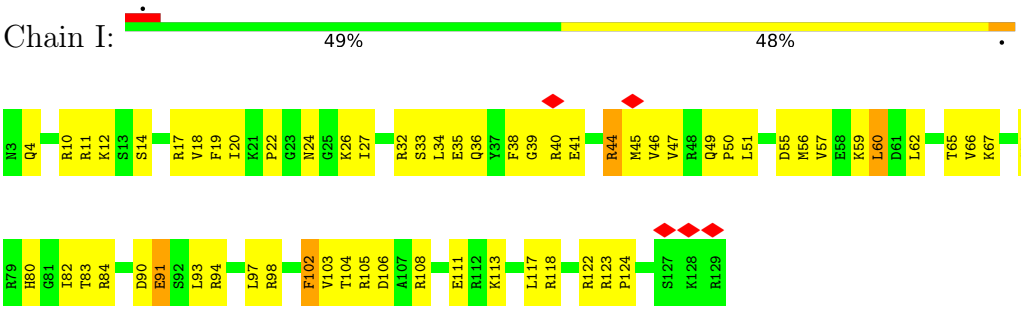
• Molecule 38: 30S ribosomal protein S8

Chain H:



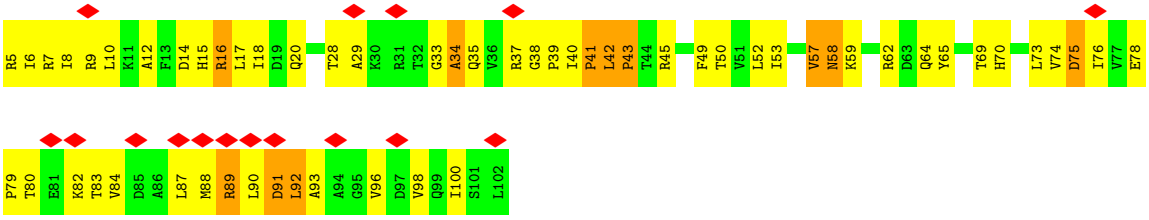
• Molecule 39: 30S ribosomal protein S9

Chain I:

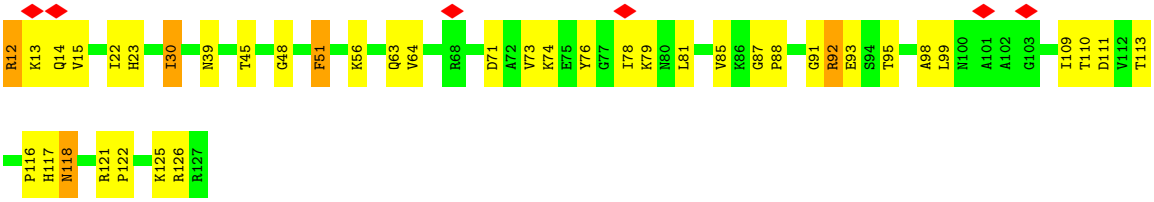


• Molecule 40: 30S ribosomal protein S10

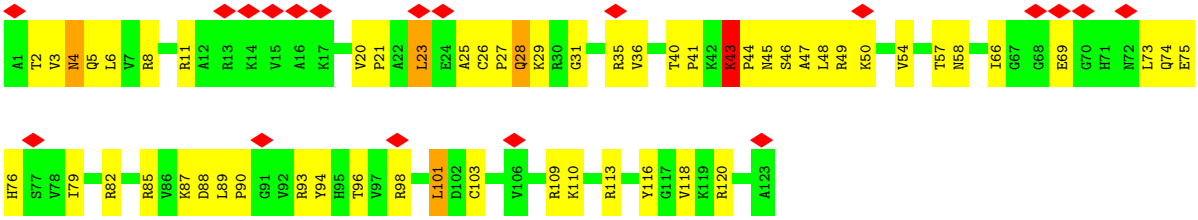
Chain J:



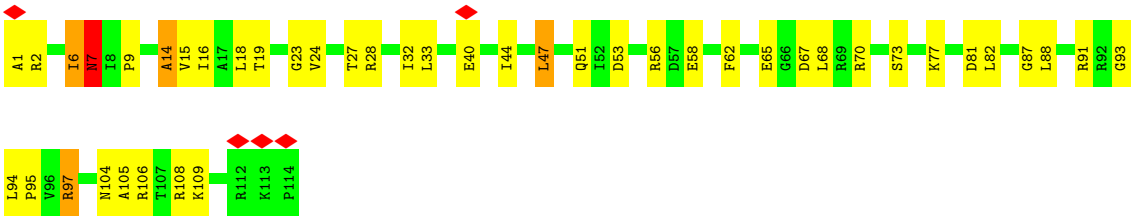
• Molecule 41: 30S ribosomal protein S11



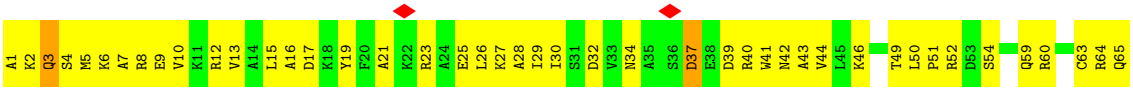
• Molecule 42: 30S ribosomal protein S12

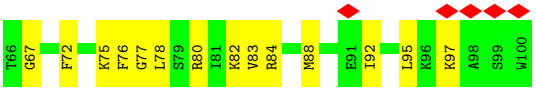


• Molecule 43: 30S ribosomal protein S13

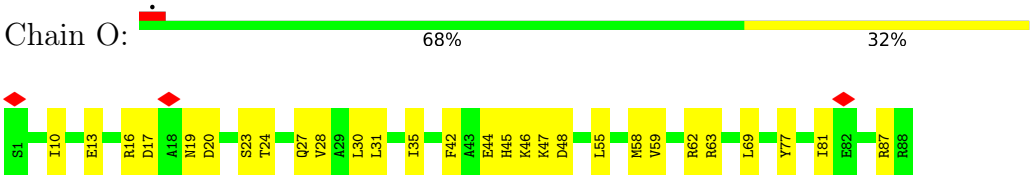


• Molecule 44: 30S ribosomal protein S14

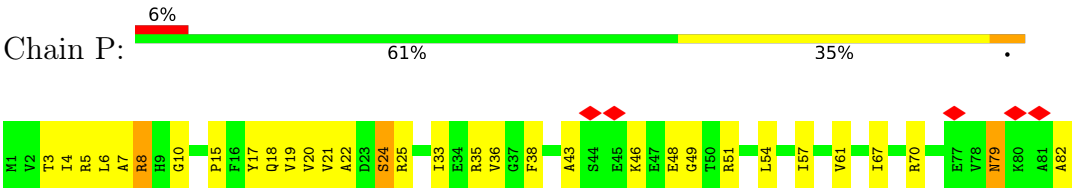




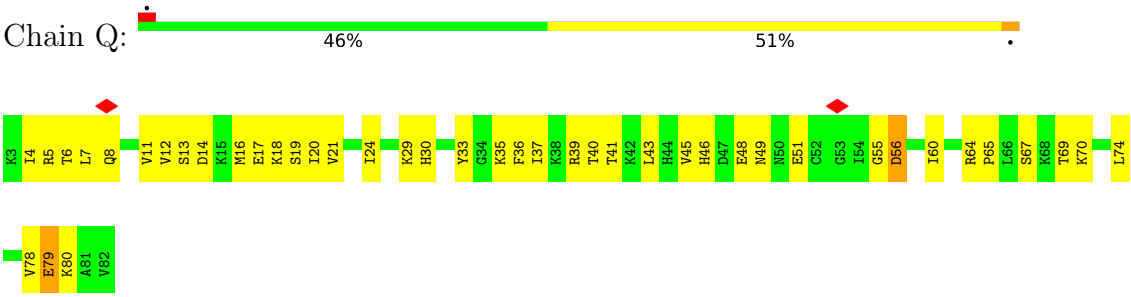
• Molecule 45: 30S ribosomal protein S15



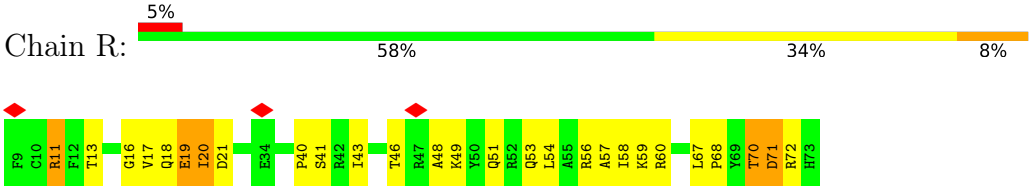
• Molecule 46: 30S ribosomal protein S16



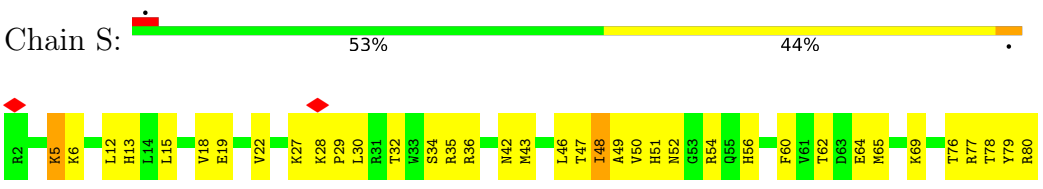
• Molecule 47: 30S ribosomal protein S17



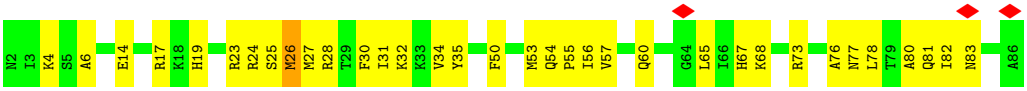
• Molecule 48: 30S ribosomal protein S18



• Molecule 49: 30S ribosomal protein S19

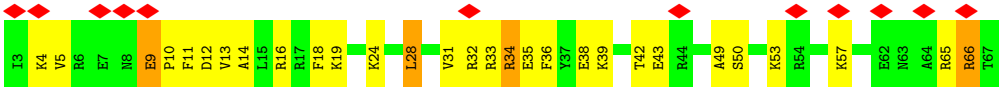


• Molecule 50: 30S ribosomal protein S20



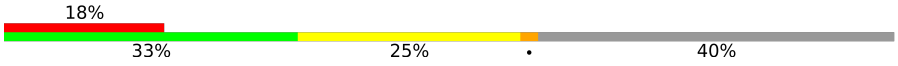
• Molecule 51: 30S ribosomal protein S21

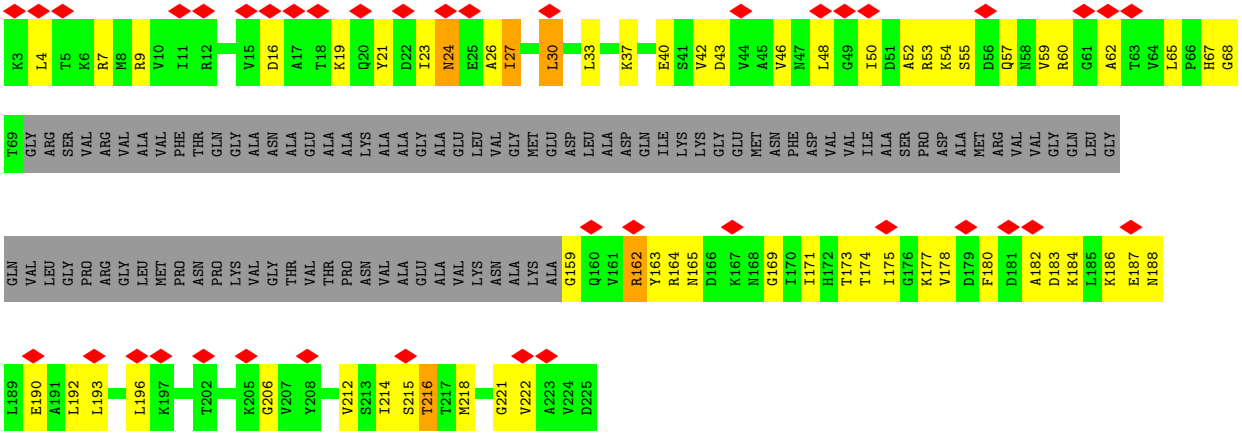
Chain U:



• Molecule 52: 50S ribosomal protein L1

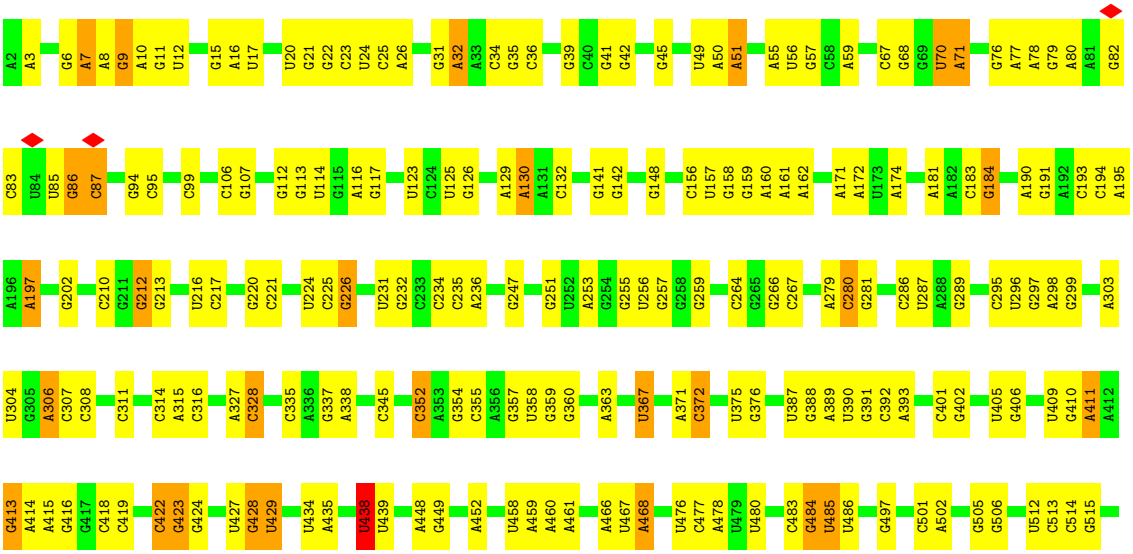
Chain 03:

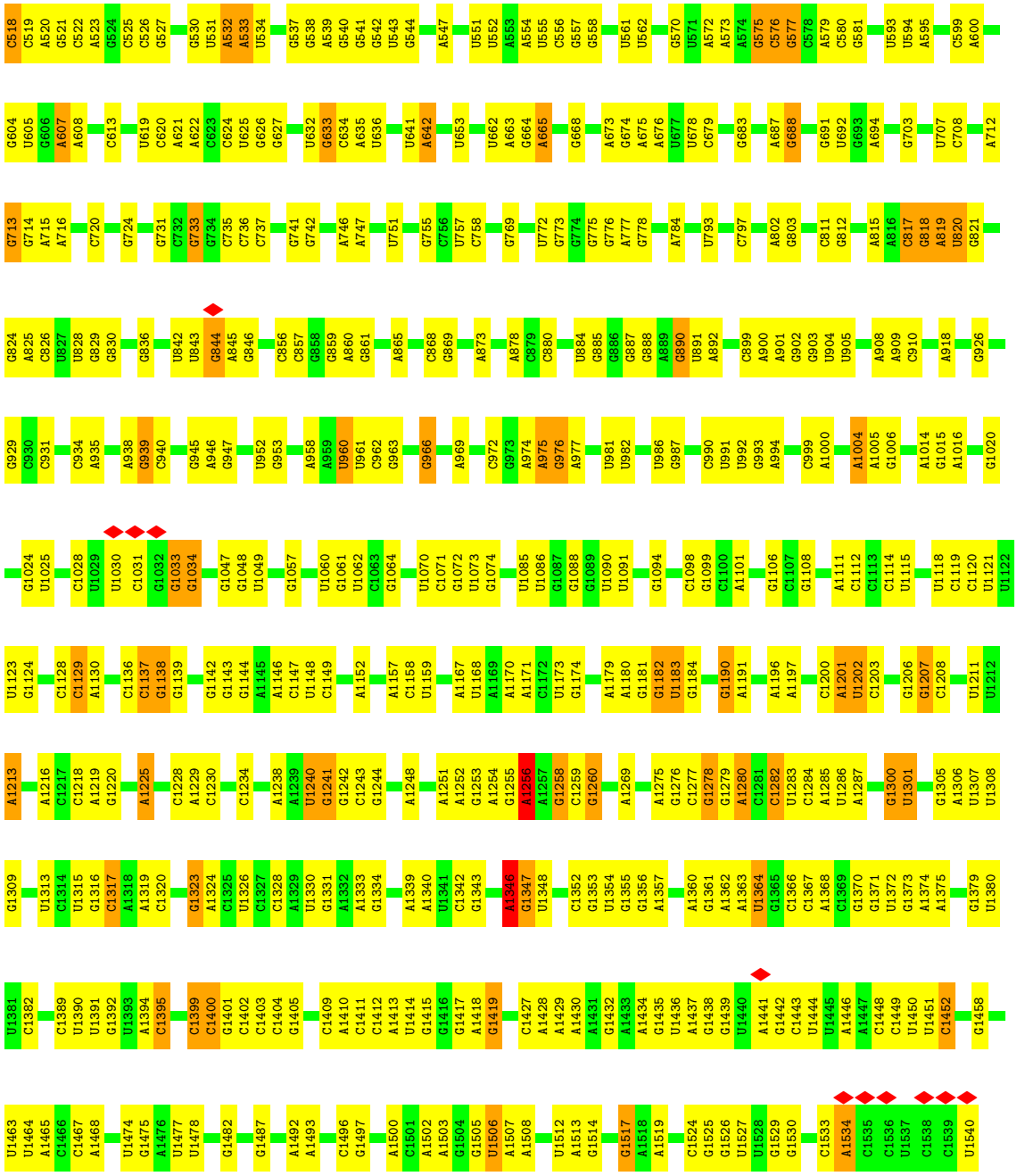




• Molecule 53: 16S ribosomal RNA

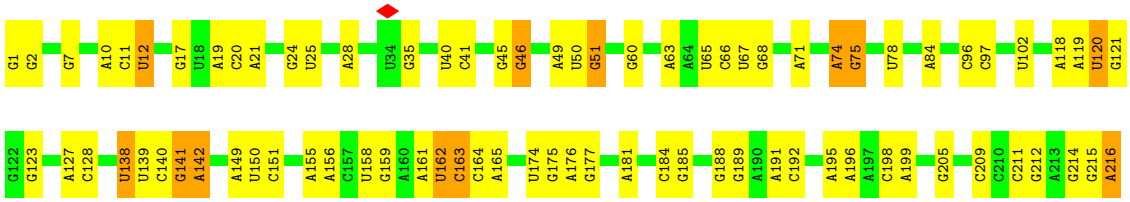
Chain A:

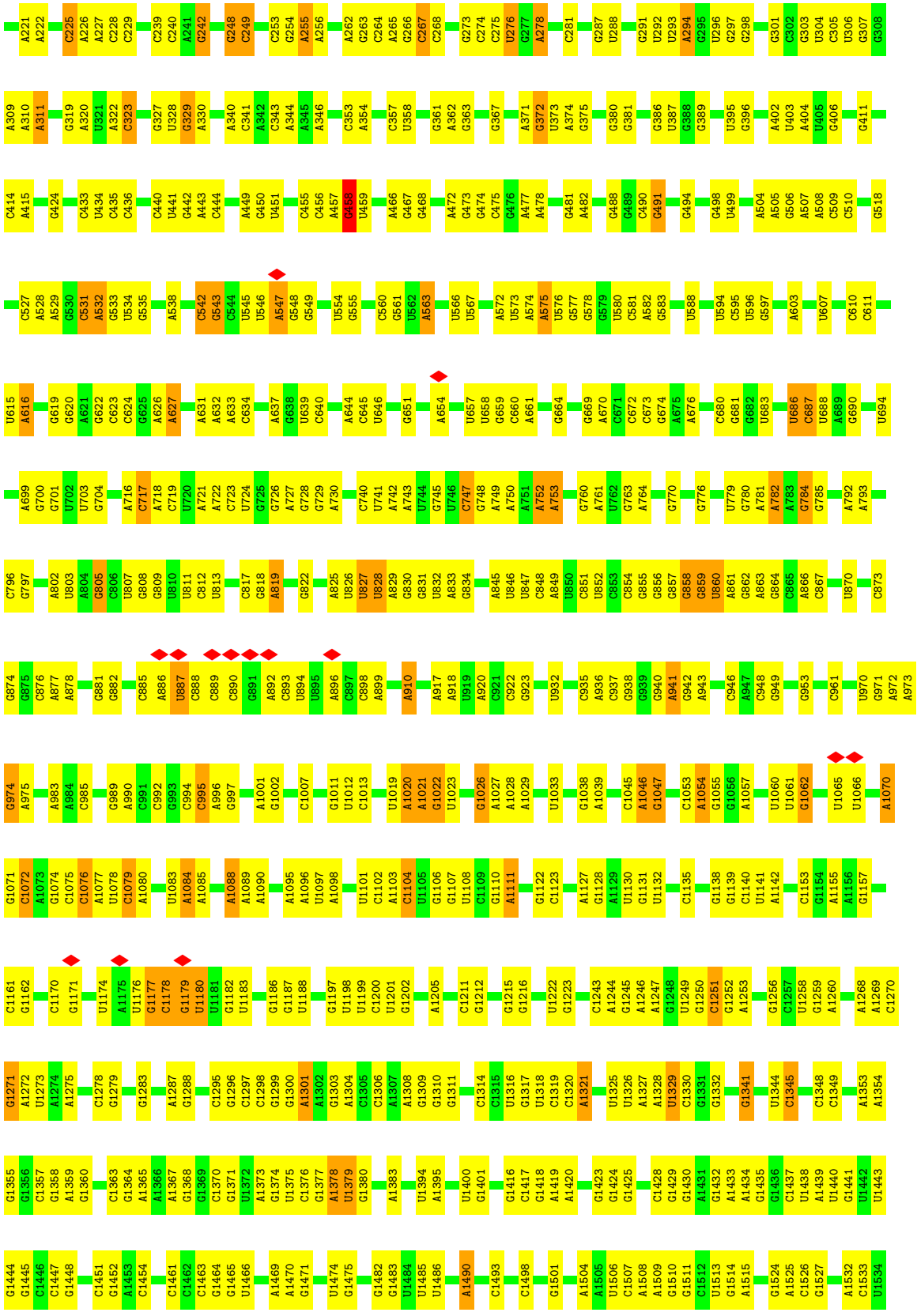


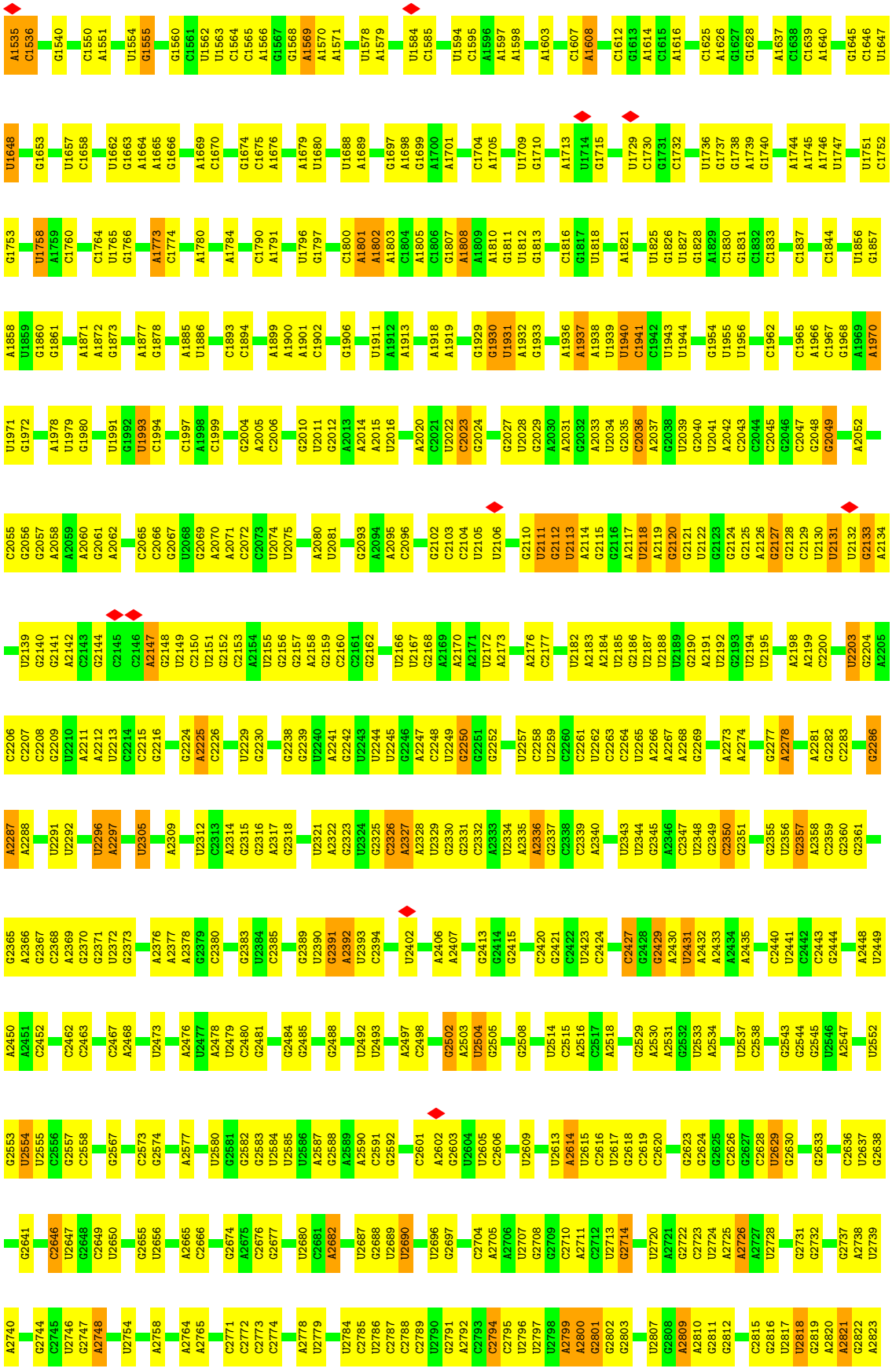


• Molecule 54: 23S ribosomal RNA

Chain 01:

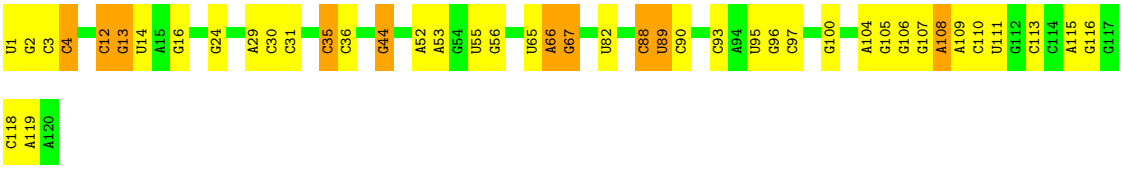






• Molecule 55: 5S ribosomal RNA

Chain 02:

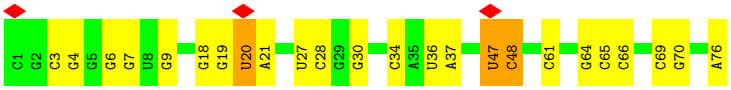


• Molecule 56: tRNAfMet

Chain X:

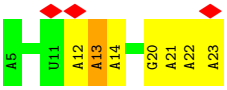
• Molecule 56: tRNAfMet

Chain W:



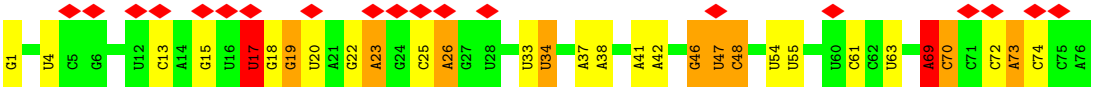
• Molecule 57: mRNA

Chain V:



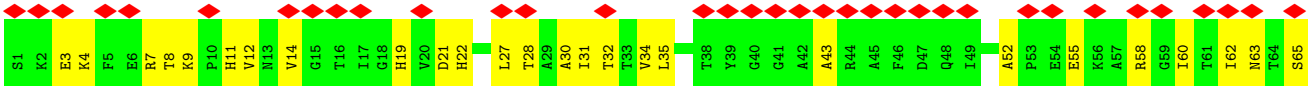
• Molecule 58: tRNALys

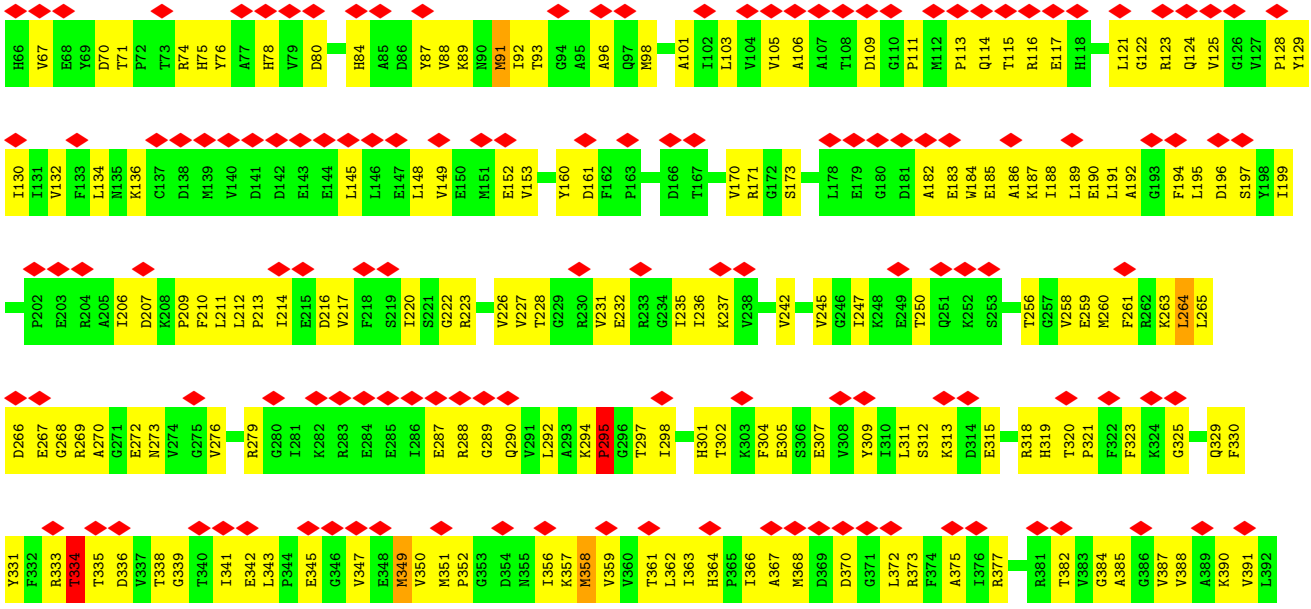
Chain Y:



• Molecule 59: Elongation factor Tu 2

Chain Z:




H66 V67 E68 Y69 D70 T71 P72 T73 R74 H75 Y76 A77 H78 V79 D80 H84 A85 D86 Y87 V88 K89 N90 N91 I92 T93 G94 A95 A96 Q97 N98 A101 I102 L103 V104 V105 A106 A107 T108 D109 G110 P111 M112 P113 Q114 T115 R116 E117 H118 L121 G122 R123 Q124 V125 G126 V127 P128 Y129
I130 I131 V132 F133 L134 N135 K136 C137 D138 M139 V140 D141 D142 E143 E144 L145 L146 E147 L148 V149 E150 M151 E152 V153 Y160 D161 F162 P163 D166 T167 V170 R171 G172 S173 L178 E179 G180 D181 A182 E183 W184 E185 A186 K187 I188 L189 E190 L191 A192 G193 F194 L195 D196 S197 Y198 I199
P202 E203 R204 A205 I206 D207 K208 P209 F210 L211 L212 P213 I214 E215 D216 V217 F218 S219 I220 S221 G222 R223 V226 V227 T228 G229 R230 V231 E232 R233 G234 I235 I236 K237 V238 V242 V245 G246 I247 K248 E249 T250 Q251 K252 S253 T256 G257 V258 E259 M260 F261 R262 K263 L264 L265
D266 E267 G268 R269 A270 G271 E272 N273 V274 G275 V276 R279 G280 I281 K282 R283 E284 E285 I286 E287 R288 G289 Q290 V291 L292 A293 K294 P295 G296 T297 I298 H301 T302 K303 F304 E305 S306 E307 V308 Y309 I310 L311 S312 K313 D314 E315 R318 H319 T320 P321 F322 F323 K324 G325 Q329 F330
Y331 F332 R333 T334 T335 D336 V337 T338 G339 T340 I341 E342 L343 P344 E345 G346 V347 E348 M349 V350 M351 P352 G353 D354 N355 I356 K357 M358 V359 V360 T361 L362 I363 H364 P365 I366 A367 M368 D369 D370 G371 L372 R373 F374 A375 I376 R377 R381 T382 V383 G384 A385 G386 V387 V388 A389 K390 V391 L392

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	6910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND3 was used to determine CTF values. FREALIGN applied CTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	60976	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	13.270	Depositor
Minimum map value	-6.345	Depositor
Average map value	-0.332	Depositor
Map value standard deviation	1.036	Depositor
Recommended contour level	2.78	Depositor
Map size (Å)	393.6, 393.6, 393.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U8U, FME, GCP

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	04	0.30	0/2122	0.59	0/2852
2	05	0.32	0/1586	0.57	0/2134
3	06	0.32	0/1571	0.59	0/2113
4	07	0.35	0/1435	0.58	0/1926
5	08	0.32	0/1343	0.62	0/1816
6	09	0.35	0/1122	0.62	1/1515 (0.1%)
7	10	0.40	0/1002	0.73	0/1350
8	11	0.37	0/1046	0.66	0/1410
9	12	0.33	0/1152	0.59	0/1551
10	13	0.31	0/948	0.58	0/1268
11	14	0.32	0/1054	0.64	0/1403
12	15	0.33	0/1093	0.59	0/1460
13	16	0.32	0/974	0.55	0/1301
14	17	0.31	0/902	0.56	0/1209
15	18	0.32	0/929	0.60	0/1242
16	19	0.33	0/960	0.52	0/1278
17	20	0.34	0/829	0.65	1/1107 (0.1%)
18	21	0.30	0/864	0.59	0/1156
19	22	0.32	0/745	0.58	0/994
20	23	0.33	0/788	0.62	0/1051
21	24	0.35	0/766	0.59	0/1025
22	25	0.33	0/582	0.54	0/769
23	26	0.31	0/635	0.55	0/848
24	27	0.32	0/510	0.60	0/677
25	28	0.30	0/453	0.58	0/605
26	29	0.35	0/532	0.64	0/709
27	30	0.32	0/450	0.56	0/599
28	31	0.35	0/417	0.57	0/554
29	32	0.33	0/380	0.60	0/498
30	33	0.31	0/513	0.58	0/676
31	34	0.32	0/303	0.60	0/397
32	B	0.36	0/1736	0.63	0/2338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	C	0.34	0/1652	0.54	0/2225
34	D	0.34	0/1665	0.58	0/2227
35	E	0.33	0/1170	0.65	1/1573 (0.1%)
36	F	0.35	0/836	0.64	0/1128
37	G	0.32	0/1196	0.57	0/1602
38	H	0.32	0/989	0.61	0/1326
39	I	0.34	0/1034	0.64	0/1375
40	J	0.34	0/797	0.65	0/1077
41	K	0.33	0/886	0.59	0/1195
42	L	0.32	0/969	0.66	1/1300 (0.1%)
43	M	0.31	0/893	0.59	0/1193
44	N	0.33	0/817	0.56	0/1088
45	O	0.31	0/722	0.53	0/964
46	P	0.33	0/659	0.58	0/884
47	Q	0.34	0/658	0.71	0/881
48	R	0.36	0/545	0.58	0/731
49	S	0.35	0/653	0.63	0/877
50	T	0.31	0/671	0.53	0/888
51	U	0.40	0/551	0.64	0/728
52	03	0.38	0/1034	0.67	0/1387
53	A	0.39	0/36963	0.69	10/57662 (0.0%)
54	01	0.39	0/69796	0.68	3/108888 (0.0%)
55	02	0.41	0/2872	0.68	1/4479 (0.0%)
56	W	0.44	0/1832	0.68	0/2855
56	X	0.48	0/1832	0.68	0/2855
57	V	0.41	0/471	0.63	0/735
58	Y	0.55	1/1780 (0.1%)	0.74	2/2767 (0.1%)
59	Z	0.38	0/3085	0.67	0/4173
All	All	0.38	1/166770 (0.0%)	0.66	20/248894 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	Y	1	G	OP3-P	-7.06	1.52	1.61

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	01	1178	C	N1-C1'-C2'	8.80	125.44	114.00
53	A	1301	U	N1-C1'-C2'	6.29	122.18	114.00
53	A	960	U	N1-C1'-C2'	6.09	121.92	114.00
17	20	50	GLY	N-CA-C	-5.95	98.23	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	1256	A	N9-C1'-C2'	5.87	121.63	114.00

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	04	2083	0	2157	88	0
2	05	1565	0	1616	53	0
3	06	1552	0	1619	48	0
4	07	1411	0	1447	59	0
5	08	1323	0	1374	55	0
6	09	1111	0	1148	52	0
7	10	989	0	1025	60	0
8	11	1032	0	1088	74	0
9	12	1129	0	1162	44	0
10	13	939	0	1012	39	0
11	14	1045	0	1117	46	0
12	15	1074	0	1157	39	0
13	16	961	0	1000	32	0
14	17	892	0	923	34	0
15	18	917	0	965	43	0
16	19	947	0	1022	34	0
17	20	816	0	839	38	0
18	21	857	0	922	36	0
19	22	739	0	807	26	0
20	23	780	0	834	40	0
21	24	753	0	780	25	0
22	25	575	0	592	24	0
23	26	625	0	655	31	0
24	27	509	0	543	23	0
25	28	449	0	491	22	0
26	29	523	0	524	11	0
27	30	444	0	461	24	0
28	31	410	0	440	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	32	377	0	418	15	0
30	33	504	0	574	19	0
31	34	302	0	343	9	0
32	B	1705	0	1732	77	0
33	C	1625	0	1699	58	0
34	D	1643	0	1710	55	0
35	E	1157	0	1199	53	0
36	F	818	0	808	44	0
37	G	1182	0	1240	56	0
38	H	979	0	1034	38	0
39	I	1022	0	1070	57	0
40	J	787	0	828	52	0
41	K	870	0	878	33	0
42	L	955	0	1019	48	0
43	M	884	0	944	42	0
44	N	805	0	847	47	0
45	O	714	0	737	17	0
46	P	649	0	666	33	0
47	Q	649	0	691	32	0
48	R	536	0	552	19	0
49	S	638	0	665	32	0
50	T	665	0	714	30	0
51	U	545	0	579	26	0
52	03	1027	0	1092	58	0
53	A	33012	0	16618	489	0
54	01	62317	0	31346	907	0
55	02	2568	0	1303	42	0
56	W	1640	0	836	14	0
56	X	1640	0	837	20	0
57	V	417	0	209	6	0
58	Y	1618	0	820	23	0
59	Z	3029	0	3043	172	0
60	W	10	0	10	0	0
61	Y	9	0	12	4	0
62	Z	32	0	14	3	0
All	All	153780	0	104807	3324	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 13.

The worst 5 of 3324 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)
54:01:45:G:H5"	54:01:46:G:H5'	1.35	1.07
54:01:1645:G:H5"	54:01:1646:C:H5'	1.42	1.00
7:10:118:ILE:HG23	7:10:119:PRO:HD3	1.43	0.99
4:07:15:LEU:HD13	4:07:28:PRO:HD2	1.41	0.98
39:I:83:THR:HG21	39:I:102:PHE:HB3	1.44	0.96

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	04	269/271 (99%)	227 (84%)	35 (13%)	7 (3%)	5 35
2	05	207/209 (99%)	171 (83%)	31 (15%)	5 (2%)	6 37
3	06	199/201 (99%)	172 (86%)	24 (12%)	3 (2%)	10 45
4	07	175/177 (99%)	150 (86%)	22 (13%)	3 (2%)	9 43
5	08	174/176 (99%)	151 (87%)	20 (12%)	3 (2%)	9 43
6	09	147/149 (99%)	119 (81%)	26 (18%)	2 (1%)	11 46
7	10	129/131 (98%)	82 (64%)	37 (29%)	10 (8%)	1 15
8	11	139/141 (99%)	109 (78%)	24 (17%)	6 (4%)	2 26
9	12	140/142 (99%)	123 (88%)	15 (11%)	2 (1%)	11 46
10	13	120/122 (98%)	94 (78%)	18 (15%)	8 (7%)	1 18
11	14	141/143 (99%)	110 (78%)	24 (17%)	7 (5%)	2 23
12	15	134/136 (98%)	112 (84%)	19 (14%)	3 (2%)	6 38
13	16	118/120 (98%)	99 (84%)	18 (15%)	1 (1%)	19 57
14	17	114/116 (98%)	98 (86%)	13 (11%)	3 (3%)	5 35
15	18	112/114 (98%)	91 (81%)	21 (19%)	0	100 100
16	19	115/117 (98%)	105 (91%)	10 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	20	101/103 (98%)	83 (82%)	17 (17%)	1 (1%)	15 52
18	21	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	8 41
19	22	91/93 (98%)	64 (70%)	24 (26%)	3 (3%)	4 31
20	23	100/102 (98%)	78 (78%)	18 (18%)	4 (4%)	3 27
21	24	92/94 (98%)	79 (86%)	13 (14%)	0	100 100
22	25	73/75 (97%)	62 (85%)	9 (12%)	2 (3%)	5 35
23	26	75/77 (97%)	70 (93%)	4 (5%)	1 (1%)	12 48
24	27	61/63 (97%)	54 (88%)	7 (12%)	0	100 100
25	28	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	8 42
26	29	64/66 (97%)	50 (78%)	11 (17%)	3 (5%)	2 24
27	30	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	8 41
28	31	48/50 (96%)	44 (92%)	4 (8%)	0	100 100
29	32	44/46 (96%)	41 (93%)	3 (7%)	0	100 100
30	33	62/64 (97%)	49 (79%)	10 (16%)	3 (5%)	2 24
31	34	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5 34
32	B	216/218 (99%)	177 (82%)	30 (14%)	9 (4%)	3 26
33	C	204/206 (99%)	188 (92%)	16 (8%)	0	100 100
34	D	203/205 (99%)	169 (83%)	26 (13%)	8 (4%)	3 28
35	E	155/157 (99%)	118 (76%)	27 (17%)	10 (6%)	1 19
36	F	98/100 (98%)	75 (76%)	17 (17%)	6 (6%)	1 20
37	G	149/151 (99%)	124 (83%)	20 (13%)	5 (3%)	3 31
38	H	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	9 44
39	I	125/127 (98%)	92 (74%)	29 (23%)	4 (3%)	4 32
40	J	96/98 (98%)	74 (77%)	11 (12%)	11 (12%)	0 7
41	K	114/116 (98%)	89 (78%)	20 (18%)	5 (4%)	2 25
42	L	121/123 (98%)	94 (78%)	19 (16%)	8 (7%)	1 19
43	M	112/114 (98%)	91 (81%)	17 (15%)	4 (4%)	3 29
44	N	98/100 (98%)	80 (82%)	16 (16%)	2 (2%)	7 40
45	O	86/88 (98%)	71 (83%)	13 (15%)	2 (2%)	6 38
46	P	80/82 (98%)	64 (80%)	13 (16%)	3 (4%)	3 28
47	Q	78/80 (98%)	57 (73%)	15 (19%)	6 (8%)	1 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
48	R	63/65 (97%)	50 (79%)	8 (13%)	5 (8%)	1 15
49	S	77/79 (98%)	62 (80%)	12 (16%)	3 (4%)	3 28
50	T	83/85 (98%)	79 (95%)	2 (2%)	2 (2%)	6 37
51	U	63/65 (97%)	39 (62%)	19 (30%)	5 (8%)	1 15
52	03	130/223 (58%)	112 (86%)	15 (12%)	3 (2%)	6 38
59	Z	390/392 (100%)	330 (85%)	53 (14%)	7 (2%)	8 42
All	All	6366/6563 (97%)	5260 (83%)	911 (14%)	195 (3%)	7 32

5 of 195 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	04	121	ALA
1	04	233	GLY
2	05	170	VAL
3	06	83	VAL
4	07	175	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	04	216/216 (100%)	211 (98%)	5 (2%)	50 71
2	05	164/164 (100%)	163 (99%)	1 (1%)	86 91
3	06	165/165 (100%)	163 (99%)	2 (1%)	71 83
4	07	148/148 (100%)	145 (98%)	3 (2%)	55 74
5	08	137/137 (100%)	137 (100%)	0	100 100
6	09	114/114 (100%)	113 (99%)	1 (1%)	78 87
7	10	100/100 (100%)	95 (95%)	5 (5%)	24 53
8	11	109/109 (100%)	108 (99%)	1 (1%)	78 87
9	12	116/116 (100%)	116 (100%)	0	100 100
10	13	103/103 (100%)	101 (98%)	2 (2%)	57 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	14	102/102 (100%)	102 (100%)	0	100	100
12	15	109/109 (100%)	107 (98%)	2 (2%)	59	77
13	16	100/100 (100%)	98 (98%)	2 (2%)	55	74
14	17	86/86 (100%)	85 (99%)	1 (1%)	71	83
15	18	99/99 (100%)	99 (100%)	0	100	100
16	19	89/89 (100%)	87 (98%)	2 (2%)	52	71
17	20	84/84 (100%)	84 (100%)	0	100	100
18	21	93/93 (100%)	91 (98%)	2 (2%)	52	71
19	22	80/80 (100%)	78 (98%)	2 (2%)	47	69
20	23	83/83 (100%)	81 (98%)	2 (2%)	49	69
21	24	78/78 (100%)	77 (99%)	1 (1%)	69	82
22	25	57/57 (100%)	56 (98%)	1 (2%)	59	77
23	26	67/67 (100%)	67 (100%)	0	100	100
24	27	55/55 (100%)	55 (100%)	0	100	100
25	28	48/48 (100%)	47 (98%)	1 (2%)	53	73
26	29	59/59 (100%)	59 (100%)	0	100	100
27	30	47/47 (100%)	46 (98%)	1 (2%)	53	73
28	31	45/45 (100%)	45 (100%)	0	100	100
29	32	38/38 (100%)	38 (100%)	0	100	100
30	33	51/51 (100%)	50 (98%)	1 (2%)	55	74
31	34	34/34 (100%)	34 (100%)	0	100	100
32	B	180/180 (100%)	170 (94%)	10 (6%)	21	51
33	C	170/170 (100%)	170 (100%)	0	100	100
34	D	172/172 (100%)	166 (96%)	6 (4%)	36	62
35	E	119/119 (100%)	115 (97%)	4 (3%)	37	62
36	F	87/87 (100%)	87 (100%)	0	100	100
37	G	124/124 (100%)	123 (99%)	1 (1%)	81	89
38	H	104/104 (100%)	104 (100%)	0	100	100
39	I	105/105 (100%)	103 (98%)	2 (2%)	57	75
40	J	86/86 (100%)	84 (98%)	2 (2%)	50	71
41	K	89/89 (100%)	85 (96%)	4 (4%)	27	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	L	103/103 (100%)	100 (97%)	3 (3%)	42 65
43	M	92/92 (100%)	89 (97%)	3 (3%)	38 63
44	N	83/83 (100%)	83 (100%)	0	100 100
45	O	76/76 (100%)	76 (100%)	0	100 100
46	P	65/65 (100%)	65 (100%)	0	100 100
47	Q	74/74 (100%)	73 (99%)	1 (1%)	67 81
48	R	56/56 (100%)	52 (93%)	4 (7%)	14 44
49	S	70/70 (100%)	70 (100%)	0	100 100
50	T	65/65 (100%)	64 (98%)	1 (2%)	65 80
51	U	55/55 (100%)	53 (96%)	2 (4%)	35 61
52	03	110/174 (63%)	105 (96%)	5 (4%)	27 56
59	Z	324/325 (100%)	315 (97%)	9 (3%)	43 66
All	All	5285/5350 (99%)	5190 (98%)	95 (2%)	61 77

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	E	163	ILE
43	M	47	LEU
39	I	44	ARG
41	K	117	HIS
48	R	21	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
33	C	122	GLN
37	G	129	ASN
33	C	184	ASN
35	E	60	GLN
39	I	125	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1538/1539 (99%)	161 (10%)	7 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	01	2902/2903 (99%)	353 (12%)	13 (0%)
55	02	119/120 (99%)	10 (8%)	2 (1%)
56	W	76/77 (98%)	8 (10%)	0
56	X	76/77 (98%)	12 (15%)	1 (1%)
57	V	18/19 (94%)	3 (16%)	0
58	Y	74/76 (97%)	14 (18%)	3 (4%)
All	All	4803/4811 (99%)	561 (11%)	26 (0%)

5 of 561 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	6	G
53	A	7	A
53	A	9	G
53	A	22	G
53	A	32	A

5 of 26 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	01	1940	U
54	01	2326	C
58	Y	19	G
54	01	2296	U
54	01	2391	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	$\#\|Z\| > 2$
58	U8U	Y	34	58	19,24,25	1.41	3 (15%)	23,34,37	1.20	2 (8%)

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
58	U8U	Y	34	58	-	3/9/28/29	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	Y	34	U8U	C6-N1	4.17	1.45	1.38
58	Y	34	U8U	C4-C5	2.43	1.50	1.45
58	Y	34	U8U	C2-N3	2.29	1.42	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	Y	34	U8U	C5-C6-N1	2.66	126.48	122.91
58	Y	34	U8U	C1'-N1-C6	-2.17	117.52	121.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	Y	34	U8U	N-C-C5-C4
58	Y	34	U8U	C2'-C1'-N1-C2
58	Y	34	U8U	N-C-C5-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	Y	34	U8U	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
61	LYS	Y	101	58	7,8,9	0.70	0	3,8,10	0.19	0
62	GCP	Z	401	-	27,34,34	1.98	7 (25%)	34,54,54	3.98	17 (50%)
60	FME	W	101	-	8,9,10	0.85	0	7,9,11	1.17	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
61	LYS	Y	101	58	-	3/6/7/9	-
62	GCP	Z	401	-	-	8/15/38/38	0/3/3/3
60	FME	W	101	-	-	4/7/9/11	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	Z	401	GCP	PB-O3A	-4.91	1.52	1.58
62	Z	401	GCP	O4'-C1'	4.66	1.47	1.41
62	Z	401	GCP	C2'-C1'	3.31	1.58	1.53
62	Z	401	GCP	C5-C6	3.30	1.47	1.41
62	Z	401	GCP	C6-N1	2.85	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	Z	401	GCP	C1'-N9-C4	14.24	151.65	126.64
62	Z	401	GCP	C5-C6-N1	-8.82	111.37	123.43
62	Z	401	GCP	O1G-PG-C3B	-7.57	94.92	111.24
62	Z	401	GCP	C2-N1-C6	6.64	126.48	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	Z	401	GCP	O4'-C1'-C2'	-4.55	100.28	106.93

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	W	101	FME	O1-CN-N-CA
60	W	101	FME	C-CA-CB-CG
60	W	101	FME	O-C-CA-CB
61	Y	101	LYS	N-CA-CB-CG
61	Y	101	LYS	C-CA-CB-CG

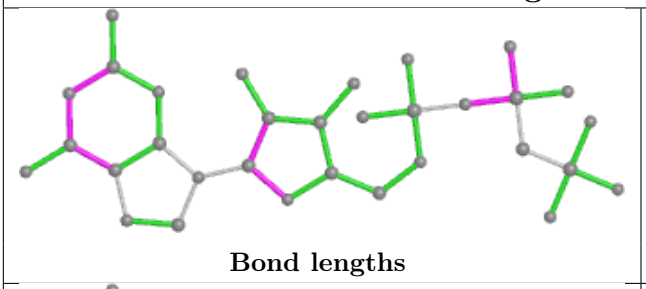
There are no ring outliers.

2 monomers are involved in 7 short contacts:

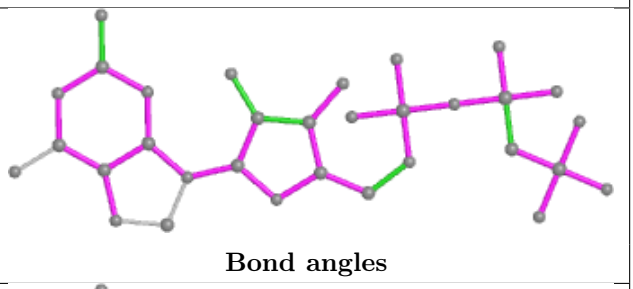
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	Y	101	LYS	4	0
62	Z	401	GCP	3	0

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.

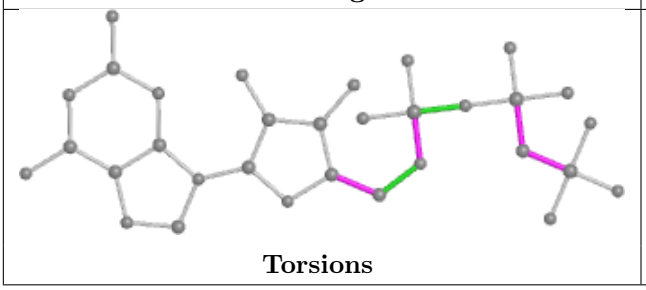
Ligand GCP Z 401



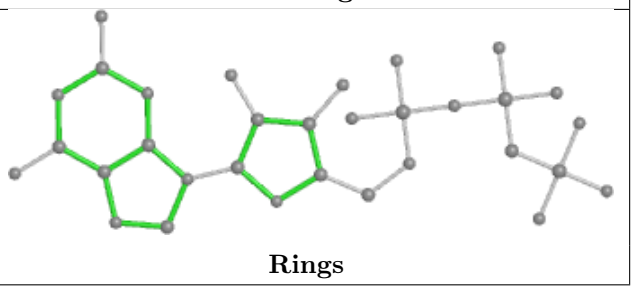
Bond lengths



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.

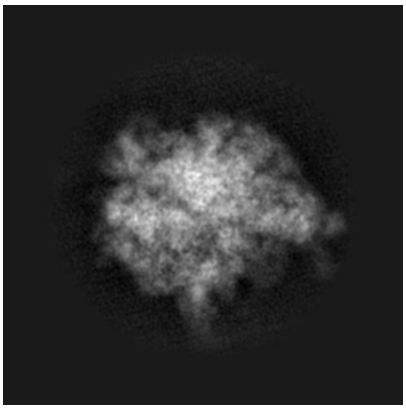
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8619. These allow visual inspection of the internal detail of the map and identification of artifacts.

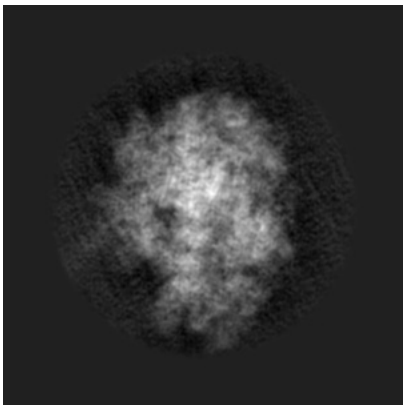
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

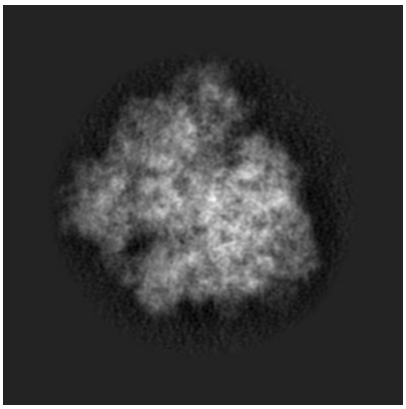
6.1.1 Primary map



X

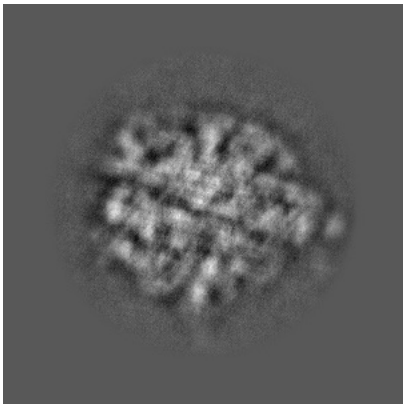


Y

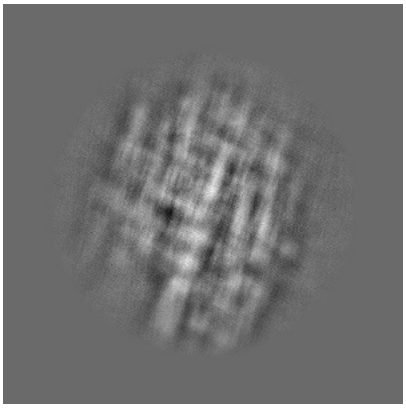


Z

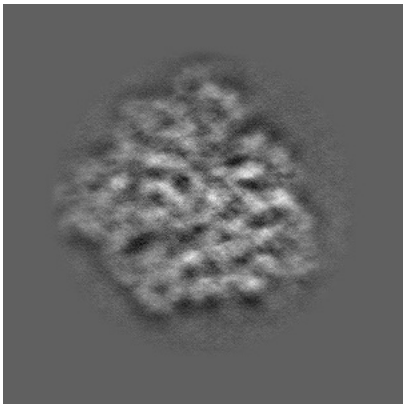
6.1.2 Raw map



X



Y

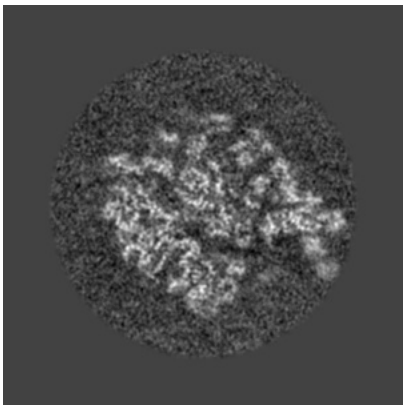


Z

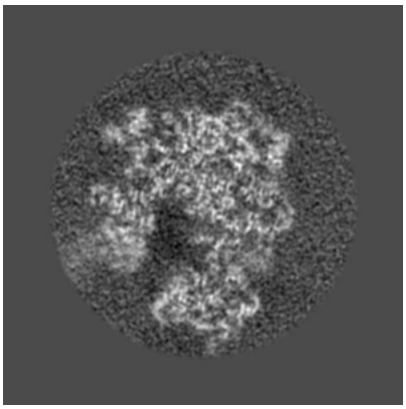
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

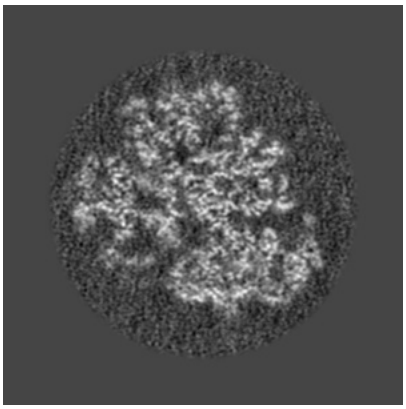
6.2.1 Primary map



X Index: 240

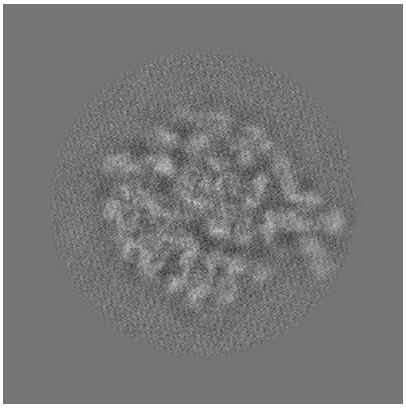


Y Index: 240

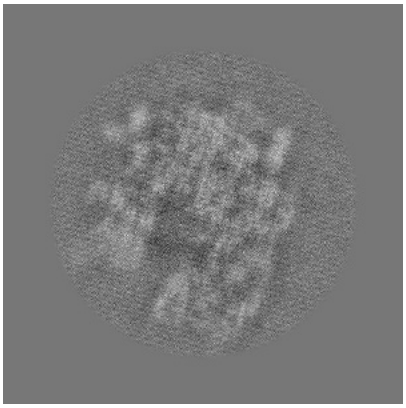


Z Index: 240

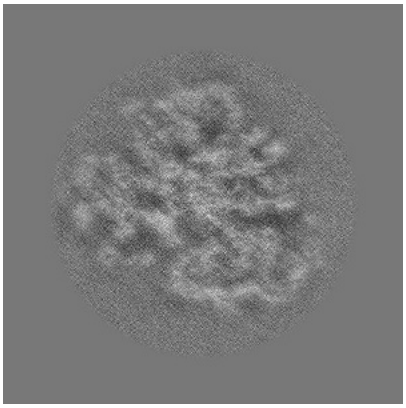
6.2.2 Raw map



X Index: 240



Y Index: 240

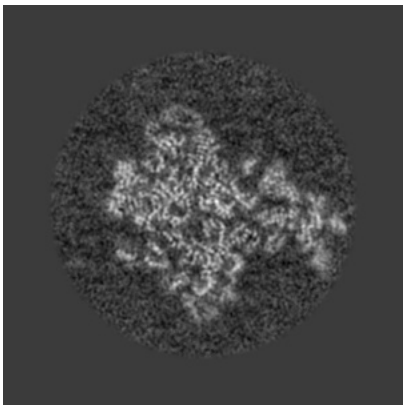


Z Index: 240

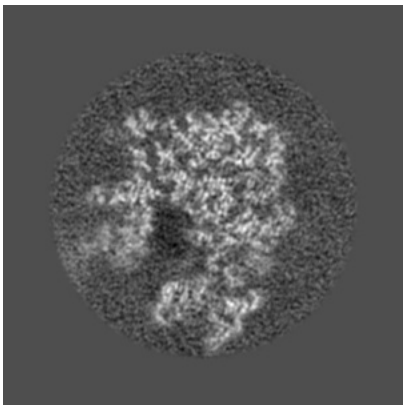
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

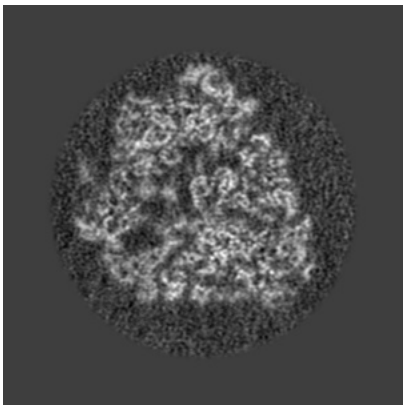
6.3.1 Primary map



X Index: 252

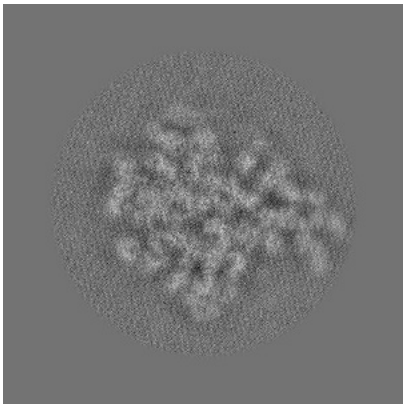


Y Index: 245

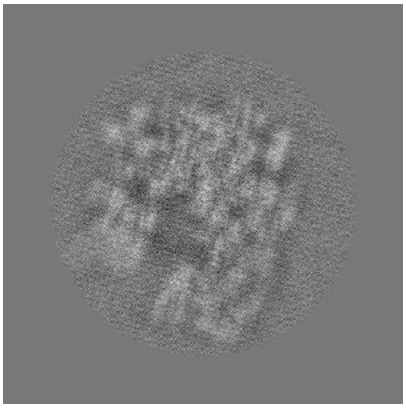


Z Index: 225

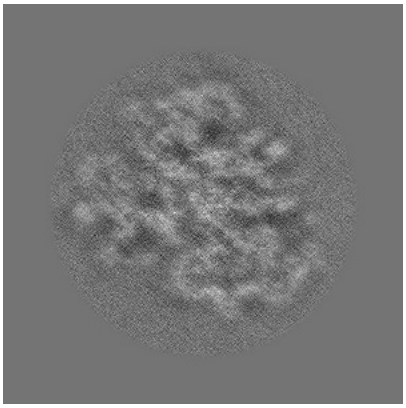
6.3.2 Raw map



X Index: 250



Y Index: 237

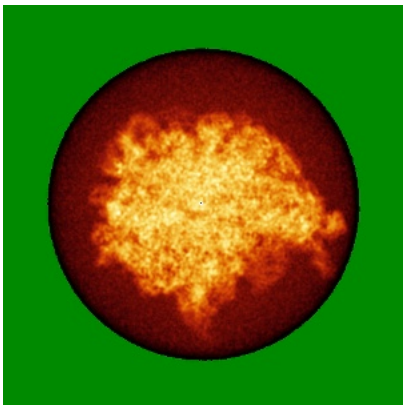


Z Index: 242

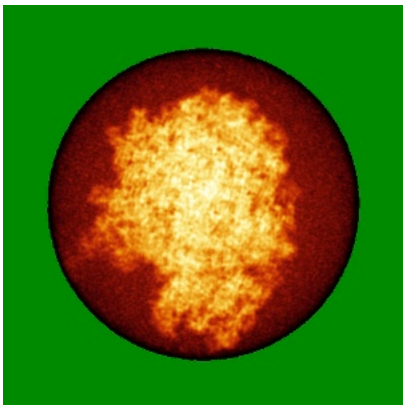
The images above show the largest variance slices of the map in three orthogonal directions.

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

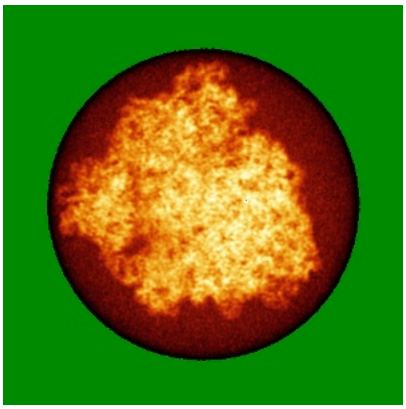
6.4.1 Primary map



X

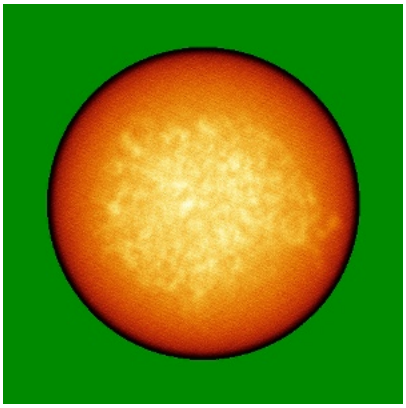


Y

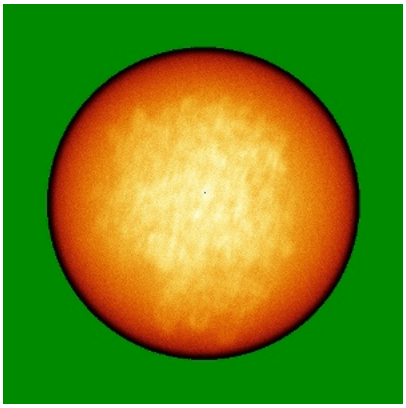


Z

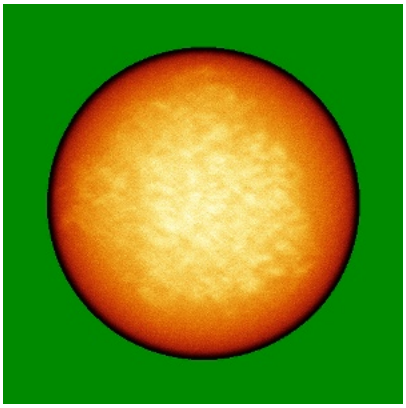
6.4.2 Raw map



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.

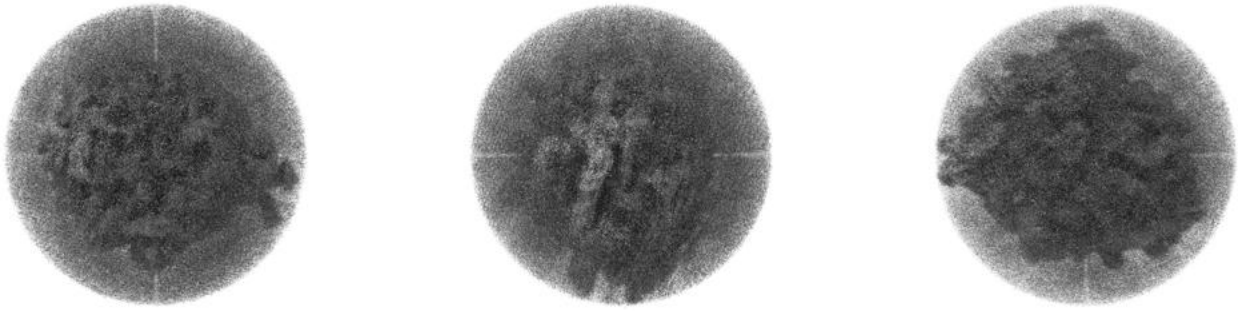
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.78. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

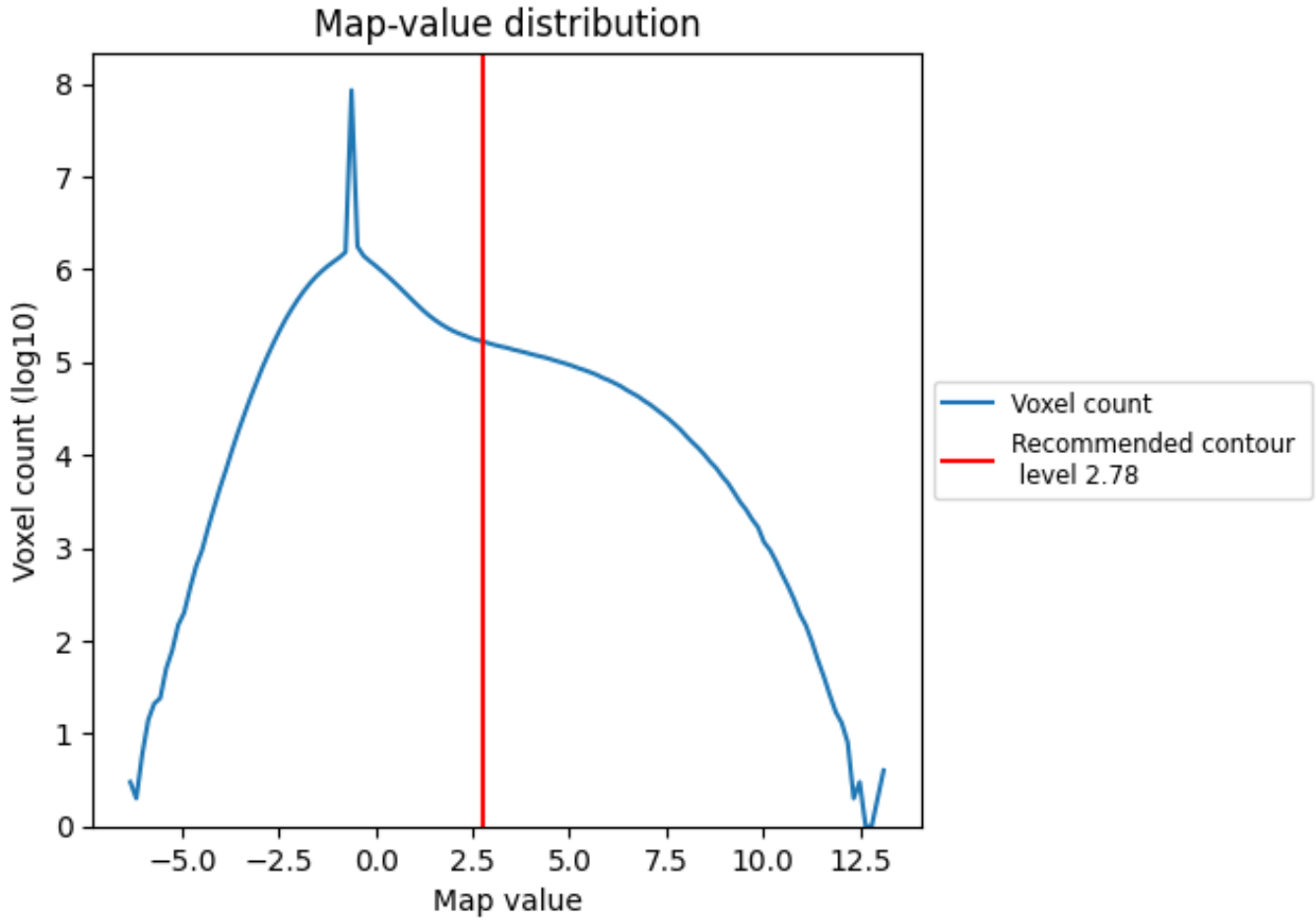
6.6 Mask visualisation (i)

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

7 Map analysis

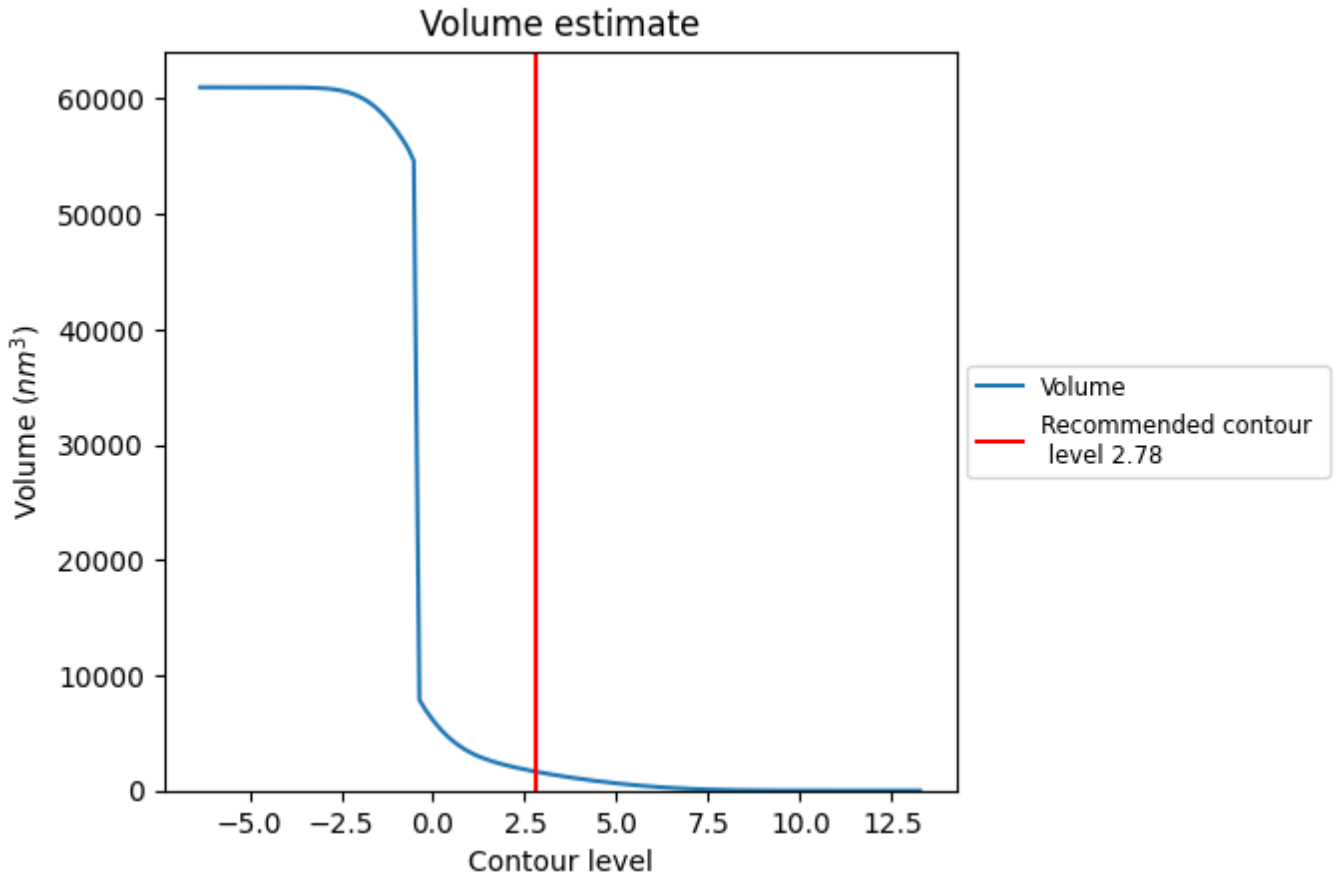
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

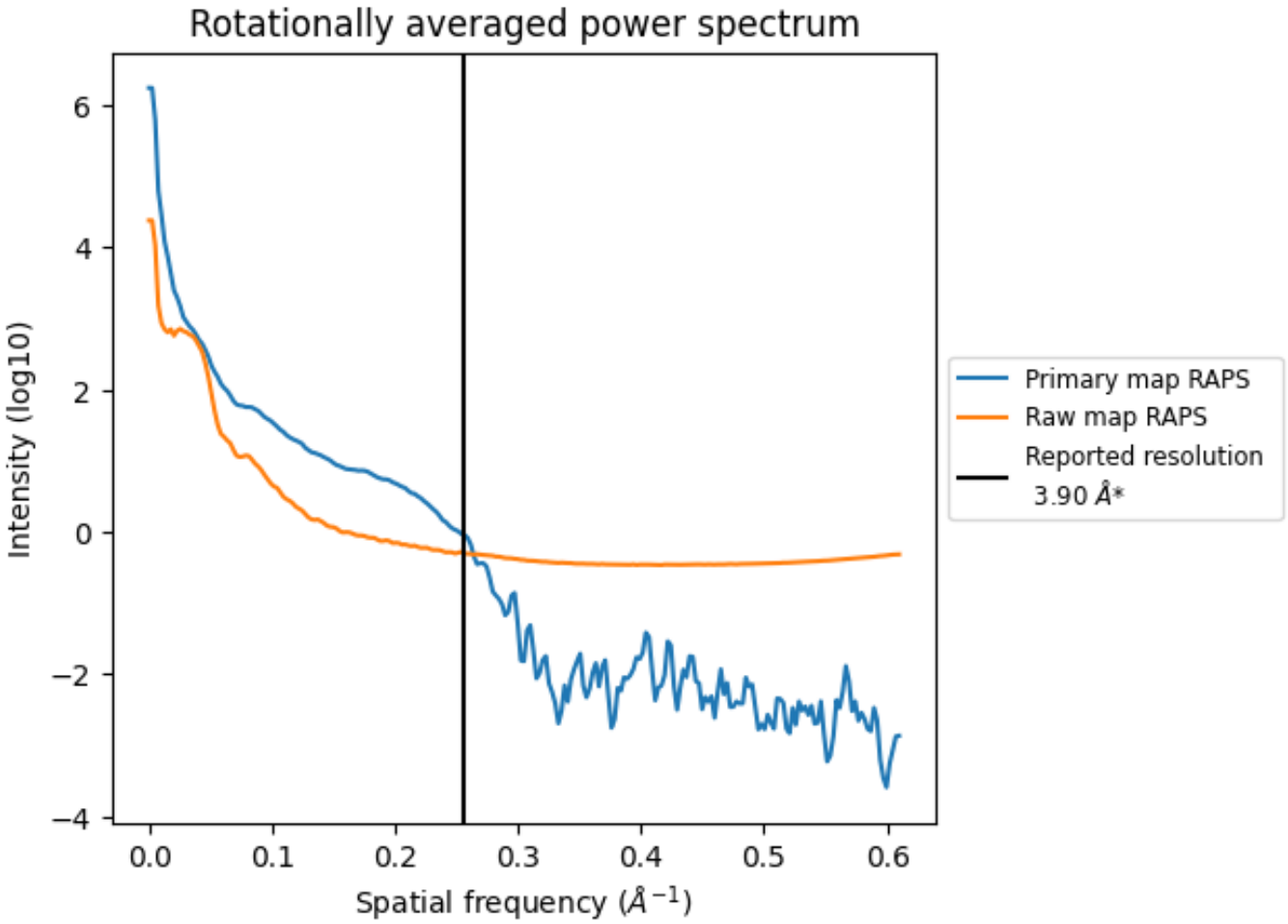
7.2 Volume estimate (i)



The volume at the recommended contour level is 1654 nm^3; this corresponds to an approximate mass of 1494 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)

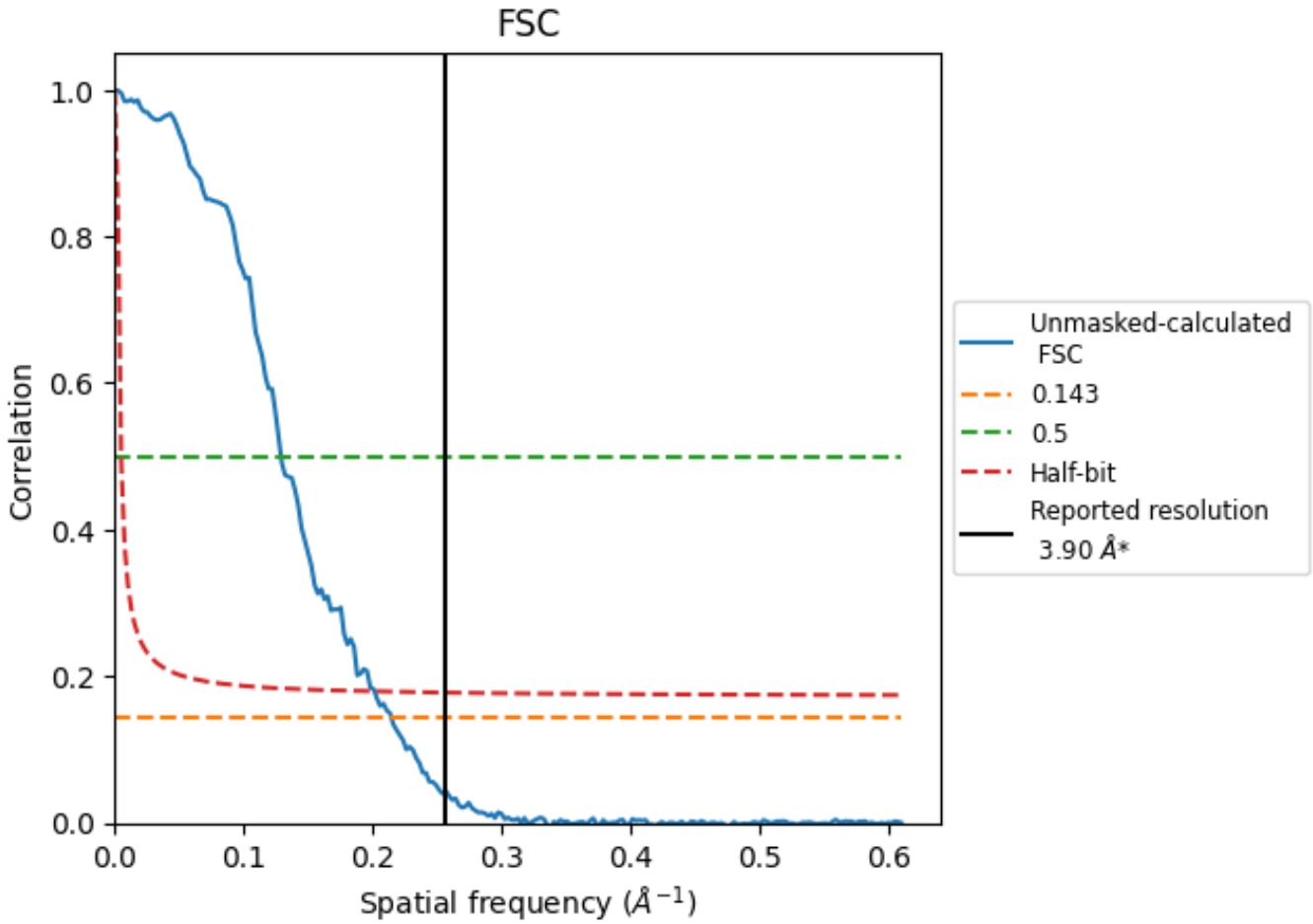


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

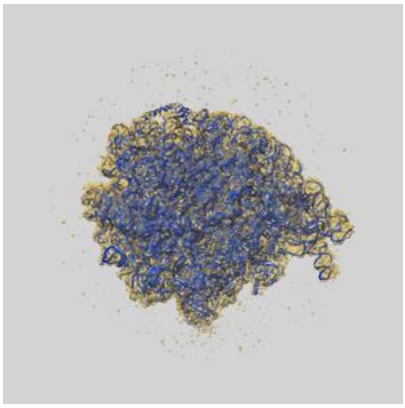
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.66	7.76	4.97

*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 4.66 differs from the reported value 3.9 by more than 10 %

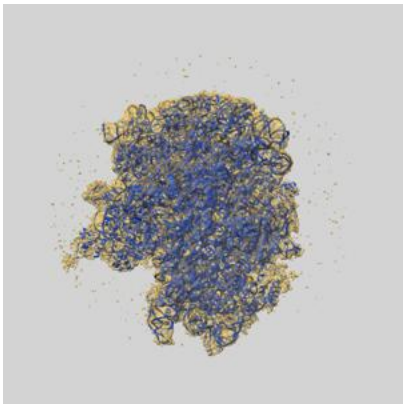
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8619 and PDB model 5UYP. Per-residue inclusion information can be found in section 3 on page 17.

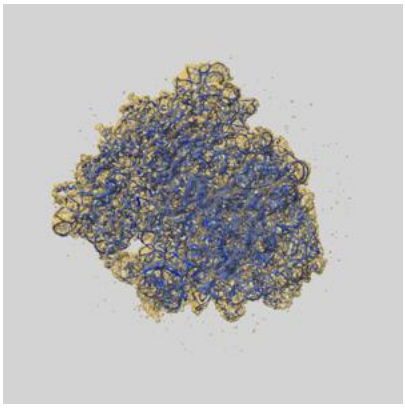
9.1 Map-model overlay



X



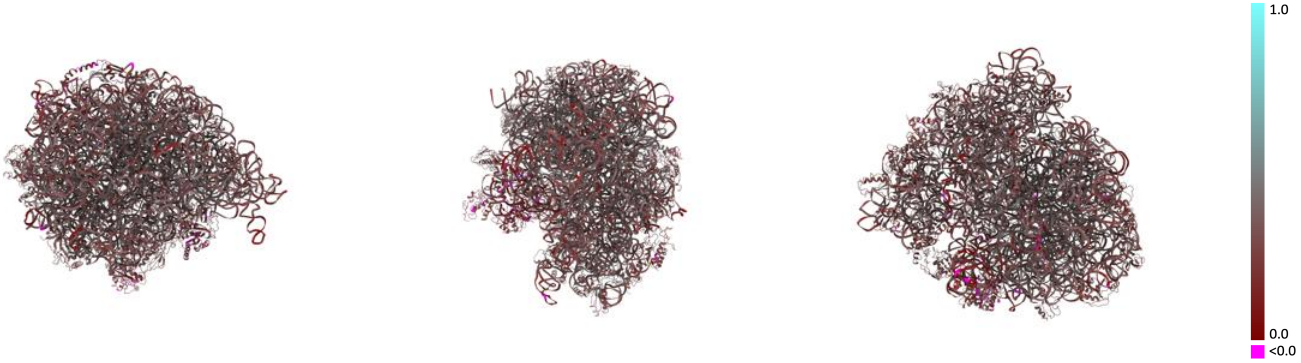
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.78 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.

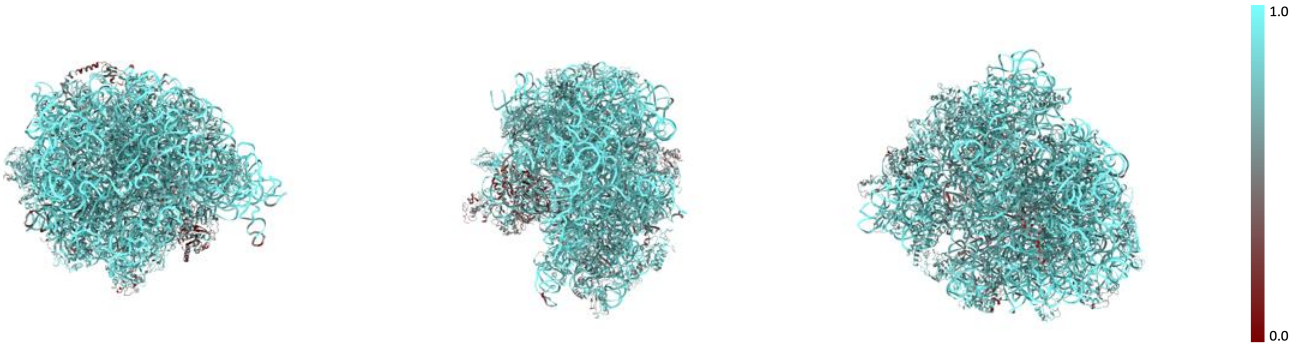
9.2 Q-score mapped to coordinate model



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.

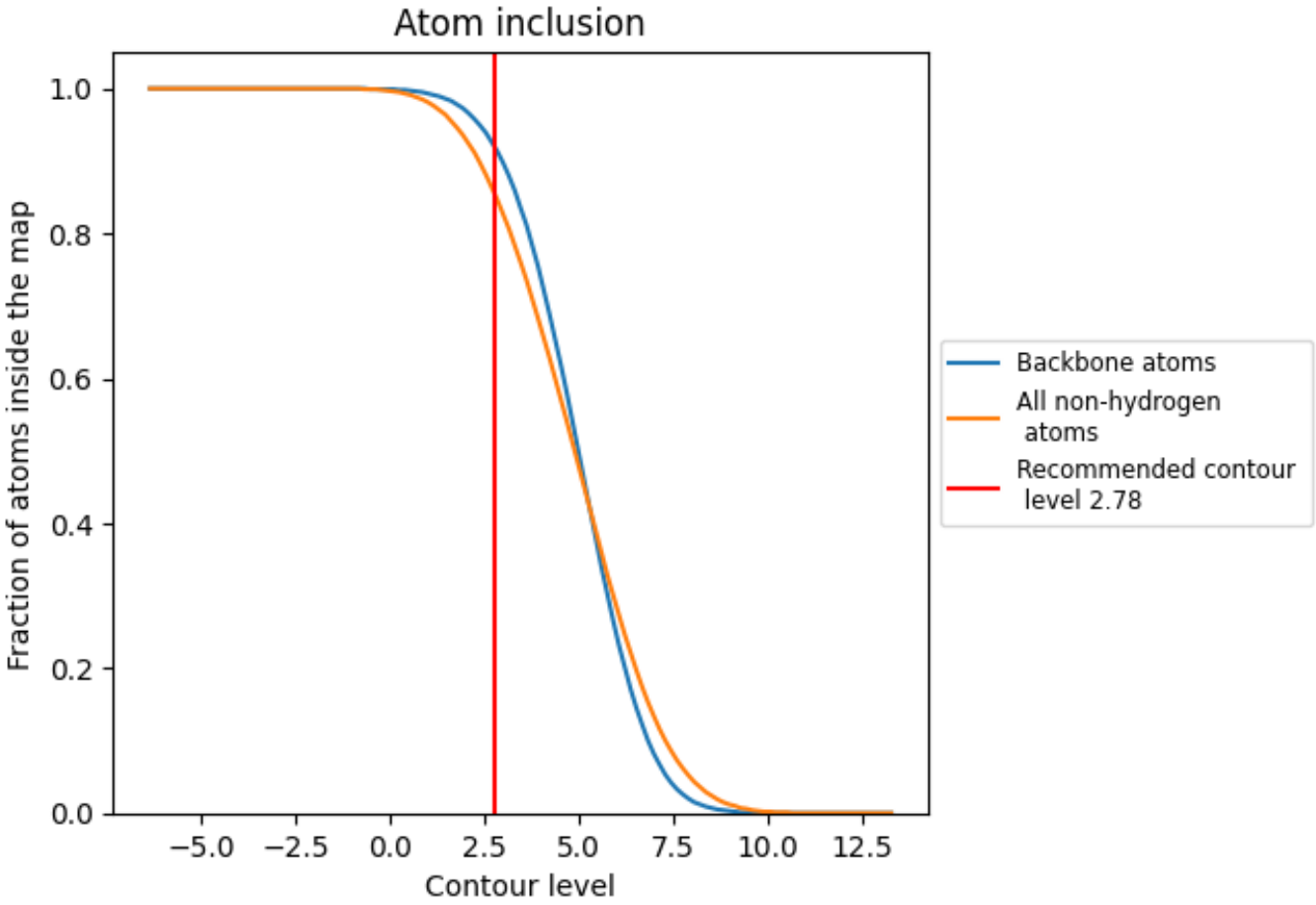
9.3 Atom inclusion mapped to coordinate model



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 (2.78).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.78) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8540	0.3380
01	0.9360	0.3520
02	0.9460	0.3400
03	0.5680	0.2060
04	0.7850	0.3870
05	0.7590	0.3810
06	0.7420	0.3480
07	0.7700	0.3230
08	0.7750	0.3350
09	0.4580	0.2710
10	0.4770	0.1730
11	0.5530	0.1990
12	0.7660	0.3710
13	0.6660	0.3750
14	0.8070	0.3590
15	0.7030	0.3730
16	0.7930	0.3510
17	0.8120	0.3460
18	0.7080	0.3650
19	0.7830	0.3500
20	0.7540	0.3540
21	0.7290	0.3450
22	0.8020	0.3590
23	0.7750	0.3140
24	0.7740	0.3580
25	0.7510	0.3800
26	0.7520	0.3600
27	0.7490	0.2860
28	0.7870	0.3610
29	0.7500	0.3190
30	0.7620	0.3640
31	0.7840	0.3330
32	0.8140	0.3800
33	0.8230	0.3910
34	0.8190	0.3770

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Chain	Atom inclusion	Q-score
A	0.9280	0.3450
B	0.7020	0.3070
C	0.6690	0.3510
D	0.7200	0.3200
E	0.7210	0.3510
F	0.7450	0.3290
G	0.7100	0.3090
H	0.7590	0.3480
I	0.7730	0.3170
J	0.6340	0.3060
K	0.7660	0.3610
L	0.6830	0.3740
M	0.7170	0.3070
N	0.7470	0.3210
O	0.7700	0.3340
P	0.8200	0.3540
Q	0.7850	0.3370
R	0.7630	0.3440
S	0.7720	0.3420
T	0.7650	0.3150
U	0.6040	0.2860
V	0.6830	0.2740
W	0.8660	0.3150
X	0.6800	0.1870
Y	0.6270	0.1960
Z	0.4480	0.2260