Full wwPDB EM Validation Report (i)

Jan 28, 2023 – 08:11 am GMT

PDB ID	:	7OYC
EMDB ID	:	EMD-13113
Title	:	Cryo-EM structure of the Xenopus egg 80S ribosome
Authors	:	Leesch, F.; Lorenzo-Orts, L.; Grishkovskaya, I.; Kandolf, S.; Belacic, K.; Meinhart, A.; Haselbach, D.; Pauli, A.
Deposited on	:	2021-06-24
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

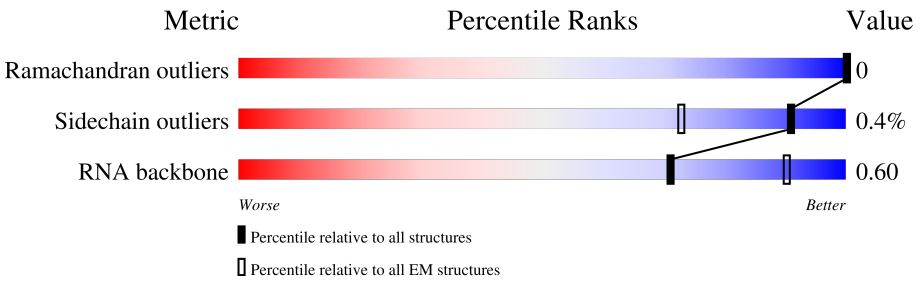
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	11	154	49%; 88%; 12%
2	22	1826	68%; 14%; 18%
3	51	4115	66%; 13%; 21%
4	71	120	91%; 8%; •
5	81	156	81%; 13%; 6%
6	A1	257	95%; 5%
7	A2	306	68%; 32%
8	B1	403	98%; •

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Mol	Chain	Length	Quality of chain
9	B2	264	80% 19%
10	C1	401	87% 12%
11	C2	281	76% 23%
12	D1	296	98%
13	D2	246	90% 9%
14	E1	258	83% 17%
15	E2	263	98%
16	F1	246	92% 8%
17	F2	203	90% 10%
18	G1	266	79% 21%
19	G2	249	89% 11%
20	H1	192	98%
21	H2	194	94%
22	I1	215	94% 6%
23	I2	208	95% 5%
24	J1	177	94% 6%
25	J2	194	92% 7%
26	K2	165	56% 44%
27	L1	211	94% 6%
28	L2	158	89% 11%
29	M1	138	97%
30	N1	204	100%
31	N2	151	99%
32	O1	231	86% 14%
33	O2	151	87% 12%

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Mol	Chain	Length	Quality of chain
34	P1	184	83% 17%
35	P2	145	80% 20%
36	Q1	188	96%
37	Q2	146	91% 8%
38	R1	197	84% 16%
39	R2	135	98%
40	S1	176	100%
41	S2	152	89% 11%
42	T1	160	98%
43	T2	146	94% 6%
44	U1	128	76% 24%
45	U2	119	70% 29%
46	V1	140	92% 8%
47	V2	83	100%
48	W1	155	39% 61%
49	W2	130	98%
50	X1	155	77% 23%
51	X2	143	96%
52	Y1	145	85% 14%
53	Y2	132	93% 7%
54	Z1	136	99%
55	Z2	125	54% 46%
56	a1	148	99%
57	a2	115	85% 15%
58	b1	75	84% 16%

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Mol	Chain	Length	Quality of chain
59	b2	84	96%
60	c1	116	81% 19%
61	c2	69	84% 14%
62	d1	125	84% 15%
63	d2	86	64% 36%
64	e1	135	93% 7%
65	e2	133	38% 62%
66	f1	110	97%
67	g1	117	87% 11%
68	g2	317	97%
69	h1	123	98%
70	i1	105	93% 7%
71	i2	378	13% 87%
72	j1	97	89% 11%
73	k1	70	97%
74	l1	51	98%
75	m1	128	39% 61%
76	n1	25	96%
77	o1	106	96%
78	p1	92	98%
79	r1	137	86% 14%
80	s1	113	13% 27% 73%
81	v2	858	6% 42% 58%

2 Entry composition (i)

There are 83 unique types of molecules in this entry. The entry contains 198947 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 Eukaryotic translation initiation factor 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	11	136	1033	644	178	200	11	0	0

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	22	1495	31922	14260	5748	10420	1494	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
22	287	C	U	conflict	GB X04025.1

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	51	3245	69603	30999	12763	22596	3245	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	71	119	2538	1133	457	830	118	0	0

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	81	147	3139	1399	564	1029	147	0	0

- Molecule 6 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A1	245	1868	1173	378	311	6	0	0

- Molecule 7 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A2	208	1643	1046	289	299	9	0	0

- Molecule 8 is a protein called Rpl3-prov protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	B1	394	3170	2021	594	541	14	0	0

- Molecule 9 is a protein called 40S ribosomal protein S3a-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B2	213	1734	1103	309	309	13	0	0

- Molecule 10 is a protein called 60S ribosomal protein L4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C1	351	2805	1763	557	469	16	0	0

- Molecule 11 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C2	215	1663	1077	285	292	9	0	0

- Molecule 12 is a protein called Rpl5-b protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D1	289	2348	1493	427	421	7	0	0

- Molecule 13 is a protein called DNA-(apurinic or apyrimidinic site) lyase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	D2	223	1732	1103	312	310	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D2	83	GLY	SER	conflict	UNP Q7ZYT3

- Molecule 14 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	E1	214	1739	1123	332	280	4	0	0

- Molecule 15 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	E2	258	2055	1312	384	351	8	0	0

- Molecule 16 is a protein called MGC130910 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	F1	227	1877	1210	358	302	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F1	134	ALA	VAL	conflict	UNP Q3B8I3

- Molecule 17 is a protein called Ribosomal_S7 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	F2	182	1439	903	271	259	6	0	0

- Molecule 18 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	G1	210	1695	1088	320	283	4	0	0

- Molecule 19 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	G2	222	1796	1120	358	312	6	0	0

- Molecule 20 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	H1	190	1517	955	285	269	8	0	0

- Molecule 21 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	H2	186	1494	952	277	264	1	0	0

- Molecule 22 is a protein called Ribosomal_L16 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	I1	202	1639	1042	316	268	13	0	0

- Molecule 23 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	I2	198	1620	1017	319	279	5	0	0

- Molecule 24 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	J1	167	1338	848	250	235	5	0	0

- Molecule 25 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	J2	180	1497	955	298	242	2	0	0

- Molecule 26 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	K2	93	779	513	133	128	5	0	0

- Molecule 27 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	L1	199	1608	1012	330	262	4	0	0

- Molecule 28 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	L2	140	1145	726	220	193	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L2	153	ALA	THR	conflict	UNP Q7SZ77

- Molecule 29 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	M1	134	1100	700	212	180	8	0	0

- Molecule 30 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	N1	203	1691	1065	351	269	6	0	0

- Molecule 31 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	N2	149	1204	770	230	203	1	0	0

- Molecule 32 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	O1	199	1627	1054	314	255	4	0	0

- Molecule 33 is a protein called Rps14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	O2	133	998	610	196	186	6	0	0

- Molecule 34 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	P1	152	1234	772	241	212	9	0	0

- Molecule 35 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	P2	116	955	607	177	163	8	0	0

- Molecule 36 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Q1	180	1454	912	299	237	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q1	116	ALA	SER	conflict	UNP A0A1L8FN04

- Molecule 37 is a protein called Rps16 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Q2	134	1054	671	197	183	3	0	0

- Molecule 38 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	R1	166	1382	858	298	217	9	0	0

- Molecule 39 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	R2	132	1066	669	199	194	4	0	0

- Molecule 40 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	S1	176	1455	934	280	232	9	0	0

- Molecule 41 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	S2	136	1129	708	228	192	1	0	0

- Molecule 42 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	T1	157	1291	814	257	215	5	0	0

- Molecule 43 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	T2	137	1059	666	199	191	3	0	0

- Molecule 44 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	U1	97	792	508	139	143	2	0	0

- Molecule 45 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	U2	85	684	429	133	118	4	0	0

- Molecule 46 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	V1	129	968	612	182	169	5	0	0

- Molecule 47 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	V2	83	643	396	118	124	5	0	0

- Molecule 48 is a protein called TRASH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	W1	60	502	321	98	81	2	0	0

- Molecule 49 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	W2	129	1035	659	193	177	6	0	0

- Molecule 50 is a protein called Ribosomal_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	X1	119	976	624	181	170	1	0	0

- Molecule 51 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	X2	139	1077	679	213	182	3	0	0

- Molecule 52 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Y1	125	1039	654	208	174	3	0	0

- Molecule 53 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Y2	123	1004	637	195	167	5	0	0

- Molecule 54 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Z1	135	1109	713	211	182	3	0	0

- Molecule 55 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Z2	67	536	345	98	92	1	0	0

- Molecule 56 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	a1	147	1164	741	233	186	4	0	0

- Molecule 57 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	a2	98	780	484	161	130	5	0	0

- Molecule 58 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	b1	63	527	328	112	84	3	0	0

- Molecule 59 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	b2	81	631	397	116	111	7	0	0

- Molecule 60 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	c1	94	732	465	130	131	6	0	0

- Molecule 61 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	c2	59	459	279	89	89	2	0	0

- Molecule 62 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	d1	106	884	558	173	152	1	0	0

- Molecule 63 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	d2	55	455	282	95	72	6	0	0

- Molecule 64 is a protein called Rpl32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	e1	126	1037	657	209	166	5	0	0

- Molecule 65 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	e2	51	407	250	90	66	1	0	0

- Molecule 66 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	f1	107	869	551	174	140	4	0	0

- Molecule 67 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	g1	104	830	520	171	133	6	0	0

- Molecule 68 is a protein called Gnb2l1-prov protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	g2	310	2410	1516	421	460	13	0	0

- Molecule 69 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
69	h1	120	995	627	203	165	0	0

- Molecule 70 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	i1	98	812	508	174	124	6	0	0

- Molecule 71 is a protein called HABP4_PAI-RBP1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	i2	51	423	255	85	81	2	0	0

- Molecule 72 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	j1	86	699	430	152	112	5	0	0

- Molecule 73 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	k1	68	558	360	99	98	1	0	0

- Molecule 74 is a protein called MGC116452 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	l1	50	441	281	96	63	1	0	0

- Molecule 75 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	m1	50	411	254	87	64	6	0	0

- Molecule 76 is a protein called Rpl41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	n1	24	231	140	63	26	2	0	0

- Molecule 77 is a protein called MGC85428 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	o1	102	835	519	173	137	6	0	0

- Molecule 78 is a protein called Rpl37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	p1	91	707	447	134	119	7	0	0

- Molecule 79 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	r1	118	945	590	193	159	3	0	0

- Molecule 80 is a protein called Death-associated protein-like 1-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	s1	31	251	158	50	42	1	0	0

- Molecule 81 is a protein called Eef2-prov protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	v2	360	2813	1776	493	530	14	0	0

- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
82	51	123	123	123	0
82	71	2	2	2	0
82	81	2	2	2	0
82	A1	1	1	1	0
82	B1	1	1	1	0
82	C1	1	1	1	0
82	V1	1	1	1	0
82	a1	1	1	1	0
82	e1	1	1	1	0
82	m1	1	1	1	0

- Molecule 83 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
83	a2	1	1	1	0
83	d2	1	1	1	0
83	g1	1	1	1	0

Continued on next page...

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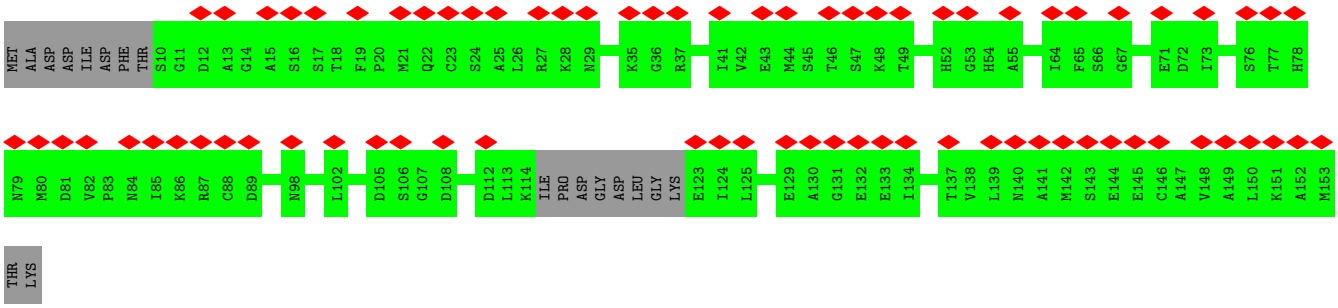
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
83	j1	1	1	1	0
			Total	Zn	
83	m1	1	1	1	0
			Total	Zn	
83	o1	1	1	1	0
			Total	Zn	
83	p1	1	1	1	0

3 Residue-property plots (i)

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

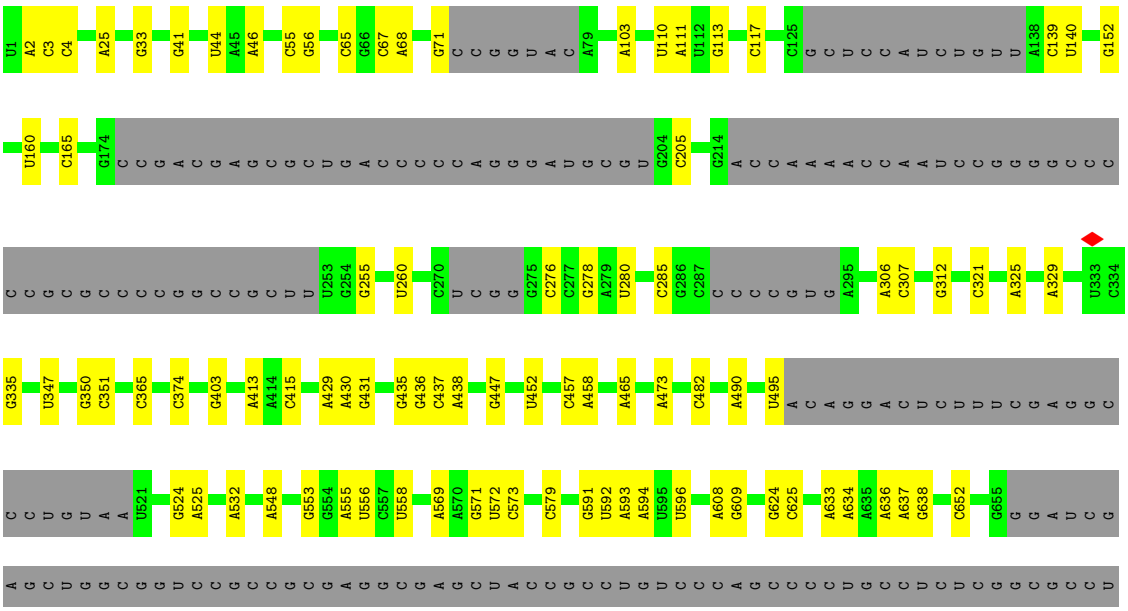
- Molecule 1: Eukaryotic translation initiation factor 5A

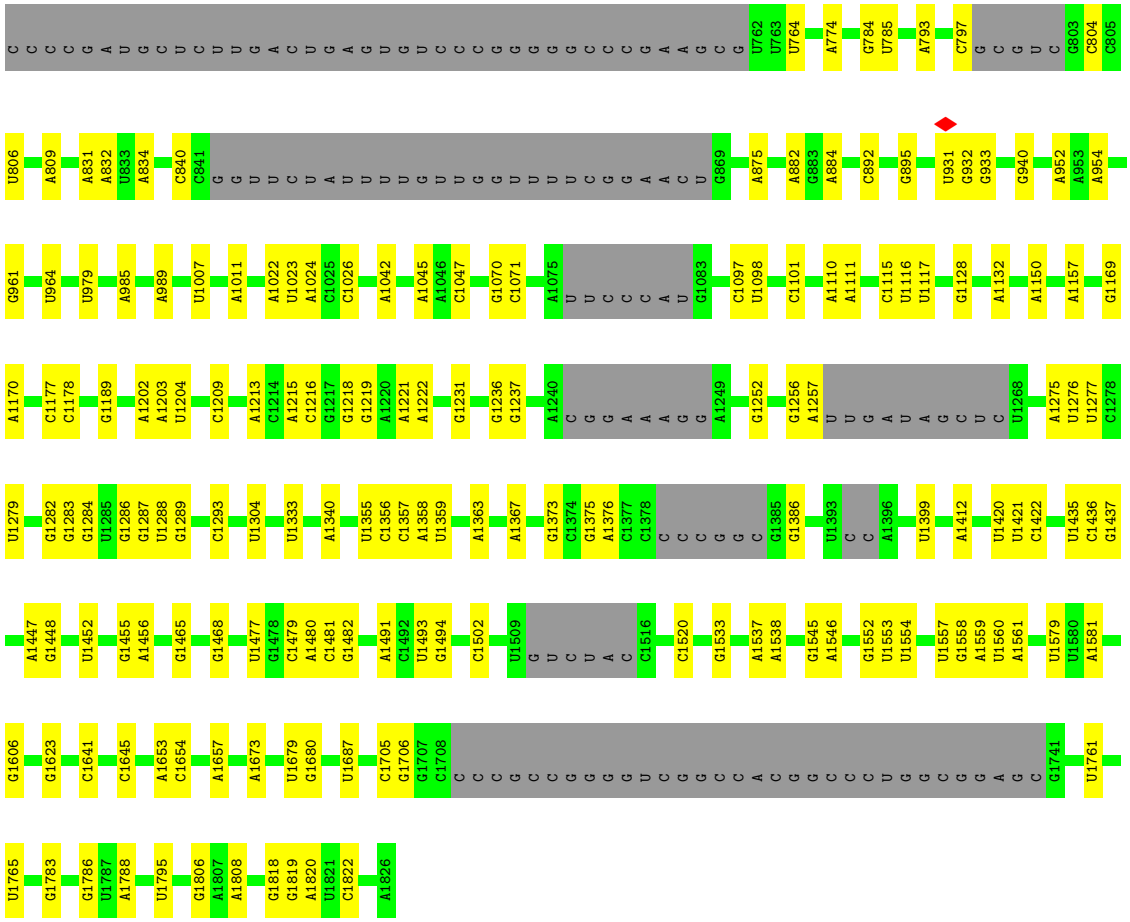
Chain 11:



- Molecule 2: 18S rRNA

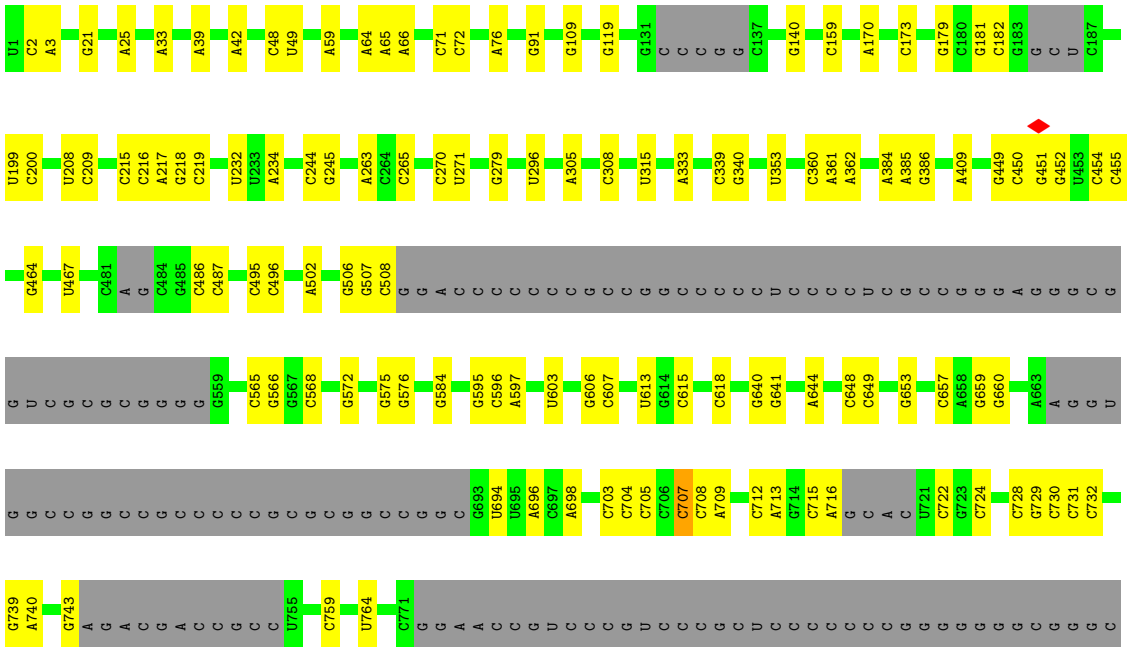
Chain 22:

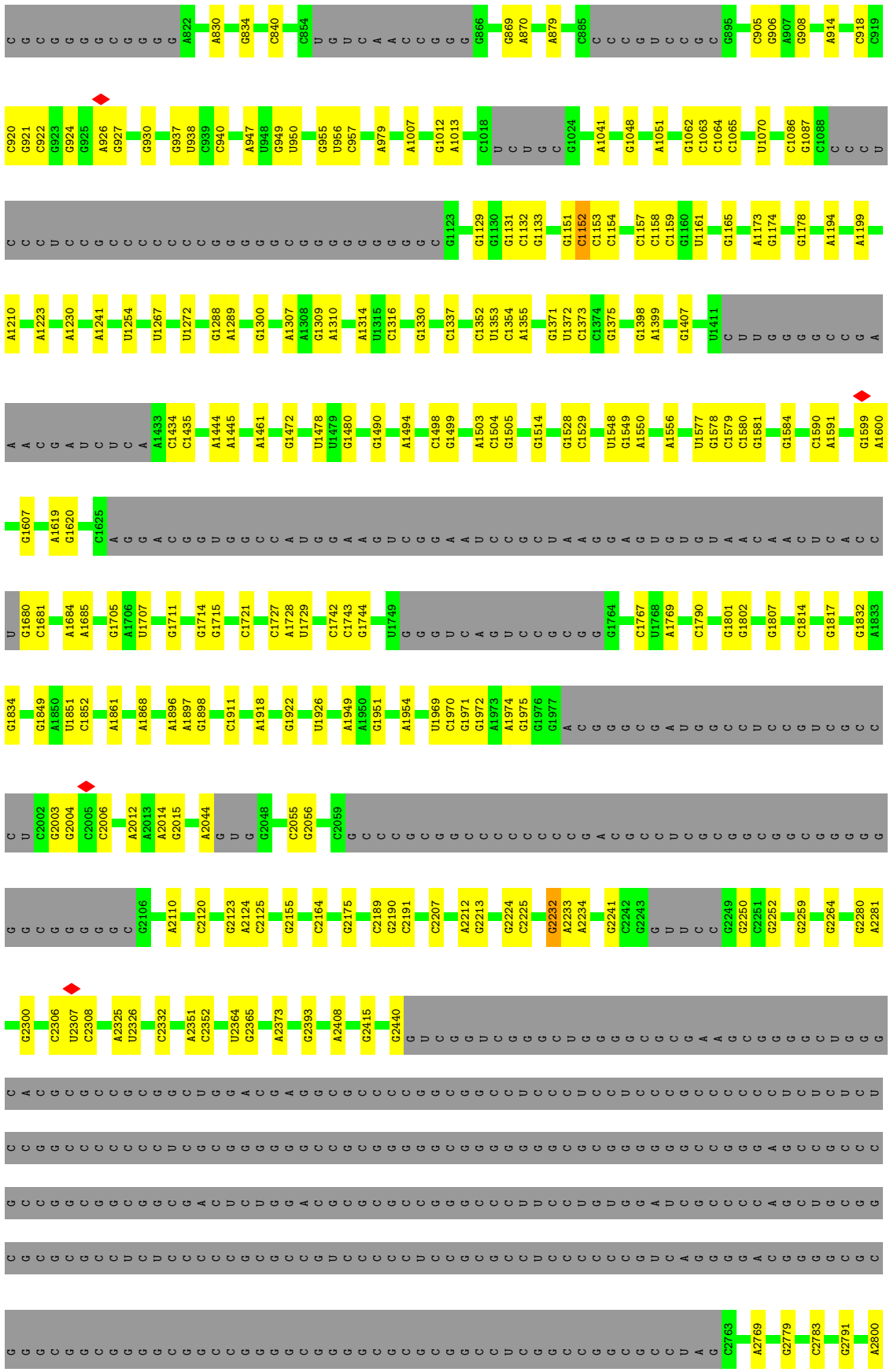


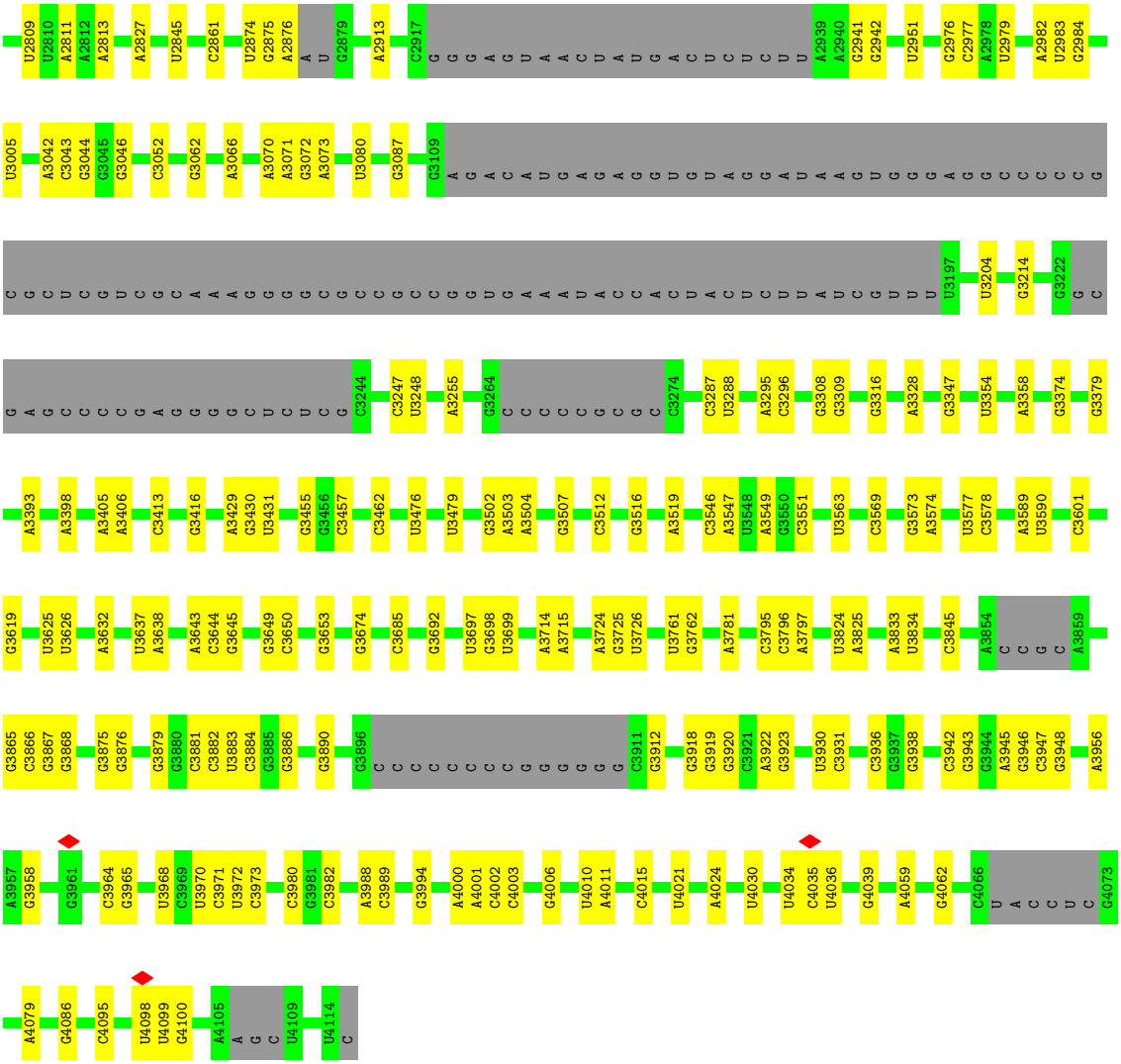


- Molecule 3: 28S rRNA

Chain 51:

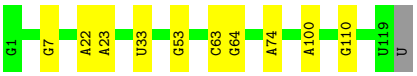



C G G C G G G G C G G G A822 A830 G834 C840 C854 U G G U C A A C C G G G G866 G869 A870 A879 C885 C C C G U C C G C G895 C905 G906 A907 G908 A914 C918 C919
C920 G921 C922 G923 G924 G925 A926 G927 G930 G937 U938 C939 C940 A947 U948 G949 U950 G955 U956 C957 A979 A1007 G1012 A1013 C1018 U C U G C G1024 A1041 G1048 A1051 G1062 C1063 C1064 C1065 U1070 C1086 G1087 C1088 C C C U
C C C C U C C C C



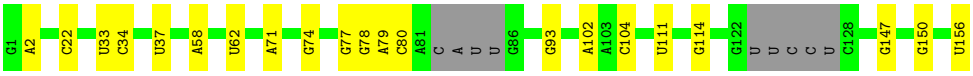
- Molecule 4: 5S rRNA

Chain 71: 91% 8%



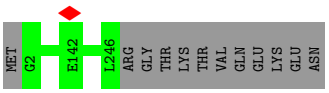
- Molecule 5: 5.8S rRNA

Chain 81: 81% 13% 6%



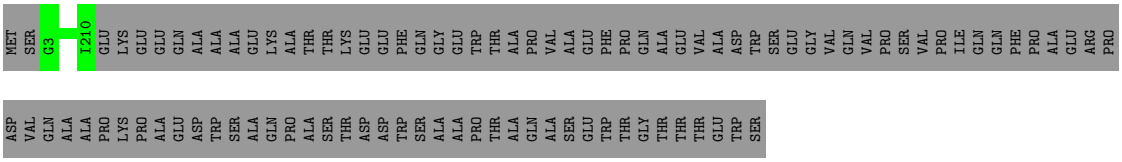
- Molecule 6: 60S ribosomal protein L8

Chain A1: 95% 5%



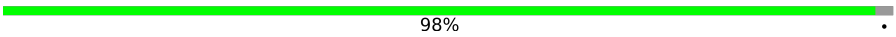
• Molecule 7: 40S ribosomal protein SA

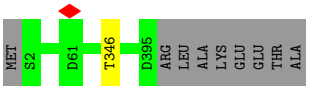
Chain A2:



• Molecule 8: Rpl3-prov protein

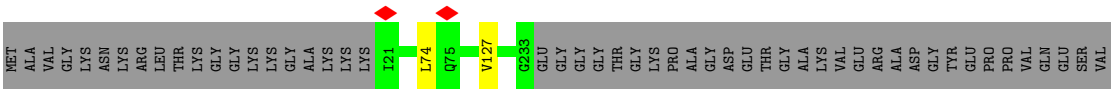
Chain B1:





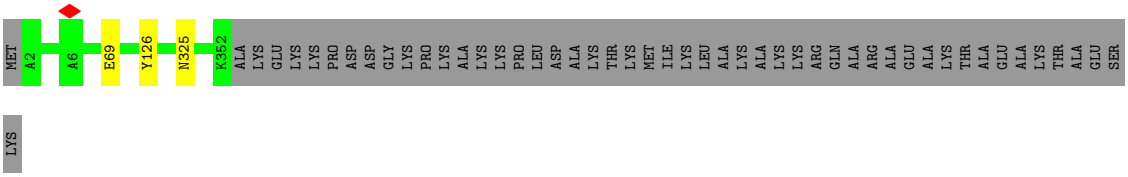
• Molecule 9: 40S ribosomal protein S3a-A

Chain B2:



• Molecule 10: 60S ribosomal protein L4-B

Chain C1:

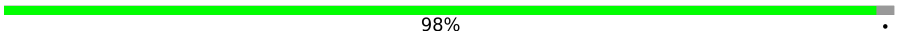


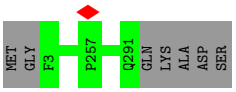
• Molecule 11: 40S ribosomal protein S2

Chain C2:

• Molecule 12: Rpl5-b protein

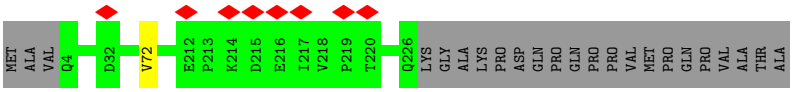
Chain D1:





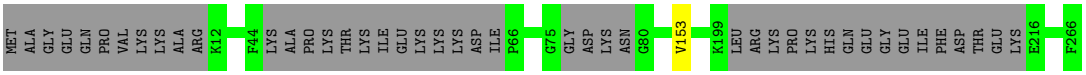
• Molecule 13: DNA-(apurinic or apyrimidinic site) lyase

Chain D2:



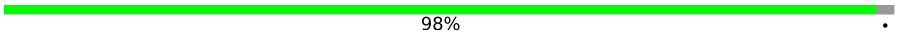
• Molecule 14: 60S ribosomal protein L6

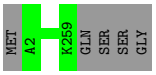
Chain E1:



• Molecule 15: 40S ribosomal protein S4

Chain E2:



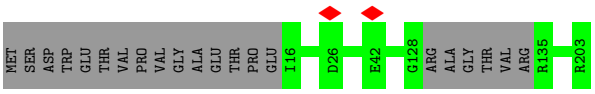


• Molecule 16: MGC130910 protein

Chain F1:

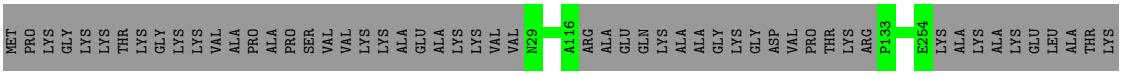
• Molecule 17: Ribosomal_S7 domain-containing protein

Chain F2:



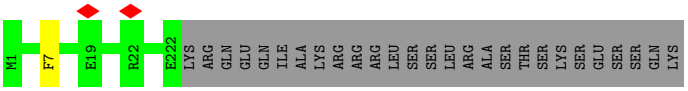
• Molecule 18: 60S ribosomal protein L7a

Chain G1:



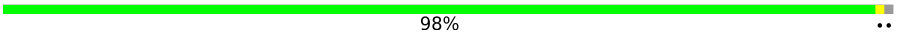
• Molecule 19: 40S ribosomal protein S6

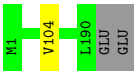
Chain G2:



• Molecule 20: 60S ribosomal protein L9

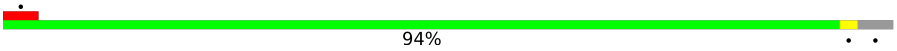
Chain H1:

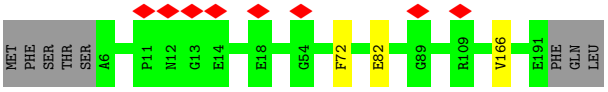




• Molecule 21: 40S ribosomal protein S7

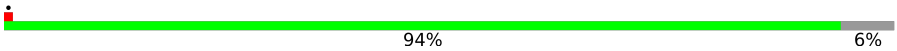
Chain H2:

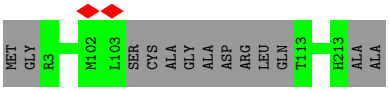




• Molecule 22: Ribosomal_L16 domain-containing protein

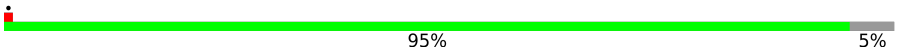
Chain I1:

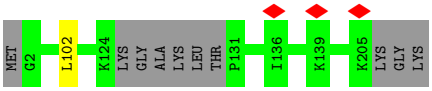




• Molecule 23: 40S ribosomal protein S8

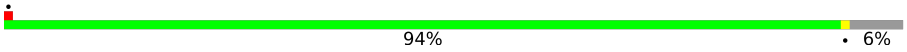
Chain I2:

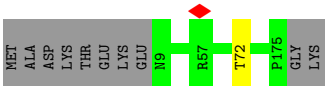




• Molecule 24: 60S ribosomal protein L11

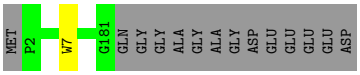
Chain J1:





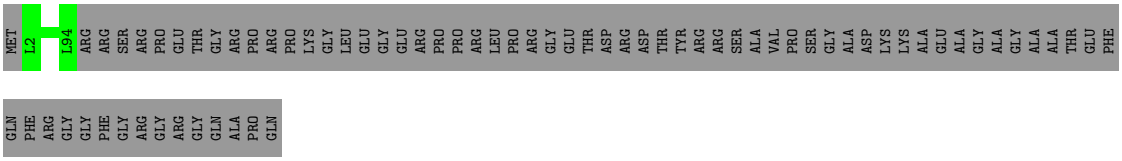
• Molecule 25: 40S ribosomal protein S9

Chain J2:



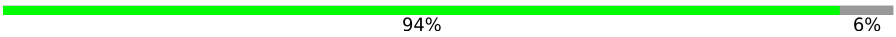
• Molecule 26: 40S ribosomal protein S10

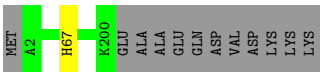
Chain K2:



• Molecule 27: 60S ribosomal protein L13

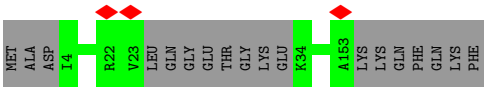
Chain L1:





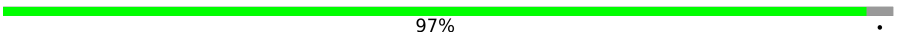
• Molecule 28: 40S ribosomal protein S11

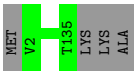
Chain L2:



• Molecule 29: 60S ribosomal protein L14

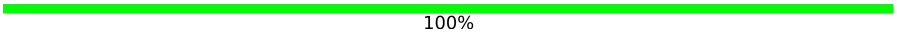
Chain M1:





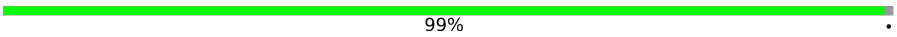
• Molecule 30: Ribosomal protein L15

Chain N1:



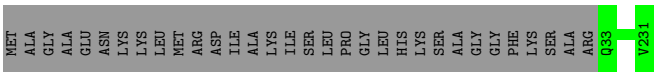
• Molecule 31: 40S ribosomal protein S13

Chain N2:



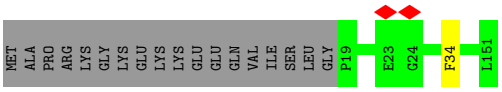
• Molecule 32: 60S ribosomal protein L13a

Chain O1:



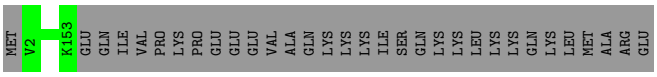
• Molecule 33: Rps14

Chain O2:



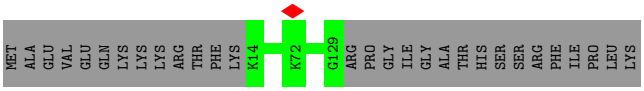
• Molecule 34: 60S ribosomal protein L17

Chain P1:



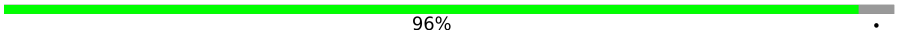
• Molecule 35: 40S ribosomal protein S15

Chain P2:



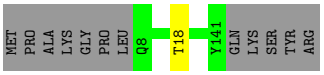
• Molecule 36: Ribosomal_L18e/L15P domain-containing protein

Chain Q1:



• Molecule 37: Rps16 protein

Chain Q2:

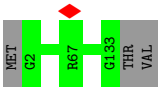


• Molecule 38: 60S ribosomal protein L19

Chain R1:

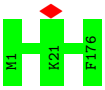
• Molecule 39: 40S ribosomal protein S17

Chain R2: 98%



• Molecule 40: 60S ribosomal protein L18a

Chain S1: 100%

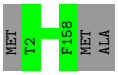


• Molecule 41: 40S ribosomal protein S18

Chain S2: 89% 11%

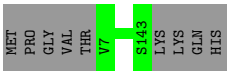
• Molecule 42: 60S ribosomal protein L21

Chain T1: 98%



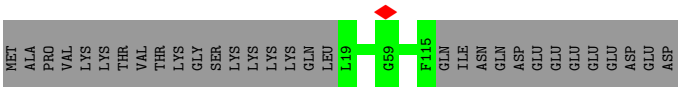
• Molecule 43: 40S ribosomal protein S19

Chain T2: 94% 6%



• Molecule 44: 60S ribosomal protein L22

Chain U1: 76% 24%

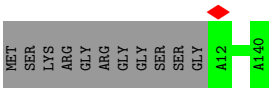


• Molecule 45: 40S ribosomal protein S20

Chain U2: 70% 29%

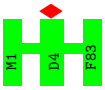
• Molecule 46: 60S ribosomal protein L23

Chain V1: 92% 8%



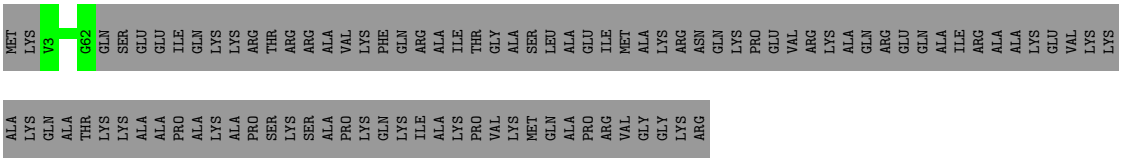
• Molecule 47: 40S ribosomal protein S21

Chain V2: 100%



• Molecule 48: TRASH domain-containing protein

Chain W1: 39% 61%

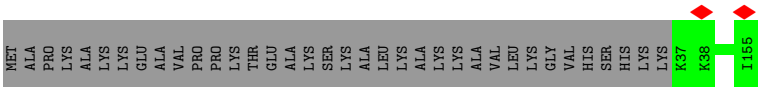


• Molecule 49: 40S ribosomal protein S15a

Chain W2: 98%

• Molecule 50: Ribosomal_L23eN domain-containing protein

Chain X1: 77% 23%

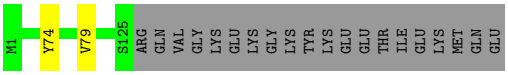


• Molecule 51: 40S ribosomal protein S23

Chain X2: 96%

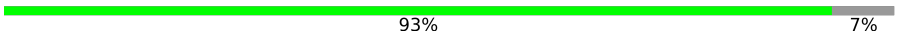
• Molecule 52: KOW domain-containing protein

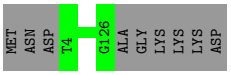
Chain Y1: 85% 14%



• Molecule 53: 40S ribosomal protein S24

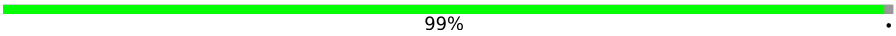
Chain Y2:





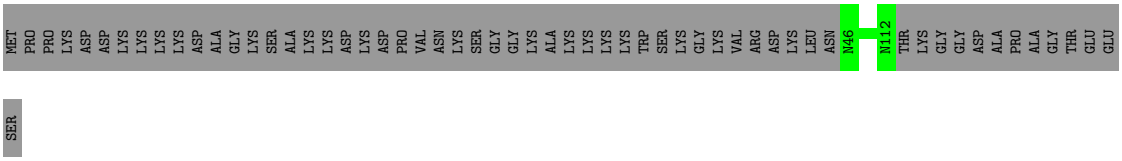
• Molecule 54: 60S ribosomal protein L27

Chain Z1:



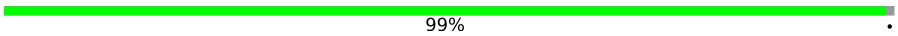
• Molecule 55: 40S ribosomal protein S25

Chain Z2:



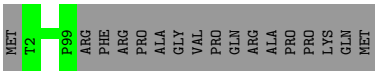
• Molecule 56: 60S ribosomal protein L27a

Chain a1:



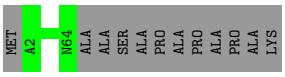
• Molecule 57: 40S ribosomal protein S26

Chain a2:



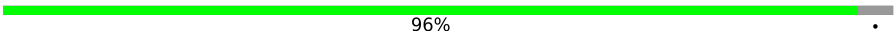
• Molecule 58: 60S ribosomal protein L29

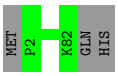
Chain b1:



• Molecule 59: 40S ribosomal protein S27

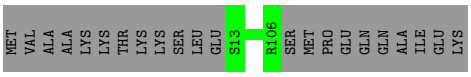
Chain b2:





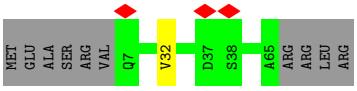
• Molecule 60: 60S ribosomal protein L30

Chain c1:



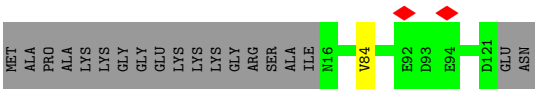
• Molecule 61: 40S ribosomal protein S28

Chain c2:



• Molecule 62: 60S ribosomal protein L31

Chain d1:

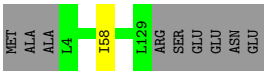


• Molecule 63: 40S ribosomal protein S29

Chain d2:

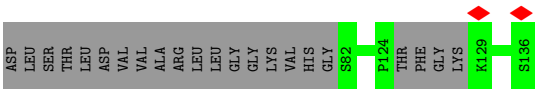
• Molecule 64: Rpl32

Chain e1:



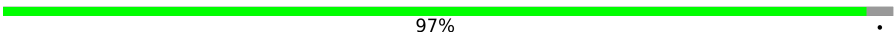
• Molecule 65: 40S ribosomal protein S30

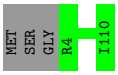
Chain e2:



• Molecule 66: 60S ribosomal protein L35a

Chain f1:



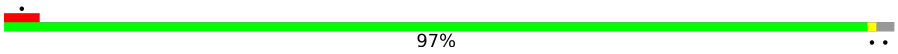


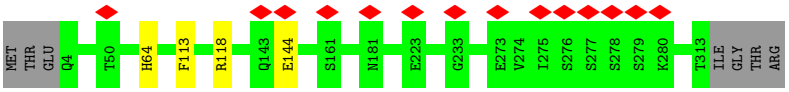
• Molecule 67: 60S ribosomal protein L34

Chain g1:

• Molecule 68: Gnb2l1-prov protein

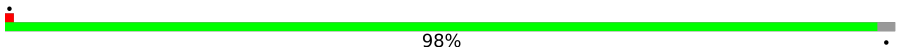
Chain g2:

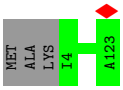




• Molecule 69: 60S ribosomal protein L35

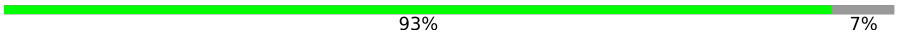
Chain h1:

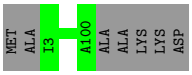




• Molecule 70: 60S ribosomal protein L36

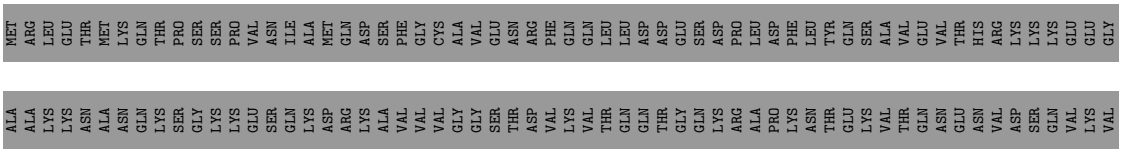
Chain i1:

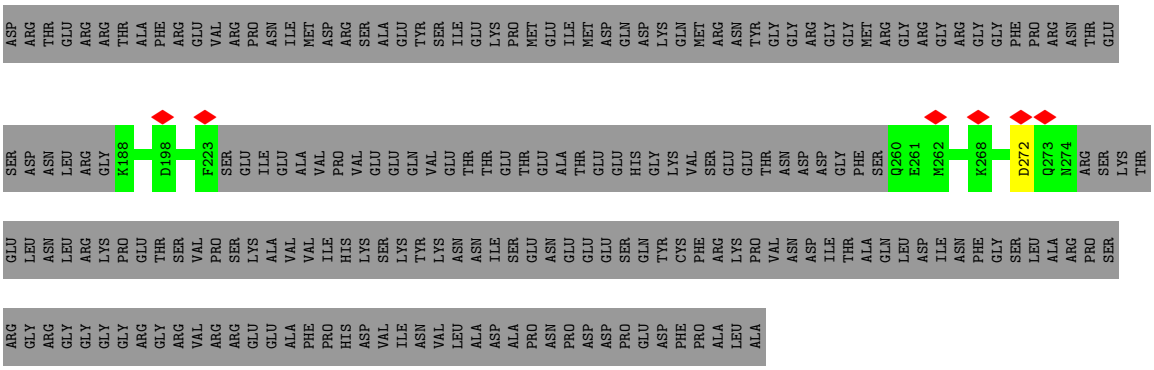




• Molecule 71: HABP4_PAI-RBP1 domain-containing protein

Chain i2:



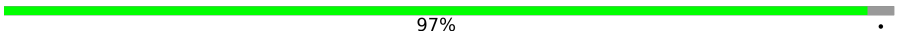


- Molecule 72: Ribosomal protein L37

Chain j1:

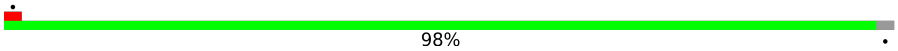
- Molecule 73: 60S ribosomal protein L38

Chain k1:



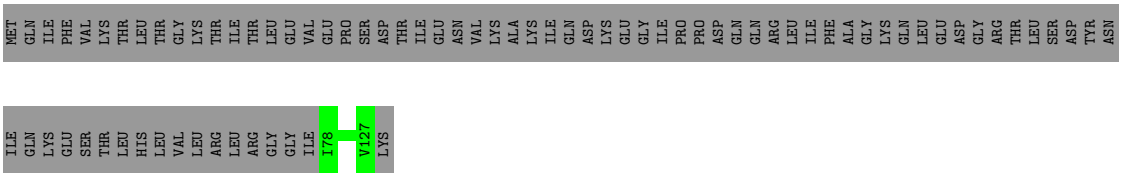
- Molecule 74: MGC116452 protein

Chain l1:



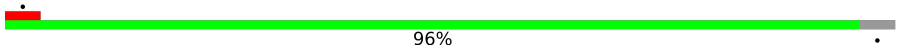
- Molecule 75: 60S ribosomal protein L40

Chain m1:



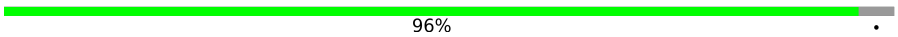
- Molecule 76: Rpl41

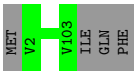
Chain n1:



- Molecule 77: MGC85428 protein

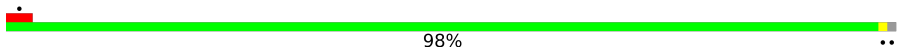
Chain o1:

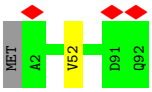




- Molecule 78: Rpl37a

Chain p1:



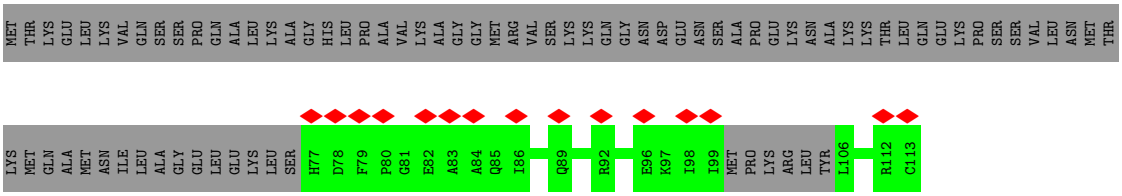


- Molecule 79: 60S ribosomal protein L28

Chain r1:

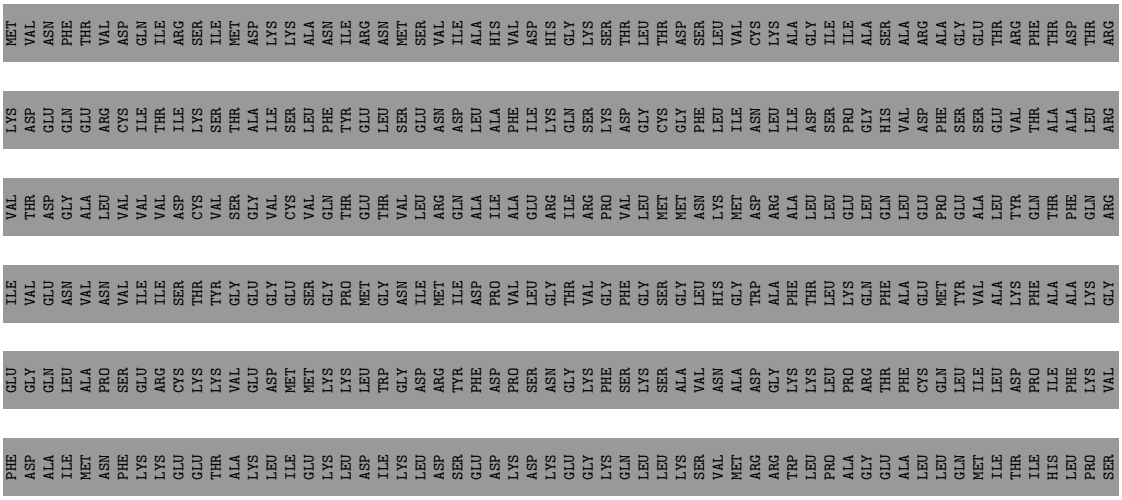
- Molecule 80: Death-associated protein-like 1-B

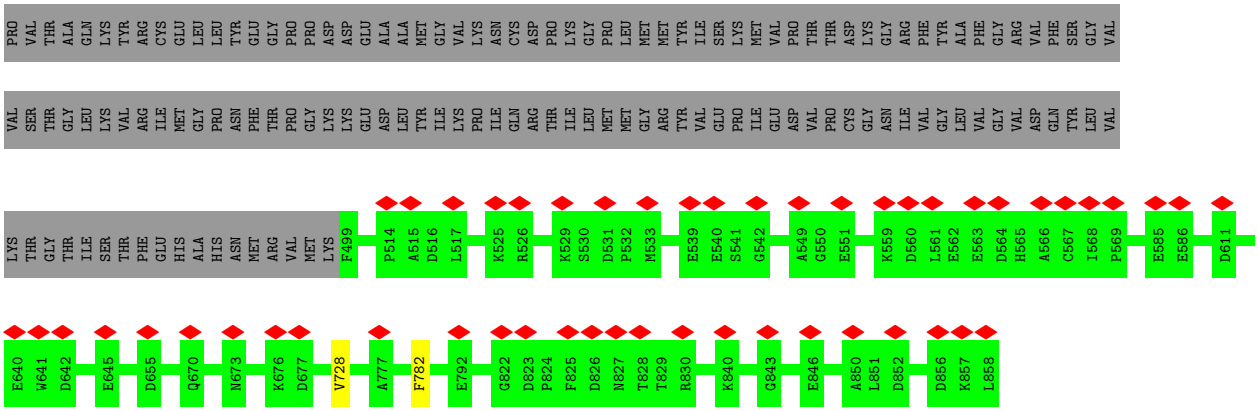
Chain s1:



- Molecule 81: Eef2-prov protein

Chain v2:




PRO VAL THR ALA GLN LYS TYR ARG CYS GLU LEU LEU TYR GLU GLY PRO PRO ASP ASP GLU ALA ALA MET GLY VAL LYS ASN CYS ASP PRO LYS GLY PRO LEU MET MET TYR ILE SER LYS MET VAL PRO THR THR ASP LYS GLY ARG PHE TYR ALA PHE GLY ARG VAL PHE SER GLY VAL
VAL SER THR GLY LEU LYS VAL ARG ILE MET GLY PRO ASN PHE THR PRO GLY LYS LYS GLU ASP LEU TYR ILE LYS PRO ILE GLN ARG THR ILE LEU MET MET GLY ARG TYR VAL GLU PRO ILE GLU ASP VAL PRO CYS GLY ASN ILE VAL GLY LEU VAL GLY VAL ASP GLN TYR LEU VAL
LYS THR GLY THR ILE SER THR PHE GLU HIS ALA HIS ASN MET ARG VAL MET LYS F499 P514 A515 D516 L517 K525 R526 K529 S530 D531 P532 M533 E539 E540 S541 G542 A549 G550 E551 K559 D560 L561 E562 E563 D564 H565 A566 C567 I568 P569 E585 E586 D611
E640 W641 D642 E645 D655 Q670 N673 K676 D677 V728 A777 F782 E792 G822 D823 P824 F825 D826 N827 T828 T829 R830 K840 G843 E846 A850 L851 D852 D856 K857 L858

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	412340	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.789	Depositor
Minimum map value	-2.088	Depositor
Average map value	0.046	Depositor
Map value standard deviation	0.188	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 5CT

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	11	0.24	0/1030	0.43	0/1381
2	22	0.19	0/35698	0.71	7/55605 (0.0%)
3	51	0.21	0/77857	0.70	13/121410 (0.0%)
4	71	0.19	0/2837	0.66	0/4422
5	81	0.19	0/3506	0.69	1/5460 (0.0%)
6	A1	0.25	0/1905	0.42	0/2554
7	A2	0.24	0/1680	0.39	0/2283
8	B1	0.25	0/3237	0.41	0/4329
9	B2	0.24	0/1762	0.42	0/2359
10	C1	0.24	0/2857	0.40	0/3836
11	C2	0.24	0/1699	0.40	0/2298
12	D1	0.24	0/2392	0.38	0/3206
13	D2	0.24	0/1760	0.41	0/2370
14	E1	0.24	0/1775	0.40	0/2373
15	E2	0.24	0/2098	0.43	0/2825
16	F1	0.24	0/1911	0.38	0/2549
17	F2	0.23	0/1459	0.38	0/1959
18	G1	0.24	0/1728	0.37	0/2328
19	G2	0.23	0/1820	0.41	0/2427
20	H1	0.24	0/1535	0.42	0/2061
21	H2	0.24	0/1516	0.42	0/2033
22	I1	0.25	0/1676	0.40	0/2238
23	I2	0.23	0/1648	0.40	0/2197
24	J1	0.24	0/1361	0.40	0/1821
25	J2	0.23	0/1522	0.37	0/2033
26	K2	0.24	0/803	0.39	0/1085
27	L1	0.24	0/1638	0.40	0/2192
28	L2	0.24	0/1165	0.42	0/1560
29	M1	0.24	0/1121	0.37	0/1496
30	N1	0.24	0/1732	0.40	0/2314
31	N2	0.23	0/1228	0.38	0/1652
32	O1	0.24	0/1659	0.38	0/2221

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	O2	0.24	0/1011	0.44	0/1355
34	P1	0.24	0/1260	0.40	0/1691
35	P2	0.24	0/972	0.38	0/1298
36	Q1	0.24	0/1476	0.41	0/1970
37	Q2	0.24	0/1070	0.40	0/1435
38	R1	0.22	0/1398	0.35	0/1849
39	R2	0.23	0/1080	0.37	0/1449
40	S1	0.25	0/1496	0.40	0/2011
41	S2	0.23	0/1146	0.40	0/1532
42	T1	0.25	0/1318	0.40	0/1761
43	T2	0.23	0/1078	0.37	0/1447
44	U1	0.24	0/807	0.42	0/1082
45	U2	0.22	0/691	0.43	0/924
46	V1	0.25	0/982	0.43	0/1317
47	V2	0.26	0/650	0.42	0/870
48	W1	0.25	0/515	0.40	0/687
49	W2	0.24	0/1052	0.41	0/1408
50	X1	0.24	0/993	0.40	0/1335
51	X2	0.24	0/1093	0.41	0/1460
52	Y1	0.24	0/1056	0.38	0/1406
53	Y2	0.24	0/1021	0.42	0/1356
54	Z1	0.25	0/1131	0.38	0/1508
55	Z2	0.23	0/542	0.39	0/729
56	a1	0.24	0/1196	0.40	0/1598
57	a2	0.24	0/793	0.41	0/1063
58	b1	0.24	0/538	0.34	0/708
59	b2	0.24	0/644	0.43	0/864
60	c1	0.24	0/742	0.39	0/996
61	c2	0.23	0/461	0.44	0/618
62	d1	0.23	0/899	0.41	0/1211
63	d2	0.23	0/466	0.37	0/619
64	e1	0.24	0/1055	0.40	0/1406
65	e2	0.24	0/410	0.38	0/537
66	f1	0.25	0/889	0.42	0/1192
67	g1	0.24	0/841	0.41	0/1121
68	g2	0.23	0/2467	0.43	0/3356
69	h1	0.22	0/1002	0.35	0/1323
70	i1	0.23	0/823	0.35	0/1089
71	i2	0.23	0/430	0.38	0/569
72	j1	0.24	0/713	0.41	0/942
73	k1	0.24	0/564	0.38	0/748
74	l1	0.23	0/451	0.36	0/596
75	m1	0.23	0/417	0.41	0/553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	n1	0.20	0/232	0.32	0/295
77	o1	0.24	0/847	0.41	0/1117
78	p1	0.23	0/717	0.41	0/951
79	r1	0.24	0/959	0.40	0/1283
80	s1	0.41	0/256	0.48	0/344
81	v2	0.24	0/2872	0.42	0/3889
All	All	0.22	0/213137	0.60	21/311745 (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
9	B2	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	51	707	C	C2-N1-C1'	8.67	128.33	118.80
3	51	707	C	N1-C2-O2	8.61	124.07	118.90
2	22	321	C	C2-N1-C1'	8.30	127.92	118.80
2	22	321	C	N1-C2-O2	8.21	123.83	118.90
2	22	321	C	N3-C2-O2	-7.08	116.94	121.90
3	51	707	C	N3-C2-O2	-6.83	117.12	121.90
2	22	321	C	C6-N1-C2	-6.03	117.89	120.30
3	51	707	C	C6-N1-C2	-5.93	117.93	120.30
3	51	707	C	C6-N1-C1'	-5.90	113.72	120.80
3	51	724	C	C2-N1-C1'	5.82	125.21	118.80
3	51	1154	C	C2-N1-C1'	5.64	125.01	118.80
2	22	321	C	C6-N1-C1'	-5.60	114.08	120.80
5	81	111	U	C2-N1-C1'	5.59	124.41	117.70
3	51	4015	C	C2-N1-C1'	5.49	124.84	118.80
3	51	1498	C	C2-N1-C1'	5.49	124.83	118.80
2	22	1520	C	N1-C2-O2	5.22	122.03	118.90
3	51	1152	C	N1-C2-O2	5.21	122.03	118.90
2	22	55	C	C2-N1-C1'	5.20	124.52	118.80
3	51	1152	C	C2-N1-C1'	5.19	124.51	118.80
3	51	3881	C	C2-N1-C1'	5.16	124.48	118.80
3	51	2232	G	P-O3'-C3'	5.13	125.86	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	B2	74	LEU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	11	131/154 (85%)	123 (94%)	8 (6%)	0	100	100
6	A1	243/257 (95%)	233 (96%)	10 (4%)	0	100	100
7	A2	206/306 (67%)	202 (98%)	4 (2%)	0	100	100
8	B1	392/403 (97%)	378 (96%)	14 (4%)	0	100	100
9	B2	211/264 (80%)	203 (96%)	8 (4%)	0	100	100
10	C1	349/401 (87%)	339 (97%)	10 (3%)	0	100	100
11	C2	213/281 (76%)	211 (99%)	2 (1%)	0	100	100
12	D1	287/296 (97%)	283 (99%)	4 (1%)	0	100	100
13	D2	221/246 (90%)	214 (97%)	7 (3%)	0	100	100
14	E1	206/258 (80%)	202 (98%)	4 (2%)	0	100	100
15	E2	256/263 (97%)	242 (94%)	14 (6%)	0	100	100
16	F1	225/246 (92%)	217 (96%)	8 (4%)	0	100	100
17	F2	178/203 (88%)	170 (96%)	8 (4%)	0	100	100
18	G1	206/266 (77%)	205 (100%)	1 (0%)	0	100	100
19	G2	220/249 (88%)	217 (99%)	3 (1%)	0	100	100
20	H1	188/192 (98%)	184 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	H2	184/194 (95%)	170 (92%)	14 (8%)	0	100	100
22	I1	198/215 (92%)	192 (97%)	6 (3%)	0	100	100
23	I2	194/208 (93%)	190 (98%)	4 (2%)	0	100	100
24	J1	165/177 (93%)	163 (99%)	2 (1%)	0	100	100
25	J2	178/194 (92%)	175 (98%)	3 (2%)	0	100	100
26	K2	91/165 (55%)	86 (94%)	5 (6%)	0	100	100
27	L1	197/211 (93%)	191 (97%)	6 (3%)	0	100	100
28	L2	136/158 (86%)	132 (97%)	4 (3%)	0	100	100
29	M1	132/138 (96%)	130 (98%)	2 (2%)	0	100	100
30	N1	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
31	N2	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
32	O1	197/231 (85%)	194 (98%)	3 (2%)	0	100	100
33	O2	131/151 (87%)	125 (95%)	6 (5%)	0	100	100
34	P1	150/184 (82%)	144 (96%)	6 (4%)	0	100	100
35	P2	114/145 (79%)	114 (100%)	0	0	100	100
36	Q1	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
37	Q2	132/146 (90%)	129 (98%)	3 (2%)	0	100	100
38	R1	164/197 (83%)	164 (100%)	0	0	100	100
39	R2	130/135 (96%)	129 (99%)	1 (1%)	0	100	100
40	S1	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
41	S2	134/152 (88%)	129 (96%)	5 (4%)	0	100	100
42	T1	155/160 (97%)	149 (96%)	6 (4%)	0	100	100
43	T2	135/146 (92%)	130 (96%)	5 (4%)	0	100	100
44	U1	95/128 (74%)	89 (94%)	6 (6%)	0	100	100
45	U2	81/119 (68%)	80 (99%)	1 (1%)	0	100	100
46	V1	127/140 (91%)	124 (98%)	3 (2%)	0	100	100
47	V2	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
48	W1	58/155 (37%)	58 (100%)	0	0	100	100
49	W2	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
50	X1	117/155 (76%)	115 (98%)	2 (2%)	0	100	100
51	X2	137/143 (96%)	131 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	Y1	123/145 (85%)	122 (99%)	1 (1%)	0	100	100
53	Y2	121/132 (92%)	112 (93%)	9 (7%)	0	100	100
54	Z1	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
55	Z2	65/125 (52%)	64 (98%)	1 (2%)	0	100	100
56	a1	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
57	a2	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
58	b1	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
59	b2	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
60	c1	92/116 (79%)	91 (99%)	1 (1%)	0	100	100
61	c2	57/69 (83%)	55 (96%)	2 (4%)	0	100	100
62	d1	104/125 (83%)	98 (94%)	6 (6%)	0	100	100
63	d2	53/86 (62%)	53 (100%)	0	0	100	100
64	e1	124/135 (92%)	123 (99%)	1 (1%)	0	100	100
65	e2	47/133 (35%)	46 (98%)	1 (2%)	0	100	100
66	f1	105/110 (96%)	104 (99%)	1 (1%)	0	100	100
67	g1	102/117 (87%)	99 (97%)	3 (3%)	0	100	100
68	g2	308/317 (97%)	287 (93%)	21 (7%)	0	100	100
69	h1	118/123 (96%)	115 (98%)	3 (2%)	0	100	100
70	i1	96/105 (91%)	96 (100%)	0	0	100	100
71	i2	47/378 (12%)	44 (94%)	3 (6%)	0	100	100
72	j1	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
73	k1	66/70 (94%)	66 (100%)	0	0	100	100
74	l1	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
75	m1	48/128 (38%)	48 (100%)	0	0	100	100
76	n1	22/25 (88%)	22 (100%)	0	0	100	100
77	o1	100/106 (94%)	98 (98%)	2 (2%)	0	100	100
78	p1	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
79	r1	116/137 (85%)	115 (99%)	1 (1%)	0	100	100
80	s1	27/113 (24%)	24 (89%)	3 (11%)	0	100	100
81	v2	358/858 (42%)	339 (95%)	19 (5%)	0	100	100
All	All	11206/13815 (81%)	10880 (97%)	326 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	11	114/129 (88%)	114 (100%)	0	100	100
6	A1	187/198 (94%)	187 (100%)	0	100	100
7	A2	175/252 (69%)	175 (100%)	0	100	100
8	B1	341/348 (98%)	340 (100%)	1 (0%)	92	97
9	B2	194/229 (85%)	193 (100%)	1 (0%)	88	95
10	C1	296/334 (89%)	293 (99%)	3 (1%)	76	88
11	C2	180/218 (83%)	179 (99%)	1 (1%)	86	94
12	D1	243/248 (98%)	243 (100%)	0	100	100
13	D2	186/204 (91%)	185 (100%)	1 (0%)	88	95
14	E1	192/230 (84%)	191 (100%)	1 (0%)	88	95
15	E2	221/225 (98%)	221 (100%)	0	100	100
16	F1	196/213 (92%)	195 (100%)	1 (0%)	88	95
17	F2	154/171 (90%)	154 (100%)	0	100	100
18	G1	182/223 (82%)	182 (100%)	0	100	100
19	G2	196/221 (89%)	195 (100%)	1 (0%)	88	95
20	H1	170/172 (99%)	169 (99%)	1 (1%)	86	94
21	H2	165/174 (95%)	162 (98%)	3 (2%)	59	76
22	I1	174/181 (96%)	174 (100%)	0	100	100
23	I2	171/178 (96%)	170 (99%)	1 (1%)	86	94
24	J1	140/149 (94%)	139 (99%)	1 (1%)	84	92
25	J2	160/168 (95%)	159 (99%)	1 (1%)	86	94
26	K2	84/136 (62%)	84 (100%)	0	100	100
27	L1	169/179 (94%)	168 (99%)	1 (1%)	86	94
28	L2	126/141 (89%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	M1	115/118 (98%)	115 (100%)	0	100	100
30	N1	172/173 (99%)	172 (100%)	0	100	100
31	N2	130/131 (99%)	130 (100%)	0	100	100
32	O1	171/194 (88%)	171 (100%)	0	100	100
33	O2	104/119 (87%)	103 (99%)	1 (1%)	76	88
34	P1	133/163 (82%)	133 (100%)	0	100	100
35	P2	104/129 (81%)	104 (100%)	0	100	100
36	Q1	157/163 (96%)	157 (100%)	0	100	100
37	Q2	109/119 (92%)	108 (99%)	1 (1%)	78	90
38	R1	147/175 (84%)	147 (100%)	0	100	100
39	R2	118/121 (98%)	118 (100%)	0	100	100
40	S1	155/155 (100%)	155 (100%)	0	100	100
41	S2	118/132 (89%)	117 (99%)	1 (1%)	81	91
42	T1	137/139 (99%)	137 (100%)	0	100	100
43	T2	110/118 (93%)	110 (100%)	0	100	100
44	U1	88/117 (75%)	88 (100%)	0	100	100
45	U2	78/106 (74%)	76 (97%)	2 (3%)	46	66
46	V1	100/107 (94%)	100 (100%)	0	100	100
47	V2	69/69 (100%)	69 (100%)	0	100	100
48	W1	52/126 (41%)	52 (100%)	0	100	100
49	W2	112/113 (99%)	110 (98%)	2 (2%)	59	76
50	X1	108/136 (79%)	108 (100%)	0	100	100
51	X2	110/114 (96%)	108 (98%)	2 (2%)	59	76
52	Y1	117/135 (87%)	115 (98%)	2 (2%)	60	78
53	Y2	107/114 (94%)	107 (100%)	0	100	100
54	Z1	116/117 (99%)	116 (100%)	0	100	100
55	Z2	59/105 (56%)	59 (100%)	0	100	100
56	a1	120/121 (99%)	120 (100%)	0	100	100
57	a2	85/99 (86%)	85 (100%)	0	100	100
58	b1	56/62 (90%)	56 (100%)	0	100	100
59	b2	73/76 (96%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	c1	79/98 (81%)	79 (100%)	0	100	100
61	c2	52/61 (85%)	51 (98%)	1 (2%)	57	75
62	d1	97/110 (88%)	96 (99%)	1 (1%)	76	88
63	d2	48/77 (62%)	48 (100%)	0	100	100
64	e1	114/121 (94%)	113 (99%)	1 (1%)	78	90
65	e2	42/113 (37%)	42 (100%)	0	100	100
66	f1	87/89 (98%)	87 (100%)	0	100	100
67	g1	90/100 (90%)	88 (98%)	2 (2%)	52	71
68	g2	270/276 (98%)	266 (98%)	4 (2%)	65	80
69	h1	107/109 (98%)	107 (100%)	0	100	100
70	i1	85/89 (96%)	85 (100%)	0	100	100
71	i2	44/327 (14%)	43 (98%)	1 (2%)	50	70
72	j1	73/80 (91%)	73 (100%)	0	100	100
73	k1	64/66 (97%)	64 (100%)	0	100	100
74	l1	47/48 (98%)	47 (100%)	0	100	100
75	m1	46/116 (40%)	46 (100%)	0	100	100
76	n1	23/24 (96%)	23 (100%)	0	100	100
77	o1	90/94 (96%)	90 (100%)	0	100	100
78	p1	74/75 (99%)	73 (99%)	1 (1%)	67	82
79	r1	103/119 (87%)	103 (100%)	0	100	100
80	s1	27/96 (28%)	27 (100%)	0	100	100
81	v2	307/735 (42%)	305 (99%)	2 (1%)	84	92
All	All	9815/11810 (83%)	9773 (100%)	42 (0%)	91	96

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	B1	346	THR
9	B2	127	VAL
10	C1	69	GLU
10	C1	126	TYR
10	C1	325	ASN
11	C2	222	PHE
13	D2	72	VAL

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Mol	Chain	Res	Type
14	E1	153	VAL
16	F1	234	ARG
19	G2	7	PHE
20	H1	104	VAL
21	H2	72	PHE
21	H2	82	GLU
21	H2	166	VAL
23	I2	102	LEU
24	J1	72	THR
25	J2	7	TRP
27	L1	67	HIS
33	O2	34	PHE
37	Q2	18	THR
41	S2	142	ARG
45	U2	65	THR
45	U2	68	THR
49	W2	105	THR
49	W2	111	MET
51	X2	82	THR
51	X2	105	PHE
52	Y1	74	TYR
52	Y1	79	VAL
61	c2	32	VAL
62	d1	84	VAL
64	e1	58	ILE
67	g1	32	TYR
67	g1	73	HIS
68	g2	64	HIS
68	g2	113	PHE
68	g2	118	ARG
68	g2	144	GLU
71	i2	272	ASP
78	p1	52	VAL
81	v2	728	VAL
81	v2	782	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166) such sidechains are listed below:

Mol	Chain	Res	Type
1	11	91	GLN
1	11	98	ASN
6	A1	8	GLN

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Mol	Chain	Res	Type
6	A1	132	ASN
6	A1	217	GLN
7	A2	111	GLN
7	A2	132	GLN
8	B1	138	GLN
8	B1	167	GLN
8	B1	354	GLN
9	B2	40	ASN
9	B2	159	GLN
9	B2	160	GLN
9	B2	163	GLN
10	C1	54	GLN
10	C1	325	ASN
10	C1	346	GLN
11	C2	258	HIS
12	D1	175	HIS
12	D1	191	ASN
12	D1	198	HIS
12	D1	229	ASN
12	D1	291	GLN
13	D2	145	GLN
13	D2	179	GLN
14	E1	14	HIS
15	E2	36	HIS
15	E2	161	GLN
15	E2	188	ASN
16	F1	22	GLN
16	F1	163	GLN
16	F1	204	ASN
16	F1	233	ASN
17	F2	109	GLN
17	F2	113	ASN
18	G1	38	ASN
18	G1	66	GLN
18	G1	90	GLN
19	G2	13	GLN
19	G2	59	GLN
19	G2	110	ASN
19	G2	197	GLN
19	G2	200	GLN
19	G2	202	ASN
20	H1	106	GLN

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Mol	Chain	Res	Type
21	H2	114	GLN
21	H2	162	GLN
22	I1	97	ASN
22	I1	166	HIS
23	I2	64	ASN
23	I2	84	ASN
23	I2	165	GLN
23	I2	168	GLN
23	I2	181	GLN
24	J1	9	ASN
24	J1	41	GLN
24	J1	64	ASN
24	J1	70	HIS
25	J2	111	GLN
26	K2	44	HIS
26	K2	66	HIS
27	L1	19	GLN
27	L1	104	ASN
27	L1	115	GLN
28	L2	5	GLN
28	L2	11	GLN
28	L2	18	GLN
28	L2	19	ASN
28	L2	85	GLN
29	M1	20	HIS
29	M1	33	GLN
30	N1	86	ASN
30	N1	90	ASN
31	N2	13	GLN
31	N2	105	ASN
32	O1	33	GLN
32	O1	42	HIS
32	O1	54	GLN
32	O1	91	ASN
32	O1	208	GLN
33	O2	32	HIS
33	O2	113	GLN
34	P1	75	GLN
34	P1	97	ASN
34	P1	137	ASN
35	P2	24	GLN
35	P2	32	GLN

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Mol	Chain	Res	Type
36	Q1	8	ASN
36	Q1	160	HIS
37	Q2	86	GLN
37	Q2	97	GLN
37	Q2	114	GLN
39	R2	29	HIS
39	R2	93	GLN
40	S1	66	GLN
40	S1	108	GLN
40	S1	163	HIS
41	S2	17	ASN
41	S2	76	GLN
41	S2	87	GLN
42	T1	112	ASN
42	T1	134	GLN
43	T2	11	ASN
43	T2	52	ASN
43	T2	86	ASN
43	T2	138	GLN
44	U1	105	ASN
45	U2	81	GLN
46	V1	77	HIS
46	V1	84	GLN
49	W2	24	GLN
49	W2	82	GLN
49	W2	113	HIS
50	X1	93	ASN
50	X1	110	GLN
50	X1	121	GLN
50	X1	124	ASN
51	X2	63	ASN
51	X2	110	HIS
52	Y1	14	ASN
52	Y1	20	ASN
52	Y1	65	GLN
53	Y2	22	GLN
53	Y2	106	GLN
56	a1	14	HIS
56	a1	67	GLN
56	a1	120	GLN
57	a2	8	ASN
58	b1	11	ASN

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Mol	Chain	Res	Type
58	b1	50	ASN
58	b1	60	ASN
59	b2	26	GLN
59	b2	65	GLN
60	c1	19	GLN
62	d1	16	ASN
63	d2	45	GLN
64	e1	23	HIS
64	e1	34	ASN
64	e1	68	HIS
64	e1	107	ASN
65	e2	99	GLN
65	e2	114	GLN
65	e2	116	ASN
66	f1	21	GLN
68	g2	20	GLN
68	g2	56	GLN
68	g2	143	GLN
69	h1	63	GLN
70	i1	80	HIS
74	l1	25	GLN
75	m1	84	GLN
75	m1	104	HIS
75	m1	109	ASN
76	n1	22	GLN
77	o1	3	ASN
77	o1	25	GLN
77	o1	45	GLN
78	p1	56	HIS
79	r1	71	GLN
80	s1	89	GLN
81	v2	535	GLN
81	v2	660	ASN
81	v2	684	GLN
81	v2	705	HIS
81	v2	710	HIS
81	v2	715	HIS

5.3.3 RNA (i)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	22	1476/1826 (80%)	244 (16%)	14 (0%)
3	51	3216/4115 (78%)	512 (15%)	34 (1%)
4	71	118/120 (98%)	10 (8%)	0
5	81	144/156 (92%)	19 (13%)	1 (0%)
All	All	4954/6217 (79%)	785 (15%)	49 (0%)

All (785) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	22	2	A
2	22	3	C
2	22	4	C
2	22	25	A
2	22	33	G
2	22	41	G
2	22	44	U
2	22	46	A
2	22	56	G
2	22	65	C
2	22	67	C
2	22	68	A
2	22	71	G
2	22	103	A
2	22	111	A
2	22	113	G
2	22	117	C
2	22	139	C
2	22	140	U
2	22	152	G
2	22	160	U
2	22	165	C
2	22	205	C
2	22	255	G
2	22	260	U
2	22	276	C
2	22	278	G
2	22	280	U
2	22	285	C
2	22	306	A
2	22	307	C
2	22	312	G

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Mol	Chain	Res	Type
2	22	325	A
2	22	329	A
2	22	335	G
2	22	347	U
2	22	350	G
2	22	351	C
2	22	365	C
2	22	374	C
2	22	403	G
2	22	413	A
2	22	415	C
2	22	429	A
2	22	430	A
2	22	431	G
2	22	435	G
2	22	436	G
2	22	437	C
2	22	438	A
2	22	447	G
2	22	452	U
2	22	457	C
2	22	458	A
2	22	465	A
2	22	473	A
2	22	482	C
2	22	490	A
2	22	495	U
2	22	524	G
2	22	525	A
2	22	532	A
2	22	548	A
2	22	553	G
2	22	555	A
2	22	556	U
2	22	558	U
2	22	569	A
2	22	571	G
2	22	572	U
2	22	573	C
2	22	579	C
2	22	591	G
2	22	592	U

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Mol	Chain	Res	Type
2	22	593	A
2	22	594	A
2	22	596	U
2	22	608	A
2	22	609	G
2	22	624	G
2	22	625	C
2	22	633	A
2	22	634	A
2	22	636	A
2	22	637	A
2	22	638	G
2	22	652	C
2	22	764	U
2	22	774	A
2	22	784	G
2	22	785	U
2	22	793	A
2	22	797	C
2	22	804	C
2	22	806	U
2	22	809	A
2	22	831	A
2	22	832	A
2	22	834	A
2	22	840	C
2	22	875	A
2	22	882	A
2	22	884	A
2	22	892	C
2	22	895	G
2	22	931	U
2	22	932	G
2	22	933	G
2	22	940	G
2	22	952	A
2	22	954	A
2	22	961	G
2	22	964	U
2	22	979	U
2	22	985	A
2	22	989	A

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Mol	Chain	Res	Type
2	22	1007	U
2	22	1011	A
2	22	1022	A
2	22	1023	U
2	22	1024	A
2	22	1026	C
2	22	1042	A
2	22	1045	A
2	22	1047	C
2	22	1070	G
2	22	1071	C
2	22	1098	U
2	22	1101	C
2	22	1110	A
2	22	1111	A
2	22	1115	C
2	22	1116	U
2	22	1117	U
2	22	1128	G
2	22	1132	A
2	22	1150	A
2	22	1157	A
2	22	1169	G
2	22	1170	A
2	22	1177	C
2	22	1178	C
2	22	1189	G
2	22	1202	A
2	22	1203	A
2	22	1204	U
2	22	1209	C
2	22	1213	A
2	22	1215	A
2	22	1216	C
2	22	1218	G
2	22	1219	G
2	22	1221	A
2	22	1222	A
2	22	1231	G
2	22	1236	G
2	22	1237	G
2	22	1252	G

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Mol	Chain	Res	Type
2	22	1257	A
2	22	1276	U
2	22	1277	U
2	22	1279	U
2	22	1282	G
2	22	1283	G
2	22	1284	G
2	22	1286	G
2	22	1287	G
2	22	1288	U
2	22	1289	G
2	22	1293	C
2	22	1304	U
2	22	1333	U
2	22	1340	A
2	22	1355	U
2	22	1356	C
2	22	1358	A
2	22	1359	U
2	22	1363	A
2	22	1367	A
2	22	1373	G
2	22	1375	G
2	22	1376	A
2	22	1386	G
2	22	1399	U
2	22	1412	A
2	22	1420	U
2	22	1421	U
2	22	1422	C
2	22	1435	U
2	22	1436	C
2	22	1437	G
2	22	1447	A
2	22	1448	G
2	22	1452	U
2	22	1455	G
2	22	1456	A
2	22	1465	G
2	22	1468	G
2	22	1477	U
2	22	1479	C

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Mol	Chain	Res	Type
2	22	1480	A
2	22	1482	G
2	22	1491	A
2	22	1493	U
2	22	1494	G
2	22	1502	C
2	22	1533	G
2	22	1537	A
2	22	1538	A
2	22	1545	G
2	22	1546	A
2	22	1553	U
2	22	1554	U
2	22	1557	U
2	22	1558	G
2	22	1559	A
2	22	1561	A
2	22	1579	U
2	22	1581	A
2	22	1606	G
2	22	1623	G
2	22	1641	C
2	22	1645	C
2	22	1653	A
2	22	1654	C
2	22	1657	A
2	22	1673	A
2	22	1679	U
2	22	1680	G
2	22	1687	U
2	22	1705	C
2	22	1706	G
2	22	1761	U
2	22	1765	U
2	22	1783	G
2	22	1786	G
2	22	1788	A
2	22	1795	U
2	22	1806	G
2	22	1808	A
2	22	1818	G
2	22	1819	G

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Mol	Chain	Res	Type
2	22	1820	A
2	22	1822	C
3	51	2	C
3	51	3	A
3	51	21	G
3	51	25	A
3	51	33	A
3	51	39	A
3	51	42	A
3	51	48	C
3	51	49	U
3	51	59	A
3	51	64	A
3	51	65	A
3	51	66	A
3	51	71	C
3	51	72	C
3	51	76	A
3	51	91	G
3	51	109	G
3	51	119	G
3	51	140	G
3	51	159	C
3	51	170	A
3	51	173	C
3	51	179	G
3	51	181	G
3	51	182	C
3	51	199	U
3	51	200	C
3	51	208	U
3	51	209	C
3	51	215	C
3	51	216	C
3	51	217	A
3	51	218	G
3	51	219	C
3	51	232	U
3	51	234	A
3	51	244	C
3	51	245	G
3	51	263	A

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Mol	Chain	Res	Type
3	51	265	C
3	51	270	C
3	51	271	U
3	51	279	G
3	51	296	U
3	51	305	A
3	51	308	C
3	51	315	U
3	51	333	A
3	51	339	C
3	51	340	G
3	51	353	U
3	51	360	C
3	51	361	A
3	51	362	A
3	51	385	A
3	51	386	G
3	51	409	A
3	51	449	G
3	51	451	G
3	51	452	G
3	51	454	C
3	51	455	C
3	51	464	G
3	51	467	U
3	51	486	C
3	51	487	C
3	51	495	C
3	51	496	C
3	51	502	A
3	51	506	G
3	51	507	G
3	51	508	C
3	51	565	C
3	51	566	G
3	51	568	C
3	51	572	G
3	51	575	G
3	51	576	G
3	51	584	G
3	51	595	G
3	51	596	C

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Mol	Chain	Res	Type
3	51	597	A
3	51	603	U
3	51	606	G
3	51	607	C
3	51	613	U
3	51	615	C
3	51	618	C
3	51	640	G
3	51	641	G
3	51	644	A
3	51	648	C
3	51	649	C
3	51	653	G
3	51	657	C
3	51	659	G
3	51	660	G
3	51	694	U
3	51	696	A
3	51	698	A
3	51	703	C
3	51	705	C
3	51	707	C
3	51	708	C
3	51	709	A
3	51	712	C
3	51	713	A
3	51	715	C
3	51	716	A
3	51	722	C
3	51	728	C
3	51	729	G
3	51	730	C
3	51	732	C
3	51	739	G
3	51	740	A
3	51	743	G
3	51	759	C
3	51	764	U
3	51	830	A
3	51	834	G
3	51	840	C
3	51	870	A

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Mol	Chain	Res	Type
3	51	879	A
3	51	905	C
3	51	906	G
3	51	908	G
3	51	914	A
3	51	918	C
3	51	920	C
3	51	921	G
3	51	922	C
3	51	924	G
3	51	926	A
3	51	927	G
3	51	930	G
3	51	937	G
3	51	938	U
3	51	940	C
3	51	947	A
3	51	949	G
3	51	950	U
3	51	955	G
3	51	956	U
3	51	957	C
3	51	979	A
3	51	1007	A
3	51	1012	G
3	51	1013	A
3	51	1041	A
3	51	1048	G
3	51	1051	A
3	51	1062	G
3	51	1063	C
3	51	1064	C
3	51	1065	C
3	51	1070	U
3	51	1087	G
3	51	1129	G
3	51	1132	C
3	51	1133	G
3	51	1152	C
3	51	1153	C
3	51	1157	C
3	51	1158	C

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Mol	Chain	Res	Type
3	51	1159	C
3	51	1161	U
3	51	1165	G
3	51	1173	A
3	51	1174	G
3	51	1178	G
3	51	1194	A
3	51	1199	A
3	51	1210	A
3	51	1223	A
3	51	1230	A
3	51	1241	A
3	51	1254	U
3	51	1267	U
3	51	1272	U
3	51	1288	G
3	51	1289	A
3	51	1300	G
3	51	1307	A
3	51	1309	G
3	51	1310	A
3	51	1314	A
3	51	1316	C
3	51	1330	G
3	51	1337	C
3	51	1352	C
3	51	1353	U
3	51	1354	C
3	51	1355	A
3	51	1372	U
3	51	1373	C
3	51	1375	G
3	51	1398	G
3	51	1399	A
3	51	1407	G
3	51	1434	C
3	51	1435	C
3	51	1444	A
3	51	1445	A
3	51	1461	A
3	51	1472	G
3	51	1478	U

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Mol	Chain	Res	Type
3	51	1480	G
3	51	1490	G
3	51	1494	A
3	51	1499	G
3	51	1503	A
3	51	1504	C
3	51	1505	G
3	51	1514	G
3	51	1528	G
3	51	1529	C
3	51	1549	G
3	51	1550	A
3	51	1556	A
3	51	1577	U
3	51	1578	G
3	51	1579	C
3	51	1580	C
3	51	1581	G
3	51	1584	G
3	51	1590	C
3	51	1591	A
3	51	1599	G
3	51	1600	A
3	51	1607	G
3	51	1619	A
3	51	1620	G
3	51	1681	C
3	51	1684	A
3	51	1685	A
3	51	1705	G
3	51	1707	U
3	51	1711	G
3	51	1714	G
3	51	1715	G
3	51	1721	C
3	51	1728	A
3	51	1729	U
3	51	1743	C
3	51	1744	G
3	51	1767	C
3	51	1769	A
3	51	1790	C

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Mol	Chain	Res	Type
3	51	1801	G
3	51	1802	G
3	51	1807	G
3	51	1814	C
3	51	1817	G
3	51	1832	G
3	51	1834	G
3	51	1849	G
3	51	1851	U
3	51	1852	C
3	51	1861	A
3	51	1868	A
3	51	1896	A
3	51	1897	A
3	51	1898	G
3	51	1911	C
3	51	1918	A
3	51	1922	G
3	51	1926	U
3	51	1949	A
3	51	1951	G
3	51	1954	A
3	51	1969	U
3	51	1970	C
3	51	1971	G
3	51	1972	G
3	51	1974	A
3	51	1975	G
3	51	2003	G
3	51	2004	G
3	51	2006	C
3	51	2012	A
3	51	2014	A
3	51	2015	G
3	51	2044	A
3	51	2055	C
3	51	2056	G
3	51	2110	A
3	51	2120	C
3	51	2123	G
3	51	2124	A
3	51	2125	C

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Mol	Chain	Res	Type
3	51	2155	G
3	51	2164	C
3	51	2175	G
3	51	2189	C
3	51	2190	G
3	51	2191	C
3	51	2207	C
3	51	2212	A
3	51	2213	G
3	51	2224	G
3	51	2225	C
3	51	2232	G
3	51	2233	A
3	51	2234	A
3	51	2241	G
3	51	2250	G
3	51	2252	G
3	51	2259	G
3	51	2264	G
3	51	2280	G
3	51	2281	A
3	51	2300	G
3	51	2306	C
3	51	2307	U
3	51	2308	C
3	51	2325	A
3	51	2326	U
3	51	2332	C
3	51	2351	A
3	51	2352	C
3	51	2364	U
3	51	2365	G
3	51	2373	A
3	51	2393	G
3	51	2408	A
3	51	2415	G
3	51	2440	G
3	51	2769	A
3	51	2779	G
3	51	2783	C
3	51	2791	G
3	51	2800	A

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Mol	Chain	Res	Type
3	51	2809	U
3	51	2811	A
3	51	2813	A
3	51	2827	A
3	51	2845	U
3	51	2861	C
3	51	2874	U
3	51	2876	A
3	51	2913	A
3	51	2941	G
3	51	2942	G
3	51	2951	U
3	51	2976	G
3	51	2977	C
3	51	2979	U
3	51	2982	A
3	51	2983	U
3	51	2984	G
3	51	3005	U
3	51	3042	A
3	51	3043	C
3	51	3044	G
3	51	3046	G
3	51	3052	C
3	51	3062	G
3	51	3066	A
3	51	3070	A
3	51	3071	A
3	51	3072	G
3	51	3073	A
3	51	3080	U
3	51	3087	G
3	51	3204	U
3	51	3214	G
3	51	3247	C
3	51	3248	U
3	51	3255	A
3	51	3287	C
3	51	3288	U
3	51	3295	A
3	51	3296	C
3	51	3308	G

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Mol	Chain	Res	Type
3	51	3309	G
3	51	3316	G
3	51	3328	A
3	51	3347	G
3	51	3354	U
3	51	3358	A
3	51	3374	G
3	51	3379	G
3	51	3393	A
3	51	3398	A
3	51	3405	A
3	51	3406	A
3	51	3413	C
3	51	3416	G
3	51	3429	A
3	51	3430	G
3	51	3431	U
3	51	3455	G
3	51	3457	C
3	51	3462	C
3	51	3476	U
3	51	3479	U
3	51	3502	G
3	51	3503	A
3	51	3504	A
3	51	3507	G
3	51	3512	C
3	51	3516	G
3	51	3519	A
3	51	3546	C
3	51	3547	A
3	51	3549	A
3	51	3551	C
3	51	3563	U
3	51	3569	C
3	51	3573	G
3	51	3574	A
3	51	3577	U
3	51	3578	C
3	51	3589	A
3	51	3590	U
3	51	3601	C

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Mol	Chain	Res	Type
3	51	3619	G
3	51	3625	U
3	51	3626	U
3	51	3632	A
3	51	3637	U
3	51	3638	A
3	51	3643	A
3	51	3644	C
3	51	3645	G
3	51	3649	G
3	51	3650	C
3	51	3653	G
3	51	3674	G
3	51	3685	C
3	51	3692	G
3	51	3697	U
3	51	3698	G
3	51	3699	U
3	51	3714	A
3	51	3715	A
3	51	3725	G
3	51	3726	U
3	51	3761	U
3	51	3762	G
3	51	3781	A
3	51	3795	C
3	51	3796	C
3	51	3797	A
3	51	3825	A
3	51	3833	A
3	51	3834	U
3	51	3845	C
3	51	3865	G
3	51	3866	C
3	51	3867	G
3	51	3868	G
3	51	3875	G
3	51	3876	G
3	51	3879	G
3	51	3882	C
3	51	3883	U
3	51	3884	C

Continued on next page...

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Mol	Chain	Res	Type
3	51	3886	G
3	51	3890	G
3	51	3912	G
3	51	3918	G
3	51	3919	G
3	51	3920	G
3	51	3922	A
3	51	3923	G
3	51	3930	U
3	51	3931	C
3	51	3936	C
3	51	3938	G
3	51	3942	C
3	51	3943	G
3	51	3945	A
3	51	3947	C
3	51	3948	G
3	51	3956	A
3	51	3958	G
3	51	3964	C
3	51	3965	G
3	51	3968	U
3	51	3970	U
3	51	3971	C
3	51	3973	C
3	51	3980	C
3	51	3982	C
3	51	3988	A
3	51	3989	C
3	51	3994	G
3	51	4000	A
3	51	4001	A
3	51	4002	C
3	51	4003	C
3	51	4006	G
3	51	4010	U
3	51	4011	A
3	51	4021	U
3	51	4024	A
3	51	4030	U
3	51	4034	U
3	51	4035	C

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Mol	Chain	Res	Type
3	51	4036	U
3	51	4039	G
3	51	4059	A
3	51	4062	G
3	51	4079	A
3	51	4086	G
3	51	4095	C
3	51	4098	U
3	51	4099	U
3	51	4100	G
4	71	7	G
4	71	22	A
4	71	23	A
4	71	33	U
4	71	53	G
4	71	63	C
4	71	64	G
4	71	74	A
4	71	100	A
4	71	110	G
5	81	2	A
5	81	22	C
5	81	33	U
5	81	34	C
5	81	37	U
5	81	58	A
5	81	62	U
5	81	71	A
5	81	74	G
5	81	78	G
5	81	79	A
5	81	80	C
5	81	93	G
5	81	102	A
5	81	104	C
5	81	114	G
5	81	147	G
5	81	150	G
5	81	156	U

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	22	110	U
2	22	430	A
2	22	1097	C
2	22	1110	A
2	22	1215	A
2	22	1221	A
2	22	1256	G
2	22	1275	A
2	22	1283	G
2	22	1357	C
2	22	1447	A
2	22	1481	C
2	22	1552	G
2	22	1560	U
3	51	218	G
3	51	244	C
3	51	384	A
3	51	450	C
3	51	454	C
3	51	595	G
3	51	704	C
3	51	731	C
3	51	869	G
3	51	920	C
3	51	1064	C
3	51	1086	C
3	51	1131	G
3	51	1151	G
3	51	1309	G
3	51	1371	G
3	51	1434	C
3	51	1548	U
3	51	1680	G
3	51	1727	C
3	51	1742	C
3	51	1974	A
3	51	2232	G
3	51	2306	C
3	51	2875	G
3	51	3697	U
3	51	3724	A
3	51	3725	G
3	51	3824	U

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Mol	Chain	Res	Type
3	51	3865	G
3	51	3866	C
3	51	3946	G
3	51	3970	U
3	51	3972	U
5	81	77	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	$\#\|Z\| > 2$
1	5CT	11	51	1	13,14,15	0.67	0	9,15,17	1.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CT	11	51	1	-	7/13/14/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	11	51	5CT	NZ-C1-C2-C3
1	11	51	5CT	NZ-C1-C2-O1
1	11	51	5CT	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	11	51	5CT	CA-CB-CG-CD
1	11	51	5CT	CD-CE-NZ-C1
1	11	51	5CT	CG-CD-CE-NZ
1	11	51	5CT	O1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 141 ligands modelled in this entry, 141 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
2	22	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	22	1268:U	O3'	1269:U	P	4.01

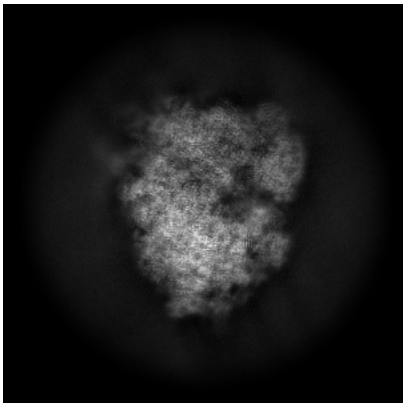
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13113. These allow visual inspection of the internal detail of the map and identification of artifacts.

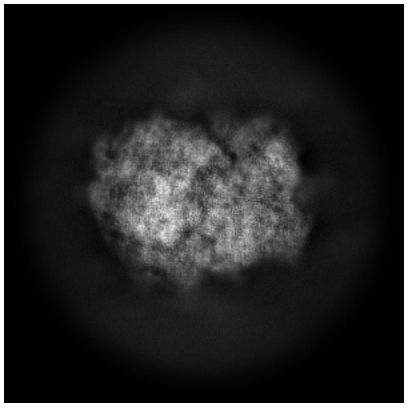
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

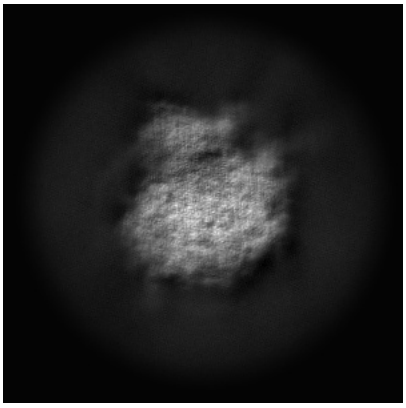
6.1.1 Primary map



X



Y

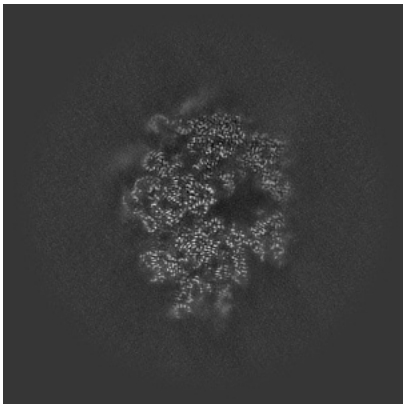


Z

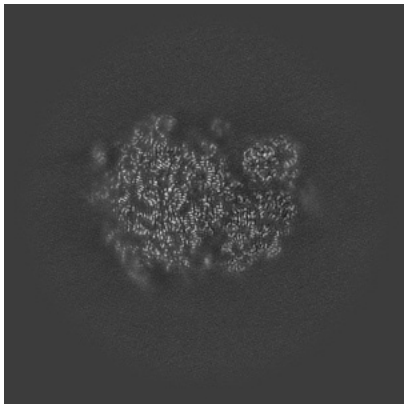
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

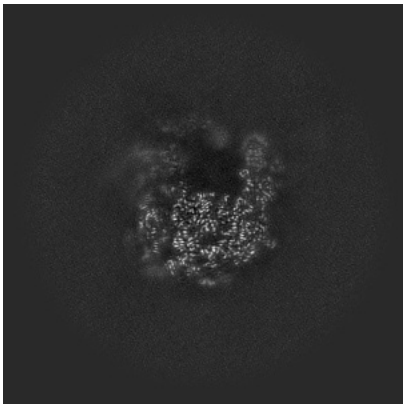
6.2.1 Primary map



X Index: 240



Y Index: 240

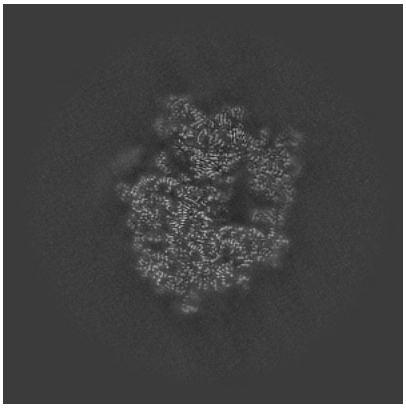


Z Index: 240

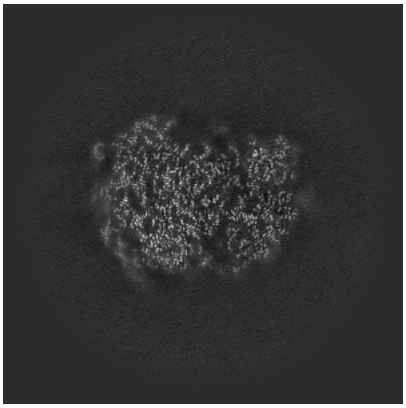
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

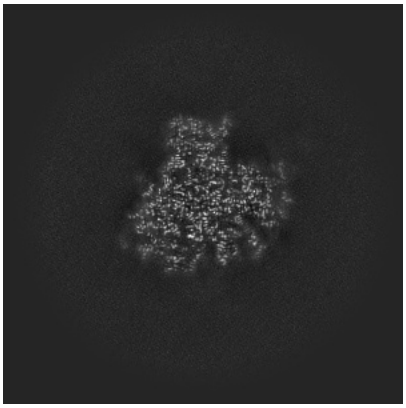
6.3.1 Primary map



X Index: 223



Y Index: 235

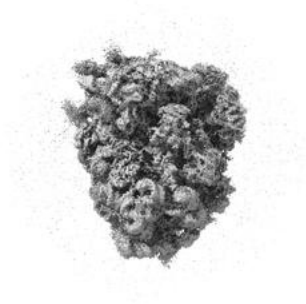


Z Index: 193

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

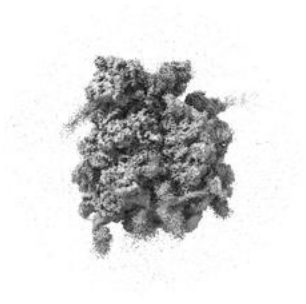
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

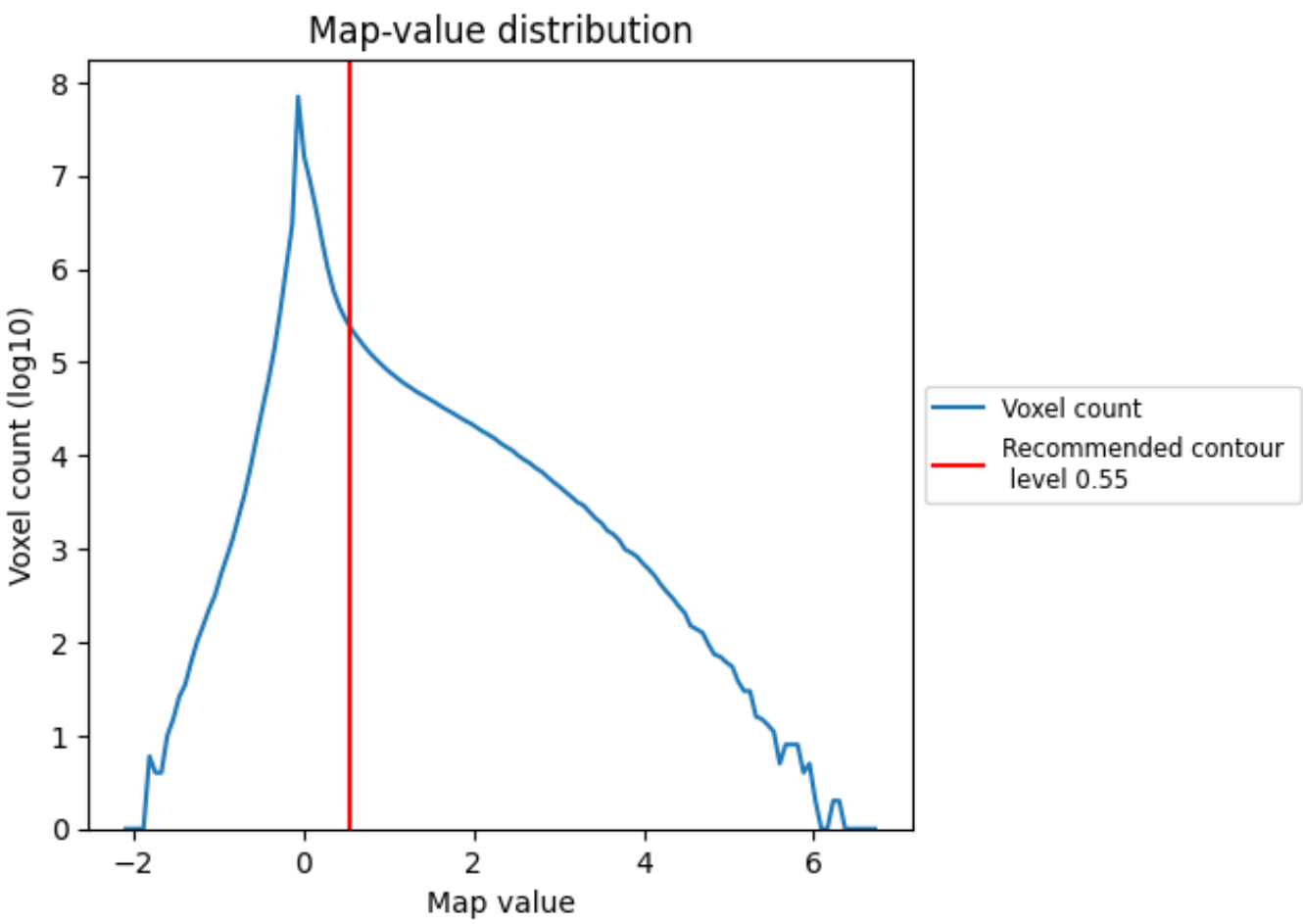
6.5 Mask visualisation (i)

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

7 Map analysis (i)

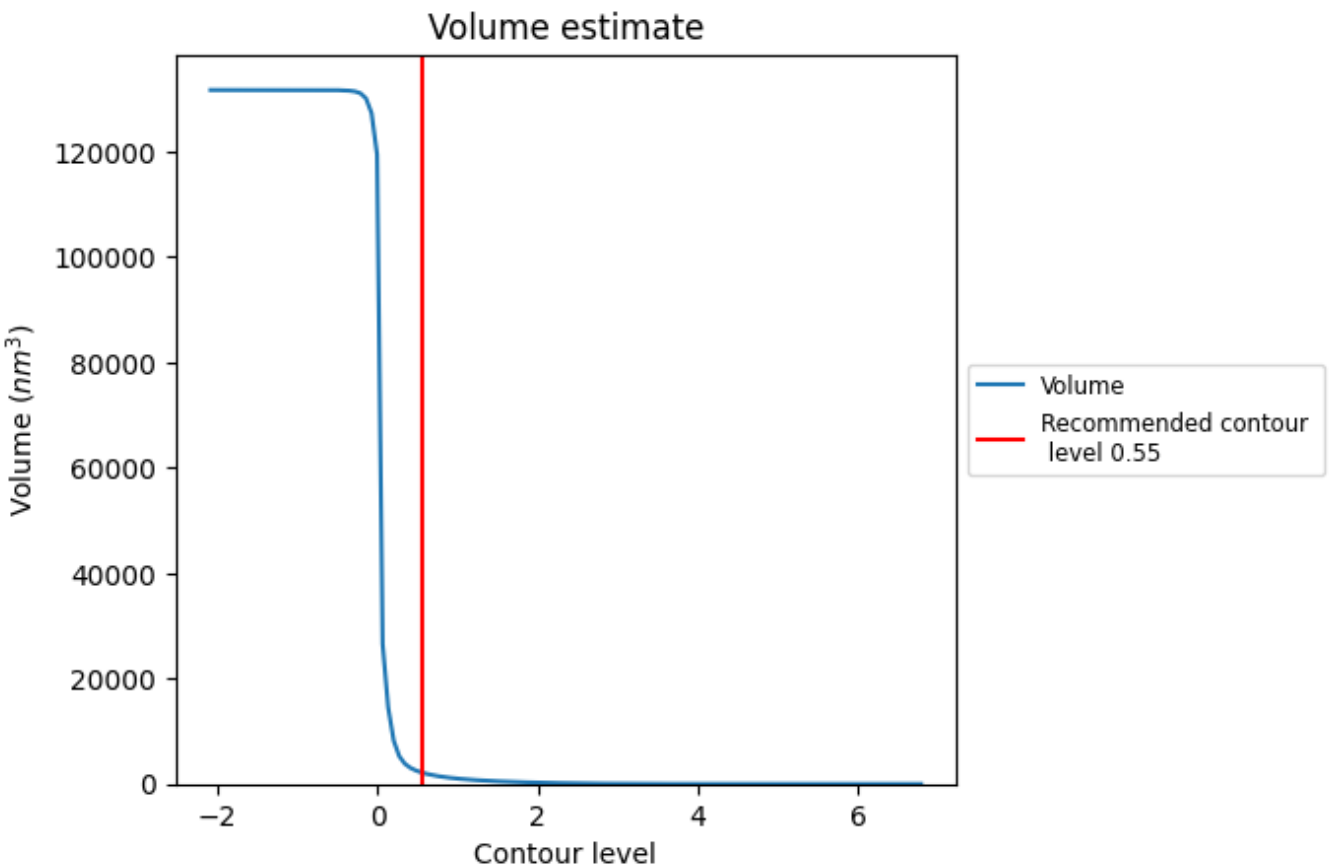
This section contains the results of statistical analysis of the map.

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.

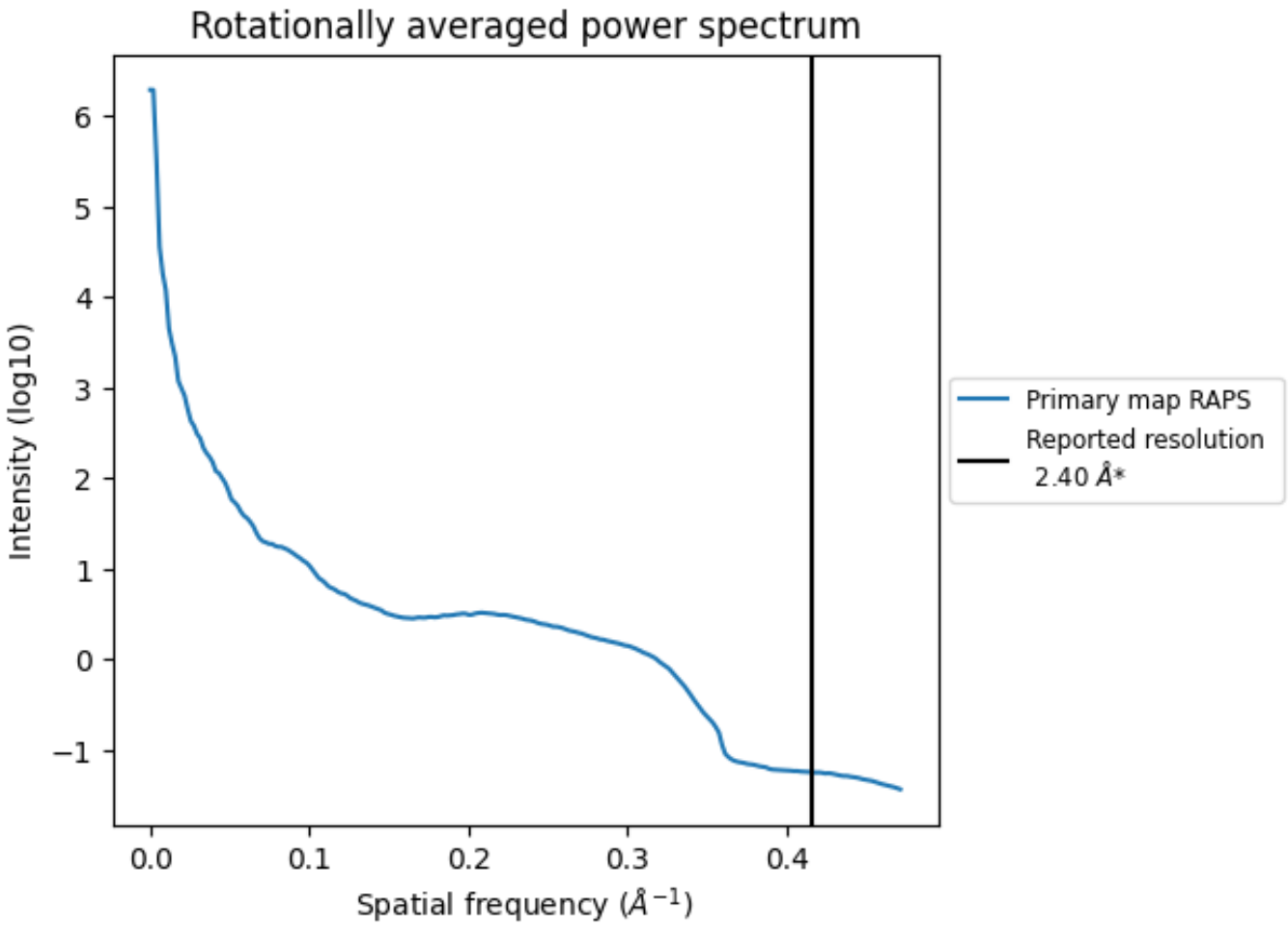
7.2 Volume estimate (i)



The volume at the recommended contour level is 2175 nm^3; this corresponds to an approximate mass of 1964 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 0.417 Å^{-1}

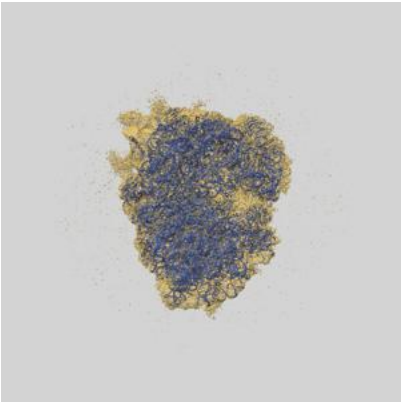
8 Fourier-Shell correlation (i)

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

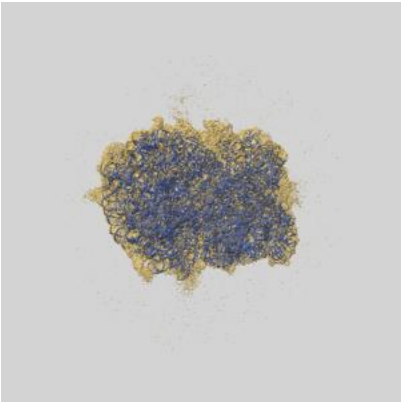
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13113 and PDB model 7OYC. Per-residue inclusion information can be found in section 3 on page 20.

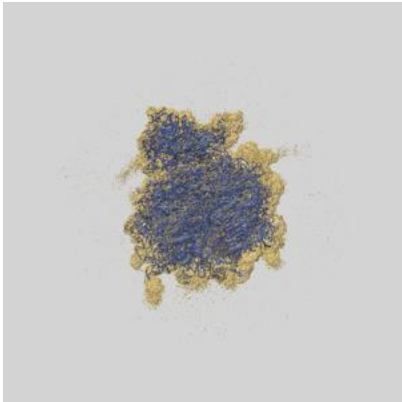
9.1 Map-model overlay (i)



X



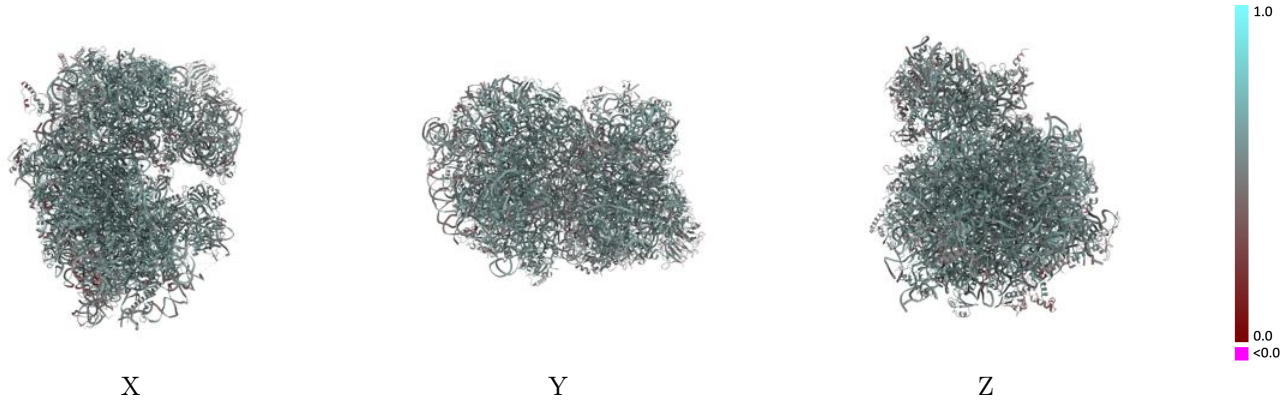
Y



Z

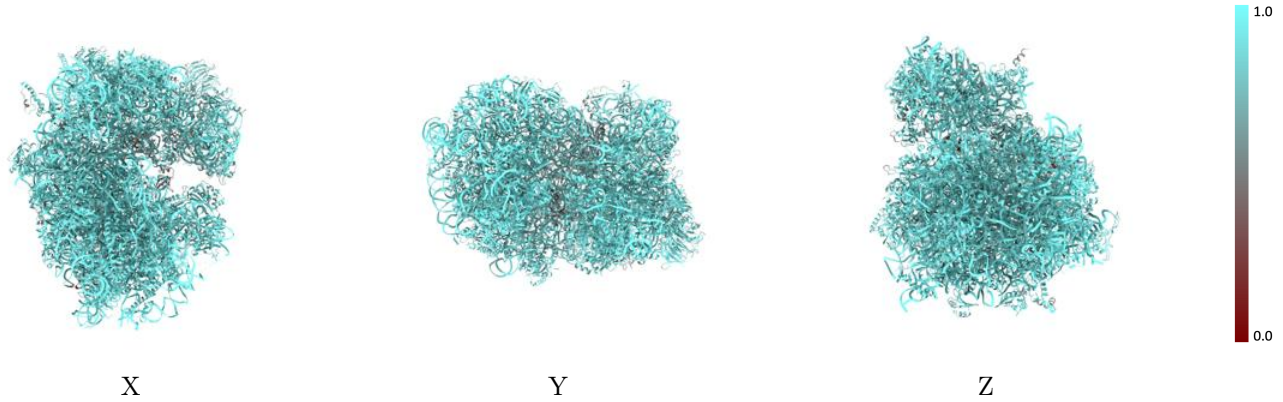
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



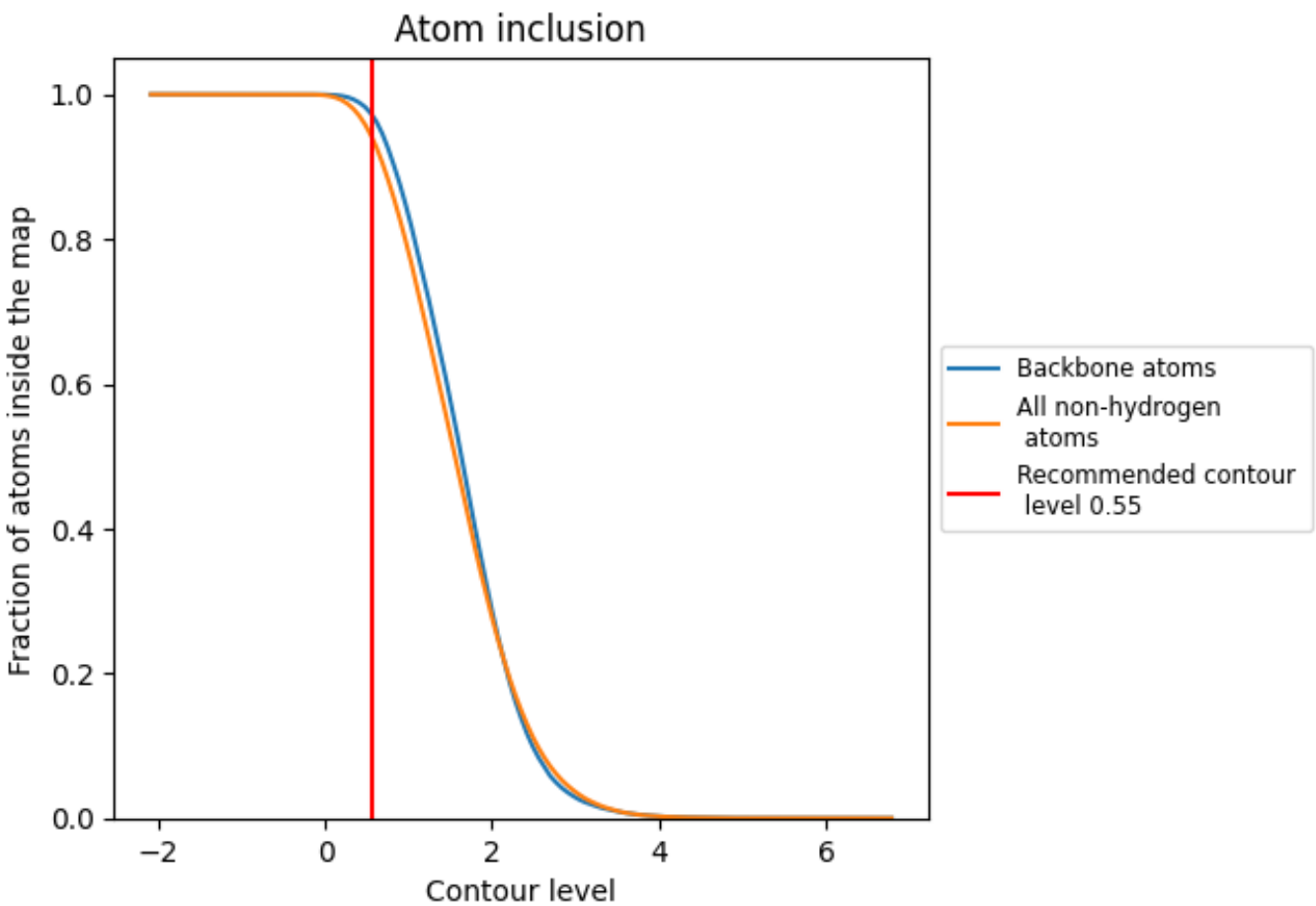
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9431	0.5570
11	0.4090	0.4890
22	0.9746	0.5620
51	0.9797	0.5630
71	0.9965	0.5760
81	0.9860	0.5640
A1	0.9415	0.5890
A2	0.9363	0.5690
B1	0.9361	0.5720
B2	0.8990	0.5410
C1	0.9554	0.5780
C2	0.9098	0.5690
D1	0.9466	0.5510
D2	0.8022	0.5210
E1	0.9432	0.5480
E2	0.9311	0.5610
F1	0.9383	0.5720
F2	0.8468	0.5130
G1	0.9375	0.5570
G2	0.8668	0.4930
H1	0.9222	0.5620
H2	0.8659	0.5030
I1	0.9327	0.5610
I2	0.8589	0.5200
J1	0.9005	0.5260
J2	0.9375	0.5630
K2	0.8966	0.5240
L1	0.9386	0.5630
L2	0.8879	0.5510
M1	0.9597	0.5670
N1	0.9740	0.6000
N2	0.9160	0.5610
O1	0.9651	0.5800
O2	0.9030	0.5480
P1	0.9599	0.5730

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Chain	Atom inclusion	Q-score
P2	0.8781	0.5190
Q1	0.9491	0.5810
Q2	0.9296	0.5570
R1	0.9063	0.5500
R2	0.8523	0.5280
S1	0.9587	0.5840
S2	0.8612	0.5120
T1	0.9271	0.5630
T2	0.9245	0.5460
U1	0.8747	0.4780
U2	0.8688	0.5220
V1	0.8976	0.5760
V2	0.9156	0.5580
W1	0.9110	0.5770
W2	0.9228	0.5770
X1	0.8948	0.5530
X2	0.8869	0.5600
Y1	0.9442	0.5620
Y2	0.9180	0.5320
Z1	0.9320	0.5490
Z2	0.8489	0.5020
a1	0.9781	0.5970
a2	0.9282	0.5680
b1	0.9223	0.5480
b2	0.9128	0.5190
c1	0.9301	0.5440
c2	0.7573	0.4720
d1	0.9188	0.5400
d2	0.9429	0.5740
e1	0.9404	0.5780
e2	0.8648	0.5310
f1	0.9580	0.5840
g1	0.9572	0.5810
g2	0.8567	0.4900
h1	0.9125	0.5490
i1	0.9278	0.5450
i2	0.6806	0.4760
j1	0.9611	0.5910
k1	0.8777	0.5280
l1	0.9336	0.5750
m1	0.9674	0.5830
n1	0.8095	0.5400

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Chain	Atom inclusion	Q-score
o1	0.9331	0.5650
p1	0.8826	0.5700
r1	0.9541	0.5730
s1	0.4735	0.4860
v2	0.6433	0.4830