wwPDB EM Validation Summary Report

Nov 20, 2022 – 07:53 am GMT

PDB ID	:	6HD7
EMDB ID	:	EMD-0202
Title	:	Cryo-EM structure of the ribosome-NatA complex
Authors	:	Knorr, A.G.; Becker, T.; Beckmann, R.
Deposited on	:	2018-08-17
Resolution	:	3.40 Å(reported)

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

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

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

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

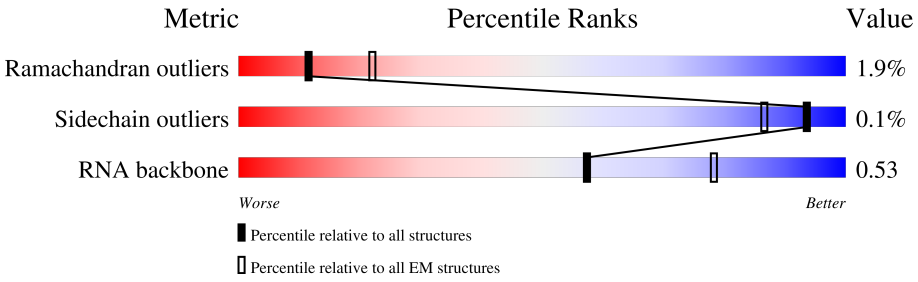
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1	3396	74% 24%
2	3	121	82% 18%
3	4	158	75% 25%
4	A	76	61% 39%
5	B	77	69% 31%
6	C	106	98%
7	D	92	98%
8	E	254	98%

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Mol	Chain	Length	Quality of chain
9	F	387	98%
10	G	362	96%
11	H	297	98%
12	I	176	88% 11%
13	J	244	88% 9%
14	K	256	89% 9%
15	L	191	98%
16	M	174	94%
17	N	199	93%
18	O	138	97%
19	P	204	98%
20	Q	199	99%
21	R	184	5% 98%
22	S	186	98%
23	T	189	98%
24	U	172	99%
25	V	160	97%
26	W	121	80% 17%
27	X	137	99%
28	Y	155	14% 63% 37%
29	Z	142	84% 15%
30	a	127	98%
31	b	136	97%
32	c	149	95% 5%
33	d	59	93% 5%

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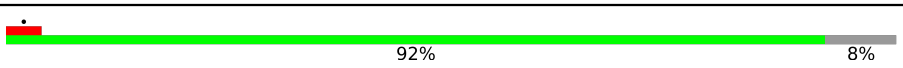
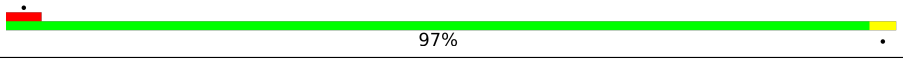
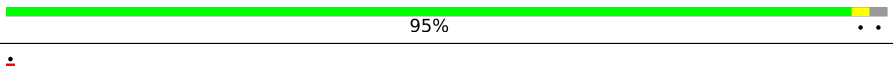
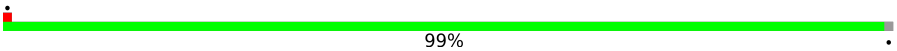
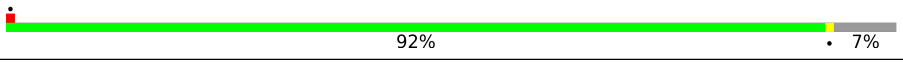
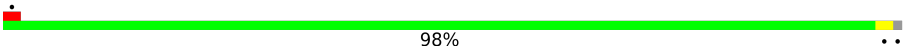
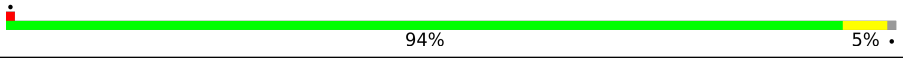
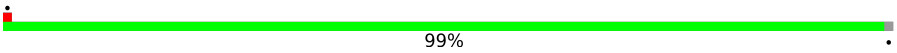
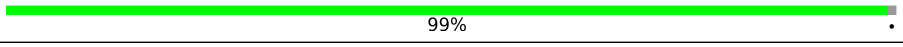
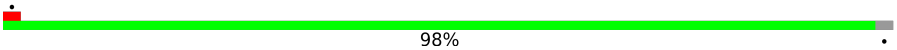
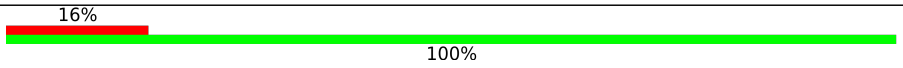
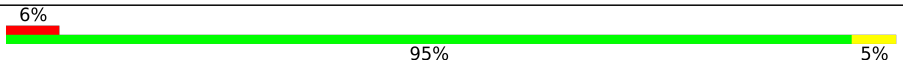
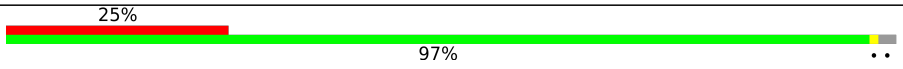
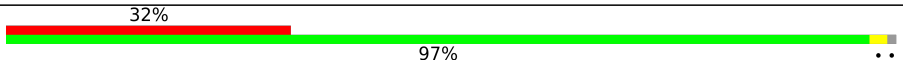
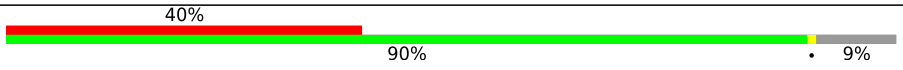
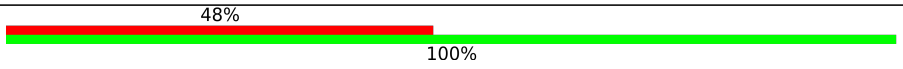
Mol	Chain	Length	Quality of chain
34	e	105	
35	f	109	
36	g	130	
37	h	107	
38	i	121	
39	j	120	
40	k	100	
41	l	88	
42	m	78	
43	n	51	
44	o	128	
45	p	25	
46	r	210	
47	s	221	
48	t	854	
49	u	238	
50	v	176	
51	z	23	

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 141153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called Saccharomyces cerevisiae S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	3335	71309	31846	12813	23315	3335	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	3	121	2579	1152	461	845	121	0	0

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	158	3353	1500	586	1109	158	0	0

- Molecule 4 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	A	76	1611	721	281	534	75	0	0

- Molecule 5 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	B	77	1644	731	290	546	77	0	0

- Molecule 6 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	105	847	534	170	138	5	0	0

- Molecule 7 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 8 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 9 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 11 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 12 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 13 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 14 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 15 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 16 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 17 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	N	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 18 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 19 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 20 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 21 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	R	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 22 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 23 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 24 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 25 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 26 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 27 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 28 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	98	Total 699	C 443	N 137	O 118	S 1	0	0

- Molecule 29 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	121	Total 964	C 620	N 169	O 173	S 2	0	0

- Molecule 30 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	a	126	Total 993	C 625	N 192	O 176	0	0

- Molecule 31 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	b	135	Total 1092	C 710	N 202	O 180	0	0

- Molecule 32 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	148	Total 1173	C 749	N 231	O 190	S 3	0	0

- Molecule 33 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	d	58	Total 462	C 289	N 100	O 73	0	0

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	97	Total 743	C 479	N 124	O 139	S 1	0	0

- Molecule 35 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	109	Total 876	C 556	N 167	O 152	S 1	0	0

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	127	Total 1020	C 647	N 205	O 167	S 1	0	0

- Molecule 37 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	106	Total 850	C 540	N 165	O 144	S 1	0	0

- Molecule 38 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	112	Total 880	C 545	N 179	O 152	S 4	0	0

- Molecule 39 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	119	Total 969	C 615	N 186	O 167	S 1	0	0

- Molecule 40 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	99	Total 771	C 481	N 156	O 132	S 2	0	0

- Molecule 41 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	87	Total 681	C 414	N 148	O 114	S 5	0	0

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	m	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 44 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 45 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 46 is a protein called ribosomal protein RPL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	r	210	Total	C	N	O	0	0
			1050	630	210	210		

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	220	Total	C	N	O	S	0	0
			1770	1121	335	307	7		

- Molecule 48 is a protein called N-terminal acetyltransferase A complex subunit NAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	838	Total	C	N	O	S	1	0
			6650	4265	1117	1246	22		

- Molecule 49 is a protein called N-terminal acetyltransferase A complex catalytic subunit ARD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	235	Total	C	N	O	S	0	0
			1798	1128	316	343	11		

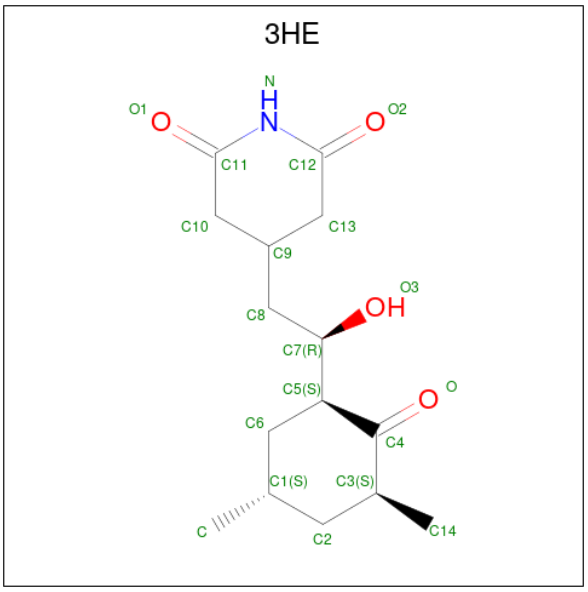
- Molecule 50 is a protein called N-alpha-acetyltransferase NAT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	161	Total	C	N	O	S	0	0
			1259	816	210	228	5		

- Molecule 51 is a protein called nascent polypeptide chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	z	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 52 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: $C_{15}H_{23}NO_4$).



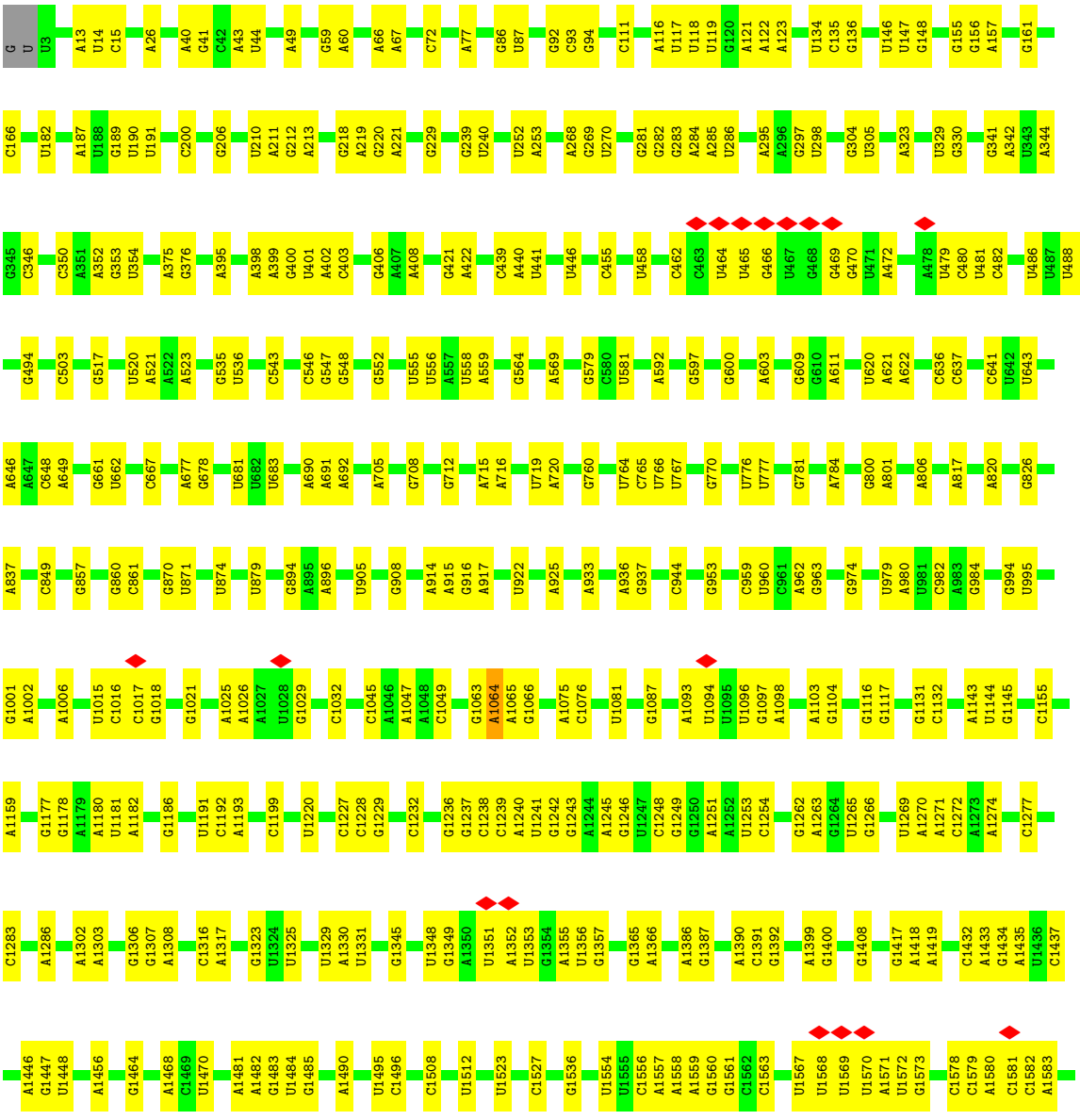
Mol	Chain	Residues	Atoms				AltConf
52	1	1	Total	C	N	O	0
			20	15	1	4	

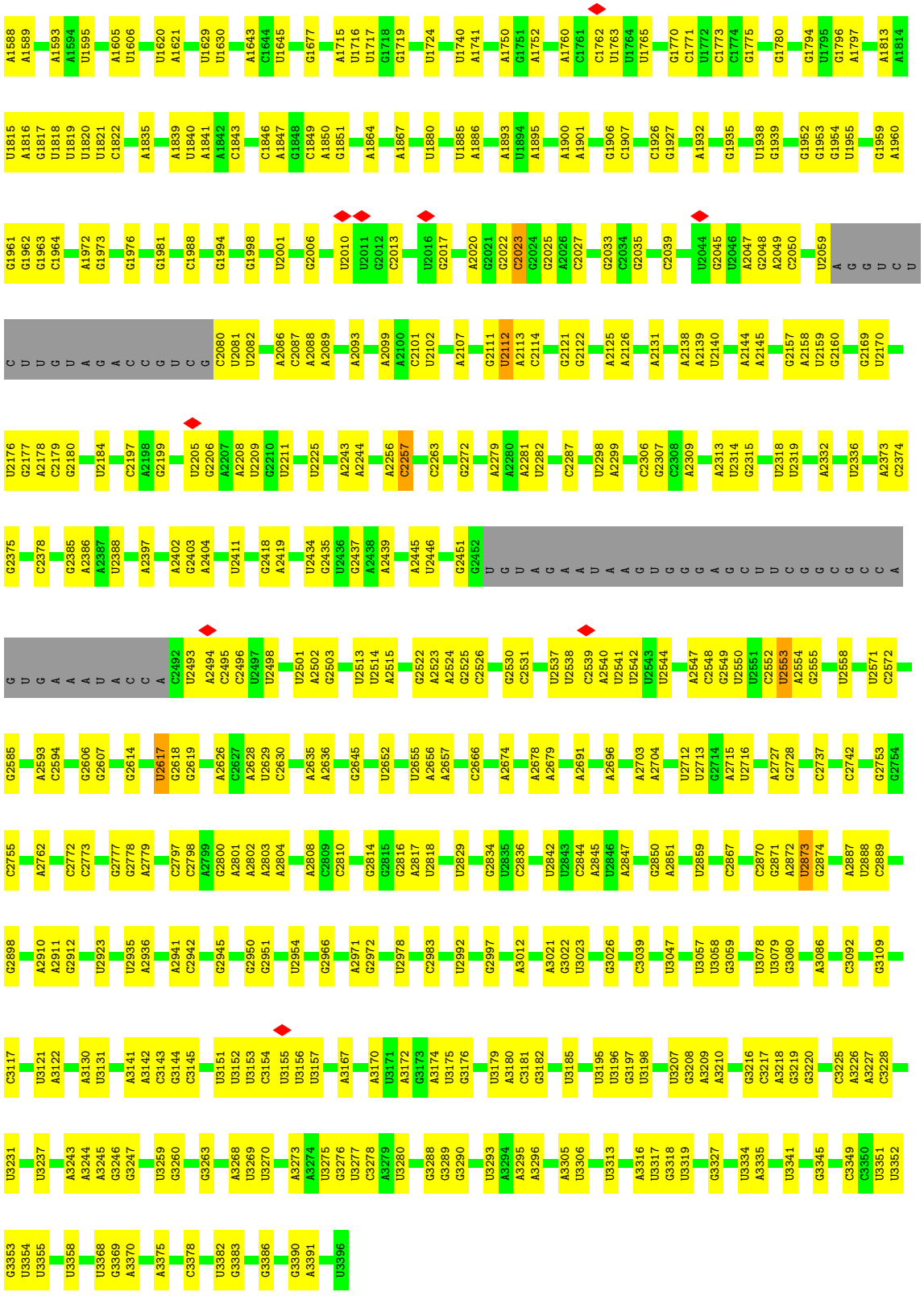
3 Residue-property plots (i)

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: Saccharomyces cerevisiae S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA

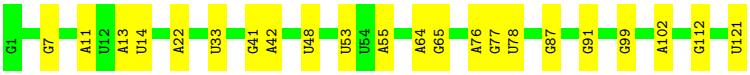
Chain 1:





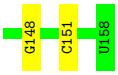
• Molecule 2: 5S rRNA

Chain 3:



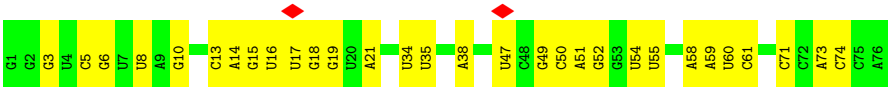
• Molecule 3: 5.8S rRNA

Chain 4:



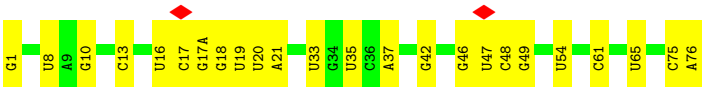
• Molecule 4: tRNA

Chain A:



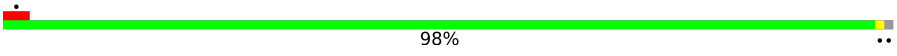
• Molecule 5: P-site tRNA

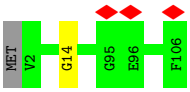
Chain B:



• Molecule 6: 60S ribosomal protein L42-A

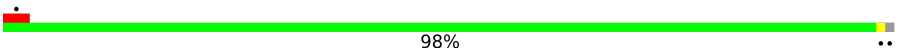
Chain C:

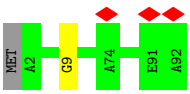




• Molecule 7: 60S ribosomal protein L43-A

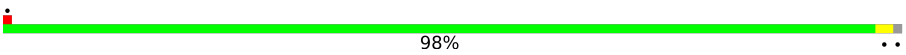
Chain D:

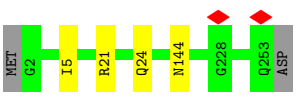




• Molecule 8: 60S ribosomal protein L2-A

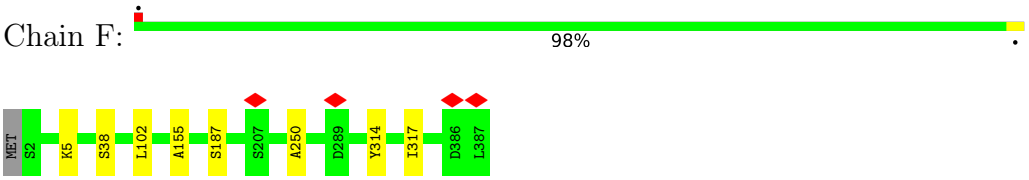
Chain E:





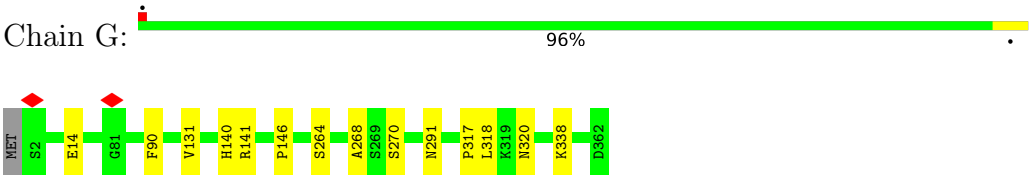
• Molecule 9: 60S ribosomal protein L3

Chain F:



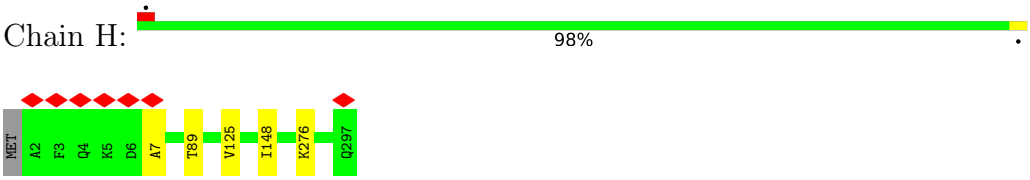
• Molecule 10: 60S ribosomal protein L4-A

Chain G:



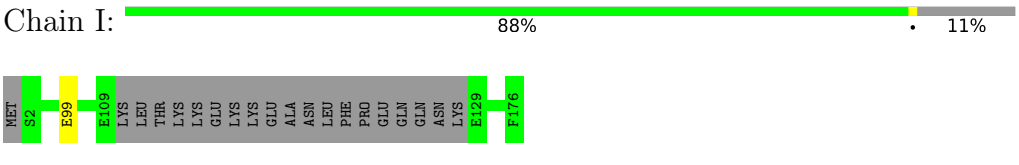
• Molecule 11: 60S ribosomal protein L5

Chain H:



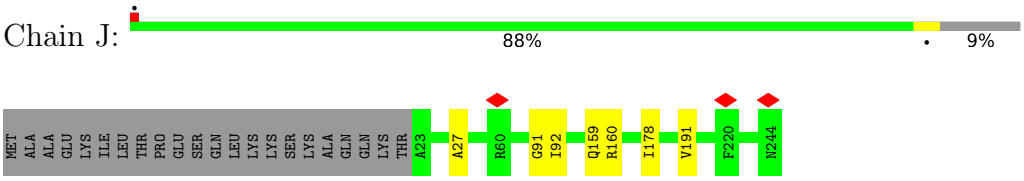
• Molecule 12: 60S ribosomal protein L6-A

Chain I:



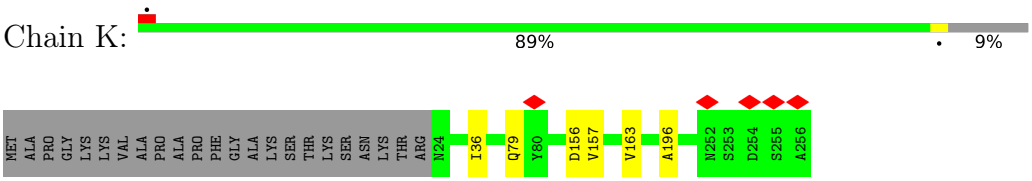
• Molecule 13: 60S ribosomal protein L7-A

Chain J:



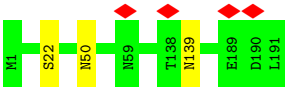
• Molecule 14: 60S ribosomal protein L8-A

Chain K:



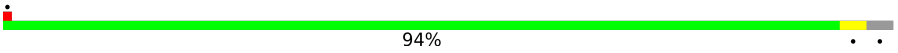
• Molecule 15: 60S ribosomal protein L9-A

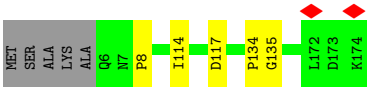
Chain L:



• Molecule 16: 60S ribosomal protein L11-A

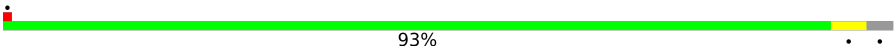
Chain M:

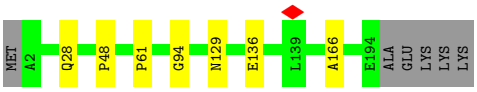




• Molecule 17: 60S ribosomal protein L13-A

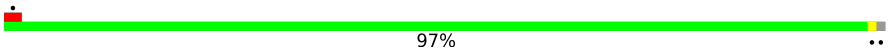
Chain N:

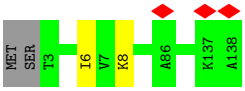




• Molecule 18: 60S ribosomal protein L14-A

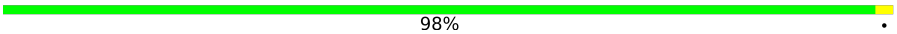
Chain O:

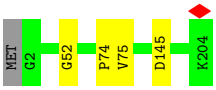




• Molecule 19: 60S ribosomal protein L15-A

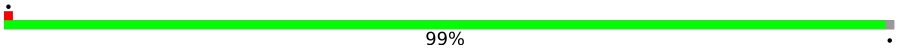
Chain P:

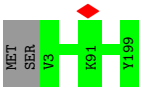




• Molecule 20: 60S ribosomal protein L16-A

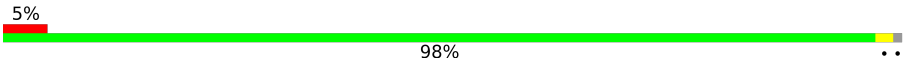
Chain Q:

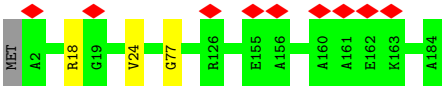




• Molecule 21: 60S ribosomal protein L17-A

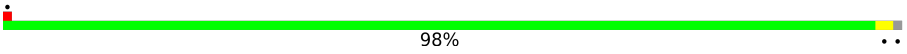
Chain R:

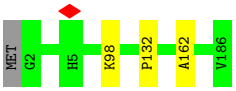




• Molecule 22: 60S ribosomal protein L18-A

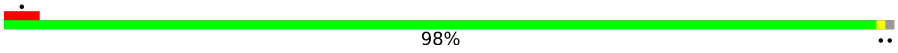
Chain S:

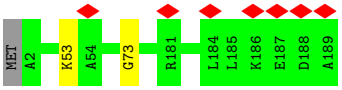




• Molecule 23: 60S ribosomal protein L19-A

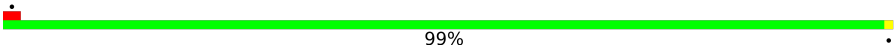
Chain T:

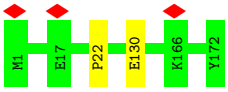




• Molecule 24: 60S ribosomal protein L20-A

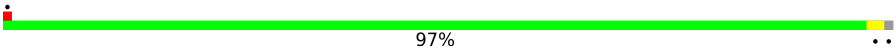
Chain U:

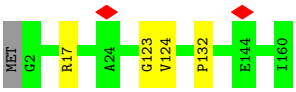




• Molecule 25: 60S ribosomal protein L21-A

Chain V:



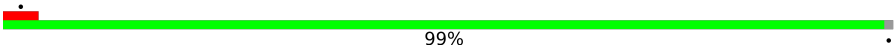


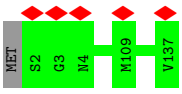
• Molecule 26: 60S ribosomal protein L22-A

Chain W:

• Molecule 27: 60S ribosomal protein L23-A

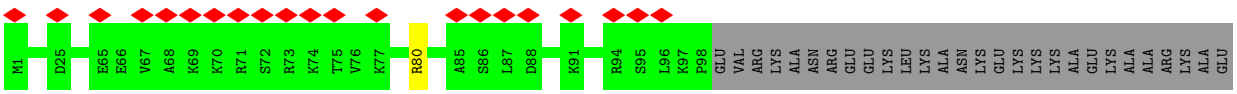
Chain X:

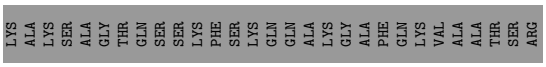




• Molecule 28: 60S ribosomal protein L24-A

Chain Y:



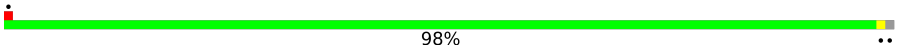


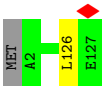
• Molecule 29: 60S ribosomal protein L25

Chain Z:

• Molecule 30: 60S ribosomal protein L26-A

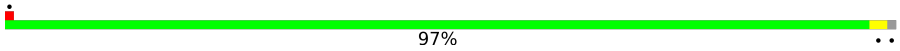
Chain a:

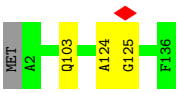




• Molecule 31: 60S ribosomal protein L27-A

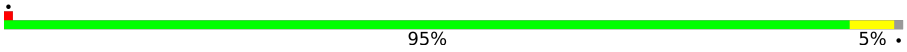
Chain b:

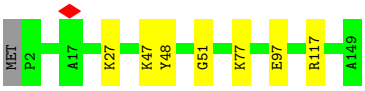




• Molecule 32: 60S ribosomal protein L28

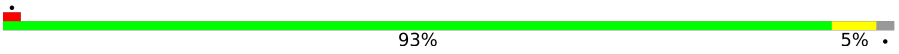
Chain c:

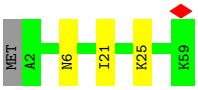




• Molecule 33: 60S ribosomal protein L29

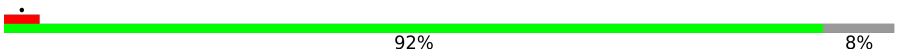
Chain d:

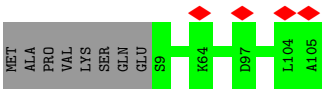




• Molecule 34: 60S ribosomal protein L30

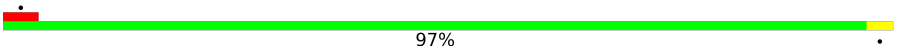
Chain e:

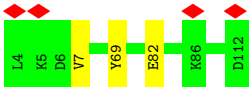




• Molecule 35: 60S ribosomal protein L31-A

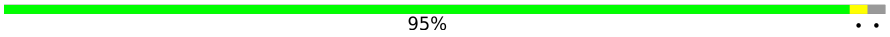
Chain f:

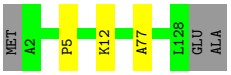




• Molecule 36: 60S ribosomal protein L32

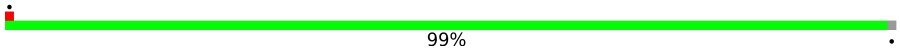
Chain g:

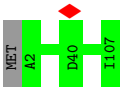




• Molecule 37: 60S ribosomal protein L33-A

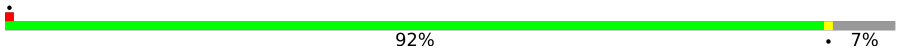
Chain h:

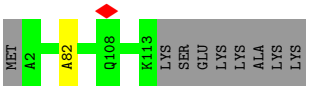




• Molecule 38: 60S ribosomal protein L34-A

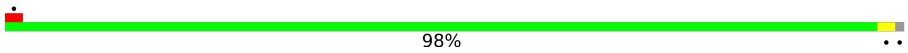
Chain i:

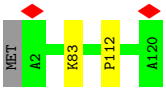




• Molecule 39: 60S ribosomal protein L35-A

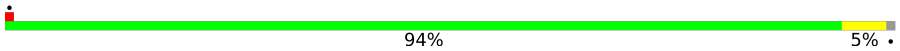
Chain j:

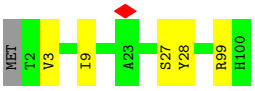




• Molecule 40: 60S ribosomal protein L36-A

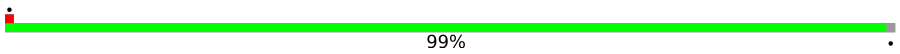
Chain k:

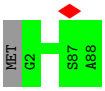




• Molecule 41: 60S ribosomal protein L37-A

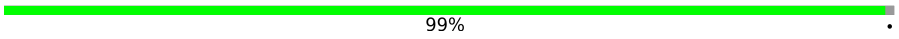
Chain l:





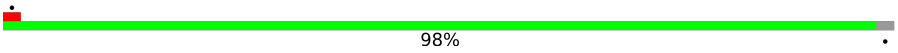
• Molecule 42: 60S ribosomal protein L38

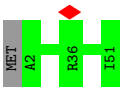
Chain m:



• Molecule 43: 60S ribosomal protein L39

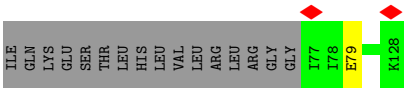
Chain n:





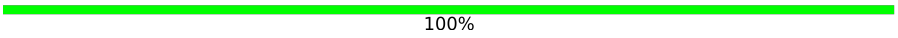
• Molecule 44: Ubiquitin-60S ribosomal protein L40

Chain o:



• Molecule 45: 60S ribosomal protein L41-A

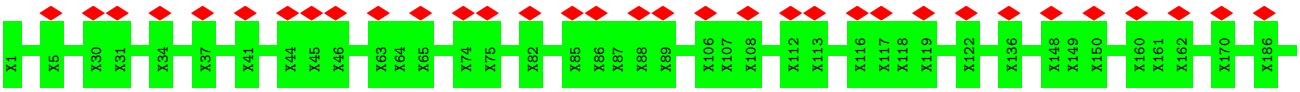
Chain p:



There are no outlier residues recorded for this chain.

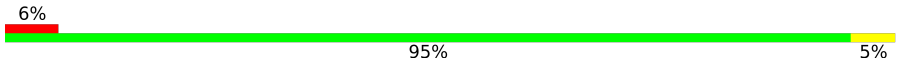
• Molecule 46: ribosomal protein RPL1

Chain r:



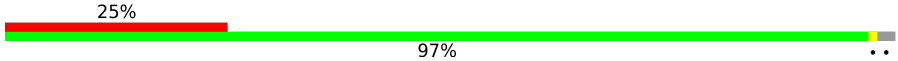
• Molecule 47: 60S ribosomal protein L10

Chain s:

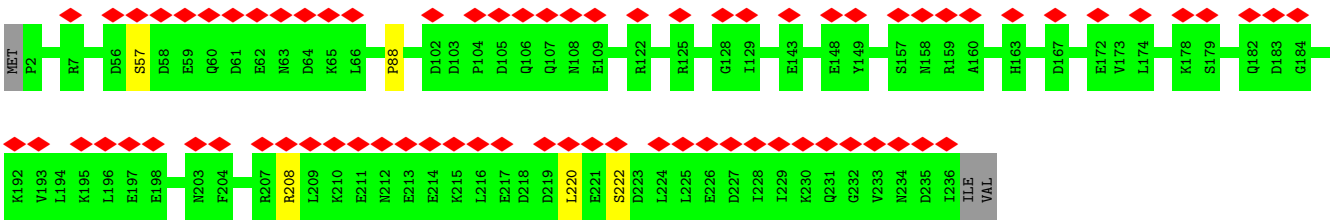


• Molecule 48: N-terminal acetyltransferase A complex subunit NAT1

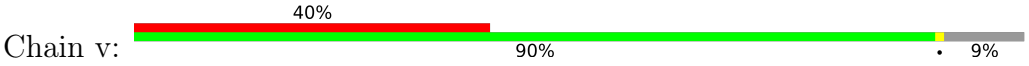
Chain t:

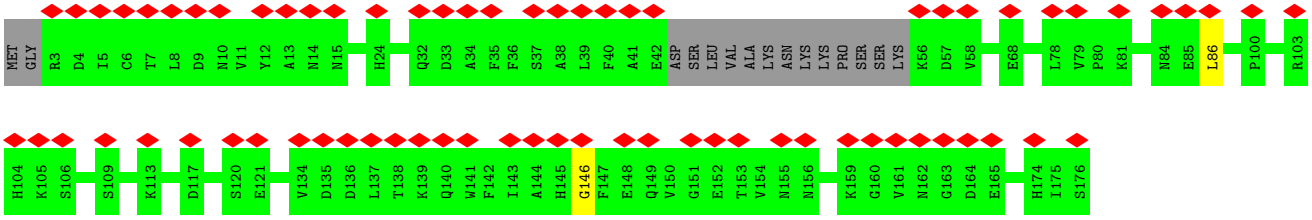


• Molecule 49: N-terminal acetyltransferase A complex catalytic subunit ARD1

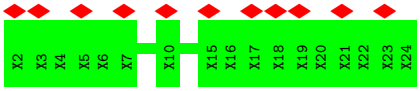


• Molecule 50: N-alpha-acetyltransferase NAT5





• Molecule 51: nascent polypeptide chain


X2
X3
X4
X5
X6
X7
X10
X15
X16
X17
X18
X19
X20
X21
X22
X23
X24

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	262507	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 ($e^-/Å^2$)	2.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.226	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0126	Depositor
Map size (Å)	455.28, 455.28, 455.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3HE

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	1	0.16	0/79803	0.76	27/124411 (0.0%)
2	3	0.15	0/2883	0.74	0/4491
3	4	0.13	0/3746	0.71	0/5832
4	A	0.16	0/1799	0.78	0/2801
5	B	0.29	1/1835 (0.1%)	0.74	0/2858
6	C	0.24	0/860	0.41	0/1136
7	D	0.22	0/701	0.41	0/934
8	E	0.23	0/1948	0.41	0/2617
9	F	0.23	0/3146	0.41	0/4228
10	G	0.23	0/2800	0.39	0/3790
11	H	0.23	0/2425	0.38	0/3271
12	I	0.24	0/1260	0.38	0/1694
13	J	0.24	0/1821	0.38	0/2451
14	K	0.23	0/1836	0.39	0/2481
15	L	0.23	0/1539	0.40	0/2073
16	M	0.23	0/1374	0.38	0/1842
17	N	0.24	0/1568	0.40	0/2106
18	O	0.23	0/1068	0.37	0/1438
19	P	0.22	0/1757	0.39	0/2354
20	Q	0.24	0/1585	0.36	0/2128
21	R	0.23	0/1443	0.41	0/1944
22	S	0.23	0/1465	0.38	0/1965
23	T	0.21	0/1538	0.34	0/2050
24	U	0.23	0/1481	0.39	0/1990
25	V	0.23	0/1300	0.38	0/1743
26	W	0.24	0/812	0.41	0/1099
27	X	0.24	0/1018	0.42	0/1369
28	Y	0.24	0/712	0.40	0/958
29	Z	0.24	0/979	0.42	0/1321
30	a	0.23	0/1004	0.40	0/1341
31	b	0.24	0/1118	0.38	0/1497
32	c	0.23	0/1204	0.39	0/1612

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	d	0.23	0/473	0.35	0/629
34	e	0.24	0/751	0.38	0/1008
35	f	0.23	0/890	0.39	0/1196
36	g	0.22	0/1041	0.38	0/1394
37	h	0.25	0/868	0.43	0/1168
38	i	0.22	0/890	0.39	0/1189
39	j	0.23	0/978	0.38	0/1301
40	k	0.23	0/778	0.40	0/1034
41	l	0.23	0/696	0.41	0/923
42	m	0.24	0/618	0.40	0/826
43	n	0.22	0/443	0.37	0/588
44	o	0.23	0/423	0.39	0/562
45	p	0.20	0/234	0.32	0/300
47	s	0.24	0/1807	0.39	0/2425
48	t	0.24	0/6792	0.35	0/9180
49	u	0.23	0/1830	0.41	0/2484
50	v	0.24	0/1287	0.37	0/1742
All	All	0.19	1/150627 (0.0%)	0.64	27/221774 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	G	OP3-P	-10.61	1.48	1.61

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2553	U	C2-N1-C1'	7.87	127.14	117.70
1	1	2553	U	N1-C2-O2	7.25	127.88	122.80
1	1	2873	U	C2-N1-C1'	7.13	126.26	117.70
1	1	2553	U	N3-C2-O2	-6.69	117.52	122.20
1	1	1227	C	N1-C2-O2	6.47	122.78	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	103/106 (97%)	84 (82%)	18 (18%)	1 (1%)	15	46
7	D	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	14	44
8	E	250/254 (98%)	212 (85%)	34 (14%)	4 (2%)	9	34
9	F	384/387 (99%)	330 (86%)	47 (12%)	7 (2%)	8	32
10	G	359/362 (99%)	308 (86%)	37 (10%)	14 (4%)	3	19
11	H	294/297 (99%)	258 (88%)	31 (10%)	5 (2%)	9	34
12	I	152/176 (86%)	135 (89%)	16 (10%)	1 (1%)	22	55
13	J	220/244 (90%)	191 (87%)	22 (10%)	7 (3%)	4	22
14	K	231/256 (90%)	203 (88%)	22 (10%)	6 (3%)	5	26
15	L	189/191 (99%)	166 (88%)	20 (11%)	3 (2%)	9	34
16	M	167/174 (96%)	132 (79%)	30 (18%)	5 (3%)	4	23
17	N	191/199 (96%)	162 (85%)	22 (12%)	7 (4%)	3	20
18	O	134/138 (97%)	114 (85%)	18 (13%)	2 (2%)	10	36
19	P	201/204 (98%)	177 (88%)	20 (10%)	4 (2%)	7	30
20	Q	195/199 (98%)	181 (93%)	14 (7%)	0	100	100
21	R	181/184 (98%)	148 (82%)	30 (17%)	3 (2%)	9	34
22	S	183/186 (98%)	164 (90%)	16 (9%)	3 (2%)	9	34
23	T	186/189 (98%)	173 (93%)	11 (6%)	2 (1%)	14	44
24	U	170/172 (99%)	137 (81%)	31 (18%)	2 (1%)	13	41
25	V	157/160 (98%)	135 (86%)	18 (12%)	4 (2%)	5	26
26	W	98/121 (81%)	77 (79%)	18 (18%)	3 (3%)	4	23
27	X	134/137 (98%)	119 (89%)	15 (11%)	0	100	100
28	Y	96/155 (62%)	83 (86%)	12 (12%)	1 (1%)	15	46
29	Z	119/142 (84%)	110 (92%)	7 (6%)	2 (2%)	9	34
30	a	124/127 (98%)	113 (91%)	10 (8%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	b	133/136 (98%)	117 (88%)	13 (10%)	3 (2%)	6 28
32	c	146/149 (98%)	121 (83%)	18 (12%)	7 (5%)	2 15
33	d	56/59 (95%)	50 (89%)	3 (5%)	3 (5%)	2 13
34	e	95/105 (90%)	92 (97%)	3 (3%)	0	100 100
35	f	107/109 (98%)	95 (89%)	9 (8%)	3 (3%)	5 24
36	g	125/130 (96%)	114 (91%)	8 (6%)	3 (2%)	6 28
37	h	104/107 (97%)	95 (91%)	9 (9%)	0	100 100
38	i	110/121 (91%)	102 (93%)	7 (6%)	1 (1%)	17 49
39	j	117/120 (98%)	102 (87%)	13 (11%)	2 (2%)	9 34
40	k	97/100 (97%)	77 (79%)	15 (16%)	5 (5%)	2 13
41	l	85/88 (97%)	70 (82%)	15 (18%)	0	100 100
42	m	75/78 (96%)	64 (85%)	11 (15%)	0	100 100
43	n	48/51 (94%)	41 (85%)	7 (15%)	0	100 100
44	o	50/128 (39%)	45 (90%)	4 (8%)	1 (2%)	7 30
45	p	23/25 (92%)	23 (100%)	0	0	100 100
47	s	218/221 (99%)	176 (81%)	33 (15%)	9 (4%)	3 18
48	t	836/854 (98%)	760 (91%)	69 (8%)	7 (1%)	19 51
49	u	233/238 (98%)	186 (80%)	43 (18%)	4 (2%)	9 34
50	v	157/176 (89%)	138 (88%)	17 (11%)	2 (1%)	12 39
All	All	7422/7847 (95%)	6461 (87%)	823 (11%)	138 (2%)	11 31

5 of 138 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	G	146	PRO
14	K	79	GLN
24	U	22	PRO
8	E	144	ASN
10	G	268	ALA

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	
6	C	90/91 (99%)	90 (100%)	0	100	100
7	D	71/72 (99%)	71 (100%)	0	100	100
8	E	193/196 (98%)	193 (100%)	0	100	100
9	F	320/323 (99%)	319 (100%)	1 (0%)	92	97
10	G	288/289 (100%)	288 (100%)	0	100	100
11	H	244/245 (100%)	244 (100%)	0	100	100
12	I	134/153 (88%)	134 (100%)	0	100	100
13	J	186/205 (91%)	186 (100%)	0	100	100
14	K	187/208 (90%)	187 (100%)	0	100	100
15	L	171/171 (100%)	171 (100%)	0	100	100
16	M	147/150 (98%)	147 (100%)	0	100	100
17	N	154/159 (97%)	154 (100%)	0	100	100
18	O	107/109 (98%)	107 (100%)	0	100	100
19	P	175/176 (99%)	175 (100%)	0	100	100
20	Q	160/162 (99%)	160 (100%)	0	100	100
21	R	140/146 (96%)	140 (100%)	0	100	100
22	S	150/151 (99%)	150 (100%)	0	100	100
23	T	153/154 (99%)	153 (100%)	0	100	100
24	U	156/156 (100%)	156 (100%)	0	100	100
25	V	136/137 (99%)	136 (100%)	0	100	100
26	W	87/107 (81%)	87 (100%)	0	100	100
27	X	104/105 (99%)	104 (100%)	0	100	100
28	Y	57/129 (44%)	57 (100%)	0	100	100
29	Z	104/118 (88%)	104 (100%)	0	100	100
30	a	109/110 (99%)	109 (100%)	0	100	100
31	b	115/116 (99%)	115 (100%)	0	100	100
32	c	118/119 (99%)	118 (100%)	0	100	100
33	d	46/47 (98%)	46 (100%)	0	100	100
34	e	81/88 (92%)	81 (100%)	0	100	100
35	f	92/96 (96%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	g	109/111 (98%)	109 (100%)	0	100 100
37	h	90/91 (99%)	90 (100%)	0	100 100
38	i	95/103 (92%)	95 (100%)	0	100 100
39	j	104/105 (99%)	104 (100%)	0	100 100
40	k	81/82 (99%)	81 (100%)	0	100 100
41	l	70/71 (99%)	70 (100%)	0	100 100
42	m	68/69 (99%)	68 (100%)	0	100 100
43	n	45/46 (98%)	45 (100%)	0	100 100
44	o	47/116 (40%)	47 (100%)	0	100 100
45	p	23/23 (100%)	23 (100%)	0	100 100
47	s	184/187 (98%)	183 (100%)	1 (0%)	88 94
48	t	683/759 (90%)	681 (100%)	2 (0%)	92 97
49	u	177/216 (82%)	176 (99%)	1 (1%)	86 94
50	v	133/153 (87%)	133 (100%)	0	100 100
All	All	6184/6620 (93%)	6179 (100%)	5 (0%)	93 98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	F	102	LEU
47	s	109	ARG
48	t	29	LYS
48	t	440	ILE
49	u	208	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
37	h	42	GLN
49	u	20	ASN
39	j	59	ASN
48	t	172	ASN
50	v	32	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3328/3396 (97%)	772 (23%)	101 (3%)
2	3	120/121 (99%)	22 (18%)	2 (1%)
3	4	157/158 (99%)	35 (22%)	5 (3%)
4	A	75/76 (98%)	27 (36%)	4 (5%)
5	B	76/77 (98%)	23 (30%)	2 (2%)
All	All	3756/3828 (98%)	879 (23%)	114 (3%)

5 of 879 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	13	A
1	1	14	U
1	1	15	C
1	1	26	A
1	1	40	A

5 of 114 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	2112	U
4	A	54	U
1	1	2514	U
4	A	15	G
1	1	3317	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
52	3HE	1	3401	-	21,21,21	4.46	7 (33%)	19,30,30	5.28	11 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3HE	1	3401	-	-	0/8/36/36	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1	3401	3HE	O-C4	11.93	1.40	1.21
52	1	3401	3HE	O1-C11	8.23	1.40	1.23
52	1	3401	3HE	C12-N	7.97	1.51	1.37
52	1	3401	3HE	O2-C12	7.93	1.39	1.23
52	1	3401	3HE	C11-N	7.07	1.49	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	1	3401	3HE	C11-N-C12	-10.23	113.38	125.78
52	1	3401	3HE	O-C4-C5	-9.76	109.08	123.28
52	1	3401	3HE	O-C4-C3	-8.83	109.00	122.15
52	1	3401	3HE	O1-C11-N	-7.27	108.77	120.28
52	1	3401	3HE	O2-C12-N	-7.24	108.81	120.28

There are no chirality outliers.

There are no torsion outliers.

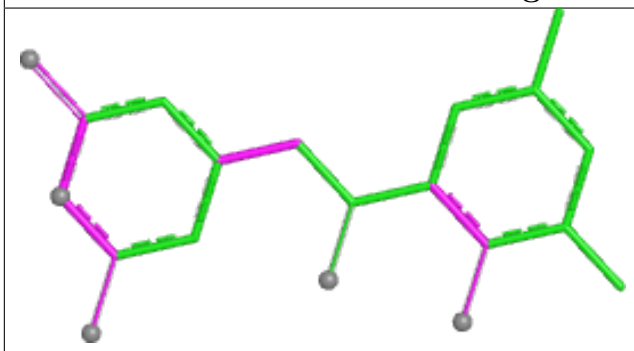
There are no ring outliers.

No monomer is involved in short contacts.

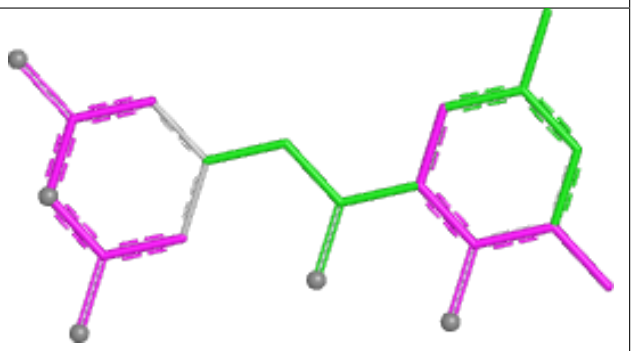
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

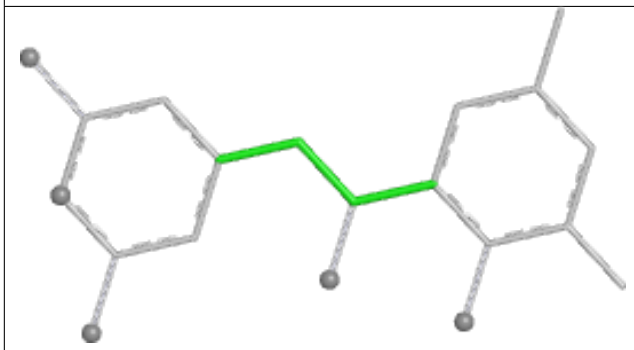
Ligand 3HE 1 3401



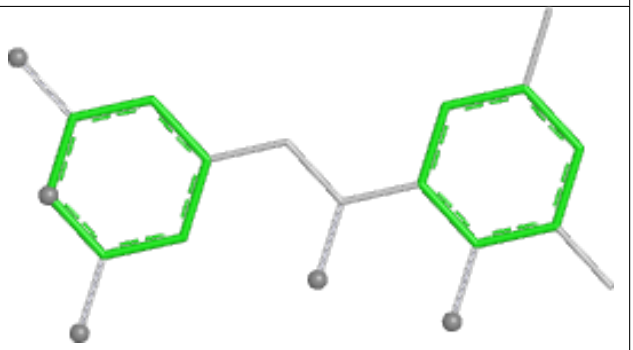
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1984:C	O3'	1985:G	P	6.36

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	615:U	O3'	616:G	P	4.31
1	1	426:G	O3'	427:C	P	3.34
1	1	1946:A	O3'	1947:G	P	3.13

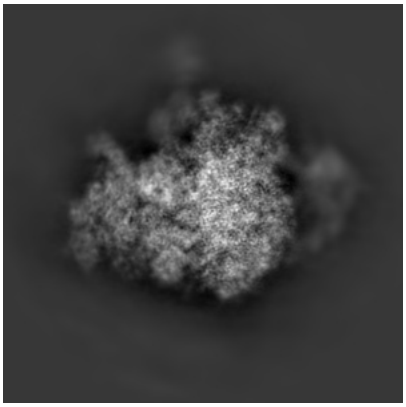
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0202. These allow visual inspection of the internal detail of the map and identification of artifacts.

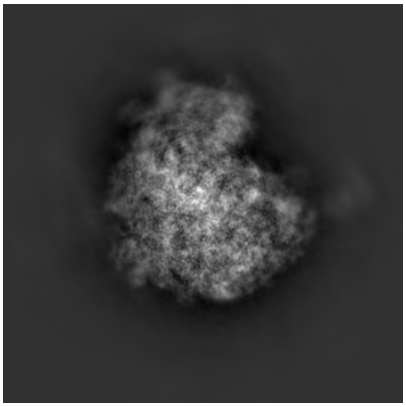
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

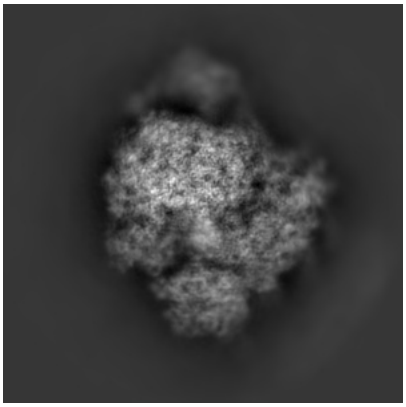
6.1.1 Primary map



X



Y

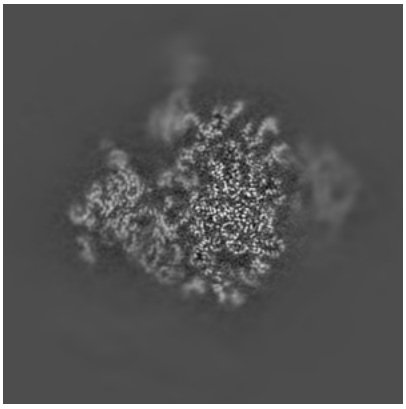


Z

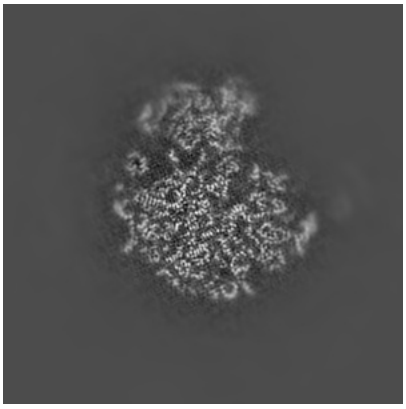
The images above show the map projected in three orthogonal directions.

6.2 Central slices

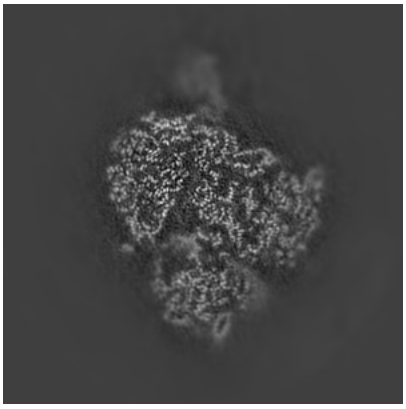
6.2.1 Primary map



X Index: 210



Y Index: 210

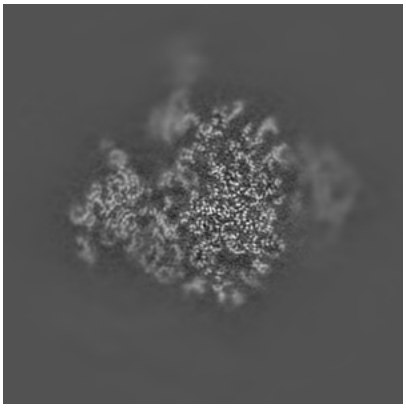


Z Index: 210

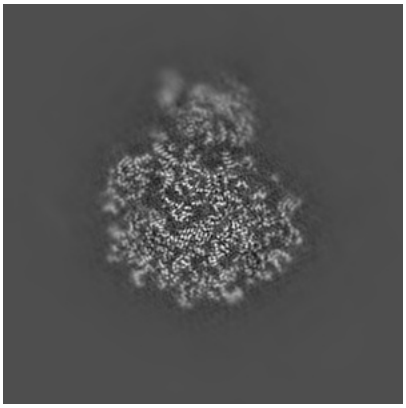
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

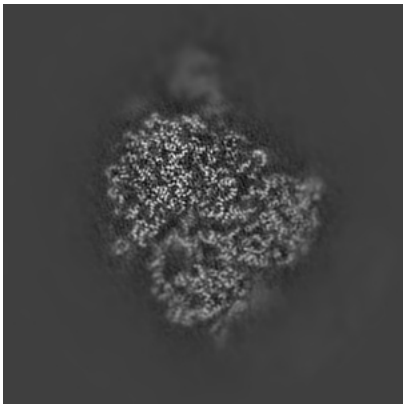
6.3.1 Primary map



X Index: 211



Y Index: 233

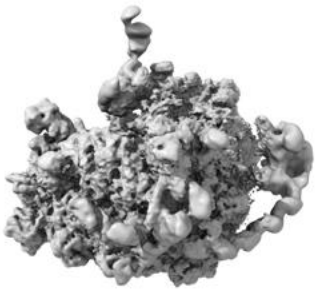


Z Index: 215

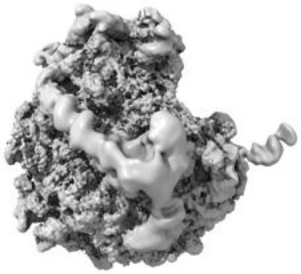
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

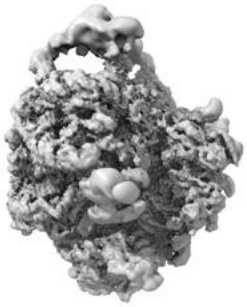
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

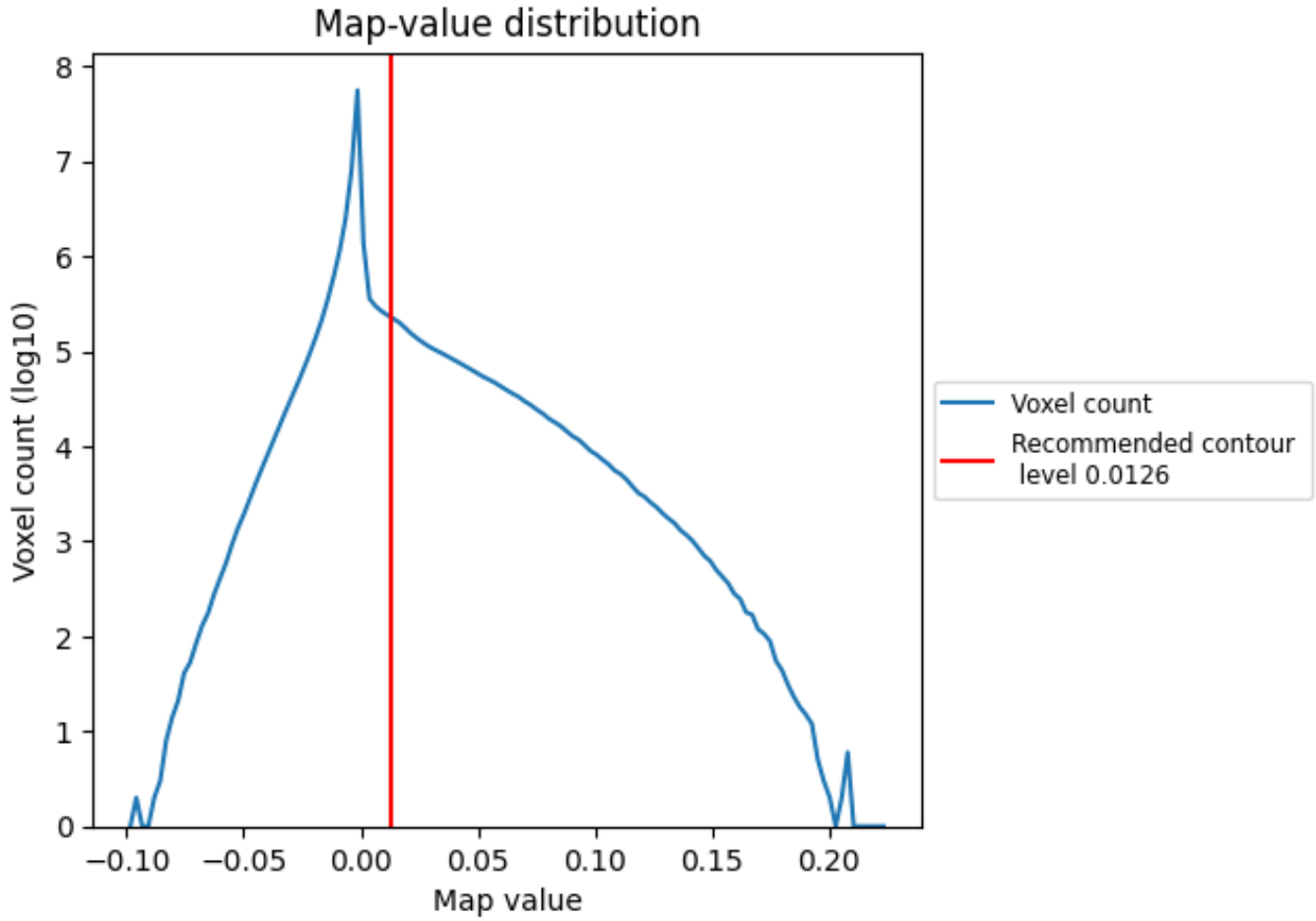
6.5 Mask visualisation (i)

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

7 Map analysis

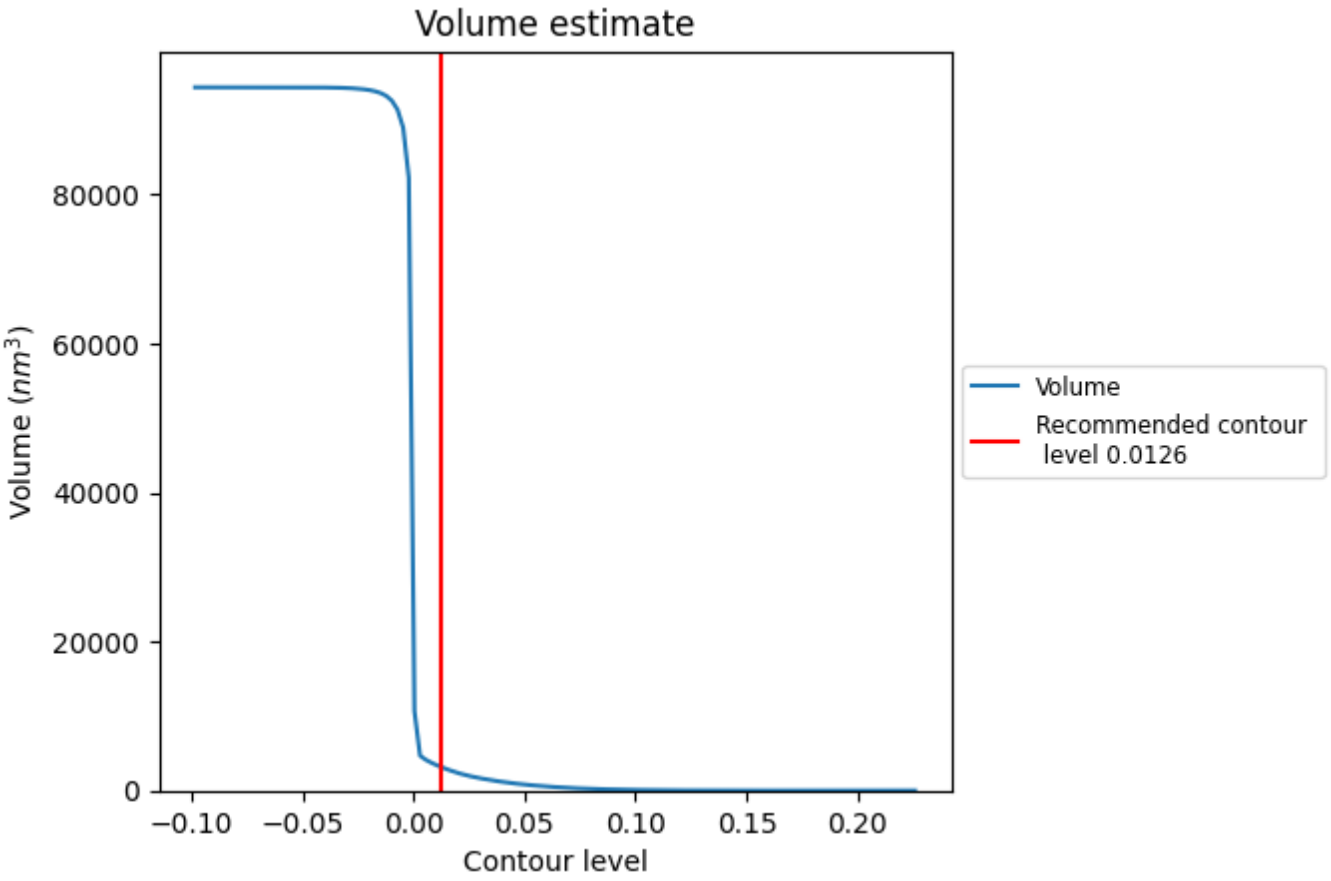
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

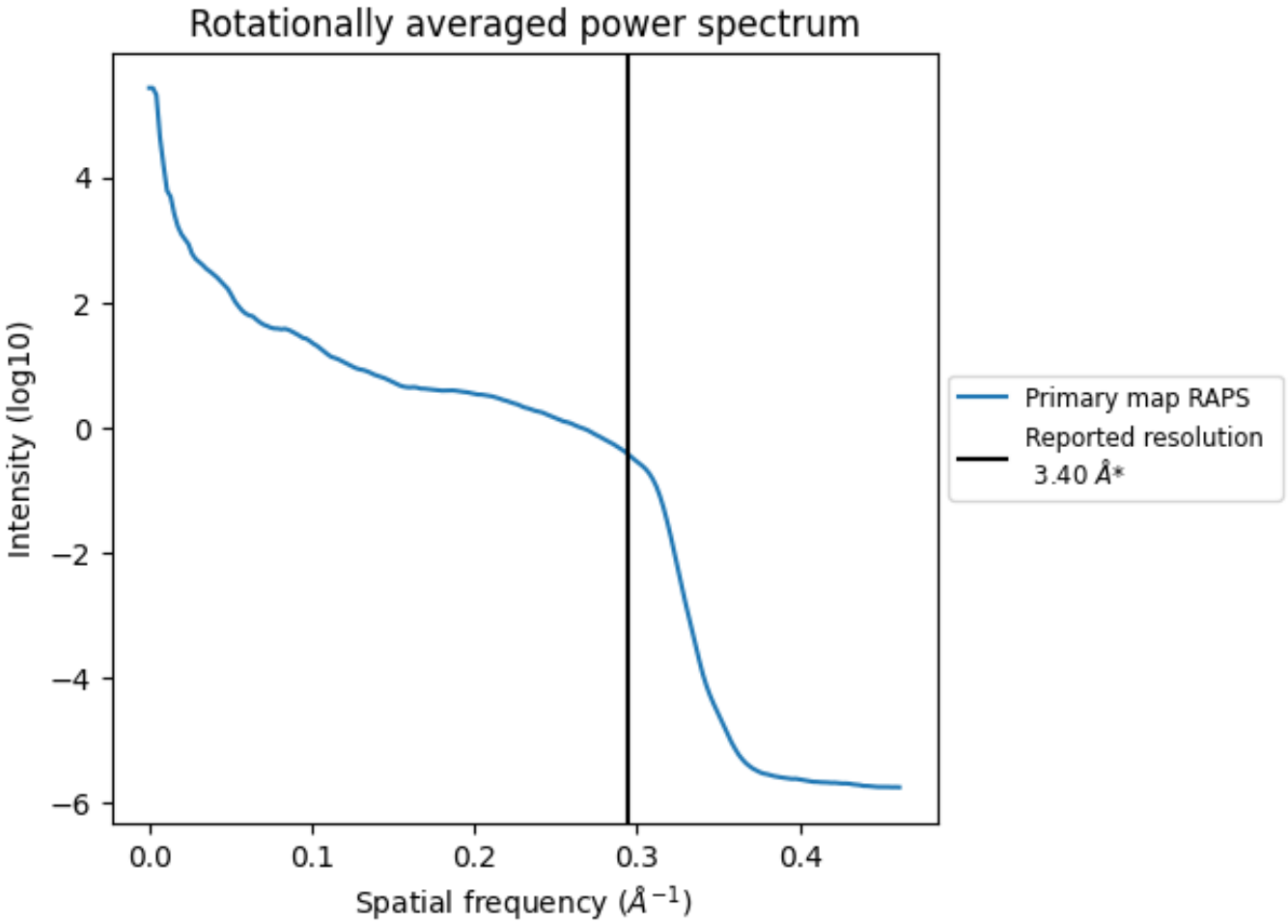
7.2 Volume estimate (i)



The volume at the recommended contour level is 3137 nm^3; this corresponds to an approximate mass of 2834 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 0.294 Å^{-1}

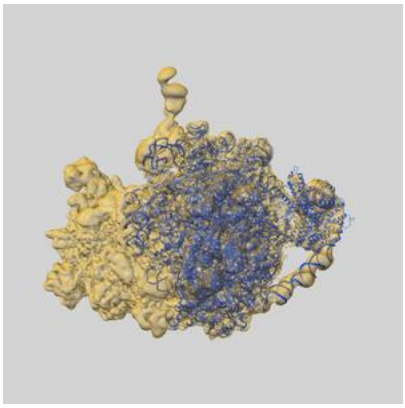
8 Fourier-Shell correlation (i)

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

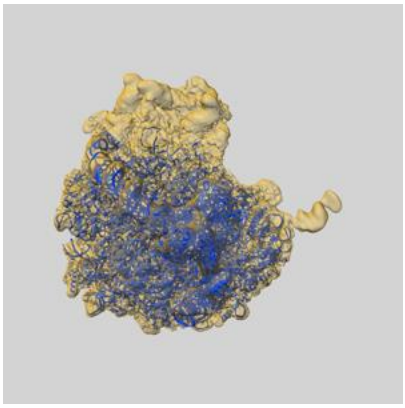
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0202 and PDB model 6HD7. Per-residue inclusion information can be found in section 3 on page 13.

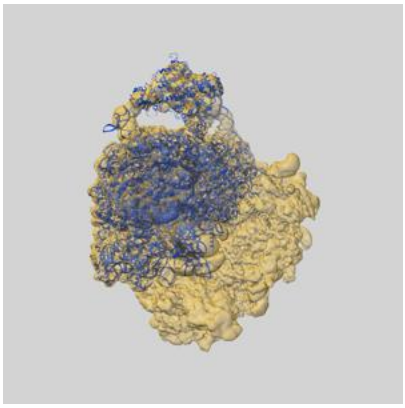
9.1 Map-model overlay



X



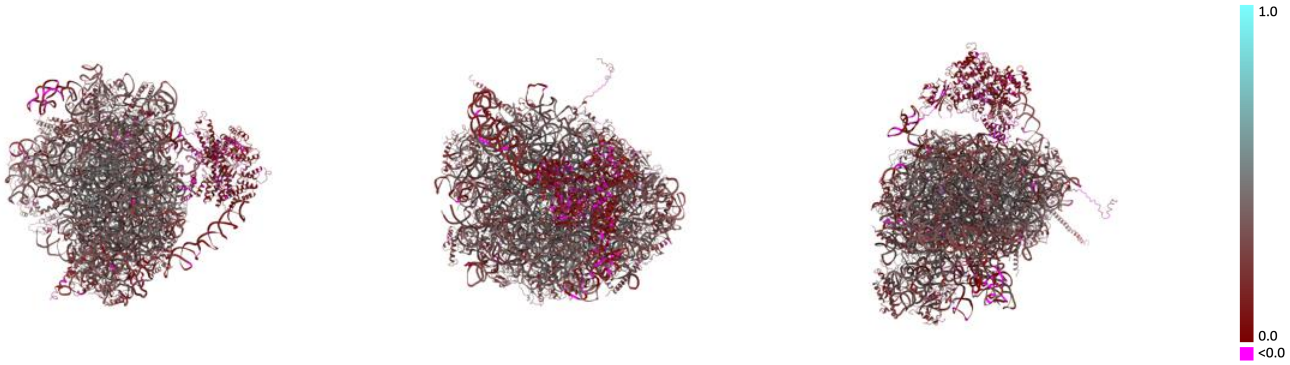
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

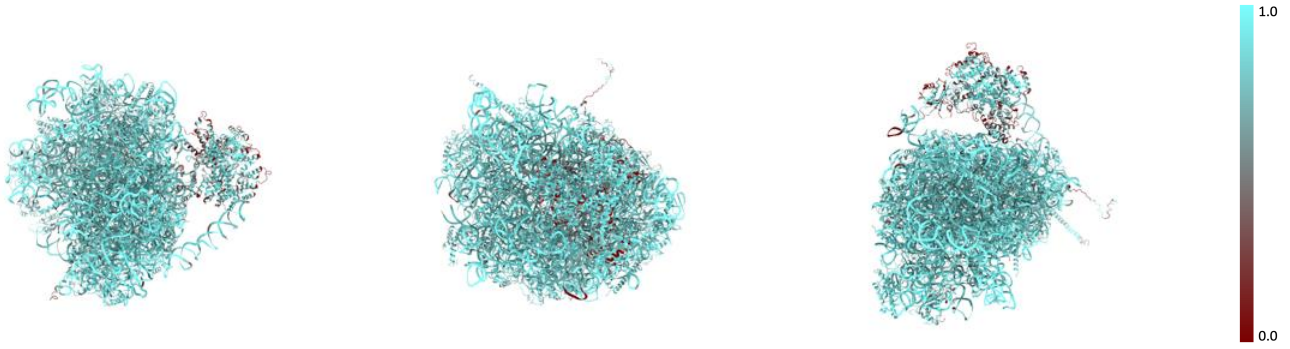
9.2 Q-score mapped to coordinate model



X Y Z

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

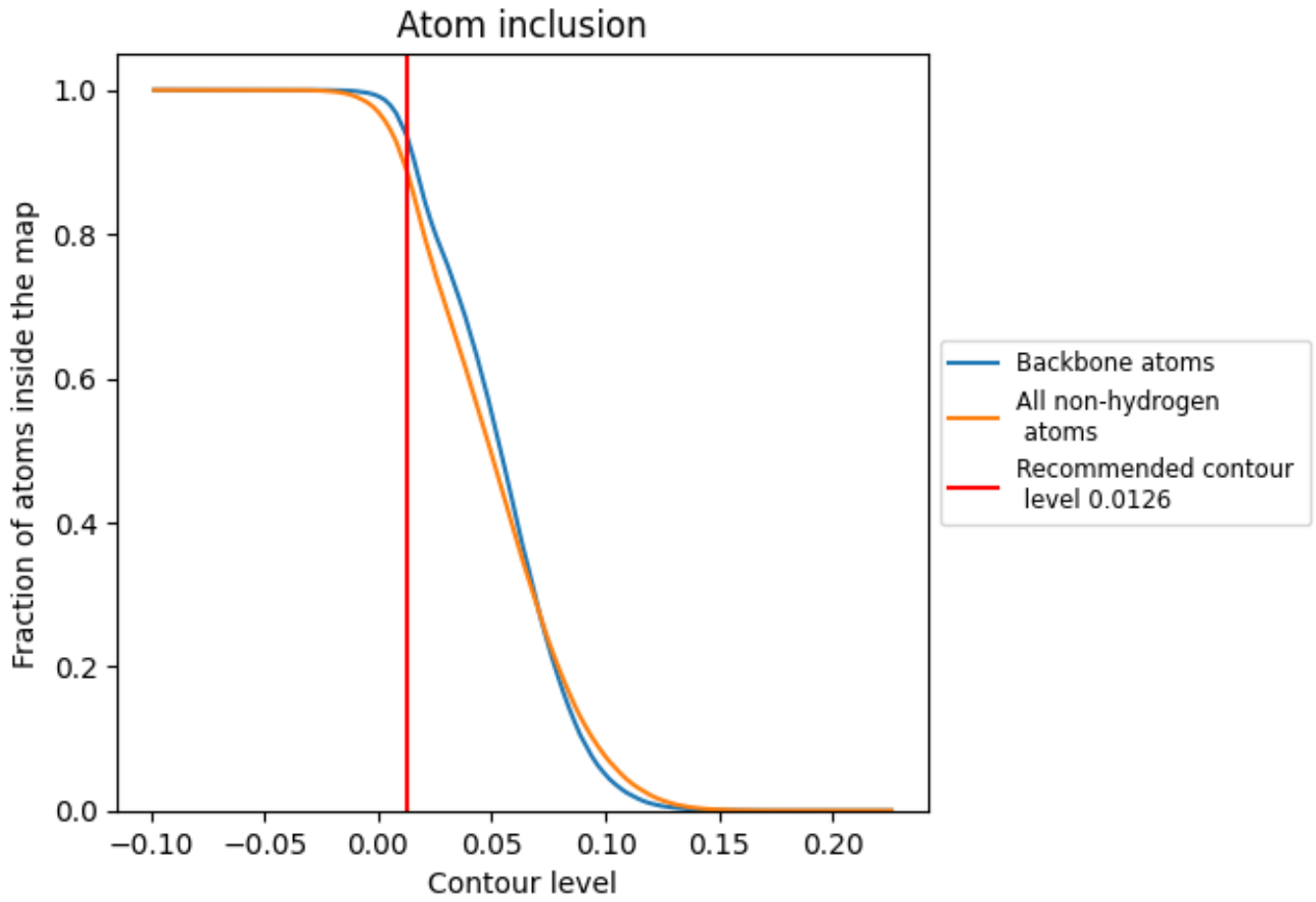
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0126).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8893	0.3130
1	0.9465	0.3410
3	0.9783	0.3350
4	0.9553	0.3470
A	0.8982	0.2670
B	0.9082	0.2840
C	0.8080	0.3230
D	0.7653	0.2980
E	0.8350	0.3650
F	0.8619	0.3470
G	0.8768	0.3590
H	0.8638	0.2830
I	0.8763	0.3290
J	0.8410	0.3080
K	0.8222	0.2400
L	0.8336	0.2840
M	0.8502	0.2560
N	0.8554	0.3140
O	0.8372	0.2750
P	0.8589	0.3640
Q	0.8415	0.3250
R	0.8001	0.3020
S	0.8466	0.3320
T	0.8245	0.3130
U	0.8338	0.2950
V	0.8347	0.3330
W	0.8708	0.2920
X	0.7926	0.3480
Y	0.7277	0.2570
Z	0.8429	0.3230
a	0.8851	0.3200
b	0.8469	0.2930
c	0.8669	0.3750
d	0.8473	0.3430
e	0.8153	0.2950

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Chain	Atom inclusion	Q-score
f	0.8388	0.3630
g	0.8370	0.3670
h	0.8648	0.3850
i	0.8331	0.3340
j	0.8314	0.2740
k	0.8188	0.2540
l	0.8611	0.3800
m	0.8631	0.2910
n	0.8843	0.3980
o	0.8164	0.3010
p	0.8255	0.3120
r	0.7676	0.2730
s	0.8058	0.2660
t	0.6982	0.0900
u	0.6765	0.0820
v	0.5224	0.0780
z	0.4870	0.1540