



## wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 02:58 AM EST

PDB ID : 6AZ1  
EMDB ID : EMD-7024  
Title : Cryo-EM structure of the small subunit of Leishmania ribosome bound to paromomycin  
Authors : Shalev-Benami, M.; Zhang, Y.; Rozenberg, H.; Matzov, D.; Zimmerman, E.; Bashan, A.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.  
Deposited on : 2017-09-09  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

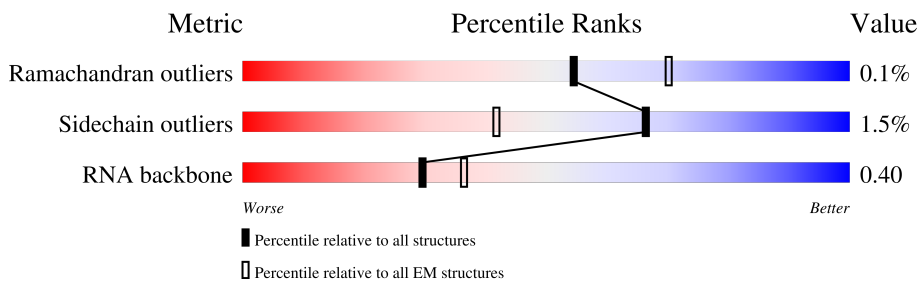
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	
2	B	246	
3	C	219	
4	D	190	
5	E	273	
6	F	265	
7	G	249	
8	H	190	

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Mol	Chain	Length	Quality of chain
9	I	200	98%
10	J	130	99%
11	K	220	83% 17%
12	L	149	94%
13	M	116	12% 88% 12%
14	N	153	7% 59% 41%
15	O	144	6% 92% 5%
16	P	143	92% 7%
17	Q	141	72% 79% 18%
18	R	153	6% 92% 7%
19	S	57	88% 7% 5%
20	T	151	93% 6%
21	U	173	6% 88% 10%
22	V	143	9% 84% 15%
23	W	152	9% 72% 28%
24	X	179	84% 15%
25	Y	159	53% 45%
26	Z	137	92% 7%
27	a	120	6% 60% 40%
28	b	112	88% 8%
29	c	86	93%
30	d	87	10% 72% 25%
31	e	66	9% 88% 11%
32	f	152	30% 34% 5% 61%
33	g	312	22% 94%

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Mol	Chain	Length	Quality of chain
34	1	2203	
35	2	76	
36	3	77	
37	4	76	
38	5	13	

## 2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 80594 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 Ribosomal protein s1e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	225	1829	1147	350	320	12	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	SER	GLY	conflict	UNP E9BRS2

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	211	1676	1066	306	292	12	2	0

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	212	1668	1059	307	289	13	5	0

- Molecule 4 is a protein called ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	182	1504	948	304	244	8	1	0

- Molecule 5 is a protein called ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	260	2029	1292	395	333	9	2	0

- Molecule 6 is a protein called ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	220	1656	1062	298	286	10	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	4	THR	ALA	conflict	UNP E9BNF0
F	8	GLN	-	insertion	UNP E9BNF0
F	10	ALA	ASN	conflict	UNP E9BNF0
F	12	ALA	GLY	conflict	UNP E9BNF0
F	13	ALA	VAL	conflict	UNP E9BNF0
F	14	ASP	GLU	conflict	UNP E9BNF0
F	15	VAL	ALA	conflict	UNP E9BNF0

- Molecule 7 is a protein called ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	238	1796	1123	366	304	3	1	0

- Molecule 8 is a protein called ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	184	1438	893	283	255	7	1	0

- Molecule 9 is a protein called ribosomal protein S7e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	200	1613	1033	303	270	7	0	0

- Molecule 10 is a protein called ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	129	1014	643	188	175	8	0	0

- Molecule 11 is a protein called ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	183	1403	885	294	222	2	0	0

- Molecule 12 is a protein called ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	143	1127	724	209	191	3	0	0

- Molecule 13 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	102	809	505	149	153	2	1	0

- Molecule 14 is a protein called ribosomal protein S10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	91	728	473	127	123	5	1	0

- Molecule 15 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	137	1032	637	205	183	7	2	0

- Molecule 16 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	142	1134	716	229	186	3	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	18	ARG	CYS	conflict	UNP E9BFB6
P	34	ALA	SER	conflict	UNP E9BFB6
P	36	LYS	ARG	conflict	UNP E9BFB6
P	127	SER	ASN	conflict	UNP E9BFB6

- Molecule 17 is a protein called ribosomal protein S12e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	115	Total	C	N	O	S	0	0
			746	462	130	149	5		

- Molecule 18 is a protein called ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	142	Total	C	N	O	S	0	0
			1080	680	210	186	4		

- Molecule 19 is a protein called ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	54	Total	C	N	O	S	0	0
			441	272	90	73	6		

- Molecule 20 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	142	Total	C	N	O	S	0	0
			1153	727	228	190	8		

- Molecule 21 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	156	Total	C	N	O	S	0	0
			1241	786	249	201	5		

- Molecule 22 is a protein called ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	122	Total	C	N	O	S	1	0
			935	587	187	156	5		

- Molecule 23 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	110	Total	C	N	O	S	0	0
			822	530	158	130	4		

- Molecule 24 is a protein called ribosomal protein S19e.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	152	1202	765	235	198	4	1	0

- Molecule 25 is a protein called ribosomal protein S21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	88	664	409	122	129	4	0	0

- Molecule 26 is a protein called ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	127	1032	664	199	166	3	1	0

- Molecule 27 is a protein called ribosomal protein S25e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	72	544	348	94	99	3	0	0

- Molecule 28 is a protein called ribosomal protein S26e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	b	103	796	496	164	129	7	0	0

- Molecule 29 is a protein called ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	84	656	407	128	113	8	0	0

- Molecule 30 is a protein called ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	d	65	466	286	94	82	4	0	0

- Molecule 31 is a protein called ribosomal protein S30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	59	Total	C	N	O	S	0	0
			449	280	97	71	1		

- Molecule 32 is a protein called ribosomal protein S31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	60	Total	C	N	O	S	0	0
			385	242	71	69	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	5	ILE	VAL	conflict	UNP E9BTC5

- Molecule 33 is a protein called LACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	300	Total	C	N	O	S	1	0
			2240	1410	395	423	12		

- Molecule 34 is a RNA chain called ribosomal RNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	1760	Total	C	N	O	P	0	0
			37613	16832	6780	12242	1759		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1539	M1Y	U	conflict	GB 322500086
1	1543	C4J	U	conflict	GB 322500086

- Molecule 35 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace	
35	2	76	Total	C	N	O	P	S	0	0
			1626	729	290	531	75	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1	G	-	expression tag	GB 1229082179

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Chain	Residue	Modelled	Actual	Comment	Reference
2	2	C	-	expression tag	GB 1229082179
2	3	G	-	expression tag	GB 1229082179
2	70	C	G	conflict	GB 1229082179

- Molecule 36 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
36	3	77	1639	732	297	534	76	0	0

- Molecule 37 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	4	76	1619	723	290	531	75	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	G	-	expression tag	GB 1229082179
4	2	C	-	expression tag	GB 1229082179
4	3	G	-	expression tag	GB 1229082179
4	70	C	G	conflict	GB 1229082179

- Molecule 38 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	5	12	251	113	43	83	12	0	0

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

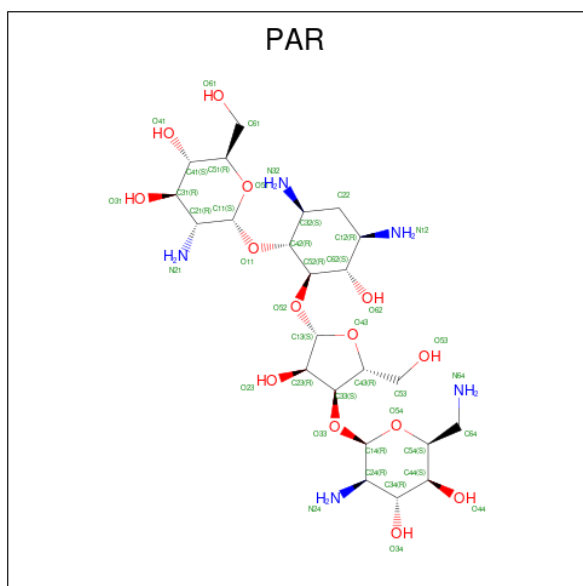
Mol	Chain	Residues	Atoms		AltConf
39	C	1	Total 1	Mg 1	0
39	D	1	Total 1	Mg 1	0
39	S	1	Total 1	Mg 1	0
39	1	20	Total 20	Mg 20	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
39	5	1	1	1	0

- Molecule 40 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
40	1	1	252	138	30	84	0
40	1	1	252	138	30	84	0
40	1	1	252	138	30	84	0
40	1	1	252	138	30	84	0
40	1	1	252	138	30	84	0
40	1	1	252	138	30	84	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
41	D	2	2	2	0
41	E	1	1	1	0

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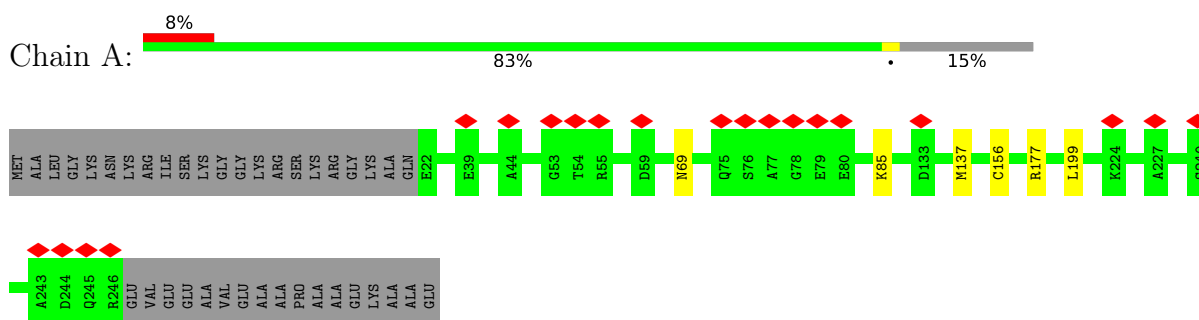
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Mol	Chain	Residues	Atoms		AltConf
41	F	3	Total 3	O 3	0
41	G	1	Total 1	O 1	0
41	H	1	Total 1	O 1	0
41	K	1	Total 1	O 1	0
41	L	1	Total 1	O 1	0
41	M	3	Total 3	O 3	0
41	O	1	Total 1	O 1	0
41	P	6	Total 6	O 6	0
41	R	2	Total 2	O 2	0
41	S	1	Total 1	O 1	0
41	T	4	Total 4	O 4	0
41	X	4	Total 4	O 4	0
41	Y	1	Total 1	O 1	0
41	Z	1	Total 1	O 1	0
41	b	1	Total 1	O 1	0
41	c	2	Total 2	O 2	0
41	f	1	Total 1	O 1	0
41	1	217	Total 217	O 217	0
41	2	2	Total 2	O 2	0
41	3	3	Total 3	O 3	0
41	5	3	Total 3	O 3	0

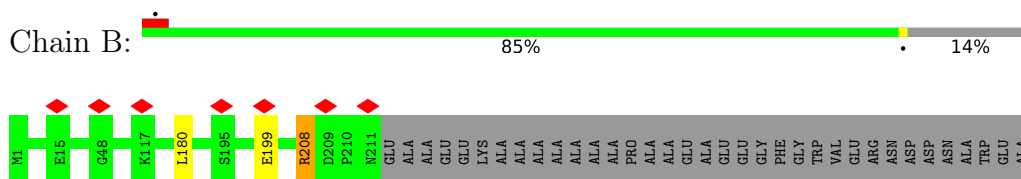
### 3 Residue-property plots [i](#)

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.

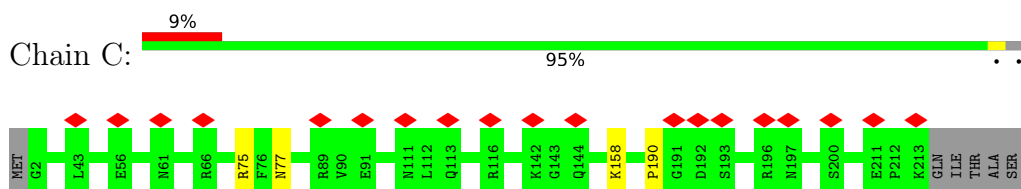
- Molecule 1: Ribosomal protein s1e



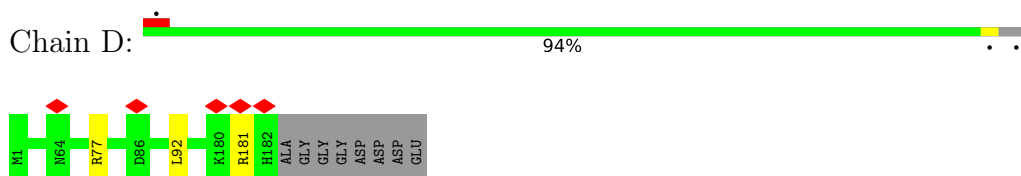
- Molecule 2: ribosomal protein S2



- Molecule 3: ribosomal protein S3

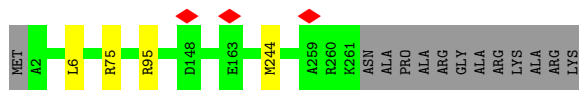


- Molecule 4: ribosomal protein S4



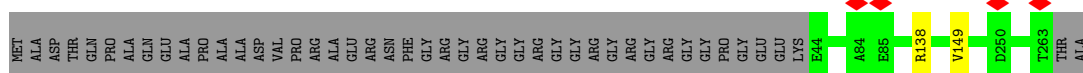
- Molecule 5: ribosomal protein S4e





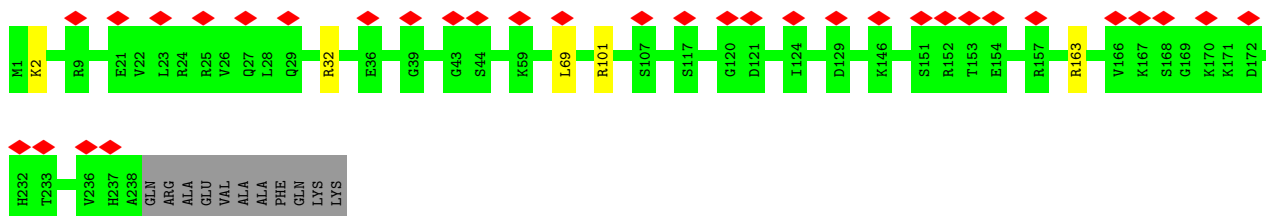
- Molecule 6: ribosomal protein S5

Chain F: 82% 17%



- Molecule 7: ribosomal protein S6e

Chain G: 13% 94%



- Molecule 8: ribosomal protein S7

Chain H: 95%



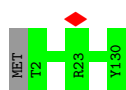
- Molecule 9: ribosomal protein S7e

Chain I: 98%



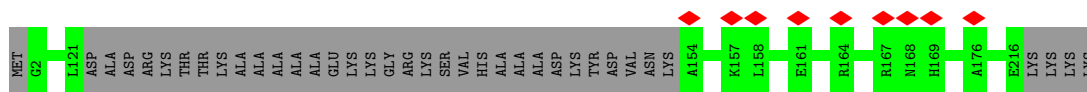
- Molecule 10: ribosomal protein S8

Chain J: 99%

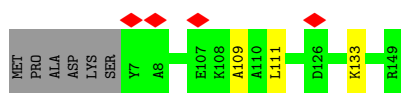


- Molecule 11: ribosomal protein S8e

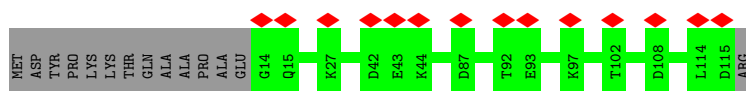
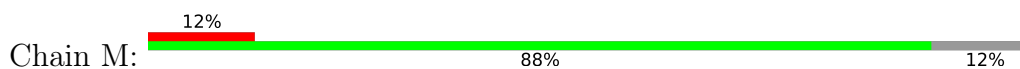
Chain K: 83% 17%



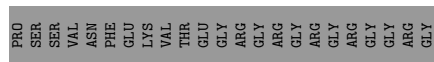
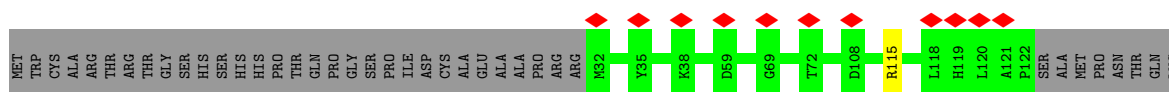
• Molecule 12: ribosomal protein S9



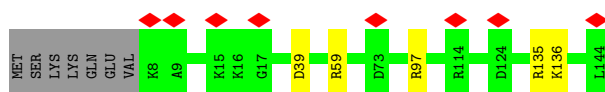
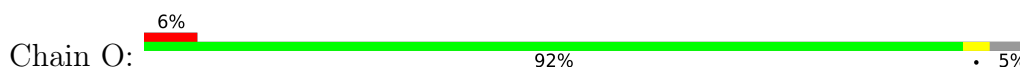
• Molecule 13: ribosomal protein S10



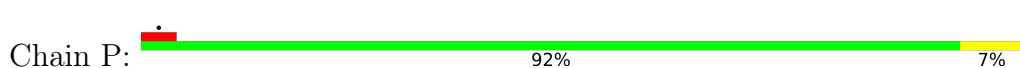
• Molecule 14: ribosomal protein S10e



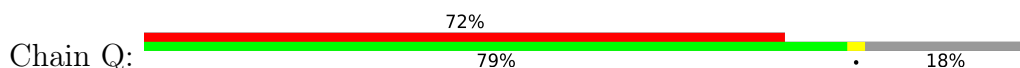
• Molecule 15: ribosomal protein S11



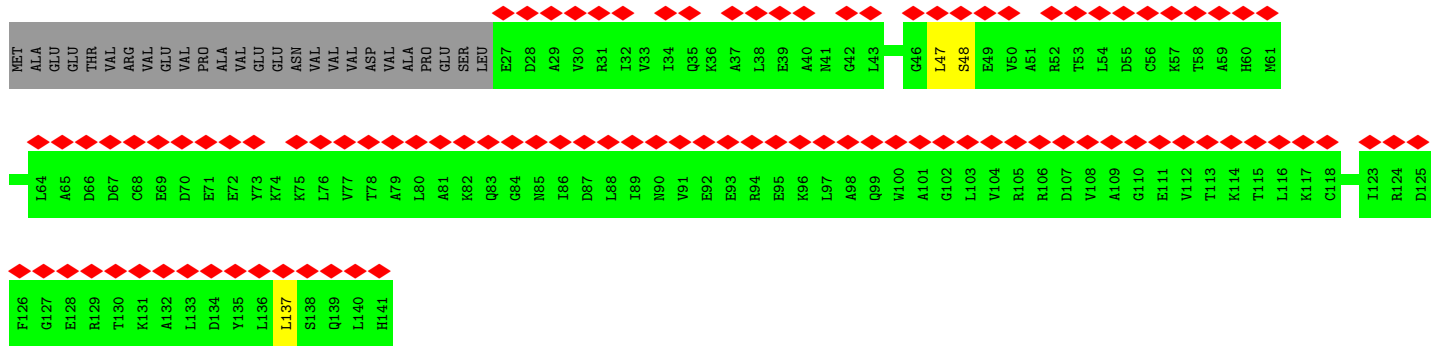
• Molecule 16: ribosomal protein S12



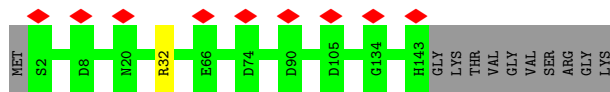
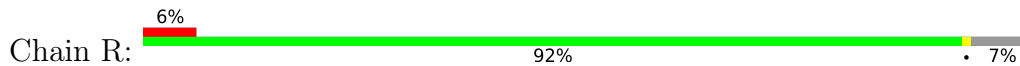
• Molecule 17: ribosomal protein S12e



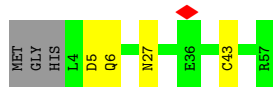
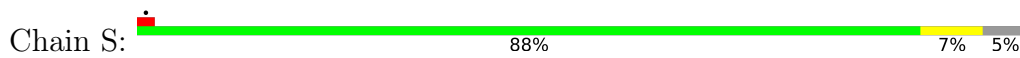




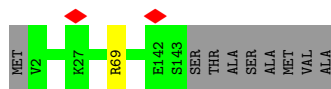
- Molecule 18: ribosomal protein S13



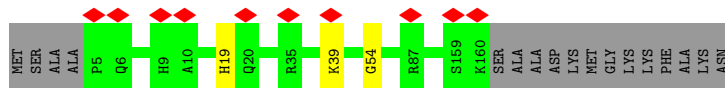
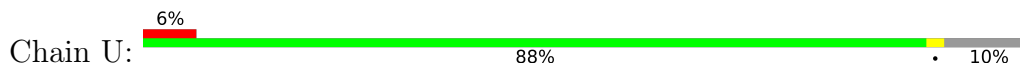
- Molecule 19: ribosomal protein S14



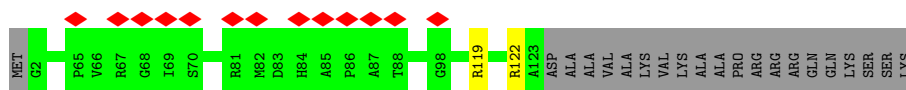
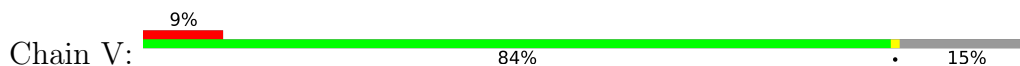
- Molecule 20: ribosomal protein S15



- Molecule 21: ribosomal protein S17

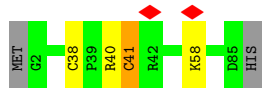
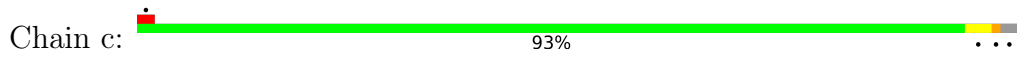


- Molecule 22: ribosomal protein S17e

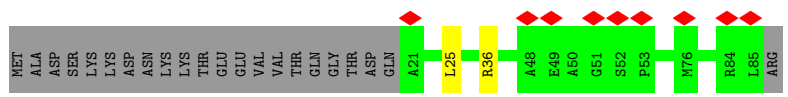
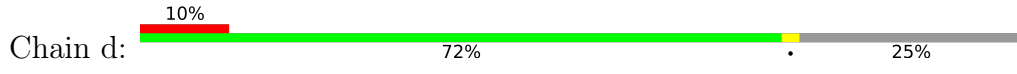


- Molecule 23: ribosomal protein S19

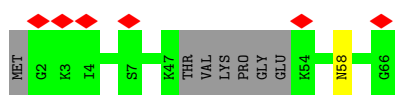
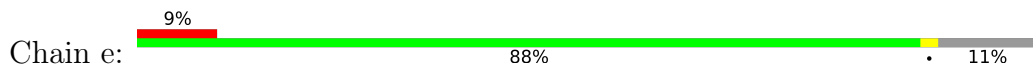




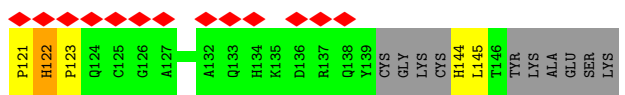
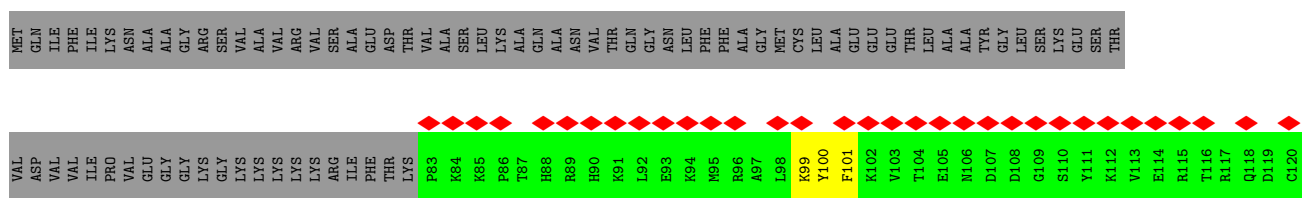
• Molecule 30: ribosomal protein S28e



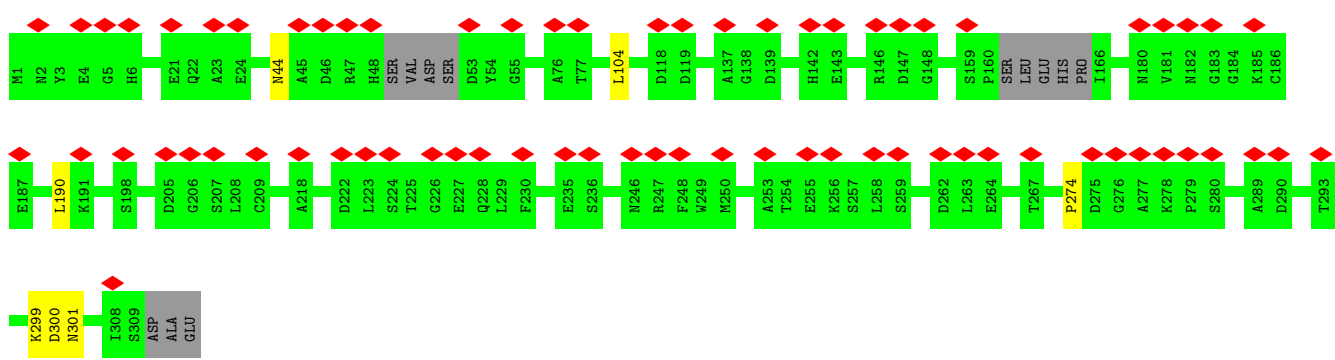
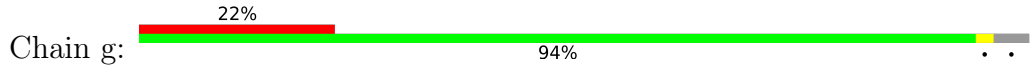
• Molecule 31: ribosomal protein S30e



• Molecule 32: ribosomal protein S31e

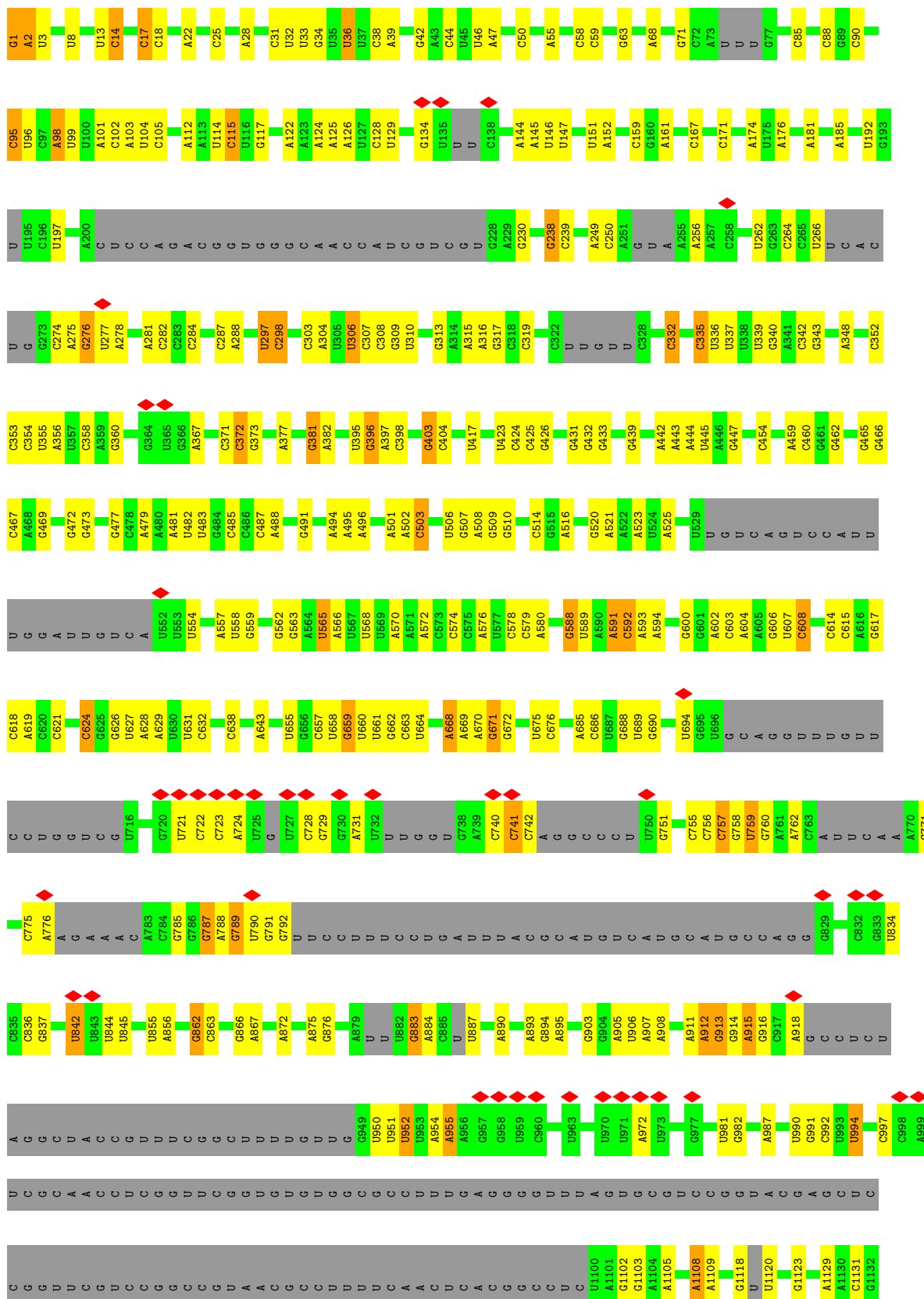


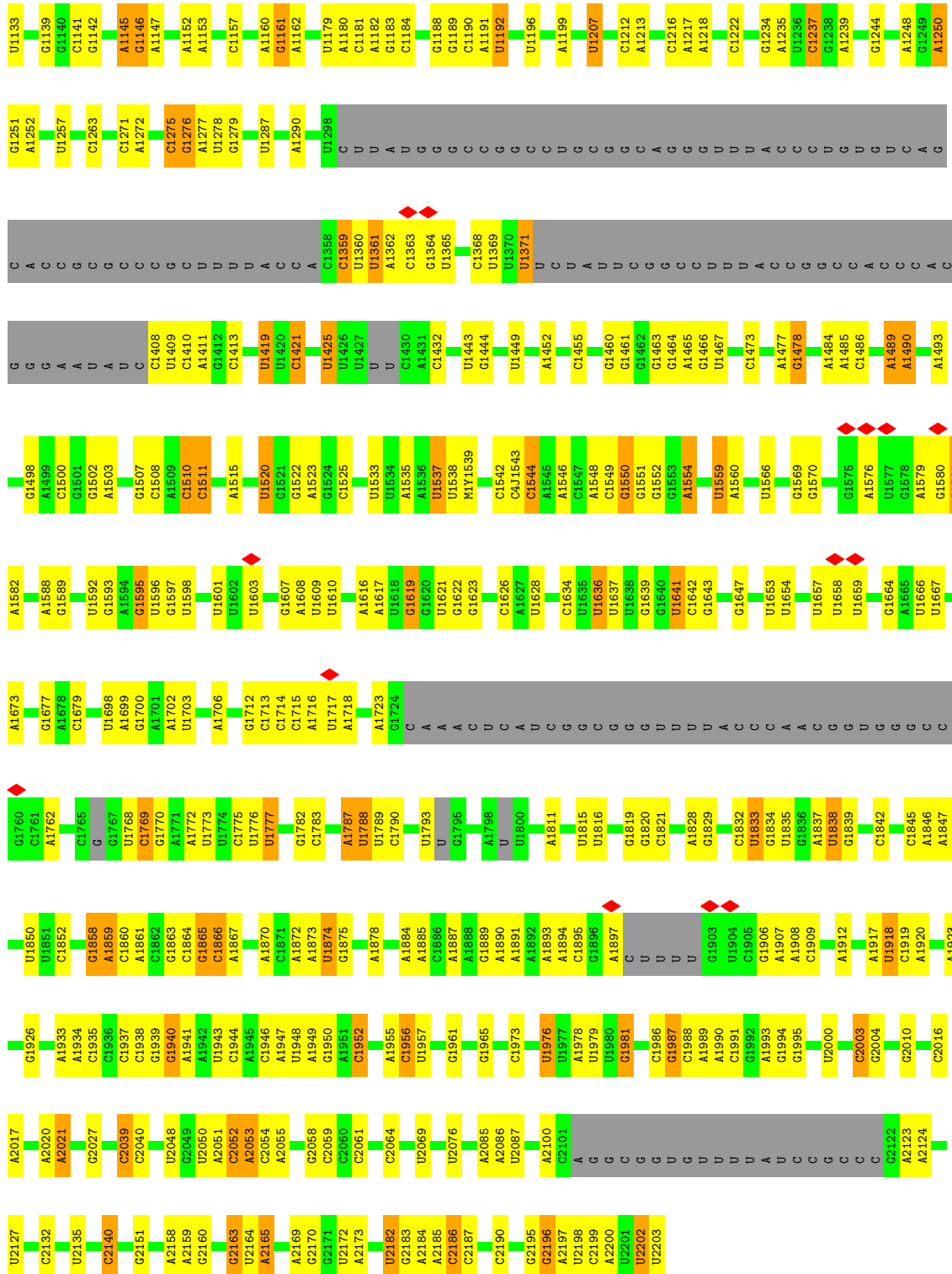
• Molecule 33: LACK1



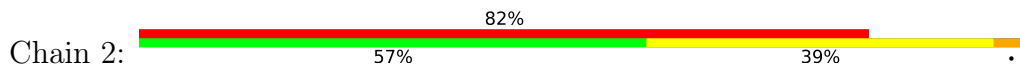
• Molecule 34: ribosomal RNA 18S

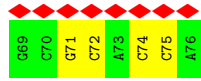
Chain 1:



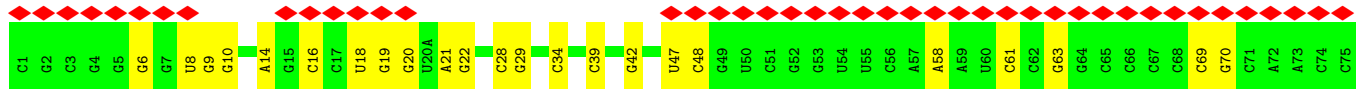


• Molecule 35: tRNA-Phe

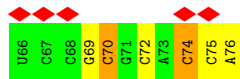
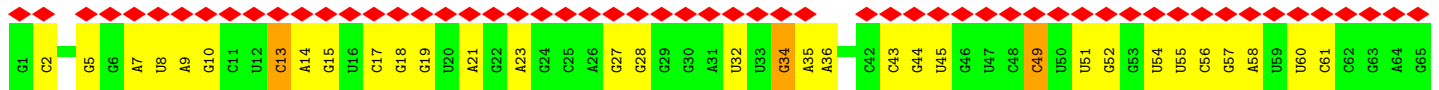
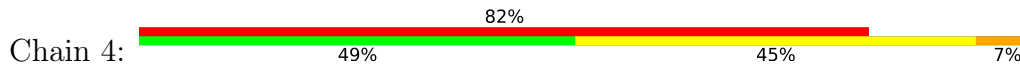




• Molecule 36: P-site tRNA



• Molecule 37: E-site tRNA



• Molecule 38: mRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141028	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.395	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	391.68, 391.68, 391.68	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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: MA6, 4OC, OMG, OMC, MG, PAR, M1Y, A2M, 5MC, 7MG, OMU, C4J, MIA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.52	0/1860	0.69	2/2503 (0.1%)
2	B	0.53	0/1713	0.64	1/2316 (0.0%)
3	C	0.46	0/1700	0.64	0/2274
4	D	0.48	0/1533	0.62	1/2057 (0.0%)
5	E	0.50	0/2074	0.70	1/2797 (0.0%)
6	F	0.51	0/1692	0.62	0/2295
7	G	0.41	0/1823	0.65	2/2449 (0.1%)
8	H	0.47	0/1460	0.68	1/1959 (0.1%)
9	I	0.58	0/1644	0.68	1/2217 (0.0%)
10	J	0.64	0/1031	0.64	0/1382
11	K	0.55	0/1425	0.68	0/1916
12	L	0.53	0/1148	0.68	1/1543 (0.1%)
13	M	0.41	0/819	0.69	0/1109
14	N	0.48	0/753	0.62	0/1024
15	O	0.57	0/1047	0.67	1/1408 (0.1%)
16	P	0.51	0/1163	0.75	4/1554 (0.3%)
17	Q	0.30	0/749	0.81	3/1028 (0.3%)
18	R	0.44	0/1099	0.65	0/1489
19	S	0.49	0/446	0.73	0/591
20	T	0.60	0/1176	0.73	0/1577
21	U	0.60	0/1270	0.66	0/1710
22	V	0.40	0/945	0.60	0/1267
23	W	0.40	0/841	0.56	0/1144
24	X	0.51	0/1236	0.67	0/1659
25	Y	0.52	0/674	0.64	0/914
26	Z	0.47	0/1056	0.67	0/1407
27	a	0.45	0/549	0.66	0/743
28	b	0.68	1/813 (0.1%)	0.80	1/1092 (0.1%)
29	c	0.65	0/669	0.72	1/897 (0.1%)
30	d	0.41	0/468	0.76	1/630 (0.2%)
31	e	0.45	0/456	0.57	0/603
32	f	0.29	0/393	0.68	1/540 (0.2%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	g	0.44	0/2294	0.72	3/3131 (0.1%)
34	1	1.06	0/41155	1.23	426/64074 (0.7%)
35	2	0.46	0/1783	0.98	6/2776 (0.2%)
36	3	0.59	0/1831	1.04	8/2853 (0.3%)
37	4	0.43	1/1809 (0.1%)	1.16	22/2819 (0.8%)
38	5	1.00	0/279	1.29	3/431 (0.7%)
All	All	0.82	2/84876 (0.0%)	1.02	490/124178 (0.4%)

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
2	B	0	2
12	L	0	1
15	O	0	1
16	P	0	3
17	Q	0	1
19	S	0	2
21	U	0	2
26	Z	0	1
29	c	0	2
32	f	0	4
33	g	0	1
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	78	CYS	CB-SG	6.89	1.94	1.82
37	4	75	C	C1'-N1	5.14	1.56	1.48

The worst 5 of 490 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	78	CYS	CA-CB-SG	13.35	138.02	114.00
34	1	1956	C	N1-C2-O2	13.04	126.72	118.90
34	1	1973	C	N1-C2-O2	11.17	125.60	118.90
34	1	1956	C	N3-C2-O2	-10.96	114.23	121.90
34	1	1510	C	C2-N1-C1'	10.23	130.05	118.80

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	208[A]	ARG	Peptide
2	B	208[B]	ARG	Peptide
12	L	109	ALA	Peptide
15	O	97	ARG	Peptide
16	P	86	PRO	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	A	226/264 (86%)	209 (92%)	17 (8%)	0	100	100
2	B	211/246 (86%)	200 (95%)	11 (5%)	0	100	100
3	C	215/219 (98%)	206 (96%)	8 (4%)	1 (0%)	29	54
4	D	181/190 (95%)	176 (97%)	5 (3%)	0	100	100
5	E	260/273 (95%)	246 (95%)	14 (5%)	0	100	100
6	F	218/265 (82%)	206 (94%)	12 (6%)	0	100	100
7	G	237/249 (95%)	222 (94%)	15 (6%)	0	100	100
8	H	181/190 (95%)	173 (96%)	8 (4%)	0	100	100
9	I	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
10	J	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
11	K	179/220 (81%)	170 (95%)	9 (5%)	0	100	100
12	L	141/149 (95%)	127 (90%)	14 (10%)	0	100	100
13	M	101/116 (87%)	94 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	90/153 (59%)	85 (94%)	5 (6%)	0	100	100
15	O	137/144 (95%)	128 (93%)	9 (7%)	0	100	100
16	P	143/143 (100%)	134 (94%)	8 (6%)	1 (1%)	22	46
17	Q	113/141 (80%)	107 (95%)	6 (5%)	0	100	100
18	R	140/153 (92%)	131 (94%)	9 (6%)	0	100	100
19	S	52/57 (91%)	50 (96%)	2 (4%)	0	100	100
20	T	140/151 (93%)	132 (94%)	8 (6%)	0	100	100
21	U	154/173 (89%)	141 (92%)	13 (8%)	0	100	100
22	V	121/143 (85%)	115 (95%)	6 (5%)	0	100	100
23	W	106/152 (70%)	100 (94%)	6 (6%)	0	100	100
24	X	151/179 (84%)	141 (93%)	10 (7%)	0	100	100
25	Y	86/159 (54%)	85 (99%)	1 (1%)	0	100	100
26	Z	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
27	a	70/120 (58%)	68 (97%)	2 (3%)	0	100	100
28	b	101/112 (90%)	96 (95%)	5 (5%)	0	100	100
29	c	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
30	d	63/87 (72%)	61 (97%)	2 (3%)	0	100	100
31	e	55/66 (83%)	52 (94%)	3 (6%)	0	100	100
32	f	56/152 (37%)	40 (71%)	14 (25%)	2 (4%)	3	7
33	g	295/312 (95%)	264 (90%)	30 (10%)	1 (0%)	41	66
All	All	4756/5531 (86%)	4466 (94%)	285 (6%)	5 (0%)	54	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	87	ASN
32	f	123	PRO
32	f	122	HIS
3	C	190	PRO
33	g	274	PRO

### 5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/223 (88%)	191 (97%)	6 (3%)	41	70
2	B	180/202 (89%)	176 (98%)	4 (2%)	52	79
3	C	176/184 (96%)	172 (98%)	4 (2%)	50	78
4	D	158/164 (96%)	156 (99%)	2 (1%)	69	87
5	E	207/225 (92%)	203 (98%)	4 (2%)	57	82
6	F	170/208 (82%)	168 (99%)	2 (1%)	71	88
7	G	171/208 (82%)	166 (97%)	5 (3%)	42	71
8	H	149/159 (94%)	146 (98%)	3 (2%)	55	81
9	I	173/187 (92%)	170 (98%)	3 (2%)	60	84
10	J	108/111 (97%)	108 (100%)	0	100	100
11	K	130/176 (74%)	130 (100%)	0	100	100
12	L	113/120 (94%)	112 (99%)	1 (1%)	78	92
13	M	93/104 (89%)	93 (100%)	0	100	100
14	N	72/129 (56%)	70 (97%)	2 (3%)	43	73
15	O	103/113 (91%)	98 (95%)	5 (5%)	25	52
16	P	117/116 (101%)	113 (97%)	4 (3%)	37	66
17	Q	60/119 (50%)	60 (100%)	0	100	100
18	R	106/130 (82%)	105 (99%)	1 (1%)	78	92
19	S	47/49 (96%)	45 (96%)	2 (4%)	29	57
20	T	124/132 (94%)	123 (99%)	1 (1%)	81	93
21	U	128/150 (85%)	127 (99%)	1 (1%)	81	93
22	V	91/124 (73%)	88 (97%)	3 (3%)	38	67
23	W	78/131 (60%)	78 (100%)	0	100	100
24	X	122/147 (83%)	120 (98%)	2 (2%)	62	85
25	Y	72/117 (62%)	68 (94%)	4 (6%)	21	45
26	Z	109/118 (92%)	109 (100%)	0	100	100
27	a	58/95 (61%)	58 (100%)	0	100	100
28	b	81/93 (87%)	78 (96%)	3 (4%)	34	63
29	c	72/76 (95%)	70 (97%)	2 (3%)	43	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	d	46/75 (61%)	45 (98%)	1 (2%)	52 79
31	e	43/54 (80%)	42 (98%)	1 (2%)	50 78
32	f	26/126 (21%)	24 (92%)	2 (8%)	13 30
33	g	232/266 (87%)	229 (99%)	3 (1%)	69 87
All	All	3812/4631 (82%)	3741 (98%)	71 (2%)	66 82

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Y	78	ILE
28	b	28	CYS
31	e	58	ASN
7	G	32	ARG
7	G	2[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	82	GLN
33	g	59	HIS
21	U	24	GLN
33	g	44	ASN
30	d	41	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	1	1725/2203 (78%)	551 (31%)	35 (2%)
35	2	74/76 (97%)	29 (39%)	2 (2%)
36	3	76/77 (98%)	20 (26%)	0
37	4	75/76 (98%)	34 (45%)	2 (2%)
38	5	11/13 (84%)	2 (18%)	0
All	All	1961/2445 (80%)	636 (32%)	39 (1%)

5 of 636 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	1	2	A

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Mol	Chain	Res	Type
34	1	3	U
34	1	14	C
34	1	17	C
34	1	22	A

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	1	1636	U
35	2	13	C
34	1	1787	A
34	1	2053	A
37	4	13	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	OMG	1	1623	34	18,26,27	1.26	2 (11%)	19,38,41	1.59	4 (21%)
34	4OC	1	2059	34	20,23,24	0.55	0	26,32,35	1.01	1 (3%)
34	OMG	1	1865	34	18,26,27	1.34	2 (11%)	19,38,41	1.64	6 (31%)
34	OMC	1	2140	34	19,22,23	1.03	1 (5%)	26,31,34	1.11	3 (11%)
34	OMG	1	1647	34	18,26,27	1.35	2 (11%)	19,38,41	1.66	6 (31%)
34	OMC	1	38	34	19,22,23	0.96	0	26,31,34	1.14	3 (11%)
34	A2M	1	28	34	18,25,26	1.71	3 (16%)	18,36,39	1.14	0
34	OMU	1	1833	34	19,22,23	0.82	1 (5%)	26,31,34	1.21	3 (11%)
34	OMU	1	2048	34	19,22,23	0.60	0	26,31,34	0.95	1 (3%)
34	A2M	1	98	34	18,25,26	1.64	2 (11%)	18,36,39	1.21	2 (11%)
34	OMG	1	1478	34	18,26,27	1.26	2 (11%)	19,38,41	1.59	5 (26%)
34	C4J	1	1543	34	24,29,30	1.73	6 (25%)	29,42,45	1.25	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	OMG	1	509	34	18,26,27	1.15	1 (5%)	19,38,41	1.25	3 (15%)
34	OMU	1	1777	34	19,22,23	0.75	0	26,31,34	0.94	1 (3%)
34	OMC	1	18	34	19,22,23	0.88	0	26,31,34	1.11	2 (7%)
34	OMC	1	115	34	19,22,23	1.03	1 (5%)	26,31,34	1.09	3 (11%)
34	OMU	1	1621	34	19,22,23	0.64	0	26,31,34	1.27	2 (7%)
34	OMG	1	1829	34	18,26,27	1.36	2 (11%)	19,38,41	1.49	3 (15%)
34	A2M	1	668	34	18,25,26	2.06	4 (22%)	18,36,39	1.09	1 (5%)
34	A2M	1	912	34	18,25,26	0.88	1 (5%)	18,36,39	1.31	2 (11%)
34	OMG	1	1550	34	18,26,27	0.99	1 (5%)	19,38,41	1.20	3 (15%)
34	OMU	1	1979	34	19,22,23	0.57	0	26,31,34	0.87	1 (3%)
34	MA6	1	2184	34	19,26,27	1.11	2 (10%)	18,38,41	2.63	2 (11%)
34	OMU	1	661	34	19,22,23	0.78	0	26,31,34	0.96	2 (7%)
34	OMG	1	2151	34	18,26,27	1.27	2 (11%)	19,38,41	1.57	4 (21%)
34	A2M	1	479	34	18,25,26	1.75	2 (11%)	18,36,39	1.07	1 (5%)
34	5MC	1	1544	34	18,22,23	1.60	5 (27%)	26,32,35	1.26	3 (11%)
34	7MG	1	1995	36,34	22,26,27	1.48	2 (9%)	29,39,42	1.36	5 (17%)
34	OMU	1	33	34	19,22,23	0.56	0	26,31,34	1.02	2 (7%)
35	MIA	2	37	35	24,31,32	1.87	3 (12%)	26,44,47	2.61	8 (30%)
34	M1Y	1	1539	34	19,22,23	1.20	3 (15%)	22,32,35	1.94	3 (13%)
34	OMC	1	1866	34	19,22,23	1.26	2 (10%)	26,31,34	1.29	3 (11%)
34	A2M	1	2021	34	18,25,26	1.72	2 (11%)	18,36,39	1.26	3 (16%)
34	MA6	1	2185	34	19,26,27	1.08	1 (5%)	18,38,41	3.06	2 (11%)
34	5MC	1	2061	34	18,22,23	1.51	4 (22%)	26,32,35	1.29	5 (19%)
34	OMG	1	1464	34	18,26,27	1.28	2 (11%)	19,38,41	1.76	6 (31%)
34	OMU	1	8	34	19,22,23	0.89	0	26,31,34	1.09	2 (7%)

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
34	OMG	1	1623	34	-	0/5/27/28	0/3/3/3
34	4OC	1	2059	34	-	2/9/29/30	0/2/2/2
34	OMG	1	1865	34	-	2/5/27/28	0/3/3/3
34	OMC	1	2140	34	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	OMG	1	1647	34	-	0/5/27/28	0/3/3/3
34	OMC	1	38	34	-	0/9/27/28	0/2/2/2
34	A2M	1	28	34	-	0/5/27/28	0/3/3/3
34	OMU	1	1833	34	-	5/9/27/28	0/2/2/2
34	OMU	1	2048	34	-	0/9/27/28	0/2/2/2
34	A2M	1	98	34	-	2/5/27/28	0/3/3/3
34	OMG	1	1478	34	-	3/5/27/28	0/3/3/3
34	C4J	1	1543	34	-	1/16/34/35	0/2/2/2
34	OMG	1	509	34	-	0/5/27/28	0/3/3/3
34	OMU	1	1777	34	-	2/9/27/28	0/2/2/2
34	OMC	1	18	34	-	0/9/27/28	0/2/2/2
34	OMC	1	115	34	-	2/9/27/28	0/2/2/2
34	OMU	1	1621	34	-	2/9/27/28	0/2/2/2
34	OMG	1	1829	34	-	0/5/27/28	0/3/3/3
34	A2M	1	668	34	-	2/5/27/28	0/3/3/3
34	A2M	1	912	34	-	2/5/27/28	0/3/3/3
34	OMG	1	1550	34	-	2/5/27/28	0/3/3/3
34	OMU	1	1979	34	-	1/9/27/28	0/2/2/2
34	MA6	1	2184	34	-	3/7/29/30	0/3/3/3
34	OMU	1	661	34	-	0/9/27/28	0/2/2/2
34	OMG	1	2151	34	-	0/5/27/28	0/3/3/3
34	A2M	1	479	34	-	0/5/27/28	0/3/3/3
34	5MC	1	1544	34	-	0/7/25/26	0/2/2/2
34	7MG	1	1995	36,34	-	2/7/37/38	0/3/3/3
34	OMU	1	33	34	-	0/9/27/28	0/2/2/2
35	MIA	2	37	35	-	5/11/33/34	0/3/3/3
34	M1Y	1	1539	34	-	2/7/25/26	0/2/2/2
34	OMC	1	1866	34	-	2/9/27/28	0/2/2/2
34	A2M	1	2021	34	-	0/5/27/28	0/3/3/3
34	MA6	1	2185	34	-	3/7/29/30	0/3/3/3
34	5MC	1	2061	34	-	0/7/25/26	0/2/2/2
34	OMG	1	1464	34	-	1/5/27/28	0/3/3/3
34	OMU	1	8	34	-	5/9/27/28	0/2/2/2

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	2	37	MIA	C13-C14	7.29	1.53	1.32
34	1	668	A2M	O5'-C5'	-6.05	1.30	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	2021	A2M	O5'-C5'	-5.37	1.31	1.44
34	1	98	A2M	O5'-C5'	-5.33	1.31	1.44
34	1	28	A2M	O5'-C5'	-5.27	1.31	1.44

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	2185	MA6	N1-C6-N6	-11.01	105.47	117.06
35	2	37	MIA	C12-C13-C14	-9.38	108.89	127.14
34	1	2184	MA6	N1-C6-N6	-9.36	107.20	117.06
34	1	2185	MA6	N3-C2-N1	-6.27	118.87	128.68
34	1	1539	M1Y	C4-N3-C2	-5.83	119.80	127.35

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	1	115	OMC	C3'-C4'-C5'-O5'
34	1	115	OMC	O4'-C4'-C5'-O5'
34	1	668	A2M	C3'-C4'-C5'-O5'
34	1	912	A2M	O4'-C4'-C5'-O5'
34	1	1464	OMG	C1'-C2'-O2'-CM2

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 30 ligands modelled in this entry, 24 are monoatomic - leaving 6 for Mogul analysis.

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
40	PAR	1	2302	-	45,45,45	3.63	10 (22%)	64,67,67	1.57	15 (23%)
40	PAR	1	2303	34	45,45,45	3.52	10 (22%)	64,67,67	1.82	13 (20%)
40	PAR	1	2305	-	45,45,45	3.45	7 (15%)	64,67,67	1.50	11 (17%)
40	PAR	1	2307	-	45,45,45	3.59	10 (22%)	64,67,67	1.08	2 (3%)
40	PAR	1	2304	-	45,45,45	3.67	9 (20%)	64,67,67	1.59	10 (15%)
40	PAR	1	2306	-	45,45,45	3.54	9 (20%)	64,67,67	1.34	9 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	PAR	1	2302	-	-	5/18/94/94	0/4/4/4
40	PAR	1	2303	34	-	5/18/94/94	0/4/4/4
40	PAR	1	2305	-	-	9/18/94/94	0/4/4/4
40	PAR	1	2307	-	-	5/18/94/94	0/4/4/4
40	PAR	1	2304	-	-	9/18/94/94	0/4/4/4
40	PAR	1	2306	-	-	10/18/94/94	0/4/4/4

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	2304	PAR	C13-C23	-17.26	1.30	1.52
40	1	2302	PAR	C13-C23	-16.70	1.31	1.52
40	1	2307	PAR	C13-C23	-16.55	1.31	1.52
40	1	2303	PAR	C13-C23	-16.11	1.32	1.52
40	1	2306	PAR	C13-C23	-16.10	1.32	1.52

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	2303	PAR	C14-O33-C33	-6.38	102.17	117.96
40	1	2303	PAR	O52-C13-C23	5.61	119.59	107.96
40	1	2304	PAR	O51-C51-C41	4.40	117.69	109.69
40	1	2303	PAR	C31-C41-C51	-4.39	102.41	110.24
40	1	2305	PAR	C13-C23-C33	4.38	107.37	102.10

There are no chirality outliers.

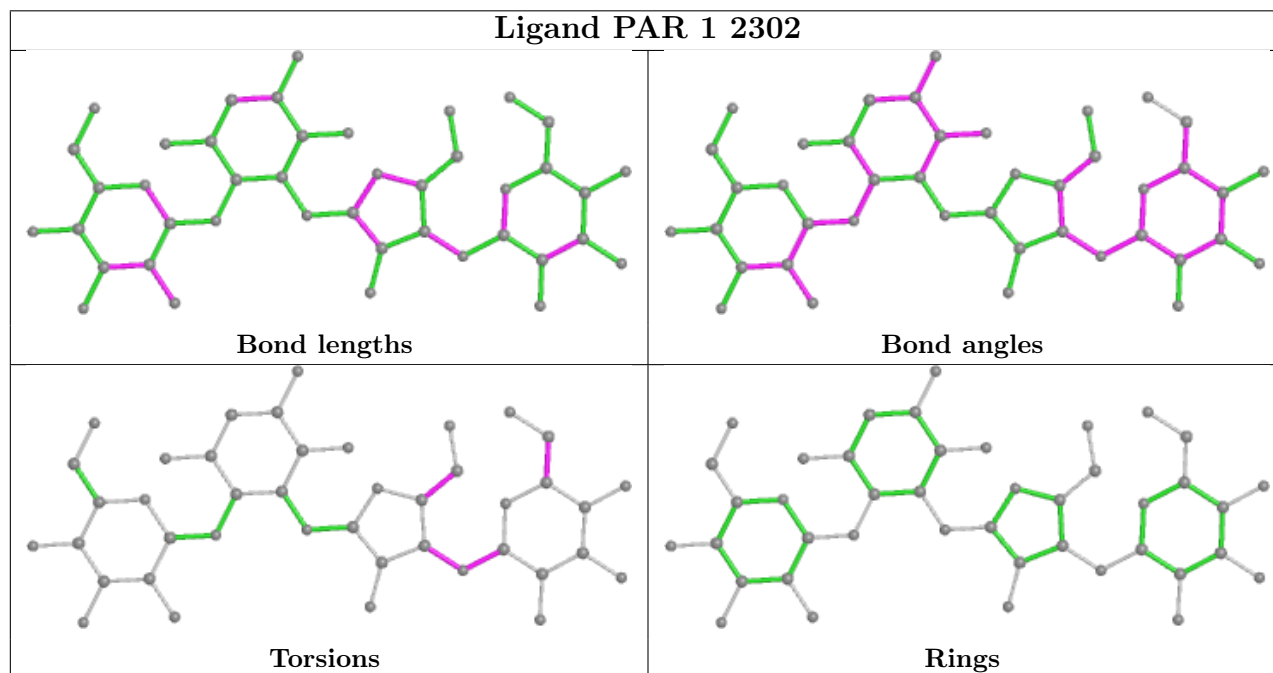
5 of 43 torsion outliers are listed below:

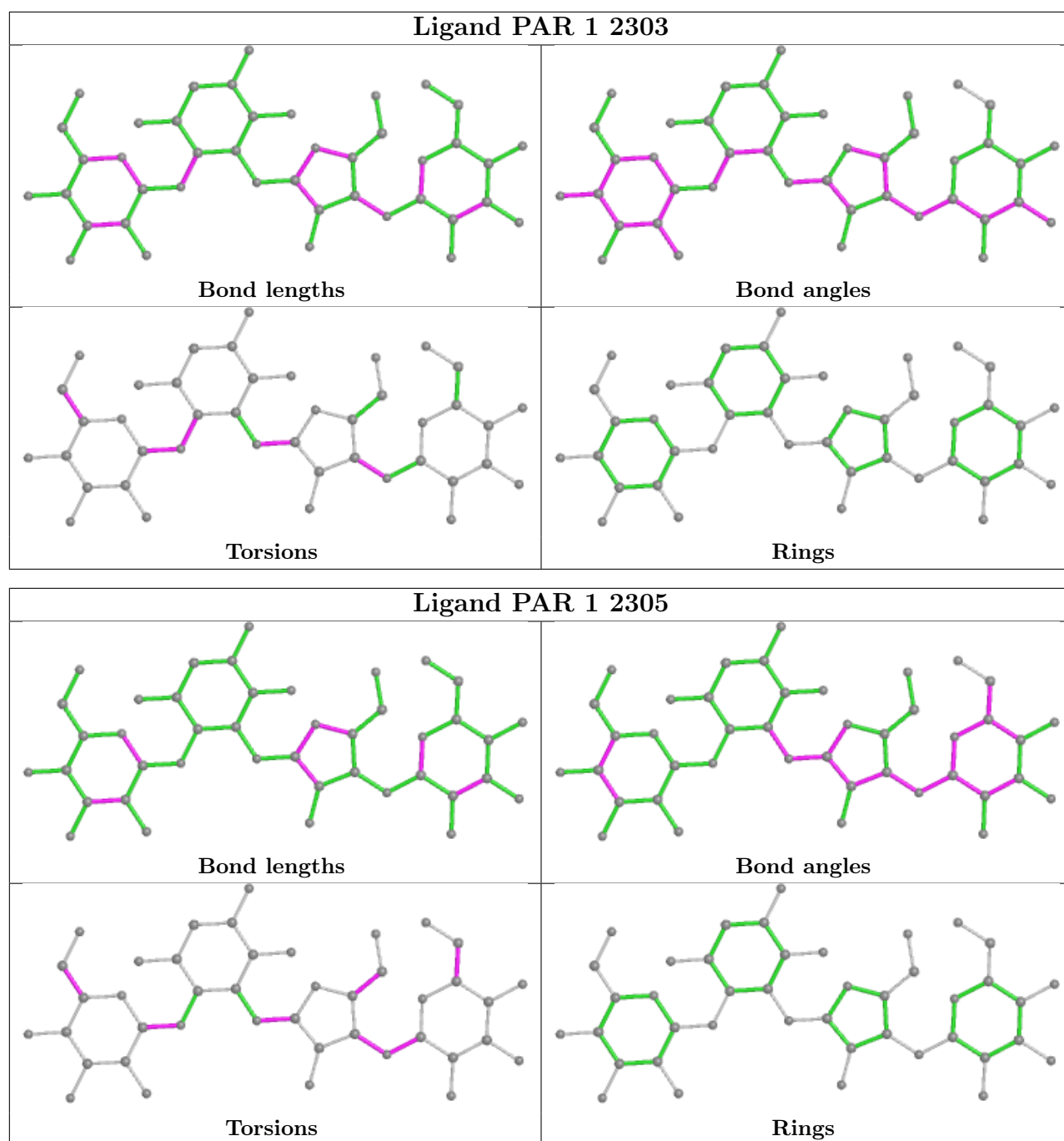
Mol	Chain	Res	Type	Atoms
40	1	2303	PAR	C23-C13-O52-C52
40	1	2304	PAR	C23-C13-O52-C52
40	1	2304	PAR	O54-C54-C64-N64
40	1	2305	PAR	C24-C14-O33-C33
40	1	2305	PAR	C33-C43-C53-O53

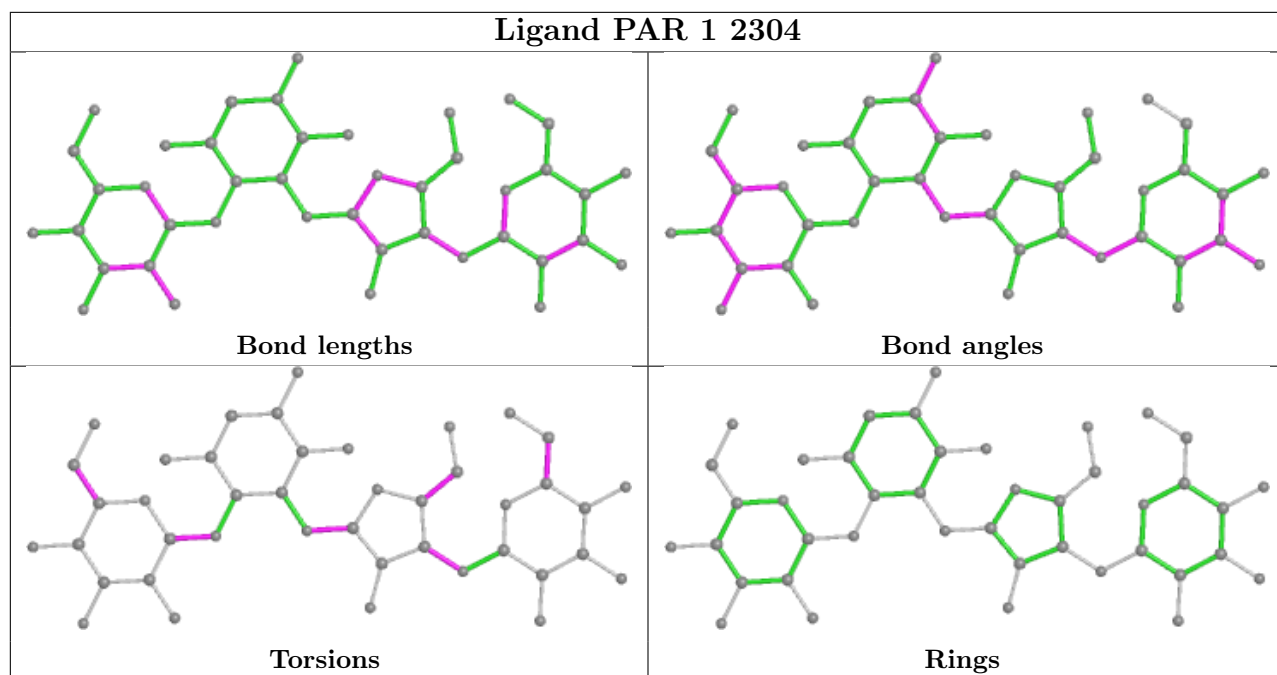
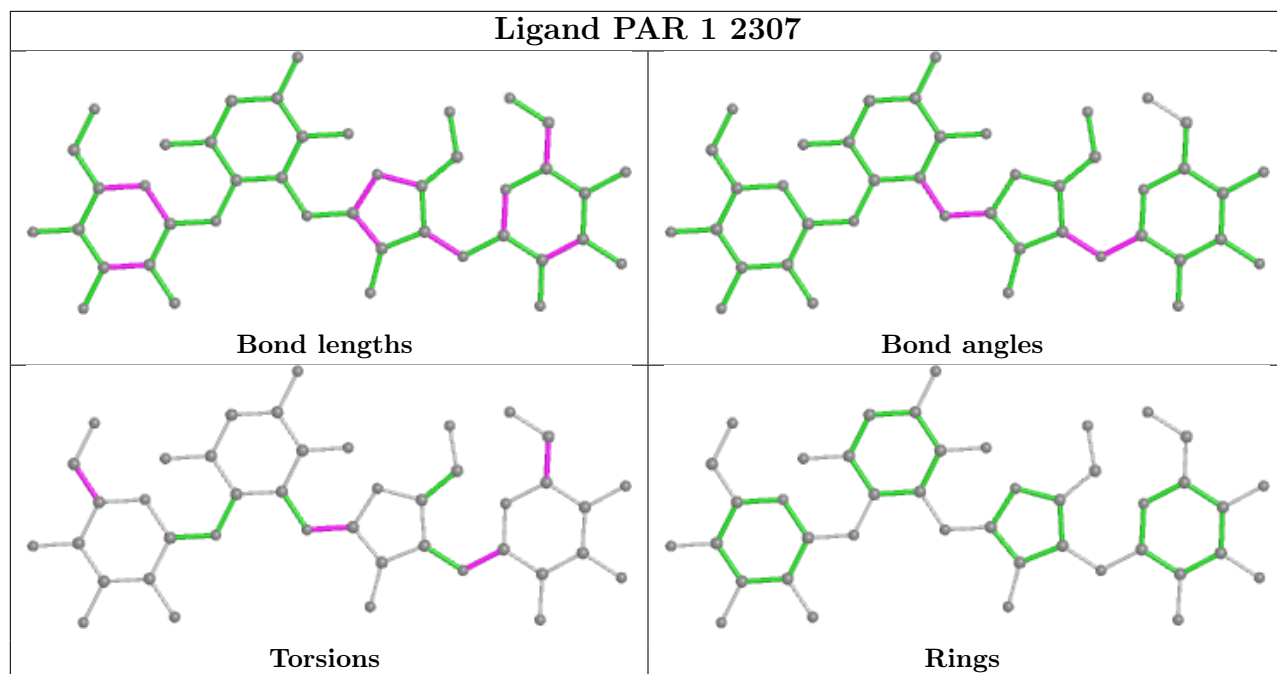
There are no ring outliers.

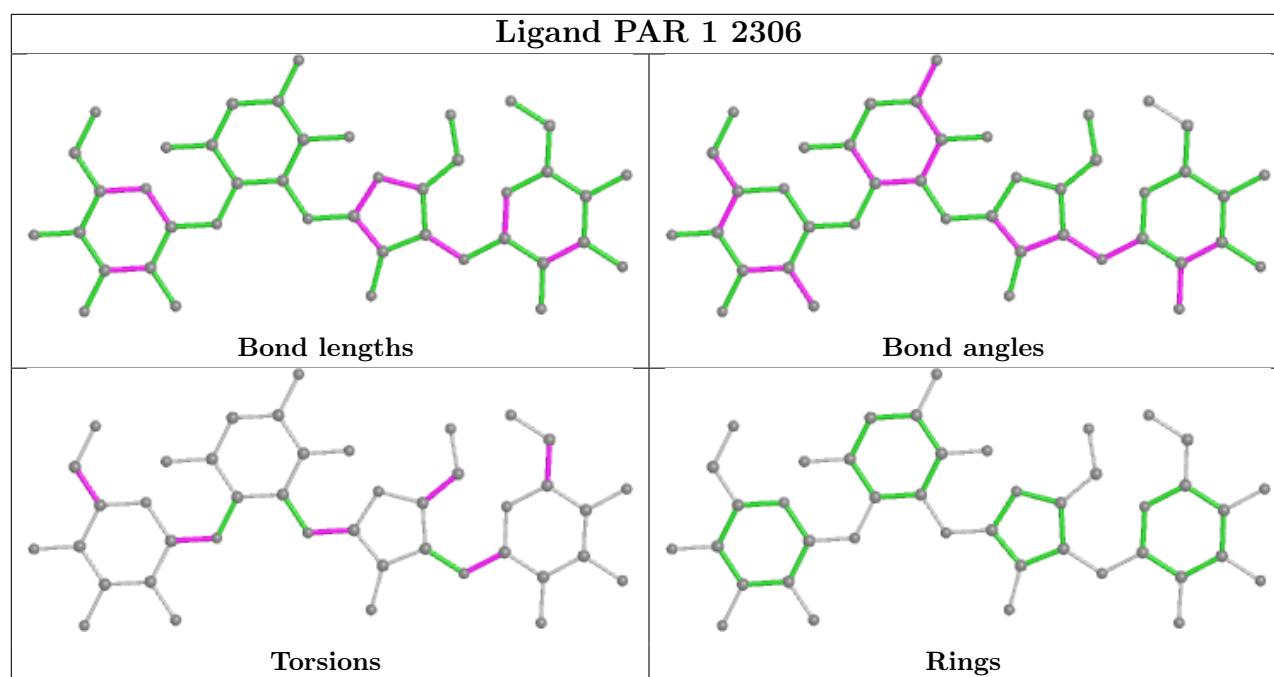
No monomer is involved in short contacts.

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	960:C	O3'	961:U	P	10.63

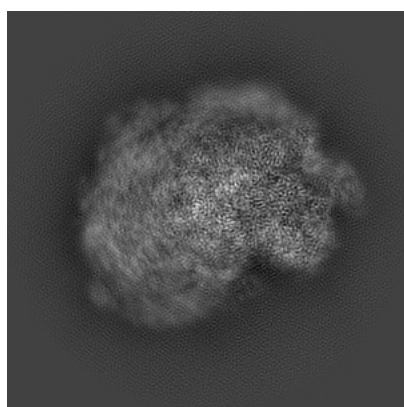
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7024. These allow visual inspection of the internal detail of the map and identification of artifacts.

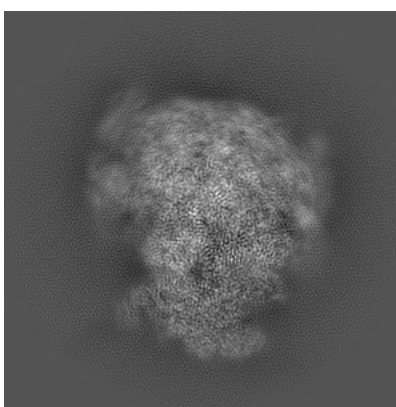
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

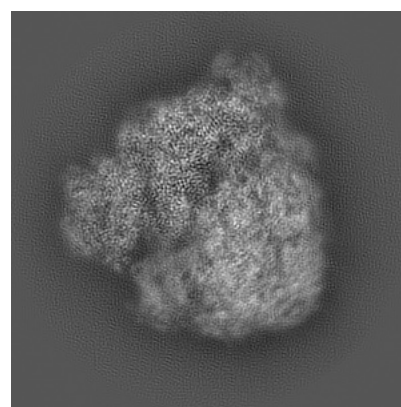
#### 6.1.1 Primary map



X



Y

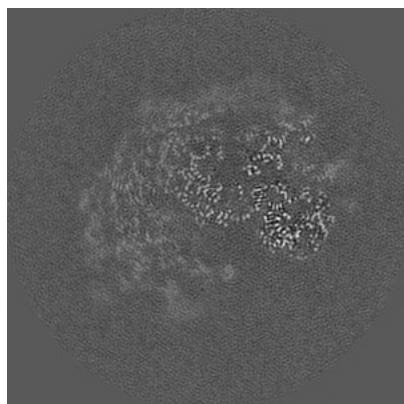


Z

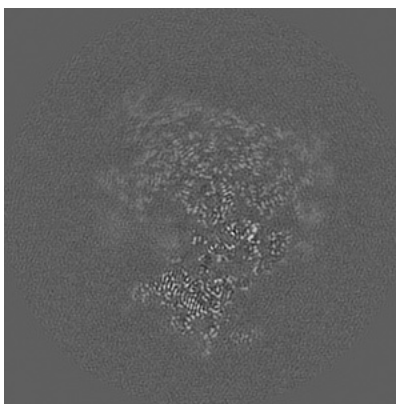
The images above show the map projected in three orthogonal directions.

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

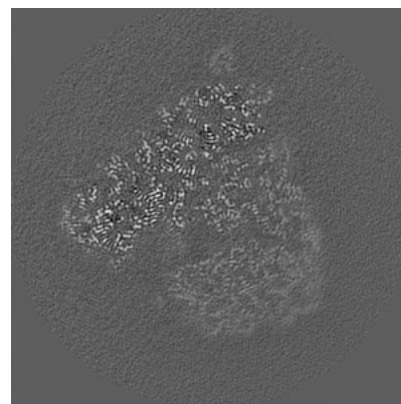
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

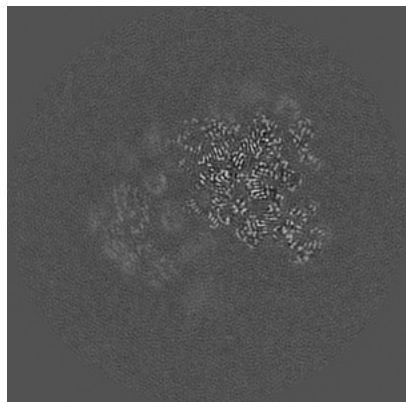


Z Index: 192

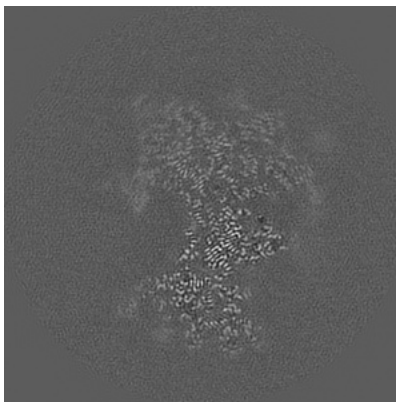
The images above show central slices of the map in three orthogonal directions.

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

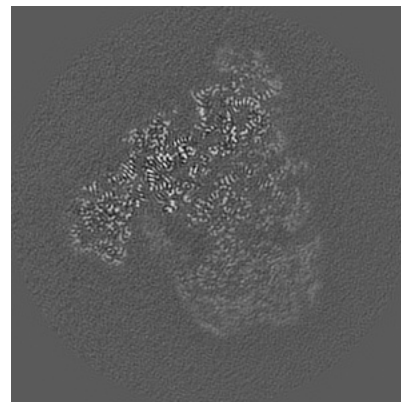
### 6.3.1 Primary map



X Index: 165



Y Index: 211



Z Index: 203

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

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

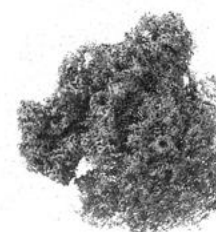
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



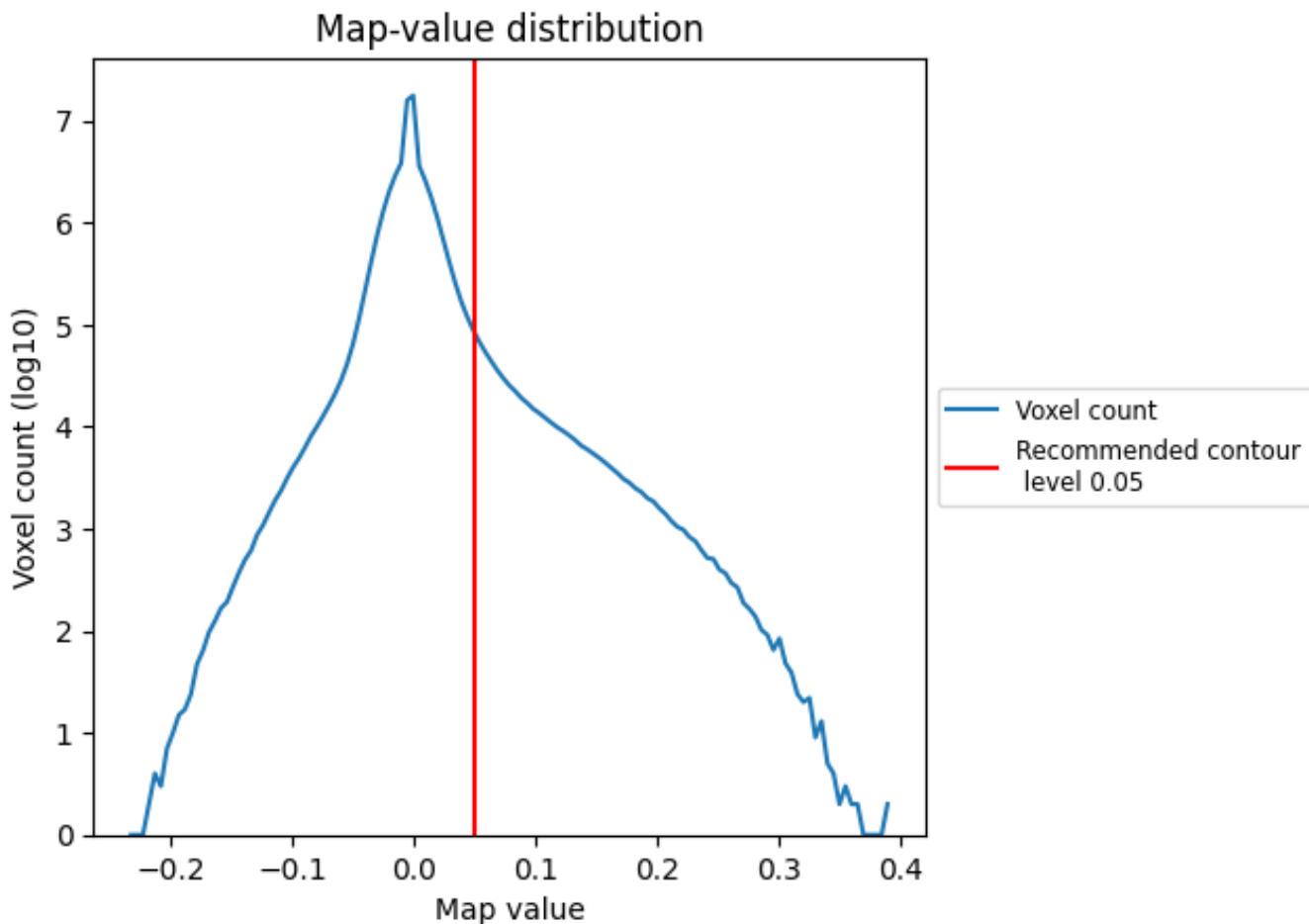
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

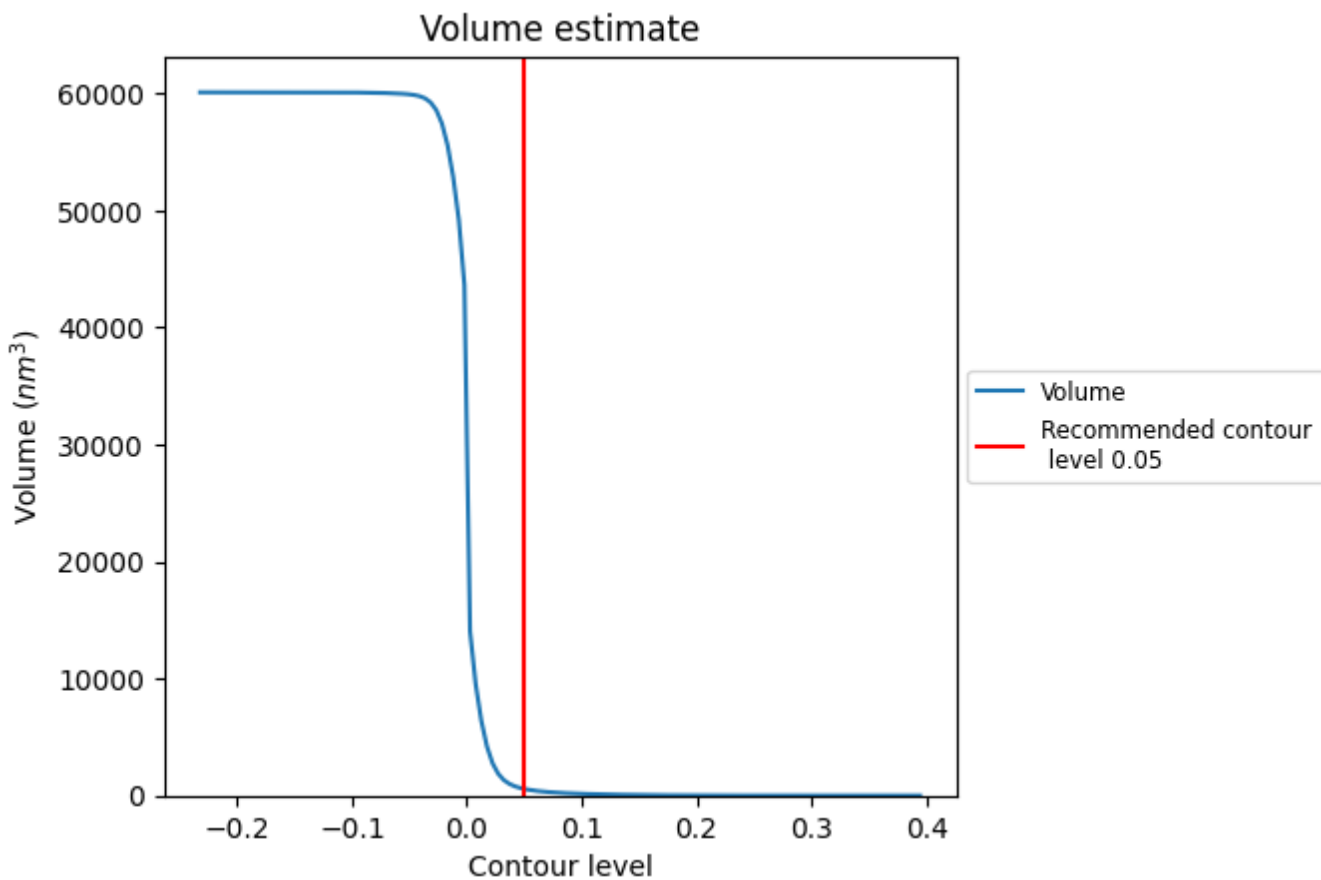
This section contains the results of statistical analysis of the map.

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



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

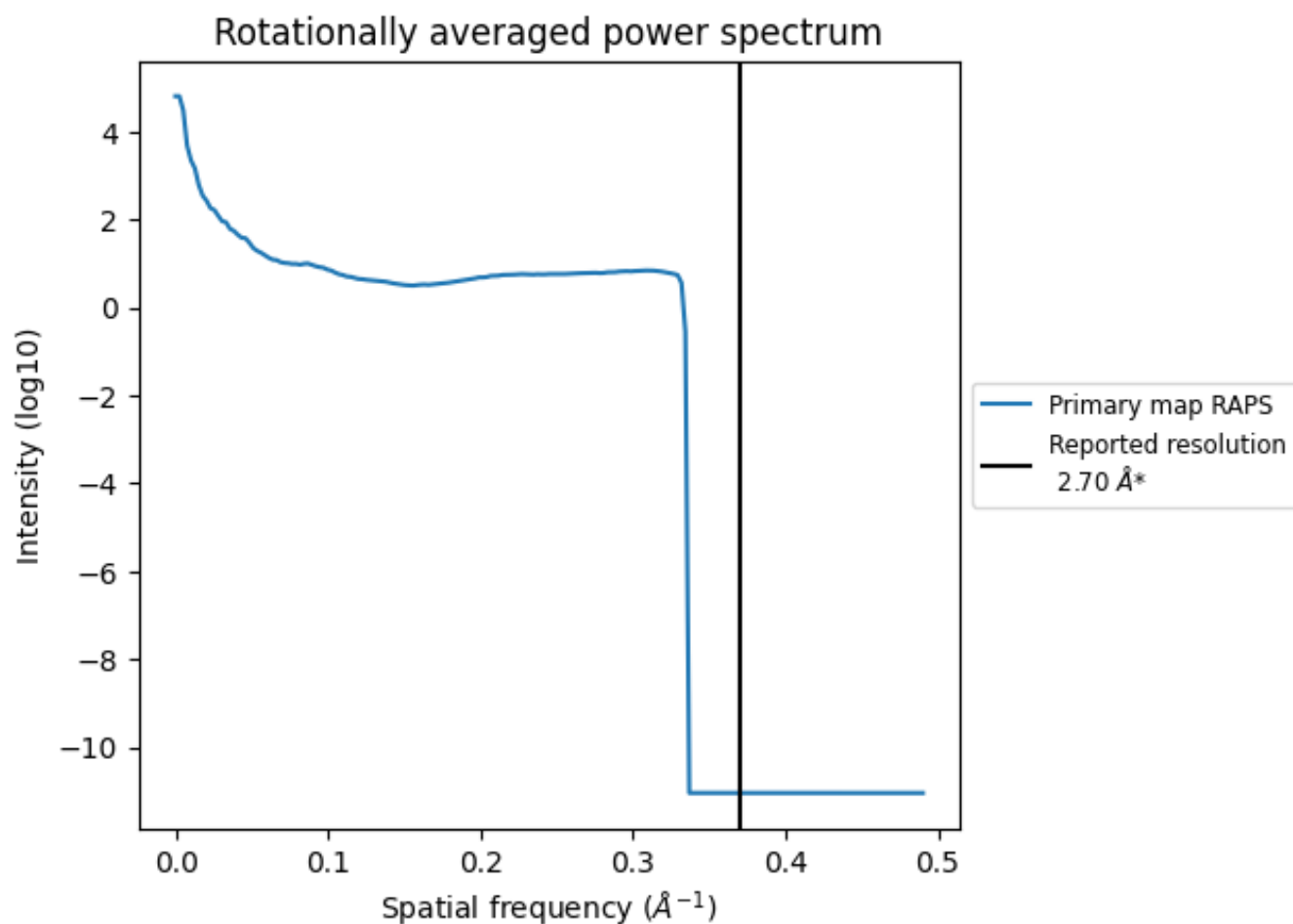
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 571 nm<sup>3</sup>; this corresponds to an approximate mass of 516 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  $0.370 \text{\AA}^{-1}$

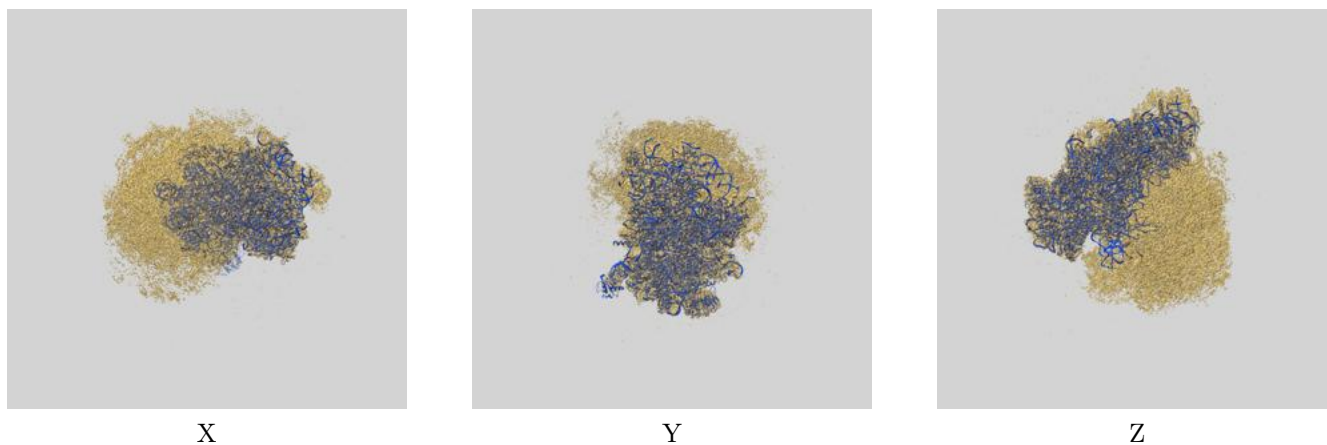
## 8 Fourier-Shell correlation

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

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

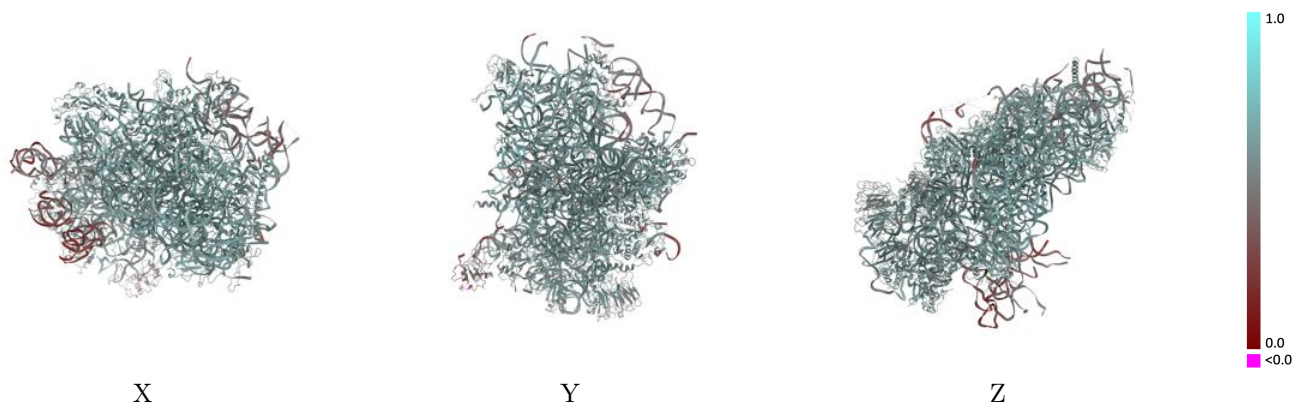
This section contains information regarding the fit between EMDB map EMD-7024 and PDB model 6AZ1. Per-residue inclusion information can be found in section 3 on page 14.

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



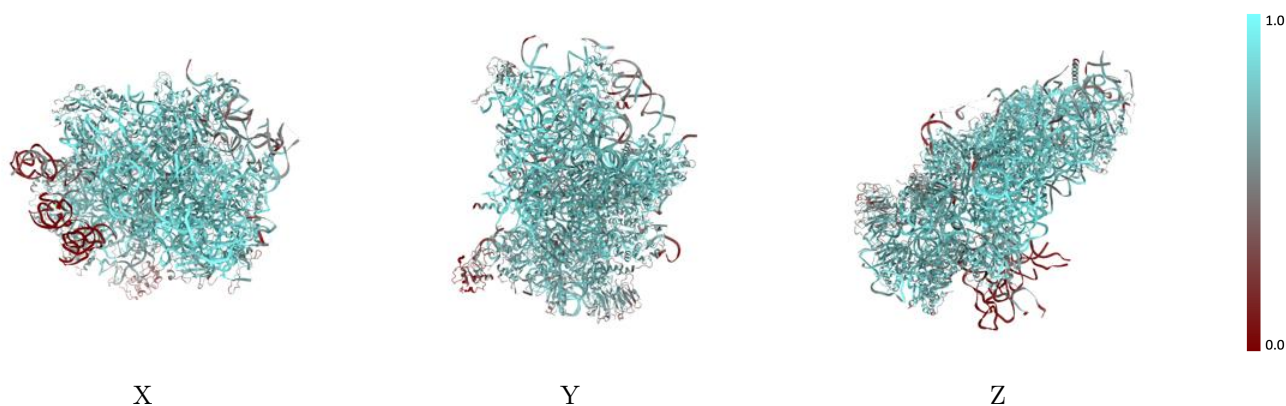
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



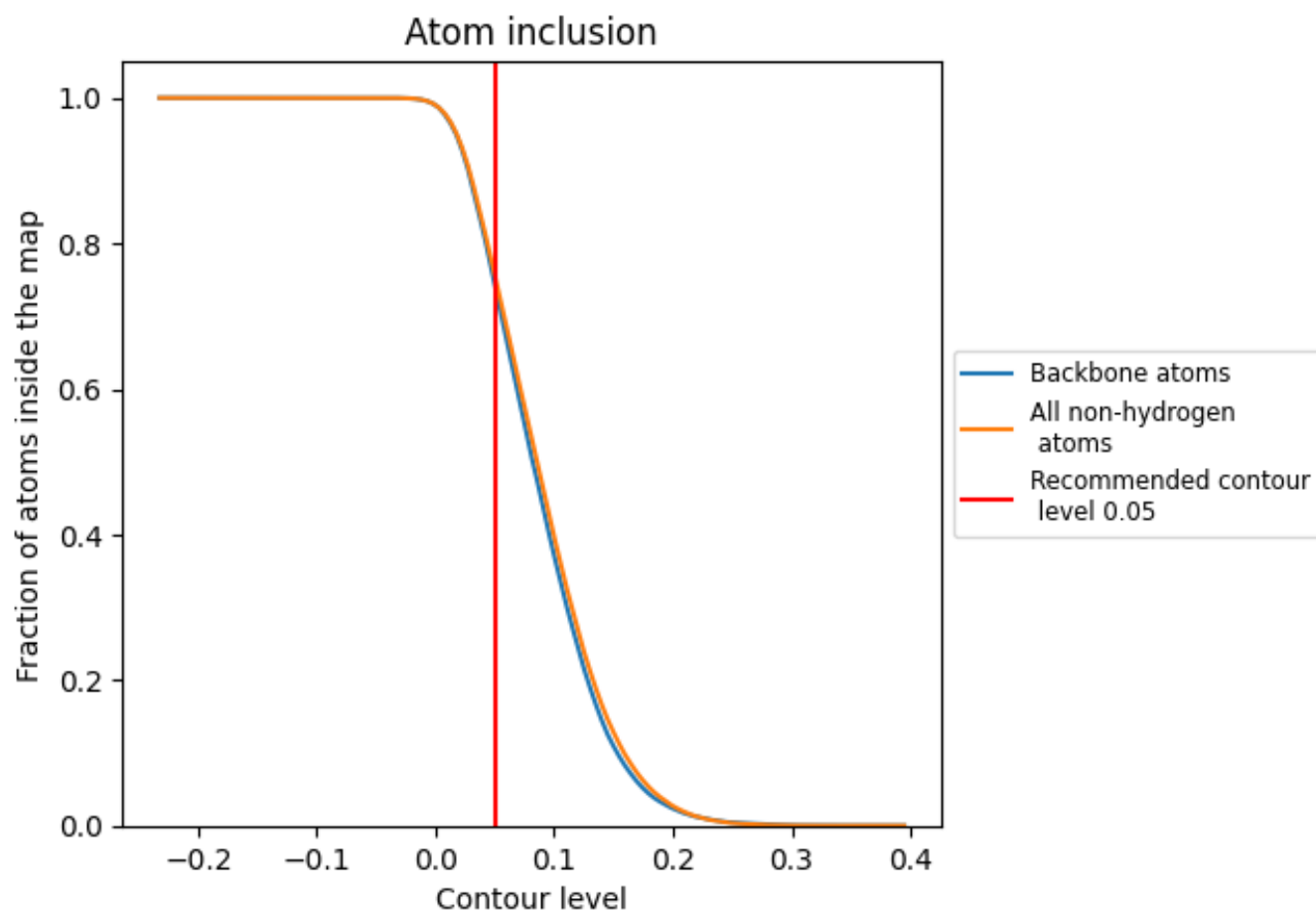
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7567	 0.5660
1	 0.8597	 0.5900
2	 0.1863	 0.3080
3	 0.3606	 0.4230
4	 0.2075	 0.3470
5	 0.8175	 0.5890
A	 0.7303	 0.5800
B	 0.7895	 0.5900
C	 0.6854	 0.5590
D	 0.7688	 0.5800
E	 0.8004	 0.5930
F	 0.8212	 0.6020
G	 0.6444	 0.5480
H	 0.7359	 0.5740
I	 0.7702	 0.5730
J	 0.8411	 0.6100
K	 0.7626	 0.5800
L	 0.7743	 0.5870
M	 0.6692	 0.5590
N	 0.6891	 0.5490
O	 0.7528	 0.5810
P	 0.7722	 0.5830
Q	 0.1691	 0.3570
R	 0.7011	 0.5680
S	 0.7934	 0.5860
T	 0.8115	 0.5950
U	 0.7832	 0.5960
V	 0.6879	 0.5600
W	 0.6675	 0.5630
X	 0.7933	 0.5830
Y	 0.7752	 0.5820
Z	 0.7578	 0.5770
a	 0.7024	 0.5630
b	 0.8214	 0.6060
c	 0.7911	 0.5920



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Chain	Atom inclusion	Q-score
d	 0.6341	 0.5650
e	 0.7156	 0.5800
f	 0.2725	 0.3930
g	 0.5701	 0.5200