



## wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 08:02 am GMT

PDB ID : 6XZB  
EMDB ID : EMD-10657  
Title : E. coli 70S ribosome in complex with dirithromycin, fMet-Phe-tRNA(Phe) and deacylated tRNA(iMet) (focused classification).  
Authors : Pichkur, E.B.; Polikanov, Y.S.; Myasnikov, A.G.; Konevega, A.L.  
Deposited on : 2020-02-03  
Resolution : 2.54 Å(reported)  
Based on initial model : 4YBB

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
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) : 2.31.3

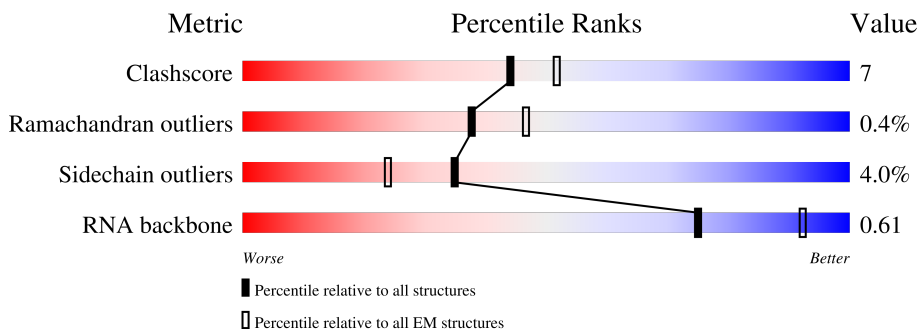
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.54 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.






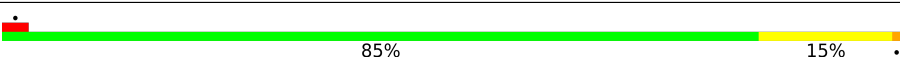
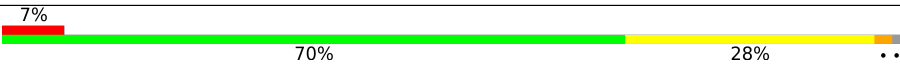

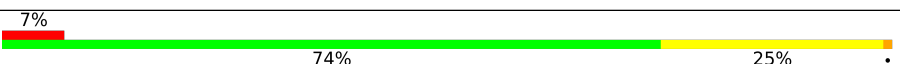
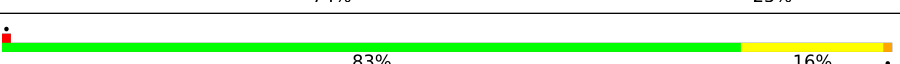
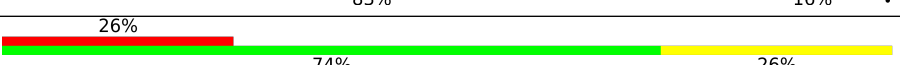
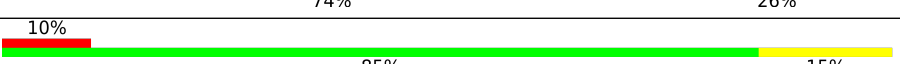
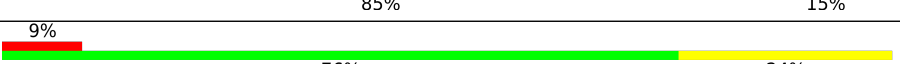
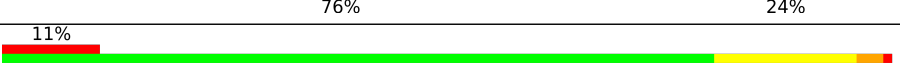

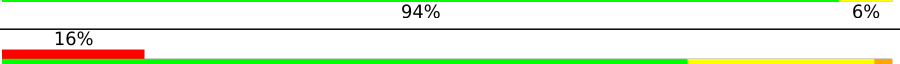



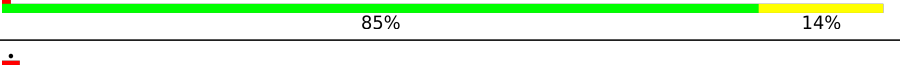

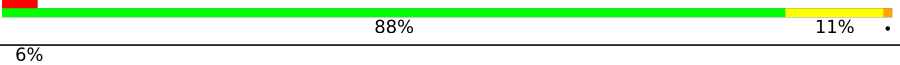
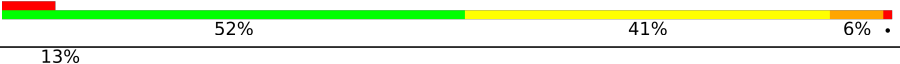
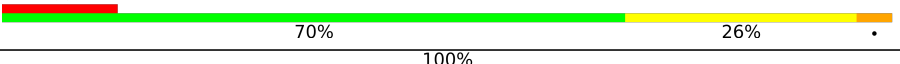
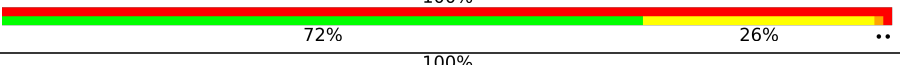
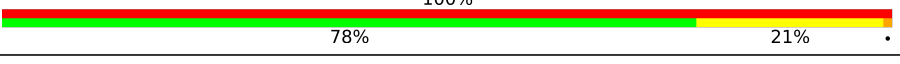

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A1	1534	
2	B1	224	
3	C1	206	
4	D1	205	
5	E1	155	
6	F1	106	
7	G1	151	



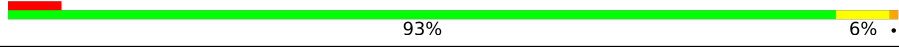


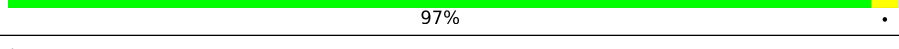
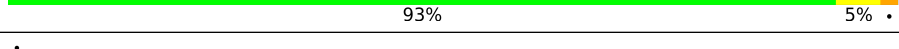
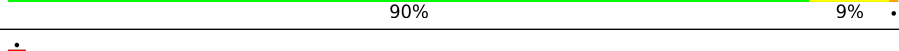
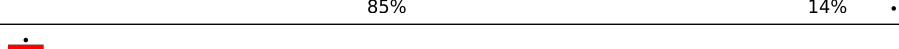
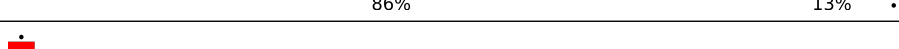
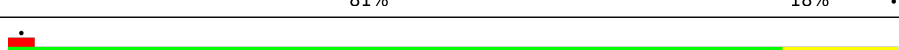

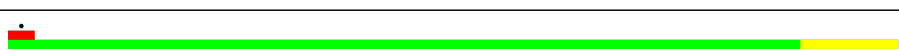

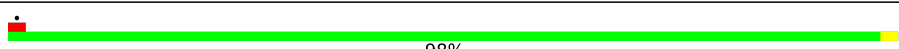

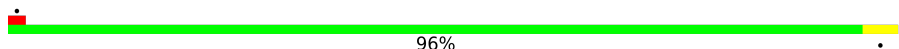
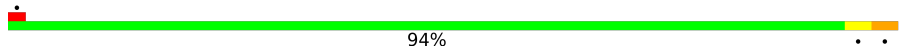
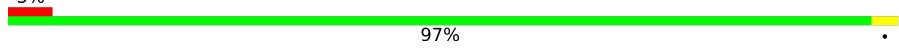

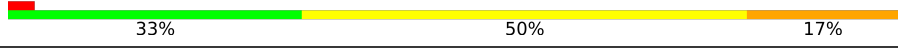

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Mol	Chain	Length	Quality of chain
8	H1	129	
9	I1	127	
10	J1	99	
11	K1	117	
12	L1	123	
13	M1	114	
14	N1	100	
15	O1	88	
16	P1	82	
17	Q1	80	
18	R1	55	
19	S1	79	
20	T1	86	
21	U1	56	
22	A2	2897	
23	B2	120	
24	C2	271	
25	D2	209	
26	E2	201	
27	F2	177	
28	G2	176	
29	H2	135	
30	I2	134	
31	J2	142	
32	K2	123	

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Mol	Chain	Length	Quality of chain
33	L2	144	 87% 13%
34	M2	136	 88% 11% .
35	N2	125	 93% 6% .
36	O2	117	 80% 19% .
37	P2	114	 83% 16% .
38	Q2	117	 97% .
39	R2	103	 93% 5% .
40	S2	110	 90% 9% .
41	T2	93	 85% 14% .
42	U2	102	 86% 13% .
43	V2	94	 81% 18% .
44	W2	76	 87% 13%
45	X2	77	 88% 12%
46	Y2	62	 89% 11%
47	Z2	58	 90% 9% .
48	a2	56	 98% .
49	b2	51	 98% .
50	c2	46	 96% .
51	d2	64	 94% . .
52	e2	38	 97% .
53	f2	76	 71% 28% .
54	g2	76	 33% 50% 17%

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 145650 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	1523	Total	C	N	O	P	0	0
			32681	14576	5998	10584	1523		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	99	Total	C	N	O	S	0	0
			796	498	152	145	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	122	Total	C	N	O	S	0	0
			947	586	195	162	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P1	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R1	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A2	2897	Total	C	N	O	P	3	0
			62252	27778	11454	20121	2899		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B2	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C2	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D2	209	Total	C	N	O	S	1	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E2	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F2	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	G2	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H2	135	Total	C	N	O	S	0	0
			1023	649	179	192	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H2	85	VAL	SER	conflict	UNP P0A7J3
H2	86	THR	MET	conflict	UNP P0A7J3

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	I2	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	J2	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K2	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L2	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M2	136	Total	C	N	O	S	1	0
			1075	686	205	178	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N2	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	O2	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	P2	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Q2	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R2	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	S2	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T2	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	U2	102	Total	C	N	O		0	0
			780	492	146	142			

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V2	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W2	76	Total	C	N	O	S	1	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X2	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y2	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Z2	58	Total	C	N	O	S	2	0
			449	281	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	a2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	b2	51	Total	C	N	O		0	0
			414	266	76	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	c2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	d2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	e2	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a RNA chain called Deacylated tRNA<sup>i</sup>(Met).

Mol	Chain	Residues	Atoms						AltConf	Trace
53	f2	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 54 is a RNA chain called fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
54	g2	76	Total	C	N	O	P	S	0	0
			1667	760	297	534	75	1		

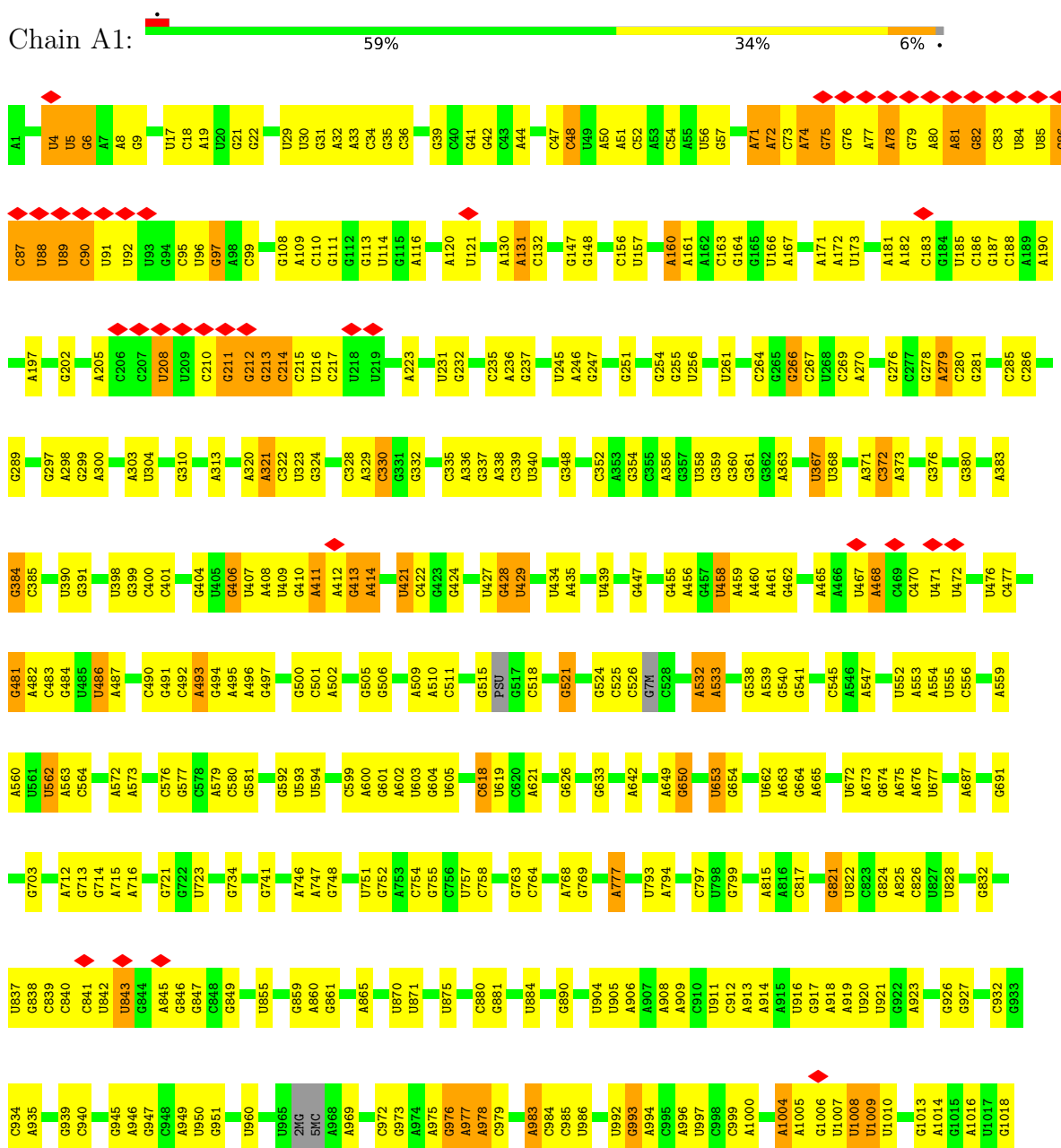
- Molecule 55 is Dirithromycin (three-letter code: DI0) (formula: C<sub>42</sub>H<sub>78</sub>N<sub>2</sub>O<sub>14</sub>).

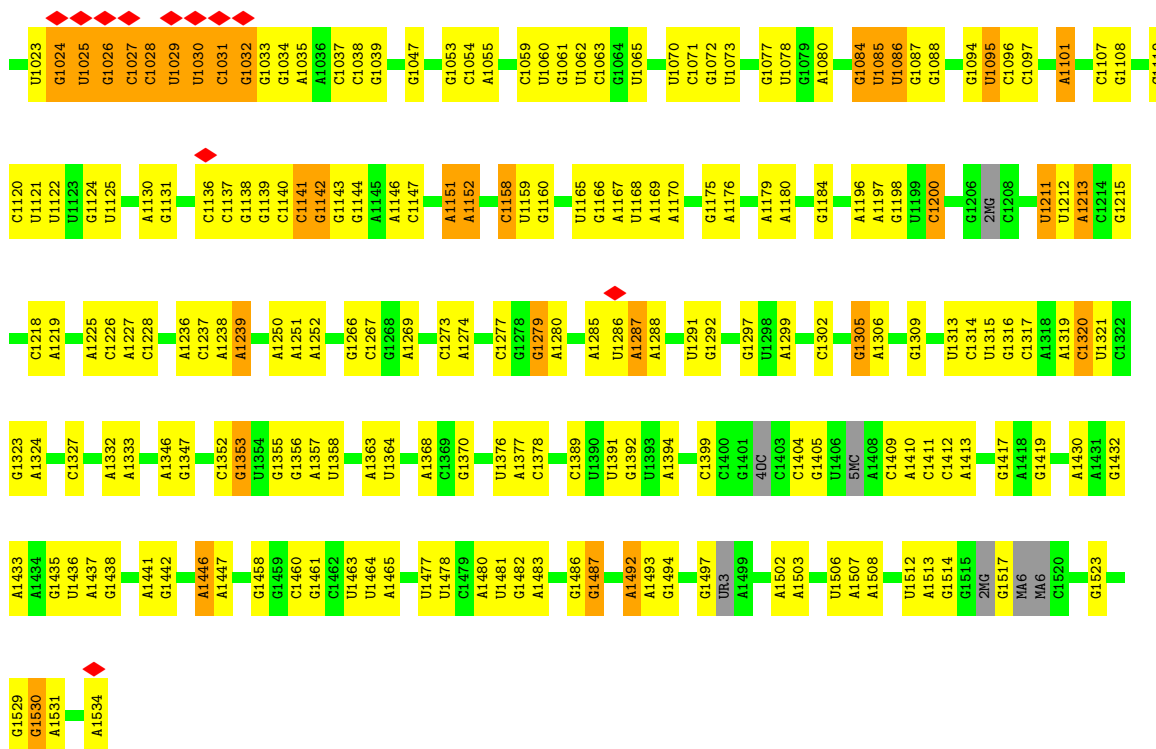


### 3 Residue-property plots

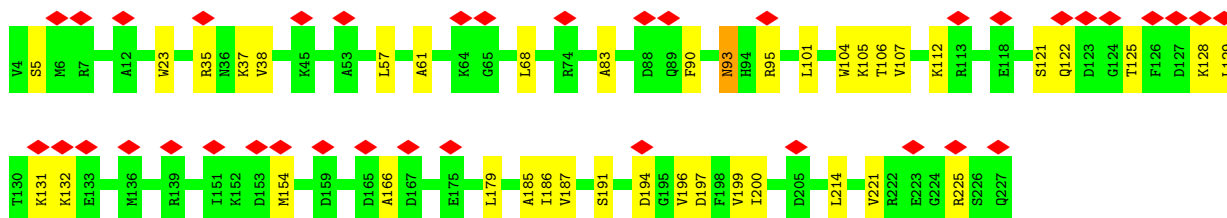
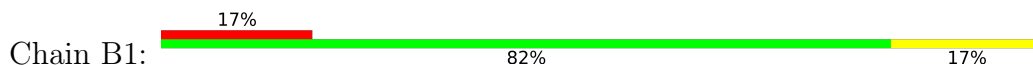
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 16S rRNA

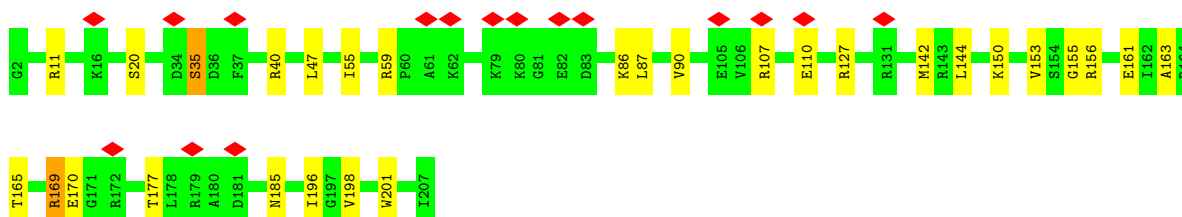
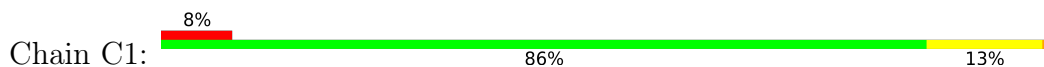




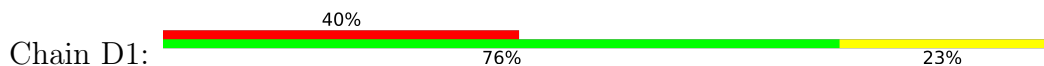
• Molecule 2: 30S ribosomal protein S2

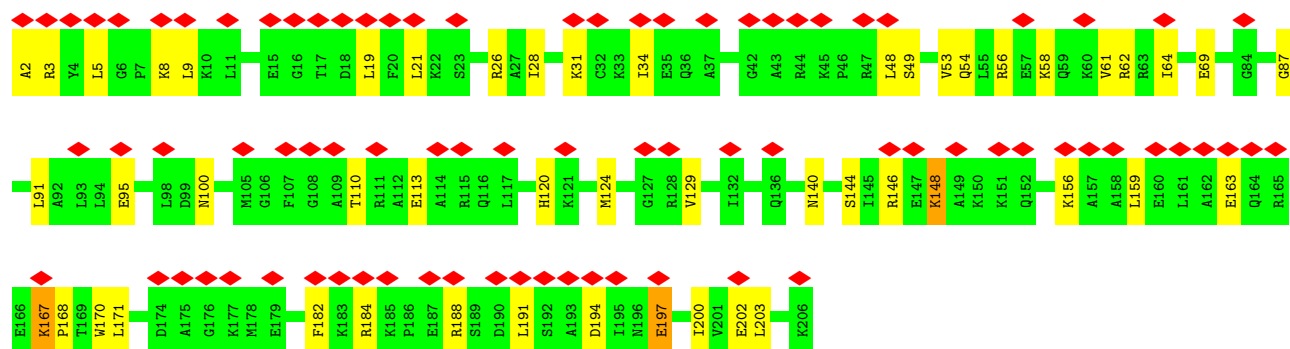


• Molecule 3: 30S ribosomal protein S3

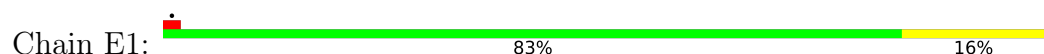


• Molecule 4: 30S ribosomal protein S4

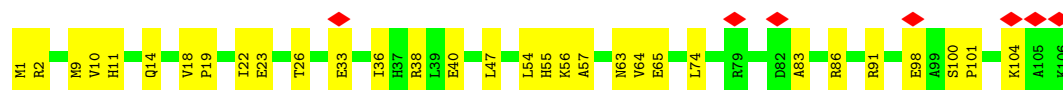
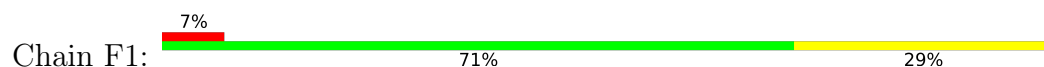




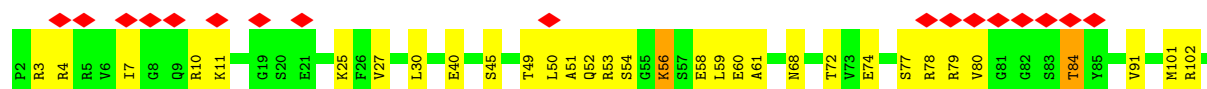
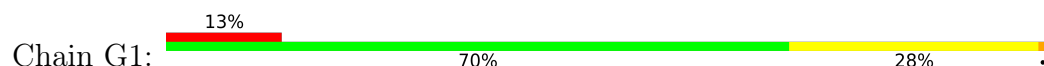
• Molecule 5: 30S ribosomal protein S5



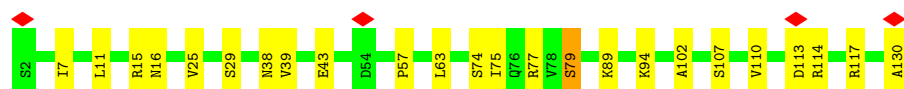
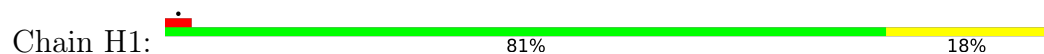
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8



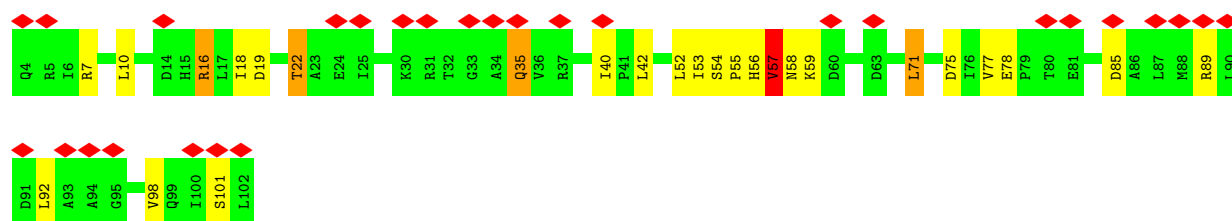
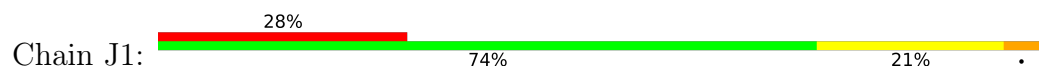
• Molecule 9: 30S ribosomal protein S9



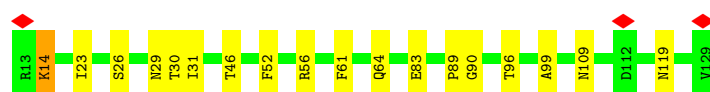
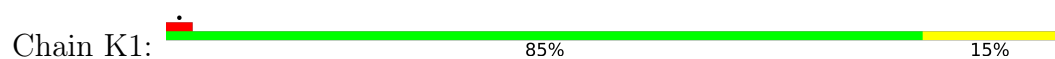




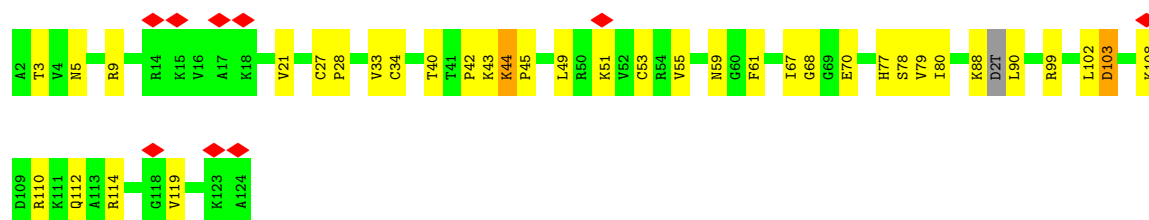
- Molecule 10: 30S ribosomal protein S10



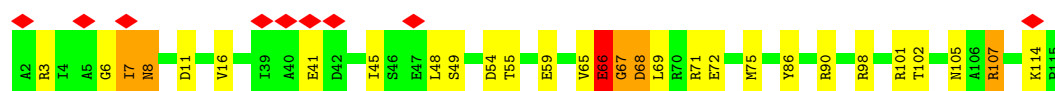
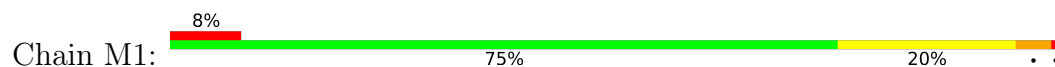
- Molecule 11: 30S ribosomal protein S11



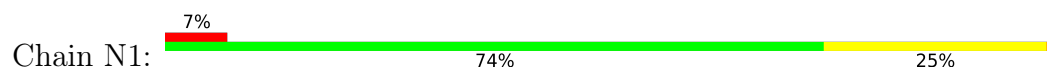
- Molecule 12: 30S ribosomal protein S12

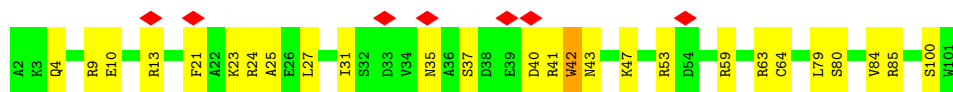


- Molecule 13: 30S ribosomal protein S13

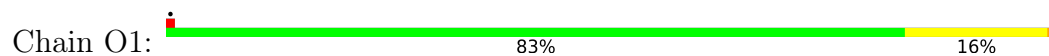


- Molecule 14: 30S ribosomal protein S14

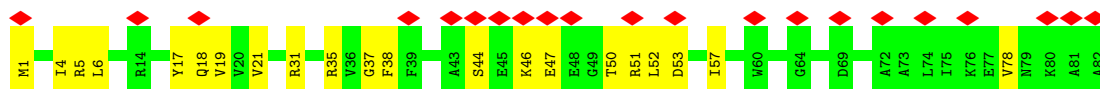
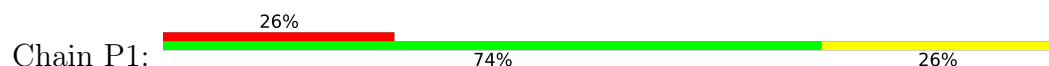




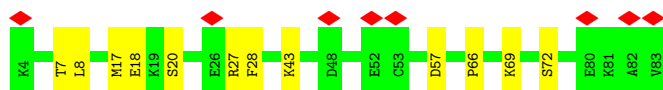
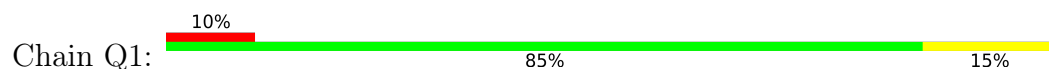
- Molecule 15: 30S ribosomal protein S15



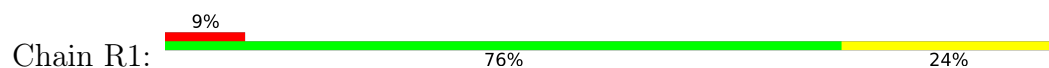
- Molecule 16: 30S ribosomal protein S16



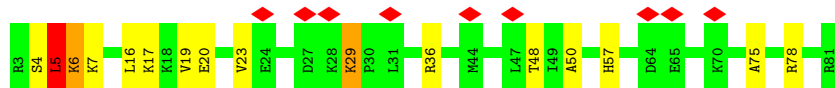
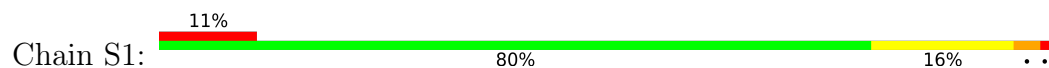
- Molecule 17: 30S ribosomal protein S17



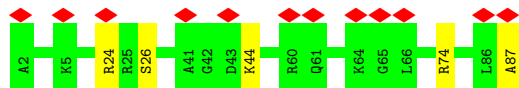
- Molecule 18: 30S ribosomal protein S18



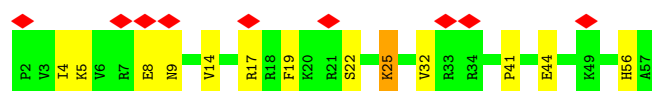
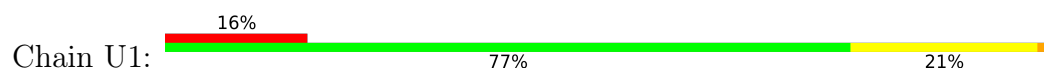
- Molecule 19: 30S ribosomal protein S19



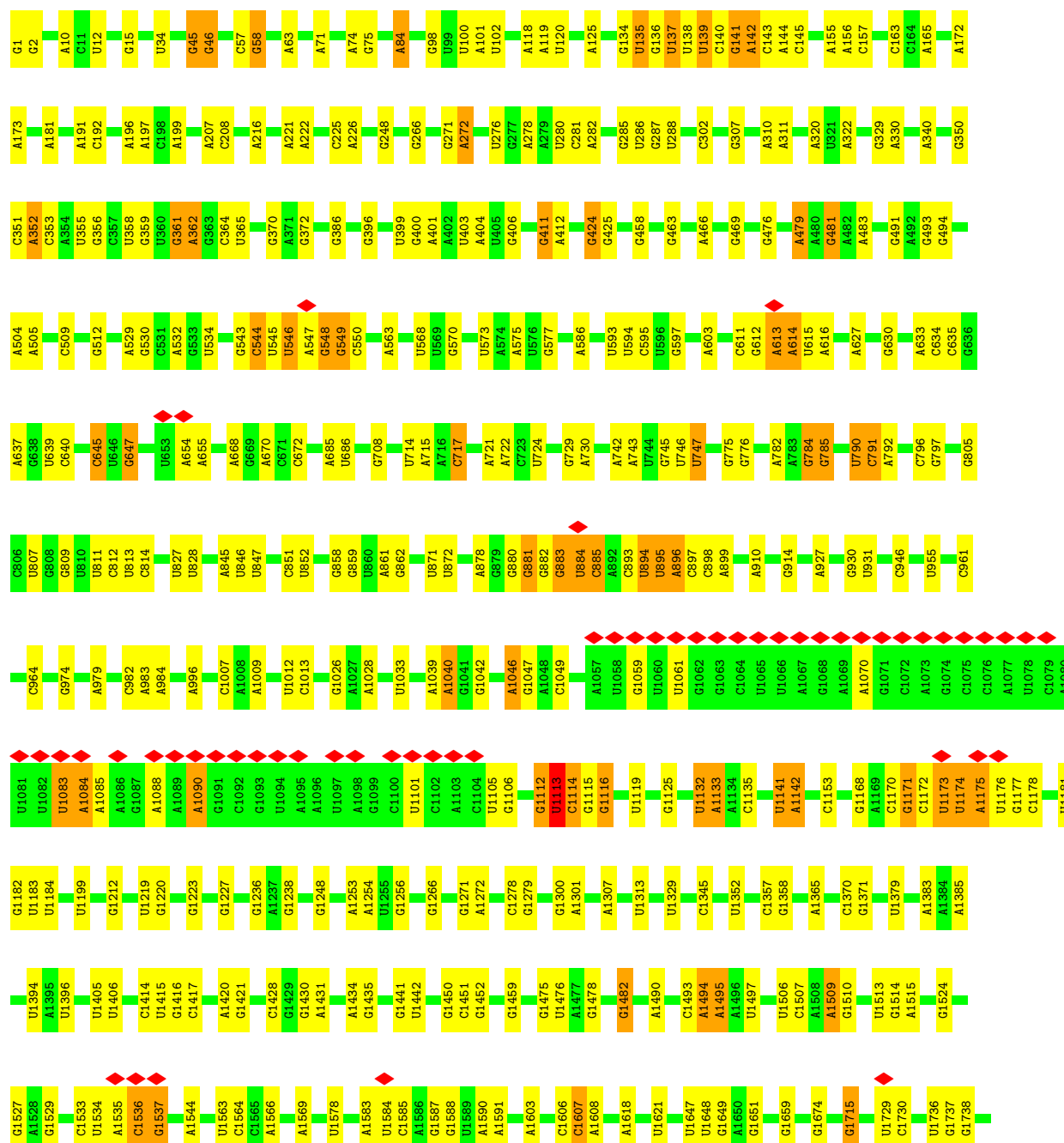
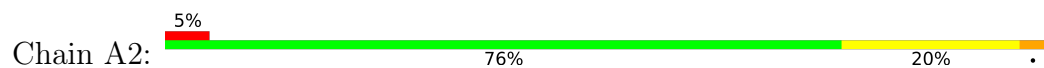
- Molecule 20: 30S ribosomal protein S20

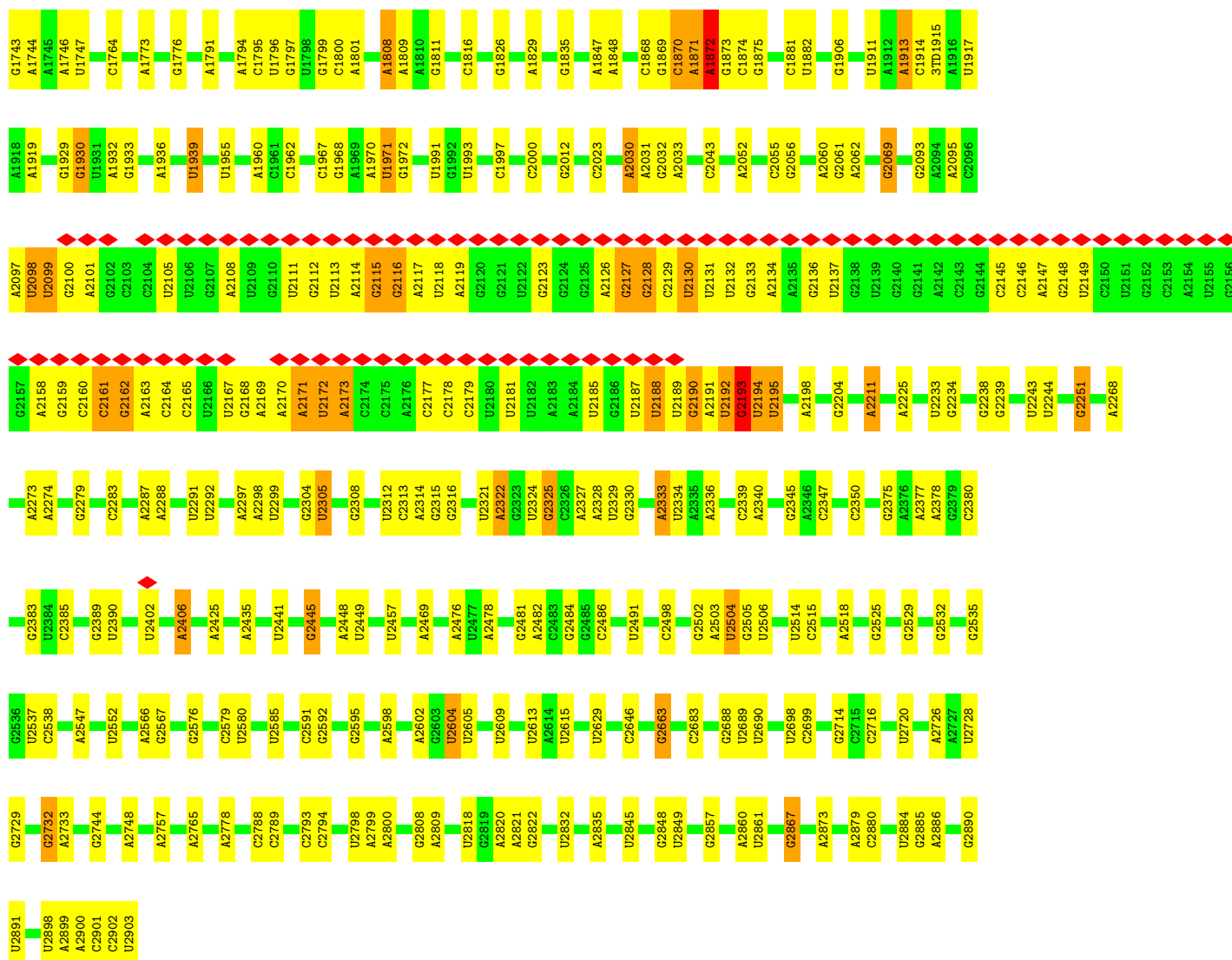


- Molecule 21: 30S ribosomal protein S21

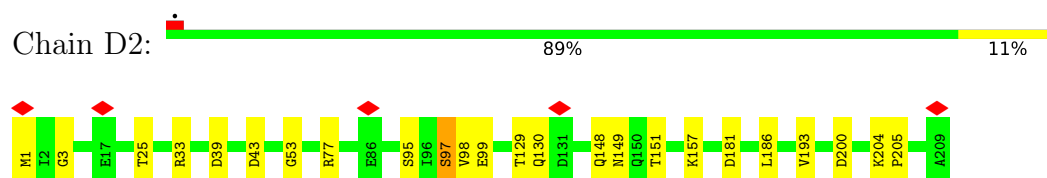


• Molecule 22: 23S rRNA

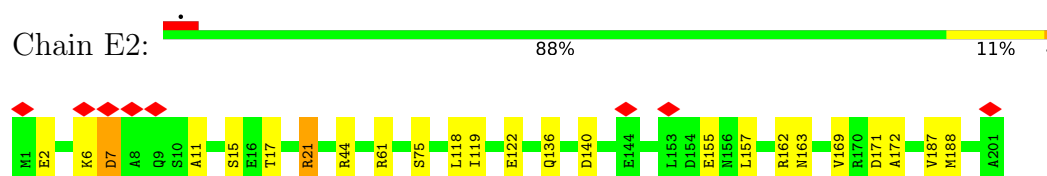




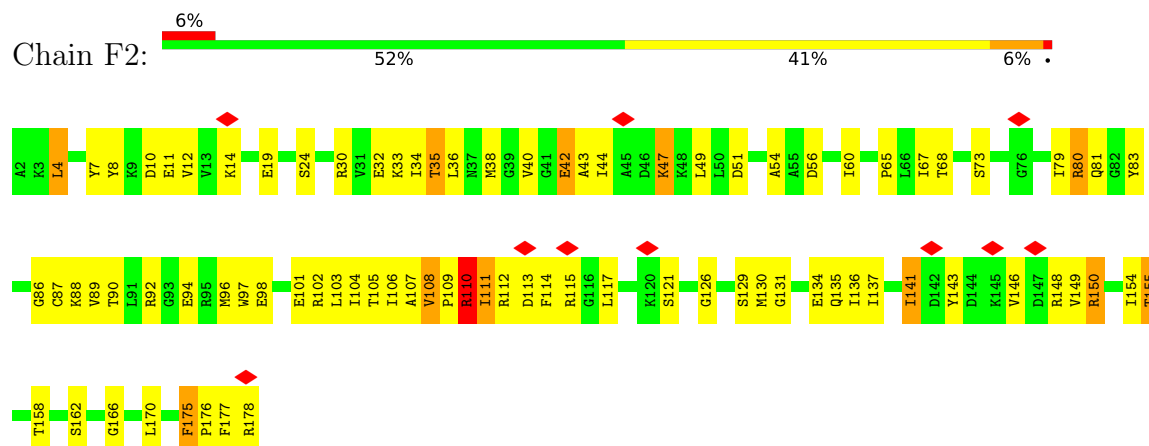
- Molecule 25: 50S ribosomal protein L3



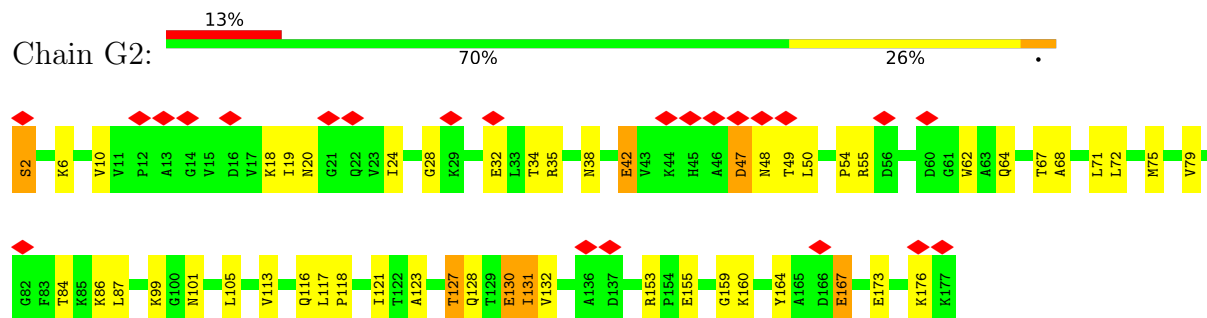
- Molecule 26: 50S ribosomal protein L4



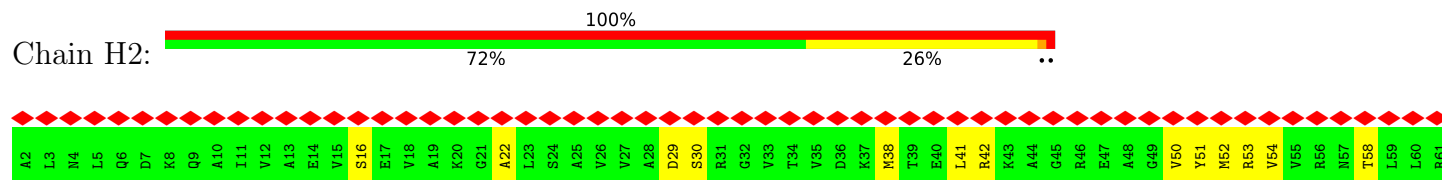
- Molecule 27: 50S ribosomal protein L5



- Molecule 28: 50S ribosomal protein L6

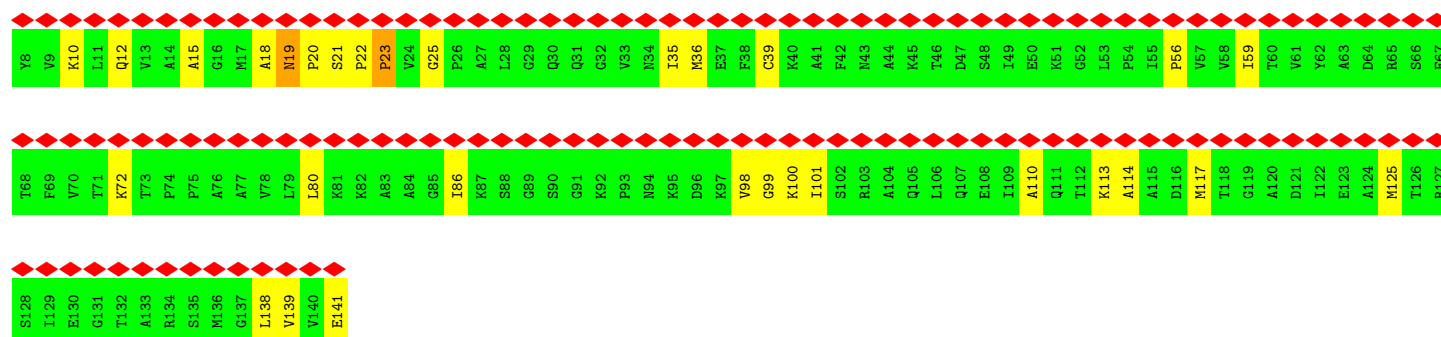
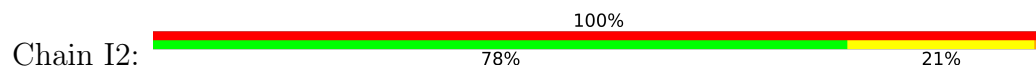


- Molecule 29: 50S ribosomal protein L10

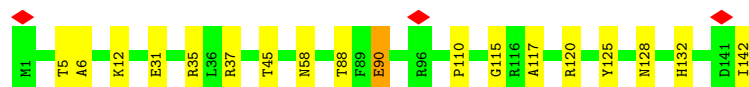




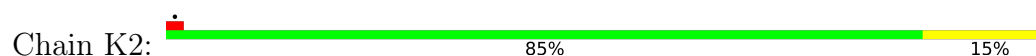
• Molecule 30: 50S ribosomal protein L11



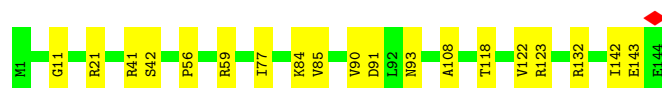
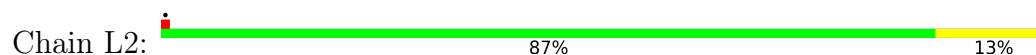
• Molecule 31: 50S ribosomal protein L13



• Molecule 32: 50S ribosomal protein L14

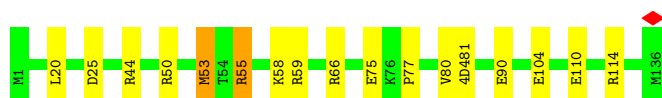


• Molecule 33: 50S ribosomal protein L15

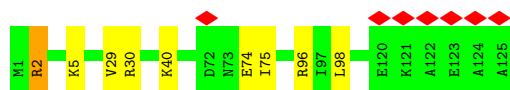


• Molecule 34: 50S ribosomal protein L16

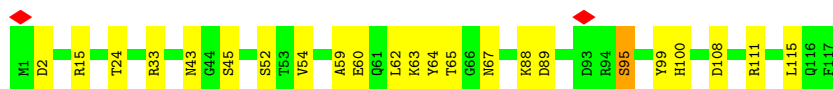
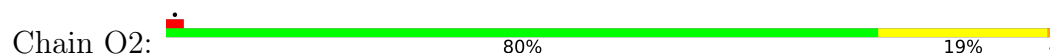




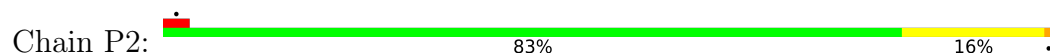
- Molecule 35: 50S ribosomal protein L17



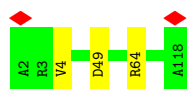
- Molecule 36: 50S ribosomal protein L18



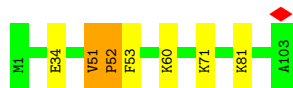
- Molecule 37: 50S ribosomal protein L19



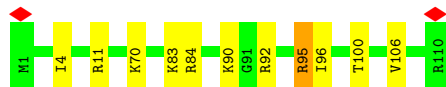
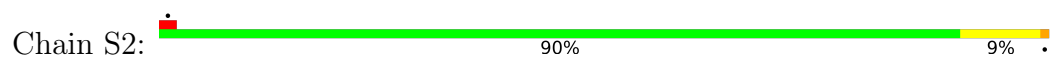
- Molecule 38: 50S ribosomal protein L20



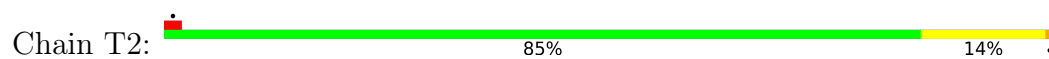
- Molecule 39: 50S ribosomal protein L21



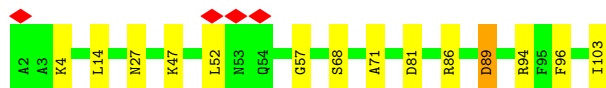
- Molecule 40: 50S ribosomal protein L22



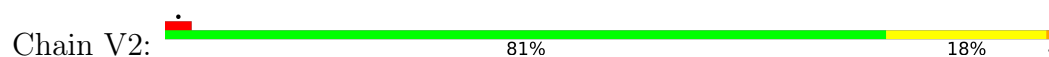
- Molecule 41: 50S ribosomal protein L23



- Molecule 42: 50S ribosomal protein L24



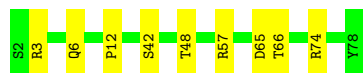
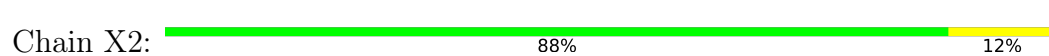
- Molecule 43: 50S ribosomal protein L25



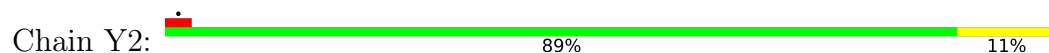
- Molecule 44: 50S ribosomal protein L27



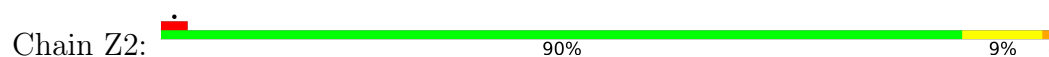
- Molecule 45: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L29



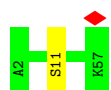
- Molecule 47: 50S ribosomal protein L30





- Molecule 48: 50S ribosomal protein L32

Chain a2:  98%



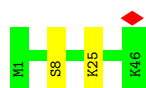
- Molecule 49: 50S ribosomal protein L33

Chain b2:  98%



- Molecule 50: 50S ribosomal protein L34

Chain c2:  96%



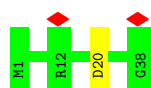
- Molecule 51: 50S ribosomal protein L35

Chain d2:  94%



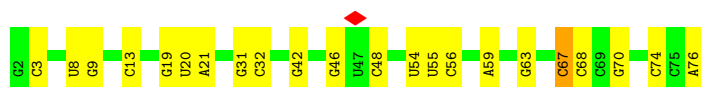
- Molecule 52: 50S ribosomal protein L36

Chain e2:  97%



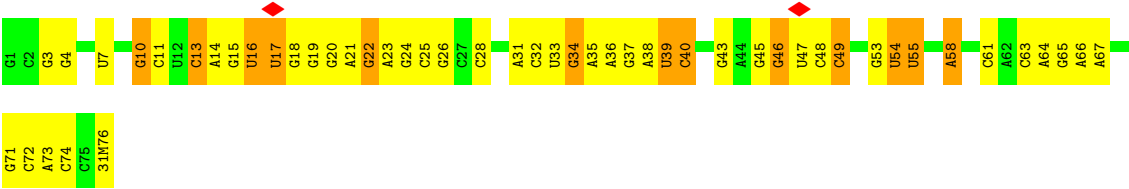
- Molecule 53: Deacylated tRNA<sup>i</sup>(Met)

Chain f2:  71% 28%



- Molecule 54: fMet-Phe-tRNA(Phe)

Chain g2:  33% 50% 17%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	117919	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	21.342	Depositor
Minimum map value	-14.160	Depositor
Average map value	-0.014	Depositor
Map value standard deviation	0.750	Depositor
Recommended contour level	2.3	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: 31M, MEQ, 4SU, H2U, OMU, 2MG, YYG, 2MA, OMG, 6MZ, 5MU, 1MG, 7MG, M2G, 5MC, 1MA, 3TD, G7M, DI0, 4D4, OMC, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A1	0.35	0/36586	0.78	1/57053 (0.0%)
2	B1	0.24	0/1784	0.41	0/2403
3	C1	0.28	0/1652	0.43	0/2225
4	D1	0.25	0/1665	0.41	0/2227
5	E1	0.27	0/1157	0.44	0/1557
6	F1	0.25	0/881	0.42	0/1189
7	G1	0.26	0/1196	0.38	0/1602
8	H1	0.26	0/989	0.43	0/1326
9	I1	0.30	0/1034	0.45	0/1375
10	J1	0.26	0/806	0.45	0/1089
11	K1	0.26	0/893	0.44	0/1205
12	L1	0.26	0/960	0.50	1/1286 (0.1%)
13	M1	0.27	0/893	0.44	0/1193
14	N1	0.27	0/817	0.40	0/1088
15	O1	0.24	0/722	0.38	0/964
16	P1	0.26	0/659	0.42	0/884
17	Q1	0.25	0/658	0.44	0/881
18	R1	0.25	0/463	0.40	0/621
19	S1	0.28	0/653	0.42	0/877
20	T1	0.25	0/676	0.37	0/895
21	U1	0.24	0/472	0.38	0/627
22	A2	0.73	1/69172 (0.0%)	0.74	7/107908 (0.0%)
23	B2	0.56	0/2872	0.71	0/4478
24	C2	0.37	0/2122	0.46	0/2852
25	D2	0.36	0/1576	0.46	0/2119
26	E2	0.34	0/1571	0.44	0/2113
27	F2	0.29	0/1435	0.45	0/1926
28	G2	0.30	0/1343	0.46	0/1816
29	H2	0.42	0/1037	0.60	0/1402
30	I2	0.48	0/993	0.66	0/1341
31	J2	0.37	0/1152	0.43	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	K2	0.36	0/955	0.47	0/1279
33	L2	0.34	0/1062	0.47	0/1413
34	M2	0.36	0/1081	0.45	0/1443
35	N2	0.35	0/1006	0.44	0/1345
36	O2	0.31	0/910	0.44	0/1219
37	P2	0.36	0/929	0.45	0/1242
38	Q2	0.40	0/960	0.38	0/1278
39	R2	0.37	0/829	0.48	0/1107
40	S2	0.32	0/864	0.44	0/1156
41	T2	0.32	0/745	0.42	0/994
42	U2	0.33	0/788	0.48	1/1051 (0.1%)
43	V2	0.33	0/766	0.42	0/1025
44	W2	0.37	0/587	0.44	0/776
45	X2	0.37	0/635	0.46	0/848
46	Y2	0.27	0/502	0.37	0/667
47	Z2	0.31	0/453	0.44	0/605
48	a2	0.35	0/450	0.45	0/599
49	b2	0.32	0/421	0.44	0/561
50	c2	0.34	0/380	0.43	0/498
51	d2	0.34	0/513	0.47	0/676
52	e2	0.35	0/303	0.44	0/397
53	f2	0.42	0/1725	1.03	3/2689 (0.1%)
54	g2	0.57	0/1458	0.83	2/2272 (0.1%)
All	All	0.55	1/157211 (0.0%)	0.69	15/235213 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
29	H2	0	1
30	I2	0	1
39	R2	0	1
51	d2	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	401	A	O3'-P	-7.84	1.51	1.61

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	f2	46	G	C6-N1-C2	-8.93	119.75	125.10
54	g2	22	G	C2'-C3'-O3'	7.83	126.72	109.50
22	A2	2193	G	C2'-C3'-O3'	6.53	124.14	113.70
22	A2	1113	U	C2'-C3'-O3'	6.50	124.10	113.70
12	L1	102	LEU	CA-CB-CG	6.10	129.33	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	H2	67	THR	Peptide
30	I2	98	VAL	Peptide
39	R2	51	VAL	Peptide
51	d2	31	HIS	Peptide

## 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	A1	32681	0	16454	398	0
2	B1	1753	0	1780	27	0
3	C1	1625	0	1696	20	0
4	D1	1643	0	1707	35	0
5	E1	1144	0	1182	24	0
6	F1	862	0	864	25	0
7	G1	1182	0	1238	21	0
8	H1	979	0	1031	15	0
9	I1	1022	0	1066	22	0
10	J1	796	0	836	18	0
11	K1	877	0	887	13	0
12	L1	947	0	1011	31	0
13	M1	884	0	940	54	0
14	N1	805	0	844	16	0
15	O1	714	0	732	17	0
16	P1	649	0	666	27	0
17	Q1	649	0	691	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R1	456	0	478	9	0
19	S1	638	0	665	10	0
20	T1	670	0	719	3	0
21	U1	465	0	491	8	0
22	A2	62252	0	31324	367	0
23	B2	2569	0	1301	13	0
24	C2	2083	0	2154	21	0
25	D2	1566	0	1617	14	0
26	E2	1552	0	1619	13	0
27	F2	1411	0	1443	124	0
28	G2	1323	0	1371	30	0
29	H2	1023	0	1052	21	0
30	I2	979	0	1028	26	0
31	J2	1129	0	1162	10	0
32	K2	946	0	1021	10	0
33	L2	1053	0	1129	12	0
34	M2	1075	0	1155	10	0
35	N2	993	0	1034	6	0
36	O2	900	0	935	18	0
37	P2	917	0	961	11	0
38	Q2	947	0	1019	3	0
39	R2	816	0	839	4	0
40	S2	857	0	922	6	0
41	T2	739	0	807	14	0
42	U2	780	0	831	7	0
43	V2	753	0	780	11	0
44	W2	580	0	593	5	0
45	X2	625	0	652	4	0
46	Y2	501	0	531	3	0
47	Z2	449	0	487	3	0
48	a2	444	0	458	0	0
49	b2	414	0	442	0	0
50	c2	377	0	418	0	0
51	d2	504	0	572	0	0
52	e2	302	0	343	0	0
53	f2	1625	0	829	0	0
54	g2	1667	0	880	0	0
55	A2	58	0	0	1	0
All	All	145650	0	97687	1410	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 7.

The worst 5 of 1410 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)
13:M1:7:ILE:HD12	27:F2:112:ARG:CG	1.30	1.59
6:F1:14:GLN:OE1	6:F1:83:ALA:CB	1.66	1.41
13:M1:7:ILE:CD1	27:F2:112:ARG:HG2	1.52	1.38
22:A2:883:G:N2	22:A2:894:U:O2	1.56	1.37
22:A2:1:G:N2	22:A2:2902:C:O2	1.64	1.30

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	
2	B1	222/224 (99%)	209 (94%)	13 (6%)	0	100	100
3	C1	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
4	D1	203/205 (99%)	201 (99%)	2 (1%)	0	100	100
5	E1	153/155 (99%)	147 (96%)	6 (4%)	0	100	100
6	F1	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
7	G1	149/151 (99%)	140 (94%)	8 (5%)	1 (1%)	22	30
8	H1	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
9	I1	125/127 (98%)	113 (90%)	12 (10%)	0	100	100
10	J1	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	22
11	K1	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
12	L1	118/123 (96%)	112 (95%)	4 (3%)	2 (2%)	9	11
13	M1	112/114 (98%)	105 (94%)	3 (3%)	4 (4%)	3	2
14	N1	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
15	O1	86/88 (98%)	84 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P1	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
17	Q1	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
18	R1	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
19	S1	77/79 (98%)	75 (97%)	1 (1%)	1 (1%)	12	16
20	T1	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
21	U1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
24	C2	269/271 (99%)	265 (98%)	4 (2%)	0	100	100
25	D2	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	29	40
26	E2	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
27	F2	175/177 (99%)	163 (93%)	11 (6%)	1 (1%)	25	34
28	G2	174/176 (99%)	168 (97%)	5 (3%)	1 (1%)	25	34
29	H2	133/135 (98%)	107 (80%)	19 (14%)	7 (5%)	2	0
30	I2	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	4	3
31	J2	140/142 (99%)	140 (100%)	0	0	100	100
32	K2	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
33	L2	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
34	M2	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
35	N2	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
36	O2	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
37	P2	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
38	Q2	115/117 (98%)	115 (100%)	0	0	100	100
39	R2	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	15	22
40	S2	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
41	T2	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
42	U2	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
43	V2	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
44	W2	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
45	X2	75/77 (97%)	75 (100%)	0	0	100	100
46	Y2	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
47	Z2	56/58 (97%)	56 (100%)	0	0	100	100
48	a2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	b2	49/51 (96%)	49 (100%)	0	0	100	100
50	c2	44/46 (96%)	44 (100%)	0	0	100	100
51	d2	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	9	12
52	e2	36/38 (95%)	36 (100%)	0	0	100	100
All	All	5630/5733 (98%)	5429 (96%)	176 (3%)	25 (0%)	38	46

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J1	57	VAL
12	L1	44	LYS
13	M1	7	ILE
13	M1	67	GLY
19	S1	5	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B1	186/186 (100%)	176 (95%)	10 (5%)	22	29
3	C1	170/170 (100%)	165 (97%)	5 (3%)	42	57
4	D1	172/172 (100%)	167 (97%)	5 (3%)	42	57
5	E1	118/118 (100%)	115 (98%)	3 (2%)	47	62
6	F1	92/92 (100%)	91 (99%)	1 (1%)	73	83
7	G1	124/124 (100%)	110 (89%)	14 (11%)	6	5
8	H1	104/104 (100%)	100 (96%)	4 (4%)	33	45
9	I1	105/105 (100%)	98 (93%)	7 (7%)	16	21
10	J1	87/87 (100%)	79 (91%)	8 (9%)	9	11
11	K1	90/90 (100%)	88 (98%)	2 (2%)	52	66
12	L1	102/102 (100%)	99 (97%)	3 (3%)	42	57
13	M1	92/92 (100%)	84 (91%)	8 (9%)	10	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N1	83/83 (100%)	79 (95%)	4 (5%)	25	34
15	O1	76/76 (100%)	75 (99%)	1 (1%)	69	80
16	P1	65/65 (100%)	64 (98%)	1 (2%)	65	77
17	Q1	74/74 (100%)	71 (96%)	3 (4%)	30	41
18	R1	48/48 (100%)	47 (98%)	1 (2%)	53	68
19	S1	70/70 (100%)	64 (91%)	6 (9%)	10	13
20	T1	65/65 (100%)	64 (98%)	1 (2%)	65	77
21	U1	48/48 (100%)	46 (96%)	2 (4%)	30	40
24	C2	216/216 (100%)	213 (99%)	3 (1%)	67	79
25	D2	163/163 (100%)	160 (98%)	3 (2%)	59	74
26	E2	165/165 (100%)	158 (96%)	7 (4%)	30	40
27	F2	148/148 (100%)	127 (86%)	21 (14%)	3	3
28	G2	137/137 (100%)	125 (91%)	12 (9%)	10	12
29	H2	103/103 (100%)	100 (97%)	3 (3%)	42	57
30	I2	104/104 (100%)	103 (99%)	1 (1%)	76	84
31	J2	116/116 (100%)	112 (97%)	4 (3%)	37	50
32	K2	104/104 (100%)	102 (98%)	2 (2%)	57	72
33	L2	103/103 (100%)	101 (98%)	2 (2%)	57	72
34	M2	108/108 (100%)	104 (96%)	4 (4%)	34	46
35	N2	102/102 (100%)	101 (99%)	1 (1%)	76	84
36	O2	87/87 (100%)	85 (98%)	2 (2%)	50	65
37	P2	99/99 (100%)	93 (94%)	6 (6%)	18	24
38	Q2	89/89 (100%)	89 (100%)	0	100	100
39	R2	84/84 (100%)	83 (99%)	1 (1%)	71	81
40	S2	93/93 (100%)	91 (98%)	2 (2%)	52	66
41	T2	80/80 (100%)	77 (96%)	3 (4%)	33	45
42	U2	83/83 (100%)	79 (95%)	4 (5%)	25	34
43	V2	78/78 (100%)	76 (97%)	2 (3%)	46	61
44	W2	57/58 (98%)	56 (98%)	1 (2%)	59	74
45	X2	67/67 (100%)	65 (97%)	2 (3%)	41	55
46	Y2	54/54 (100%)	52 (96%)	2 (4%)	34	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	Z2	48/48 (100%)	46 (96%)	2 (4%)	30	40
48	a2	47/47 (100%)	46 (98%)	1 (2%)	53	68
49	b2	45/46 (98%)	44 (98%)	1 (2%)	52	66
50	c2	38/38 (100%)	36 (95%)	2 (5%)	22	30
51	d2	51/51 (100%)	47 (92%)	4 (8%)	12	16
52	e2	34/34 (100%)	33 (97%)	1 (3%)	42	57
All	All	4674/4676 (100%)	4486 (96%)	188 (4%)	35	43

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	F2	111	ILE
32	K2	91	SER
27	F2	155	THR
28	G2	130	GLU
34	M2	59	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
28	G2	111	HIS
38	Q2	81	ASN
28	G2	115	HIS
36	O2	100	HIS
42	U2	27	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1513/1534 (98%)	227 (15%)	6 (0%)
22	A2	2888/2897 (99%)	380 (13%)	15 (0%)
23	B2	119/120 (99%)	7 (5%)	0
53	f2	75/76 (98%)	17 (22%)	0
54	g2	74/76 (97%)	47 (63%)	0
All	All	4669/4703 (99%)	678 (14%)	21 (0%)

5 of 678 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	4	U
1	A1	5	U
1	A1	6	G
1	A1	9	G
1	A1	32	A

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	A2	1535	A
22	A2	2127	G
22	A2	2193	G
22	A2	2130	U
22	A2	2118	U

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

45 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
54	31M	g2	76	22	38,44,45	4.34	18 (47%)	38,61,64	2.23	13 (34%)
22	PSU	A2	2504	22	18,21,22	2.39	8 (44%)	22,30,33	1.89	4 (18%)
54	7MG	g2	46	54	22,26,27	2.13	4 (18%)	29,39,42	3.15	10 (34%)
53	5MU	f2	54	53	19,22,23	1.44	5 (26%)	28,32,35	1.92	5 (17%)
54	OMC	g2	32	54	19,22,23	1.39	3 (15%)	26,31,34	2.13	2 (7%)
22	OMU	A2	2552	22	19,22,23	2.68	7 (36%)	26,31,34	1.86	6 (23%)
22	2MG	A2	2445	22	18,26,27	3.39	7 (38%)	16,38,41	1.30	3 (18%)
53	PSU	f2	55	53	18,21,22	1.31	2 (11%)	22,30,33	1.91	4 (18%)
22	PSU	A2	1917	22	18,21,22	2.32	8 (44%)	22,30,33	1.82	4 (18%)
22	PSU	A2	1911	22	18,21,22	2.32	8 (44%)	22,30,33	1.84	4 (18%)
54	OMG	g2	34	54	18,26,27	1.57	3 (16%)	19,38,41	1.52	4 (21%)
54	2MG	g2	10	54	18,26,27	1.53	3 (16%)	16,38,41	1.64	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	1MA	g2	58	54	16,25,26	1.62	3 (18%)	18,37,40	1.87	5 (27%)
54	PSU	g2	39	54	18,21,22	1.84	5 (27%)	22,30,33	2.49	7 (31%)
22	6MZ	A2	2030	22	18,25,26	1.98	1 (5%)	16,36,39	2.59	4 (25%)
22	5MC	A2	1962	22	18,22,23	2.01	6 (33%)	26,32,35	1.16	2 (7%)
25	MEQ	D2	150[A]	25	8,9,10	0.95	0	5,10,12	0.66	0
22	PSU	A2	746	22	18,21,22	2.37	9 (50%)	22,30,33	1.80	4 (18%)
22	OMC	A2	2498	22	19,22,23	1.90	6 (31%)	26,31,34	0.96	1 (3%)
54	M2G	g2	26	54	20,27,28	1.57	3 (15%)	22,40,43	1.06	2 (9%)
22	H2U	A2	2449	22	18,21,22	4.07	5 (27%)	21,30,33	5.20	7 (33%)
22	G7M	A2	2069	22	20,26,27	2.24	5 (25%)	17,39,42	0.71	0
22	PSU	A2	2457	22	18,21,22	2.46	8 (44%)	22,30,33	1.90	4 (18%)
54	5MC	g2	49	54	18,22,23	1.05	1 (5%)	26,32,35	1.59	4 (15%)
54	5MU	g2	54	54	19,22,23	1.54	3 (15%)	28,32,35	2.42	7 (25%)
22	OMG	A2	2251	53,22	18,26,27	2.46	5 (27%)	19,38,41	1.15	3 (15%)
34	4D4	M2	81	34	9,11,12	2.03	2 (22%)	8,13,15	2.10	4 (50%)
54	PSU	g2	55	54	18,21,22	1.65	4 (22%)	22,30,33	2.11	4 (18%)
22	1MG	A2	745	22	18,26,27	2.80	4 (22%)	19,39,42	1.28	3 (15%)
53	4SU	f2	8	53	18,21,22	2.17	5 (27%)	26,30,33	1.70	6 (23%)
22	2MA	A2	2503	22	17,25,26	1.59	3 (17%)	17,37,40	1.04	2 (11%)
22	3TD	A2	1915	22	18,22,23	2.73	7 (38%)	22,32,35	1.89	2 (9%)
54	5MC	g2	40	54	18,22,23	1.27	1 (5%)	26,32,35	2.12	10 (38%)
22	5MU	A2	747	22	19,22,23	2.58	7 (36%)	28,32,35	3.81	11 (39%)
54	H2U	g2	17	54	18,21,22	1.00	2 (11%)	21,30,33	1.92	2 (9%)
22	PSU	A2	2605	22	18,21,22	2.39	8 (44%)	22,30,33	1.87	4 (18%)
22	6MZ	A2	1618	22	18,25,26	1.98	1 (5%)	16,36,39	2.19	4 (25%)
54	YYG	g2	37	54	31,42,43	2.16	7 (22%)	33,62,65	2.03	10 (30%)
53	5MC	f2	32	53	18,22,23	0.97	2 (11%)	26,32,35	1.29	3 (11%)
22	PSU	A2	2604	22	18,21,22	2.40	8 (44%)	22,30,33	1.87	4 (18%)
22	5MU	A2	1939	22	19,22,23	2.67	7 (36%)	28,32,35	3.95	10 (35%)
54	H2U	g2	16	54	18,21,22	0.99	2 (11%)	21,30,33	1.90	2 (9%)
22	PSU	A2	955	22	18,21,22	2.44	8 (44%)	22,30,33	1.85	4 (18%)
22	PSU	A2	2580	22	18,21,22	2.47	10 (55%)	22,30,33	1.90	5 (22%)
22	2MG	A2	1835	22	18,26,27	3.37	7 (38%)	16,38,41	1.35	3 (18%)

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	31M	g2	76	22	-	6/27/49/50	0/4/4/4
22	PSU	A2	2504	22	-	2/7/25/26	0/2/2/2
54	7MG	g2	46	54	-	3/7/37/38	0/3/3/3
53	5MU	f2	54	53	-	0/7/25/26	0/2/2/2
54	OMC	g2	32	54	-	0/9/27/28	0/2/2/2
22	OMU	A2	2552	22	-	0/9/27/28	0/2/2/2
22	2MG	A2	2445	22	-	2/5/27/28	0/3/3/3
53	PSU	f2	55	53	-	0/7/25/26	0/2/2/2
22	PSU	A2	1917	22	-	0/7/25/26	0/2/2/2
22	PSU	A2	1911	22	-	0/7/25/26	0/2/2/2
54	OMG	g2	34	54	-	3/5/27/28	0/3/3/3
54	2MG	g2	10	54	-	0/5/27/28	0/3/3/3
54	1MA	g2	58	54	-	2/3/25/26	0/3/3/3
54	PSU	g2	39	54	-	3/7/25/26	0/2/2/2
22	6MZ	A2	2030	22	-	2/5/27/28	0/3/3/3
22	5MC	A2	1962	22	-	2/7/25/26	0/2/2/2
25	MEQ	D2	150[A]	25	-	4/8/9/11	-
22	PSU	A2	746	22	-	2/7/25/26	0/2/2/2
22	OMC	A2	2498	22	-	0/9/27/28	0/2/2/2
54	M2G	g2	26	54	-	0/7/29/30	0/3/3/3
22	H2U	A2	2449	22	-	0/7/38/39	0/2/2/2
22	G7M	A2	2069	22	-	1/3/25/26	0/3/3/3
22	PSU	A2	2457	22	-	0/7/25/26	0/2/2/2
54	5MC	g2	49	54	-	3/7/25/26	0/2/2/2
54	5MU	g2	54	54	-	2/7/25/26	0/2/2/2
22	OMG	A2	2251	53,22	-	1/5/27/28	0/3/3/3
34	4D4	M2	81	34	-	3/11/12/14	-
54	PSU	g2	55	54	-	0/7/25/26	0/2/2/2
22	1MG	A2	745	22	-	0/3/25/26	0/3/3/3
53	4SU	f2	8	53	-	0/7/25/26	0/2/2/2
22	2MA	A2	2503	22	-	1/3/25/26	0/3/3/3
22	3TD	A2	1915	22	-	0/7/25/26	0/2/2/2
54	5MC	g2	40	54	-	0/7/25/26	0/2/2/2
22	5MU	A2	747	22	-	0/7/25/26	0/2/2/2
54	H2U	g2	17	54	-	5/7/38/39	0/2/2/2
22	PSU	A2	2605	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	6MZ	A2	1618	22	-	0/5/27/28	0/3/3/3
54	YYG	g2	37	54	-	16/20/42/43	0/3/4/4
53	5MC	f2	32	53	-	0/7/25/26	0/2/2/2
22	PSU	A2	2604	22	-	0/7/25/26	0/2/2/2
22	5MU	A2	1939	22	-	0/7/25/26	0/2/2/2
54	H2U	g2	16	54	-	3/7/38/39	0/2/2/2
22	PSU	A2	955	22	-	0/7/25/26	0/2/2/2
22	PSU	A2	2580	22	-	0/7/25/26	0/2/2/2
22	2MG	A2	1835	22	-	0/5/27/28	0/3/3/3

The worst 5 of 231 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	g2	76	31M	C2'-C1'	-16.92	1.28	1.53
54	g2	76	31M	O4'-C1'	12.06	1.57	1.41
22	A2	2449	H2U	O4-C4	10.10	1.43	1.23
54	g2	76	31M	O4'-C4'	-9.47	1.23	1.45
22	A2	1835	2MG	O6-C6	9.24	1.42	1.23

The worst 5 of 206 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A2	2449	H2U	C4-N3-C2	-15.23	113.16	125.79
22	A2	2449	H2U	O2-C2-N1	-11.49	108.68	123.11
54	g2	46	7MG	N9-C4-N3	10.82	141.66	125.47
54	g2	32	OMC	C2'-C1'-N1	-9.28	96.21	114.22
22	A2	1939	5MU	C4-N3-C2	-9.13	115.53	127.35

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	D2	150[A]	MEQ	N-CA-CB-CG
34	M2	81	4D4	NE-CD-CG-CB
22	A2	746	PSU	C2'-C1'-C5-C4
22	A2	2251	OMG	C1'-C2'-O2'-CM2
54	g2	17	H2U	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 4 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A2	2030	6MZ	2	0
22	A2	2251	OMG	1	0
22	A2	2604	PSU	1	0
22	A2	1939	5MU	1	0

## 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	$\# Z  > 2$
55	DI0	A2	3001	-	58,61,61	1.62	11 (18%)	77,92,92	1.65	20 (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
55	DI0	A2	3001	-	-	10/70/121/121	0/3/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A2	3001	DI0	CAF-CAE	-5.60	1.39	1.51
55	A2	3001	DI0	OBI-CAG	-4.12	1.33	1.43
55	A2	3001	DI0	OAU-CBG	-3.41	1.38	1.44
55	A2	3001	DI0	OAY-CAC	-3.13	1.35	1.43
55	A2	3001	DI0	CBC-CBB	2.86	1.58	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A2	3001	DI0	OAL-CAW-CBT	4.88	116.70	107.40
55	A2	3001	DI0	CBT-CAW-CAD	-4.69	106.31	115.20
55	A2	3001	DI0	OBK-CAN-CAX	4.22	110.07	103.81
55	A2	3001	DI0	CAP-CAH-CAJ	-3.35	109.30	114.05
55	A2	3001	DI0	CBR-CAP-CBC	-2.75	106.45	111.09

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

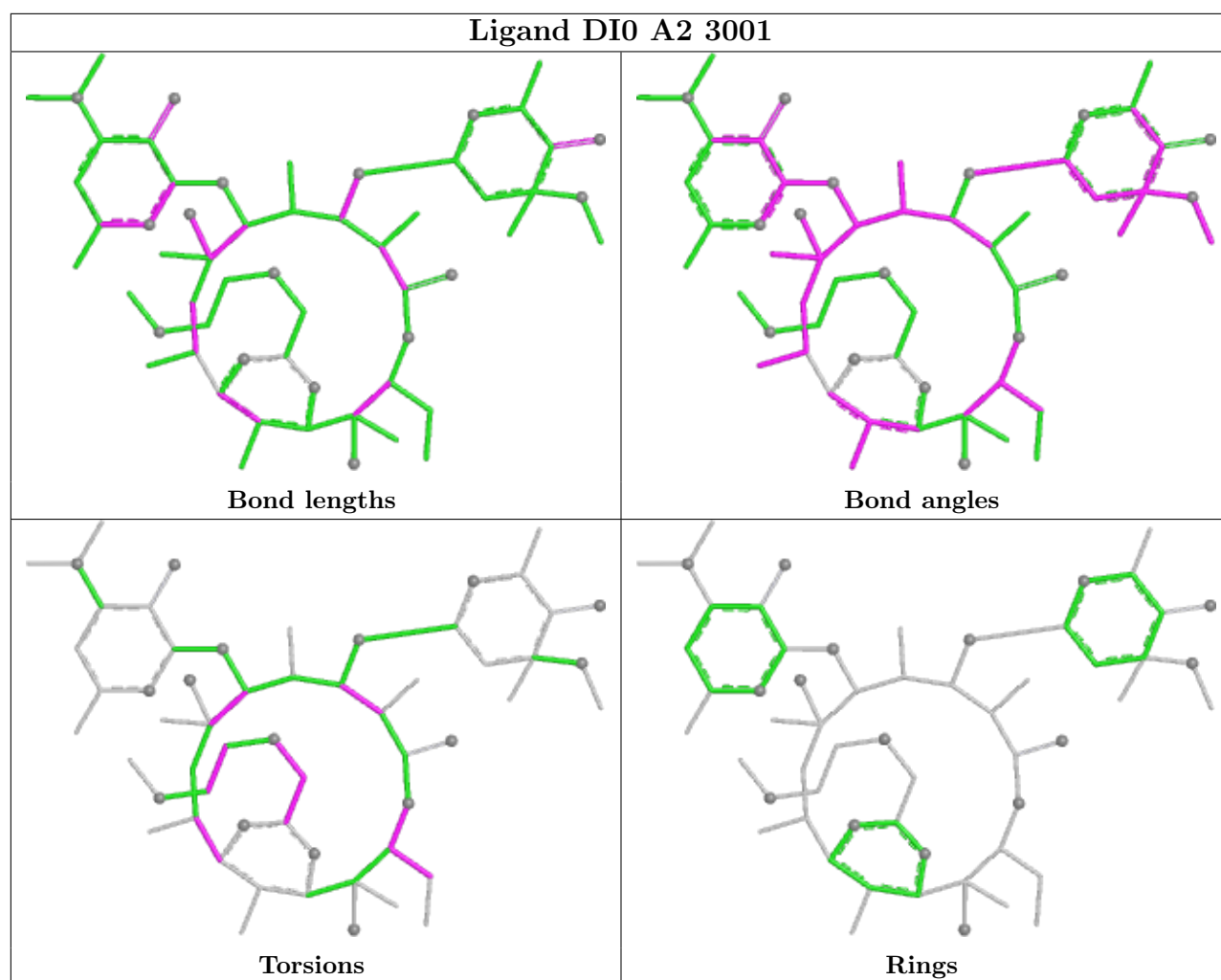
Mol	Chain	Res	Type	Atoms
55	A2	3001	DI0	NAQ-CBA-CBS-OBW
55	A2	3001	DI0	NAQ-CAK-CBB-CBC
55	A2	3001	DI0	CAJ-CAH-CAP-OBJ
55	A2	3001	DI0	OBX-CCC-CCD-OBW
55	A2	3001	DI0	OAL-CAW-CBT-CCF

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	A2	3001	DI0	1	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	A2	1
54	g2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	885:C	O3'	892:A	P	11.25
1	g2	75:C	O3'	76:31M	P	1.09

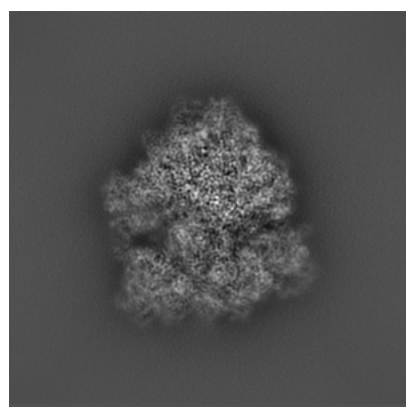
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10657. These allow visual inspection of the internal detail of the map and identification of artifacts.

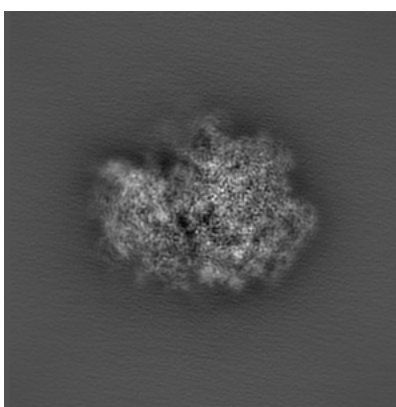
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

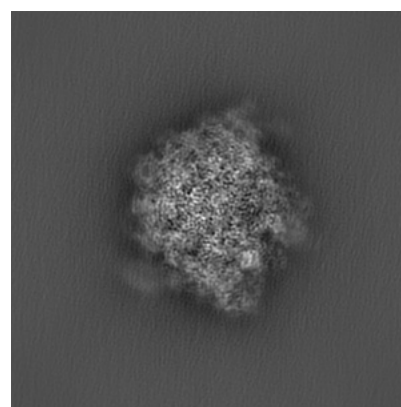
#### 6.1.1 Primary map



X



Y

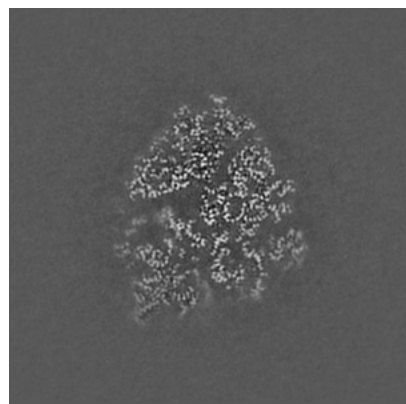


Z

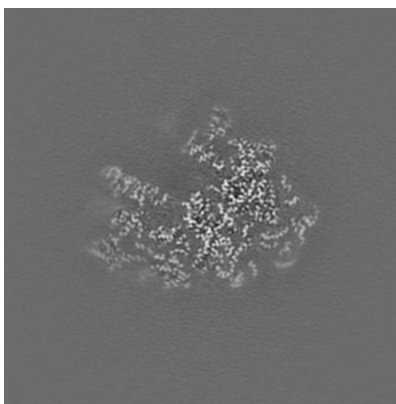
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

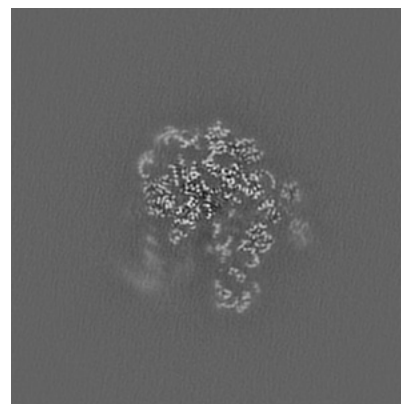
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

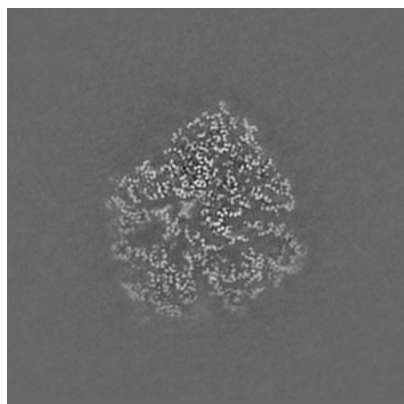


Z Index: 256

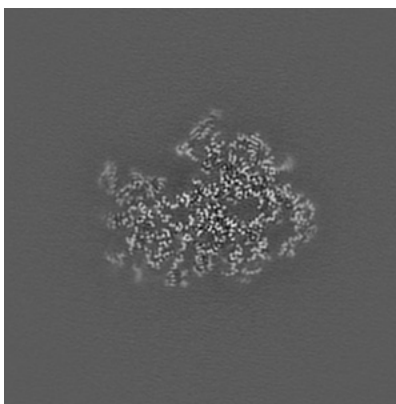
The images above show central slices of the map in three orthogonal directions.

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

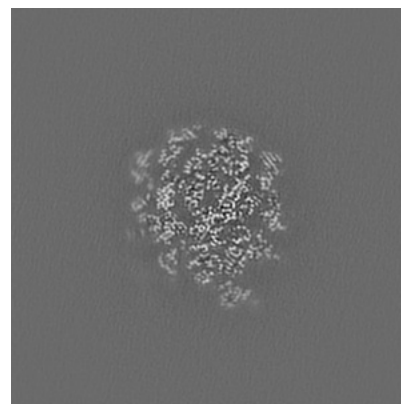
### 6.3.1 Primary map



X Index: 266



Y Index: 271

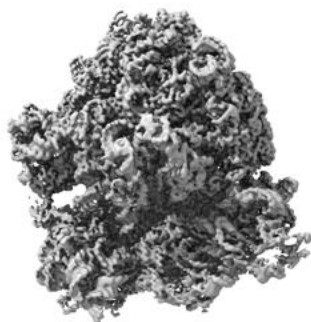


Z Index: 297

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

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

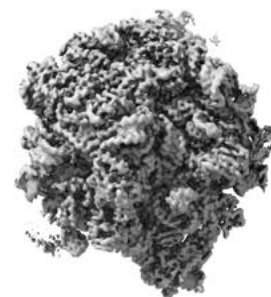
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

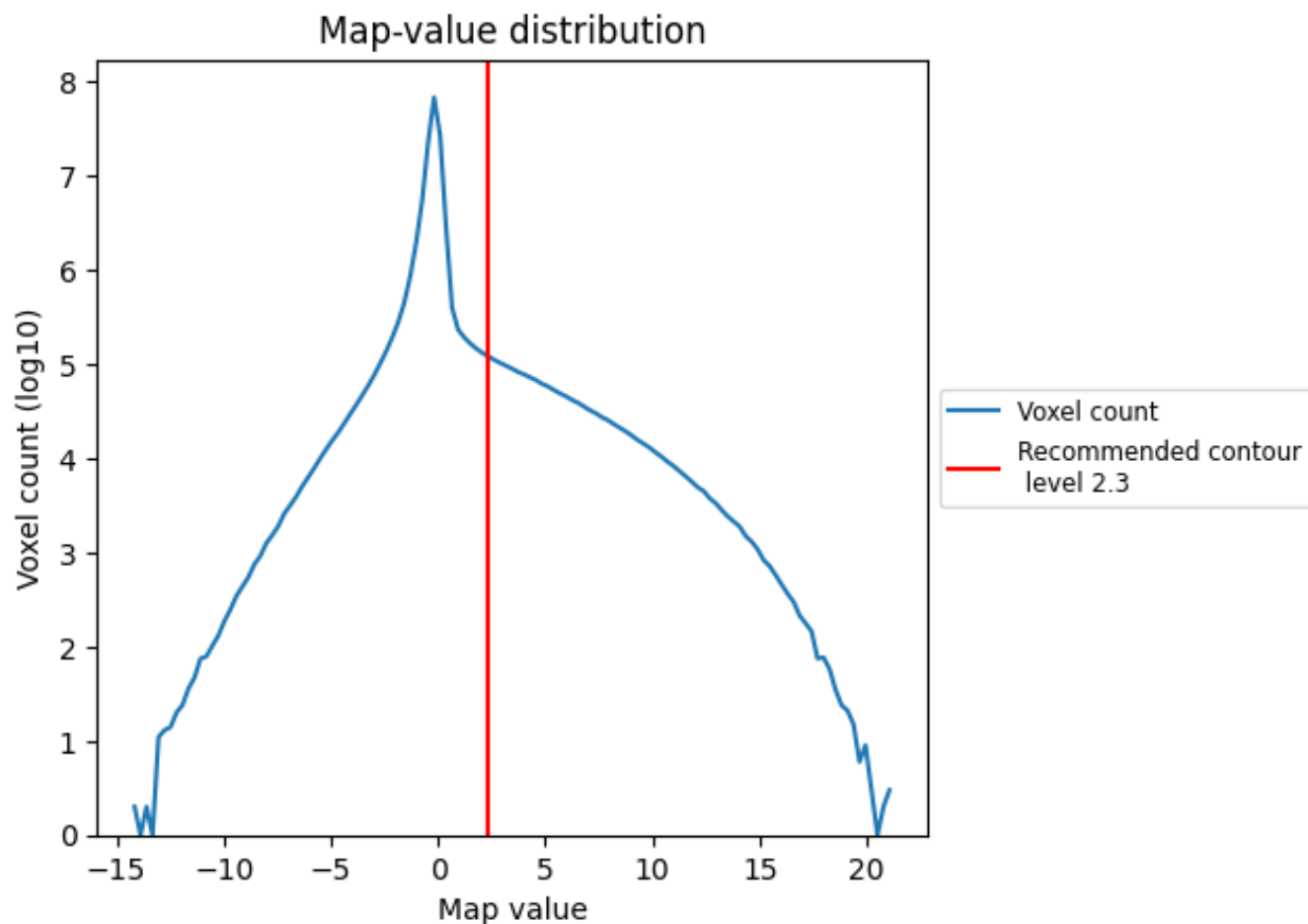
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

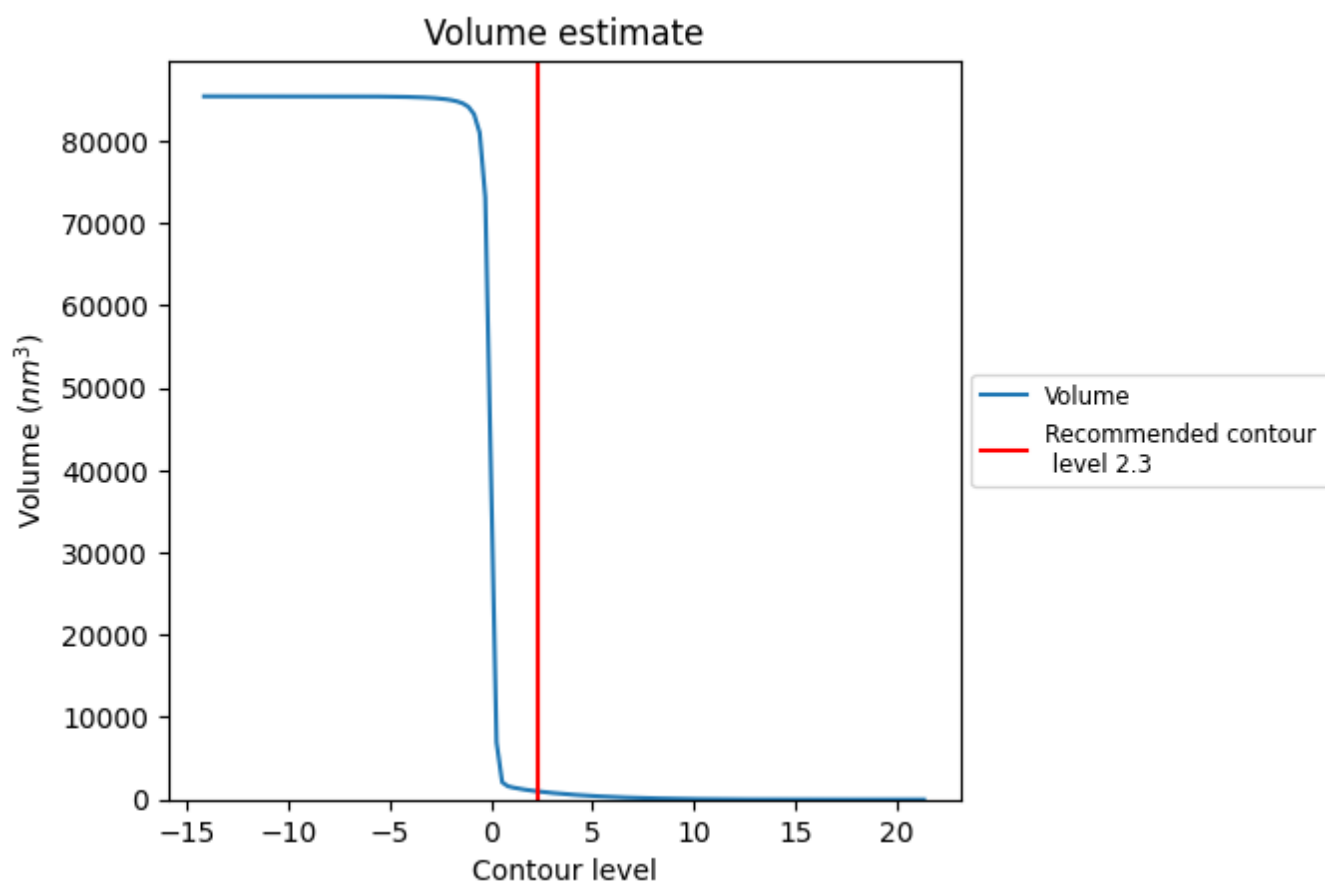
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

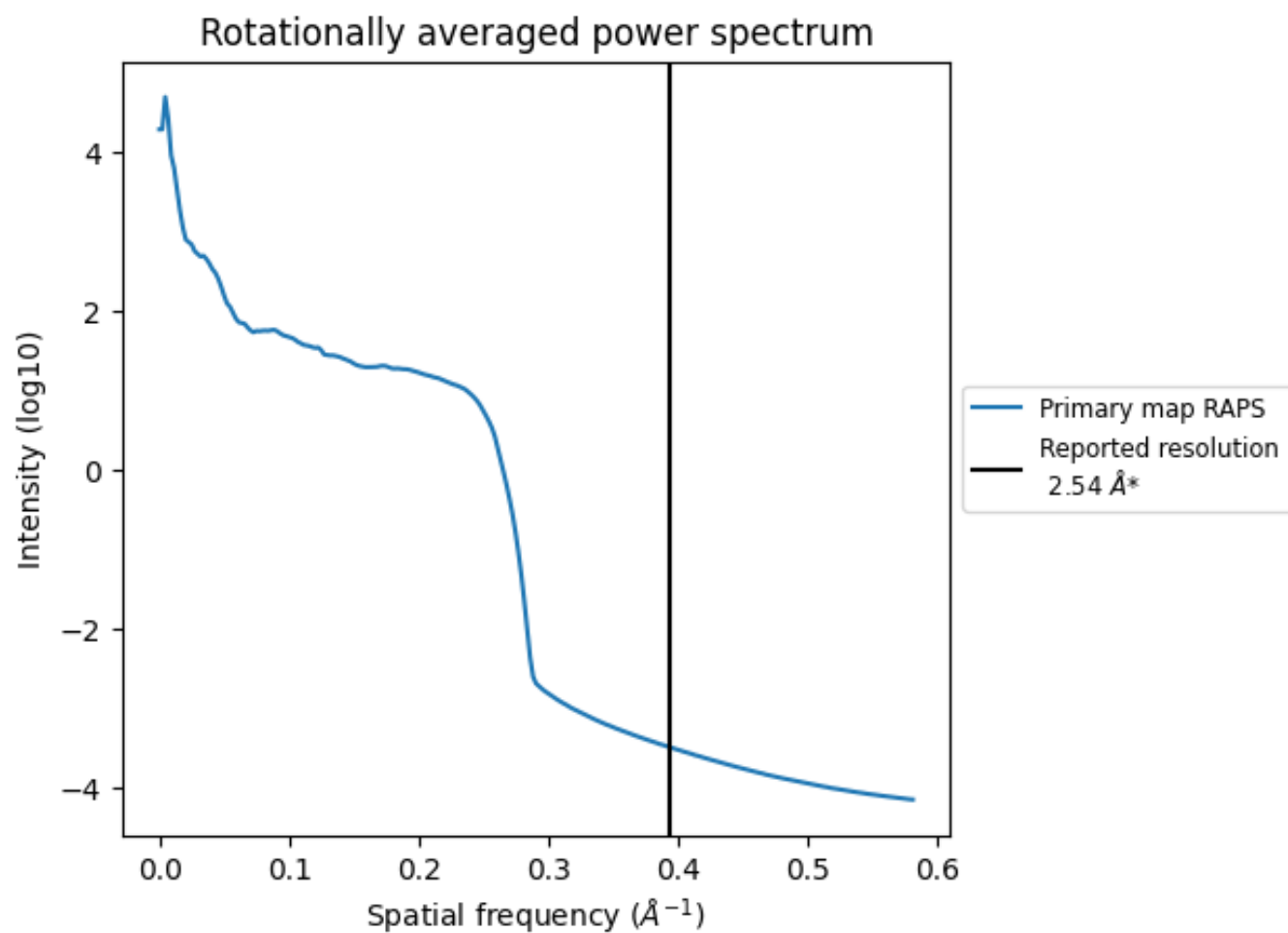


The volume at the recommended contour level is 994 nm<sup>3</sup>; this corresponds to an approximate mass of 898 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.394 Å<sup>-1</sup>

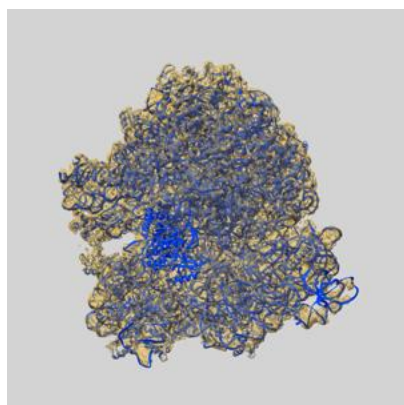
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

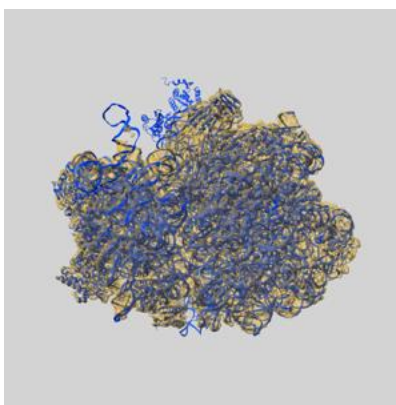
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10657 and PDB model 6XZB. Per-residue inclusion information can be found in section 3 on page 14.

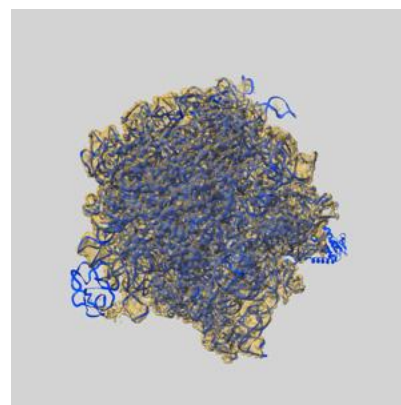
### 9.1 Map-model overlay [i](#)



X



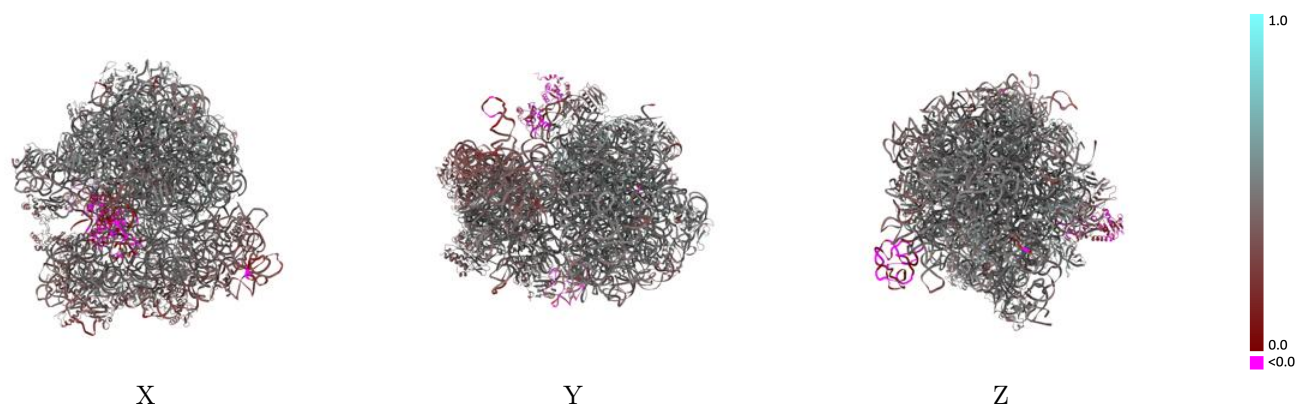
Y



Z

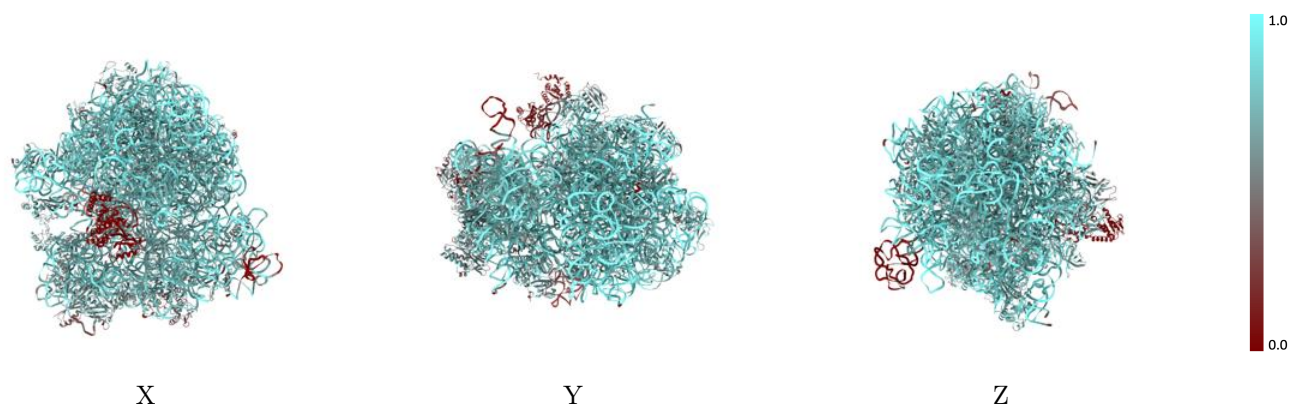
The images above show the 3D surface view of the map at the recommended contour level 2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



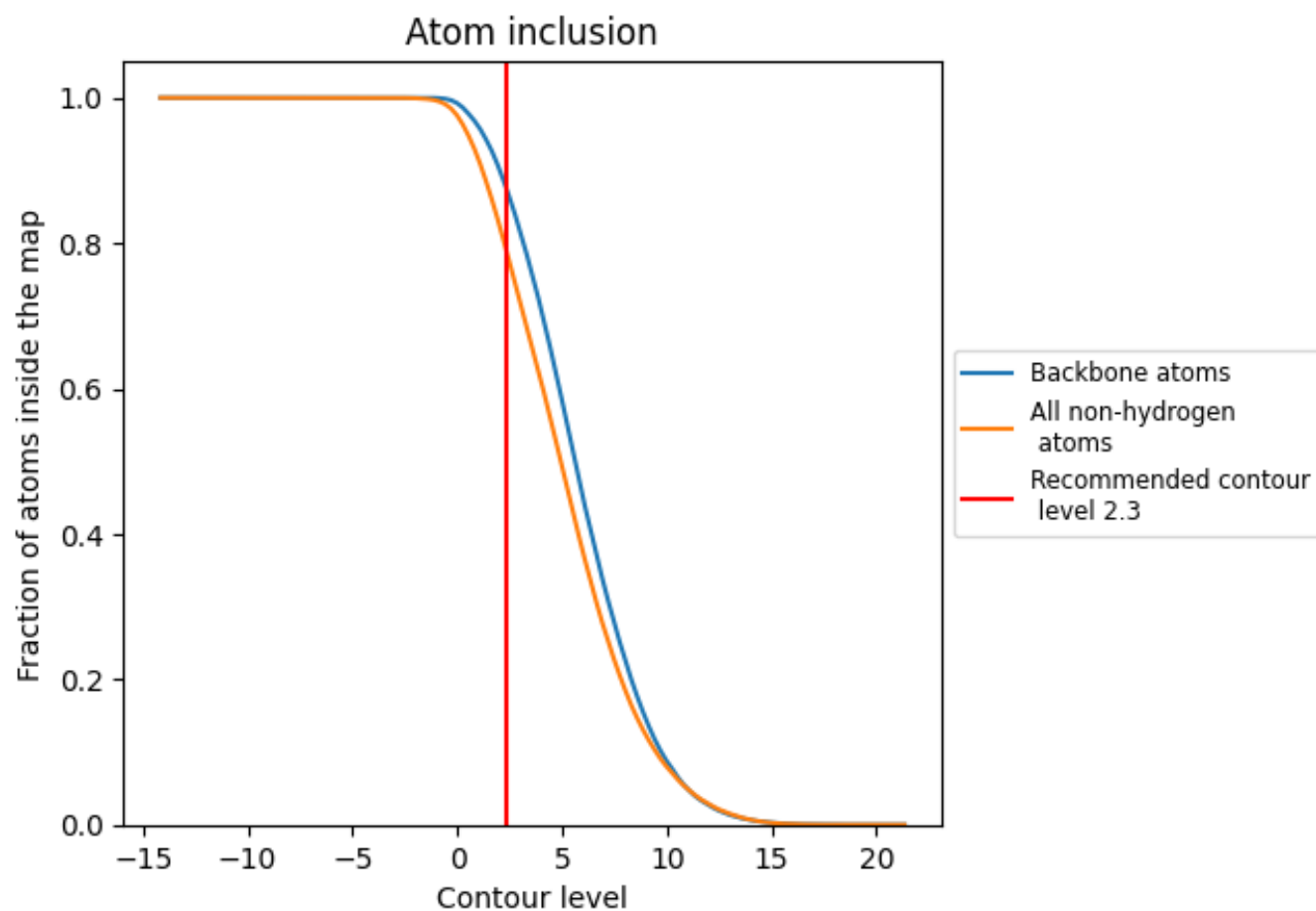
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.3).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 79% 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 (2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7946	 0.4320
A1	 0.8394	 0.4140
A2	 0.8665	 0.4430
B1	 0.5639	 0.4060
B2	 0.9089	 0.4490
C1	 0.6238	 0.4270
C2	 0.7685	 0.5050
D1	 0.4642	 0.3420
D2	 0.7485	 0.4980
E1	 0.6818	 0.4620
E2	 0.7138	 0.4780
F1	 0.6790	 0.4130
F2	 0.6718	 0.4080
G1	 0.5773	 0.3840
G2	 0.6384	 0.4210
H1	 0.6729	 0.4560
H2	 0.0010	 0.0450
I1	 0.5567	 0.4020
I2	 0.0000	 0.0500
J1	 0.5097	 0.3820
J2	 0.7573	 0.4840
K1	 0.6882	 0.4350
K2	 0.7318	 0.5000
L1	 0.6616	 0.4370
L2	 0.7598	 0.4830
M1	 0.6491	 0.4020
M2	 0.7632	 0.4990
N1	 0.6085	 0.3990
N2	 0.7455	 0.4830
O1	 0.7203	 0.4330
O2	 0.7176	 0.4420
P1	 0.5120	 0.3770
P2	 0.7365	 0.4850
Q1	 0.6398	 0.4170
Q2	 0.7786	 0.4980



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Chain	Atom inclusion	Q-score
R1	 0.6957	 0.4440
R2	 0.7629	 0.4900
S1	 0.6158	 0.3880
S2	 0.7165	 0.4890
T1	 0.5817	 0.3540
T2	 0.6957	 0.4640
U1	 0.5360	 0.4000
U2	 0.6953	 0.4670
V2	 0.7425	 0.4690
W2	 0.7748	 0.5040
X2	 0.7737	 0.4860
Y2	 0.6871	 0.4250
Z2	 0.7437	 0.4880
a2	 0.7547	 0.4790
b2	 0.6749	 0.4790
c2	 0.7634	 0.4950
d2	 0.7882	 0.5130
e2	 0.7295	 0.4930
f2	 0.8769	 0.4150
g2	 0.8452	 0.4310