



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 05:49 AM UTC

PDB ID : 7NFX / pdb_00007nfx
EMDB ID : EMD-12303
Title : Mammalian ribosome nascent chain complex with SRP and SRP receptor in early state A
Authors : Jomaa, A.; Lee, J.H.; Shan, S.; Ban, N.
Deposited on : 2021-02-08
Resolution : 3.20 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:

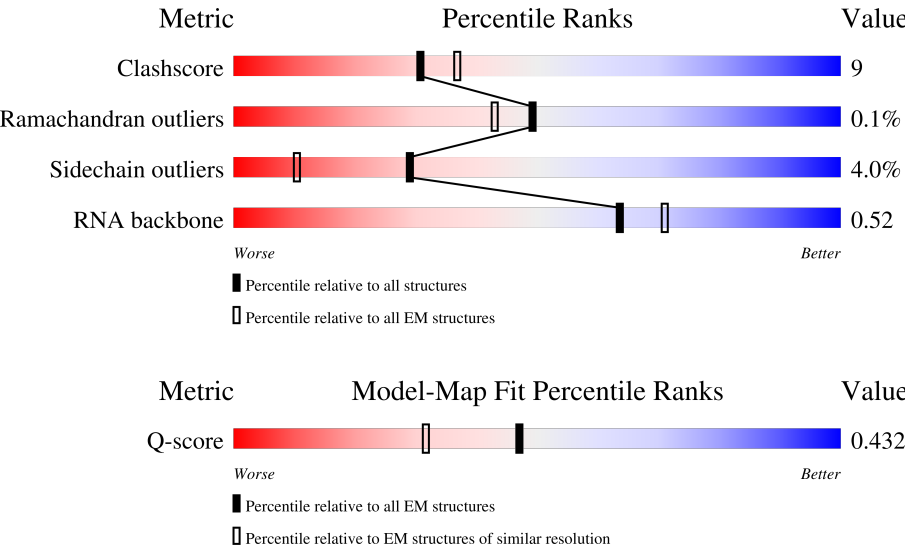
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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 $\leq 5\%$. 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	1	299	83% 41% 38% 17%
2	5	3493	13% 47% 43% 10%
3	7	120	62% 31% 8%

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Mol	Chain	Length	Quality of chain
4	8	156	
5	A	245	
6	B	403	
7	C	413	
8	D	297	
9	E	291	
10	F	225	
11	G	319	
12	H	192	
13	I	214	
14	J	178	
15	L	210	
16	M	218	
17	N	204	
18	O	199	
19	P	153	
20	Q	187	
21	R	180	
22	S	175	
23	T	160	
24	U	99	
25	V	140	
26	W	63	
27	X	156	
28	Y	145	

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Mol	Chain	Length	Quality of chain
29	Z	136	
30	a	148	
31	b	223	
32	c	94	
33	d	125	
34	e	128	
35	f	110	
36	g	129	
37	h	123	
38	i	104	
39	j	97	
40	k	69	
41	l	51	
42	m	52	
43	n	25	
44	o	105	
45	p	92	
46	q	144	
47	r	137	
48	s	21	
49	t	136	
50	u	627	
51	v	271	
52	w	86	
53	x	504	

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Mol	Chain	Length	Quality of chain
54	y	638	23% 19% 77%
55	z	671	97%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 148232 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 SRP RNA 7SL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	249	Total	C	N	O	P	0	0
			5341	2377	977	1738	249		

- Molecule 2 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	3493	Total	C	N	O	P	0	0
			74854	33335	13681	24346	3492		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 4 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 5 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	244	Total	C	N	O	S	0	0
			1868	1171	382	309	6		

- Molecule 6 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	394	Total	C	N	O	S	0	0
			3148	2007	591	537	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 7 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	292	Total	C	N	O	S	0	0
			2386	1509	437	426	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	236	Total	C	N	O	S	0	0
			1898	1215	362	318	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	126	ARG	LYS	conflict	UNP G1SKF7
E	217	GLN	LYS	conflict	UNP G1SKF7

- Molecule 10 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	175	ALA	THR	conflict	UNP G1SV32
F	185	GLY	ASN	conflict	UNP G1SV32
F	202	ARG	HIS	conflict	UNP G1SV32
F	233	GLU	GLY	conflict	UNP G1SV32

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	241	Total	C	N	O	S	0	0
			1934	1233	371	326	4		

- Molecule 12 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 13 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	204	Total	C	N	O	S	0	0
			1655	1051	319	272	13		

- Molecule 14 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 15 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	210	Total	C	N	O	S	0	0
			1703	1065	354	280	4		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0

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Chain	Residue	Modelled	Actual	Comment	Reference
L	51	ALA	-	insertion	UNP G1TPV0
L	52	SER	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0
L	55	LEU	-	insertion	UNP G1TPV0

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 17 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 18 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	199	Total	C	N	O	S	0	0
			1638	1056	321	256	5		

- Molecule 19 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 20 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	187	Total	C	N	O	S	0	0
			1506	941	311	249	5		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	6	ARG	LEU	conflict	UNP G1TX70
Q	14	ARG	TRP	conflict	UNP G1TX70

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	23	ILE	MET	conflict	UNP G1TX70
Q	24	TYR	CYS	conflict	UNP G1TX70
Q	38	ARG	HIS	conflict	UNP G1TX70
Q	57	ASN	LYS	conflict	UNP G1TX70
Q	66	MET	VAL	conflict	UNP G1TX70
Q	74	GLY	ASP	conflict	UNP G1TX70
Q	75	ARG	PRO	conflict	UNP G1TX70
Q	77	GLY	ASN	conflict	UNP G1TX70
Q	106	SER	THR	conflict	UNP G1TX70
Q	110	ARG	HIS	conflict	UNP G1TX70
Q	117	GLY	GLU	conflict	UNP G1TX70
Q	124	ASP	HIS	conflict	UNP G1TX70
Q	134	CYS	ARG	conflict	UNP G1TX70
Q	150	ARG	GLN	conflict	UNP G1TX70
Q	172	ARG	GLY	conflict	UNP G1TX70
Q	184	ARG	TRP	conflict	UNP G1TX70

- Molecule 21 is a protein called 60S RIBOSOMAL PROTEIN EL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 22 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	175	Total	C	N	O	S	0	0
			1454	925	284	235	10		

- Molecule 23 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 24 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	32	GLY	ARG	variant	UNP G1TSG1
U	36	ALA	GLU	variant	UNP G1TSG1
U	39	PHE	SER	variant	UNP G1TSG1
U	54	GLY	ARG	variant	UNP G1TSG1
U	60	VAL	ALA	variant	UNP G1TSG1
U	97	ARG	HIS	variant	UNP G1TSG1

- Molecule 25 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 26 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 27 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 28 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 29 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 30 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	-	initiating methionine	UNP G1SNY0

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	75	Total	C	N	O	S	0	0
			609	378	130	98	3		

- Molecule 32 is a protein called eL30.

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

- Molecule 33 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 34 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 35 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 36 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 37 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 38 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 39 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 40 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 41 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN EL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 43 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 44 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 45 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 46 is a protein called Signal recognition particle 19 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	104	Total	C	N	O	S	0	0
			842	534	152	150	6		

- Molecule 47 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	125	Total	C	N	O	S	0	0
			1001	621	206	168	6		

- Molecule 48 is a protein called Signal Sequence.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	s	21	Total	C	N	O	0	0
			105	63	21	21		

- Molecule 49 is a protein called Signal recognition particle 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	88	Total	C	N	O	S	0	0
			693	438	122	128	5		

- Molecule 50 is a protein called Signal recognition particle subunit SRP68.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	196	Total	C	N	O	S	0	0
			1637	1028	307	294	8		

- Molecule 51 is a protein called Signal recognition particle receptor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	186	Total	C	N	O	S	0	0
			1455	923	252	274	6		

- Molecule 52 is a protein called Signal recognition particle 9 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	75	Total	C	N	O	S	1	0
			623	397	108	112	6		

- Molecule 53 is a protein called Signal recognition particle 54 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	417	Total	C	N	O	S	0	0
			3236	2042	552	620	22		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	226	GLU	GLY	engineered mutation	UNP P61011

- Molecule 54 is a protein called Signal recognition particle receptor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	147	Total	C	N	O	S	0	0
			1133	724	194	213	2		

- Molecule 55 is a protein called Signal recognition particle subunit SRP72.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	19	Total	C	N	O	S	0	0
			161	106	26	28	1		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	g	1	Total	Zn	0
			1	1	
56	j	1	Total	Zn	0
			1	1	
56	m	1	Total	Zn	0
			1	1	

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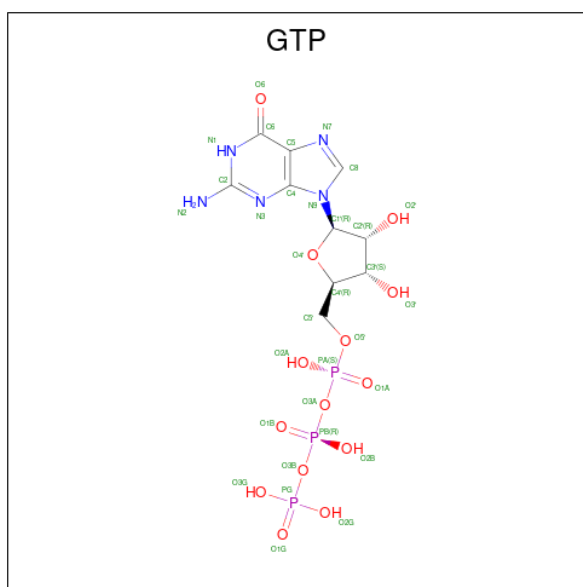
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Mol	Chain	Residues	Atoms		AltConf
56	o	1	Total	Zn	0
			1	1	
56	p	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

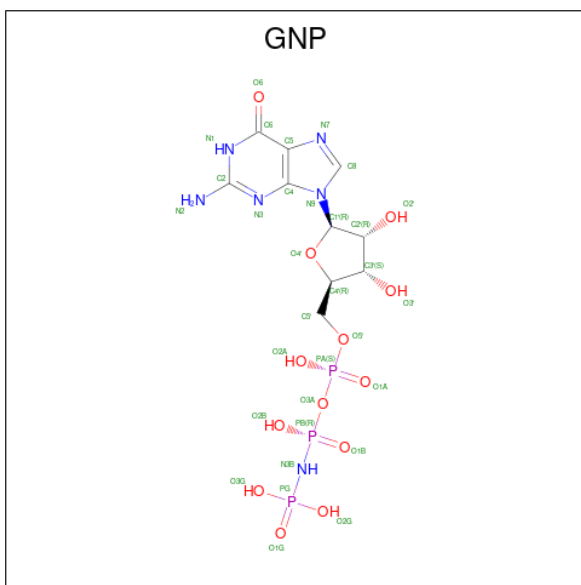
Mol	Chain	Residues	Atoms		AltConf
57	v	1	Total	Mg	0
			1	1	
57	x	1	Total	Mg	0
			1	1	

- Molecule 58 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
58	v	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 59 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

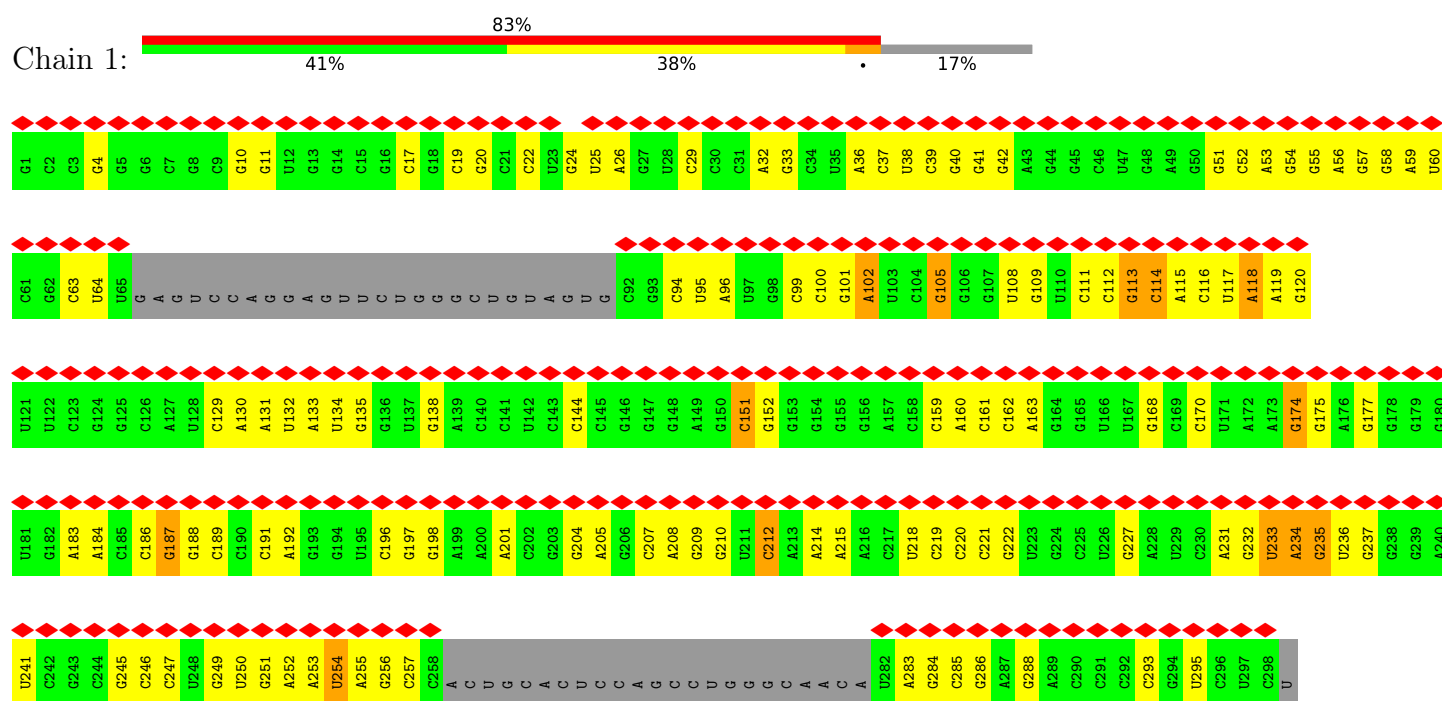


Mol	Chain	Residues	Atoms					AltConf
59	x	1	Total	C	N	O	P	0
			32	10	6	13	3	

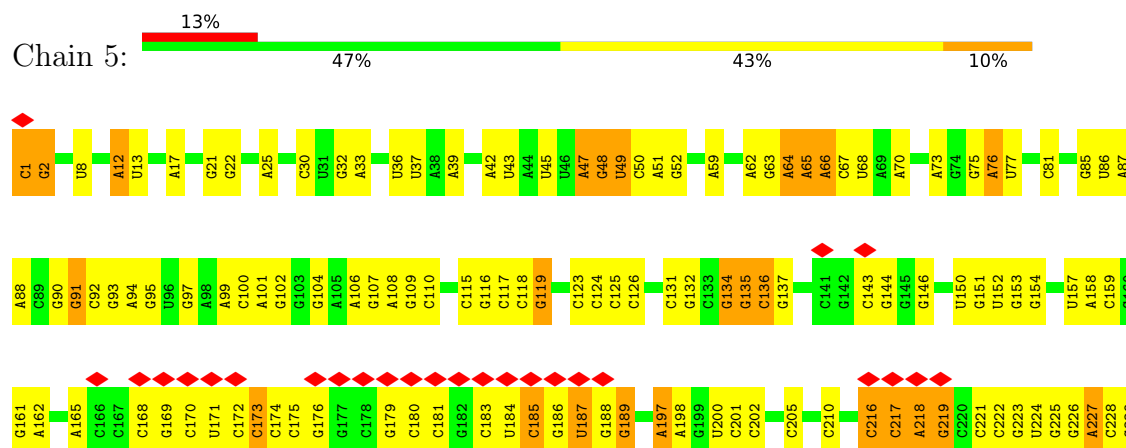
3 Residue-property plots

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

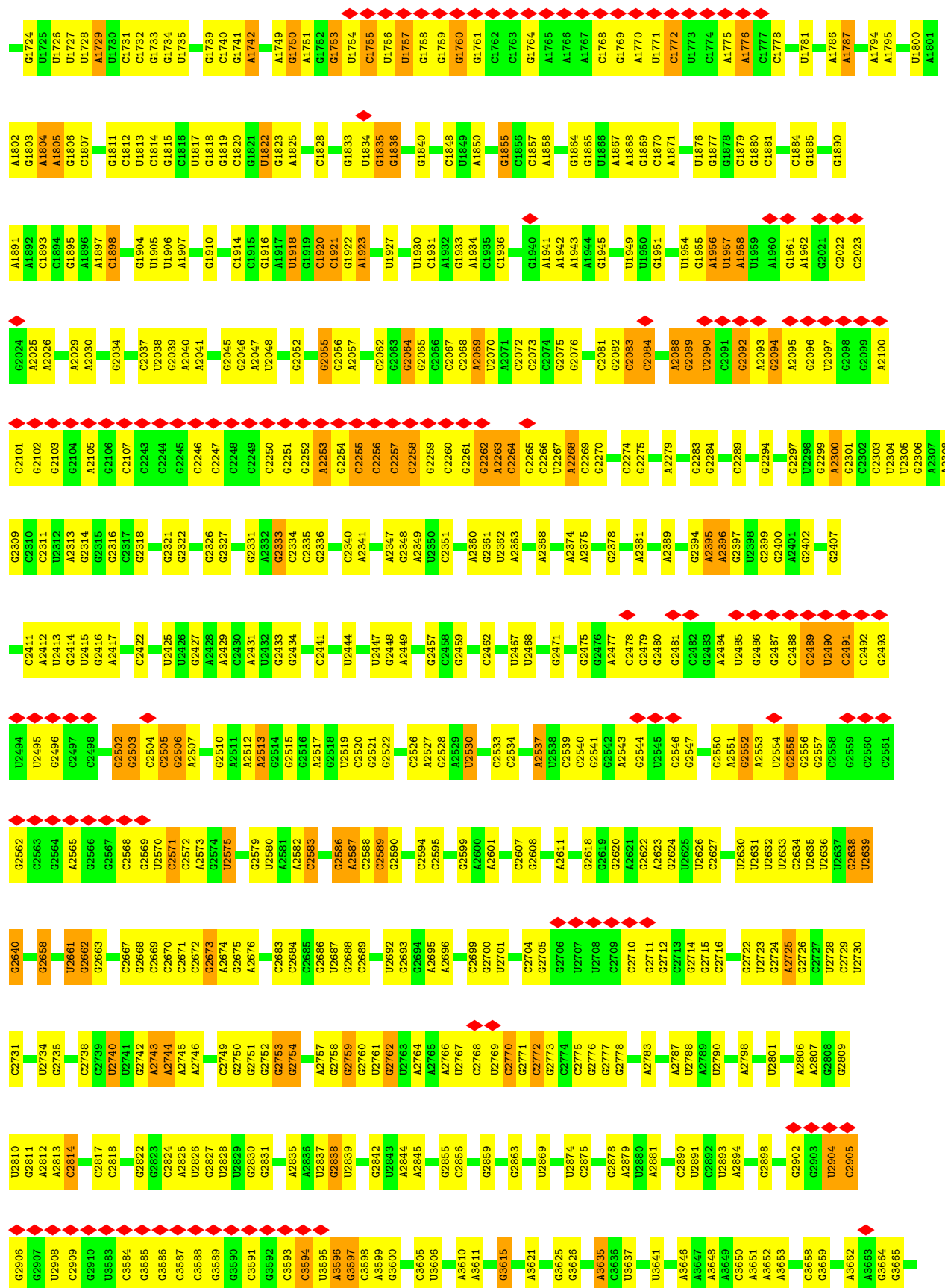
• Molecule 1: SRP RNA 7SL

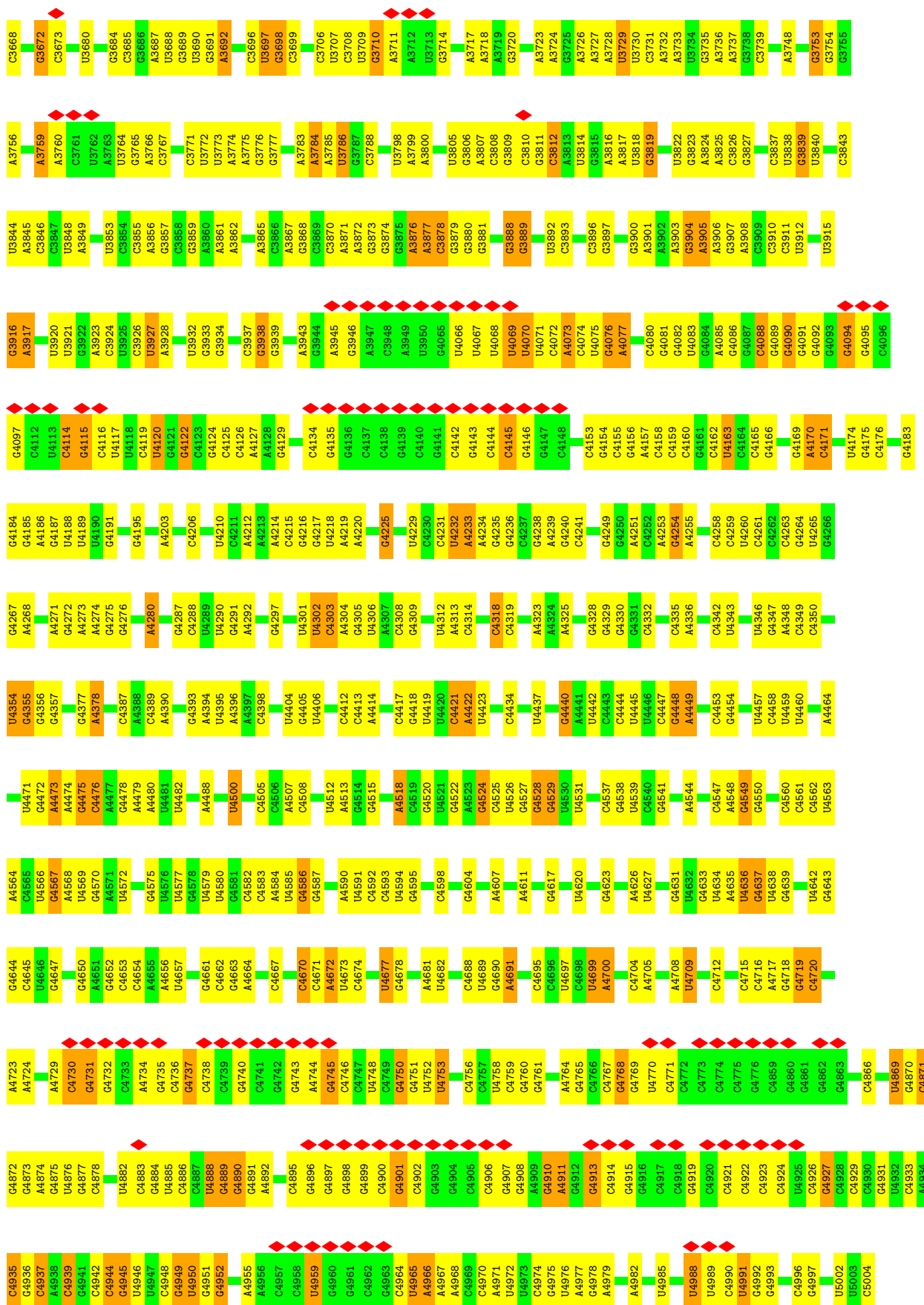


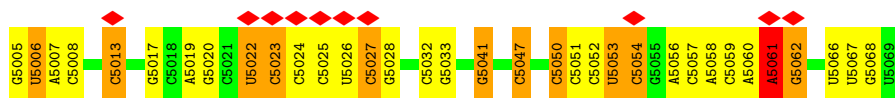
• Molecule 2: 28S ribosomal RNA







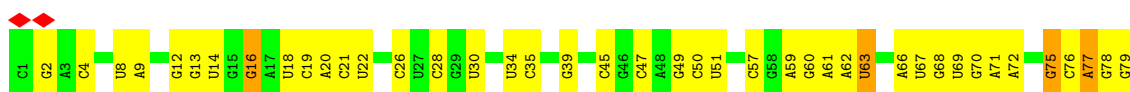




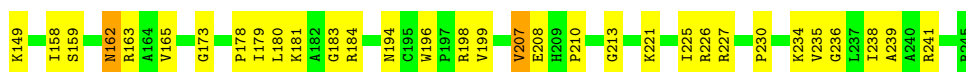
• Molecule 3: 5S ribosomal RNA



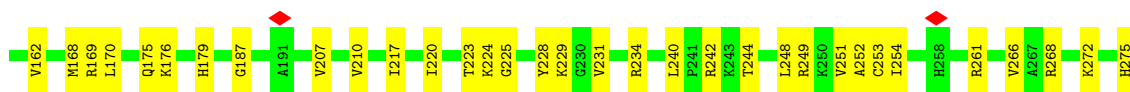
• Molecule 4: 5.8S ribosomal RNA



• Molecule 5: uL2

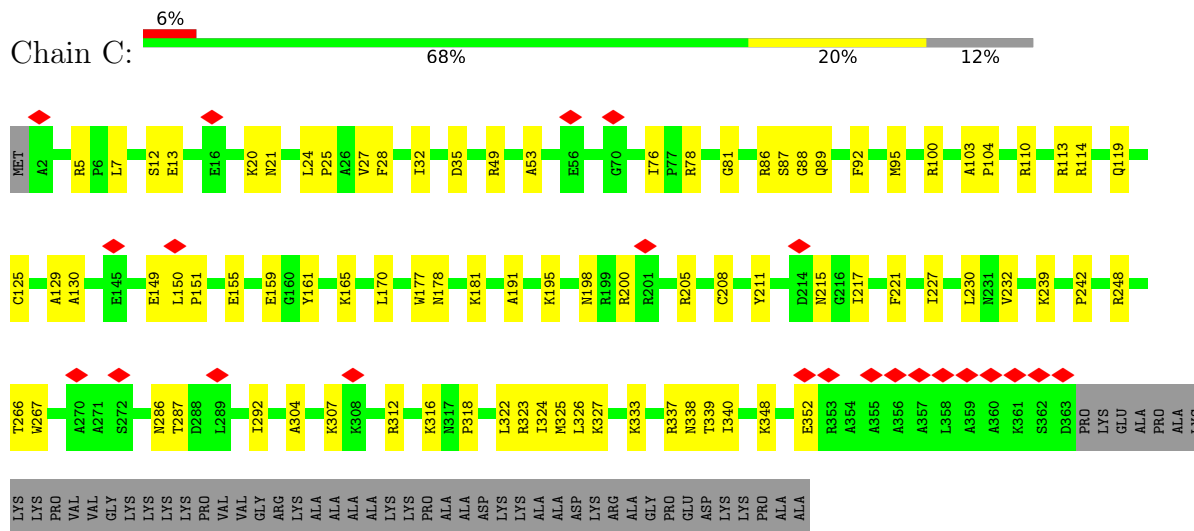


• Molecule 6: uL3

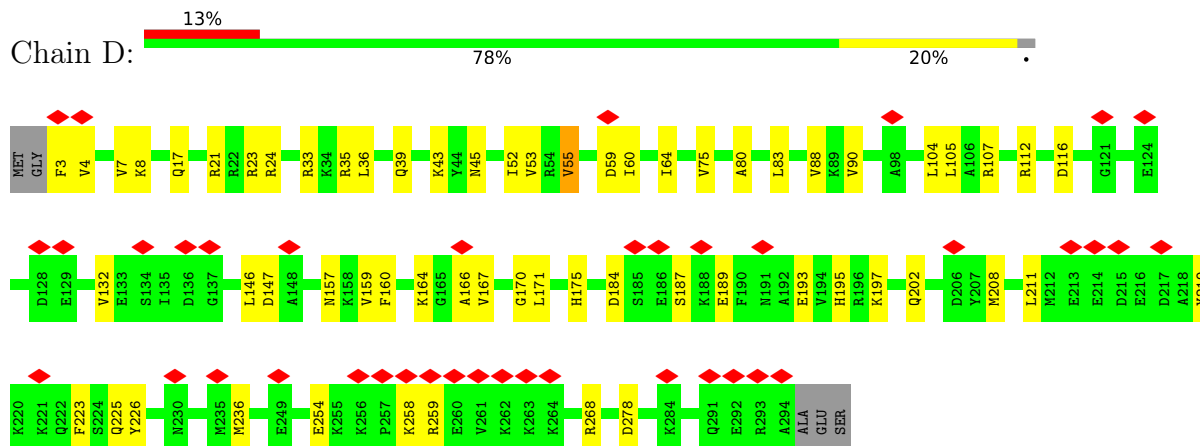


ILE
ALA
LYS
GLU
GLY
GLY
ALA

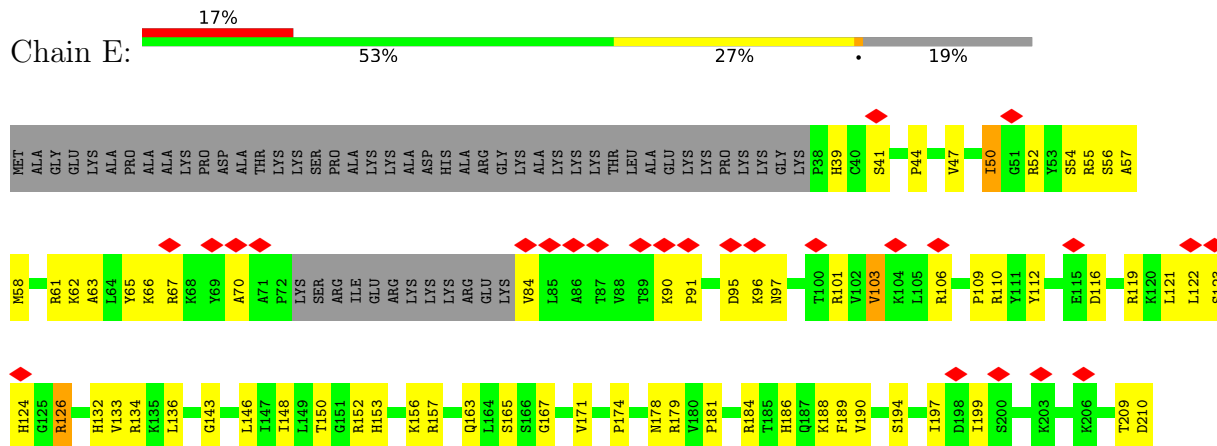
• Molecule 7: 60S ribosomal protein L4

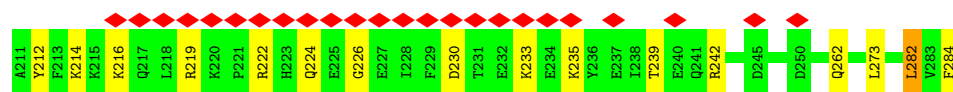


• Molecule 8: 60S ribosomal protein L5

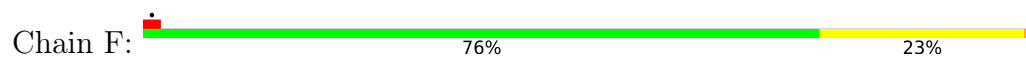


• Molecule 9: 60S ribosomal protein L6

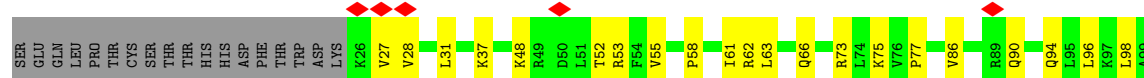
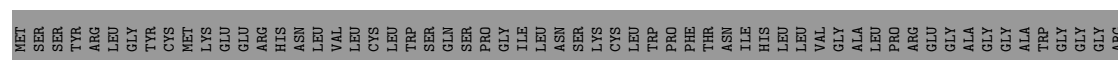




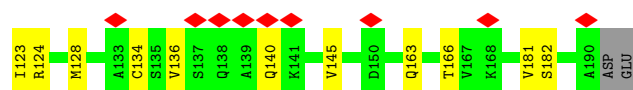
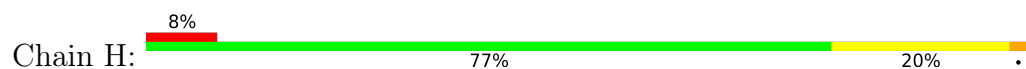
• Molecule 10: uL30



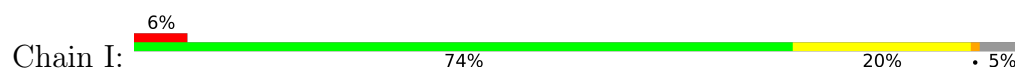
• Molecule 11: 60S ribosomal protein L7a



• Molecule 12: 60S ribosomal protein L9

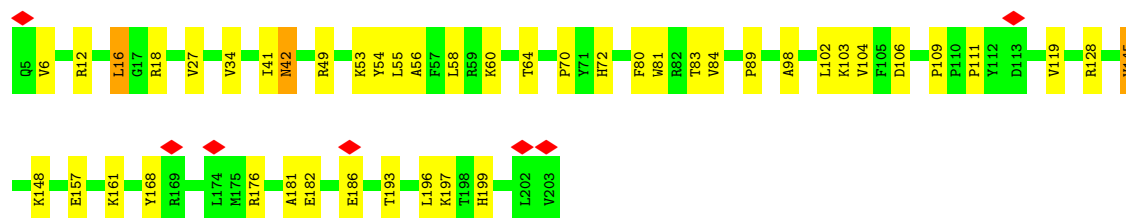


• Molecule 13: 60S ribosomal protein L10



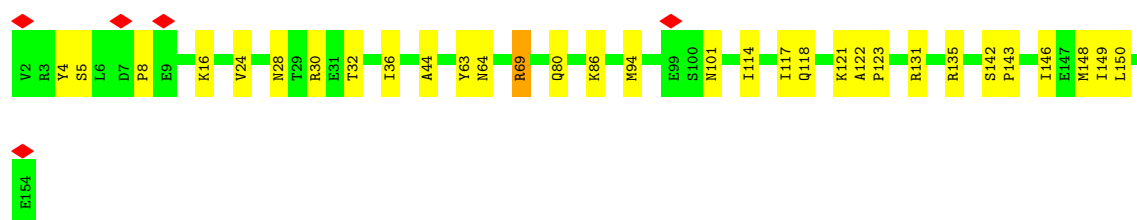
- Molecule 18: uL13

Chain O: 



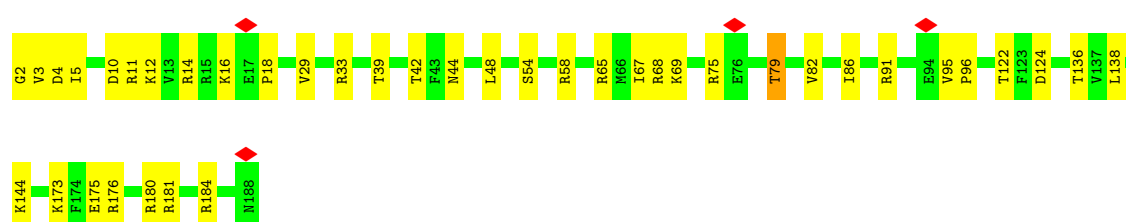
- Molecule 19: uL22

Chain P: 



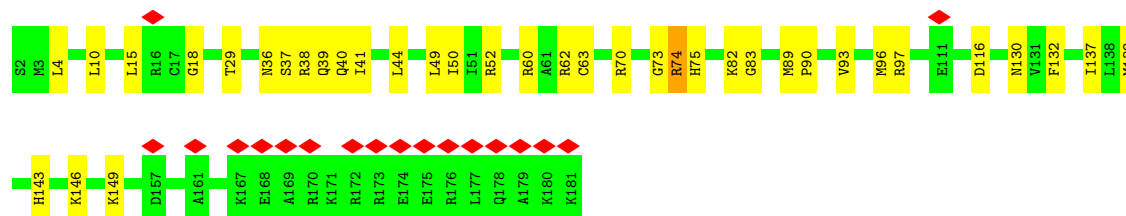
- Molecule 20: eL18

Chain Q: 



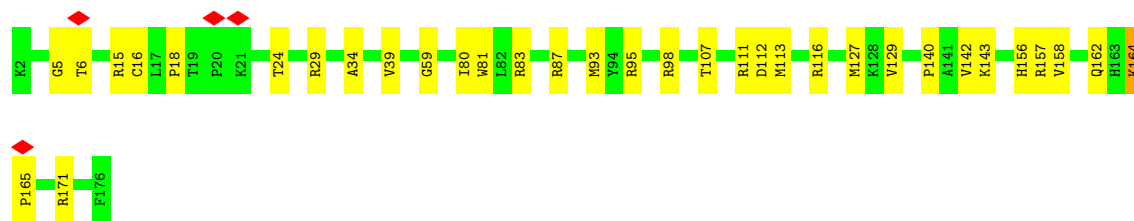
- Molecule 21: 60S RIBOSOMAL PROTEIN EL19

Chain R: 

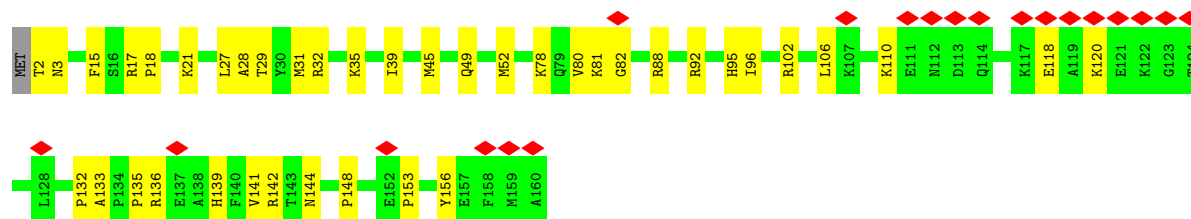
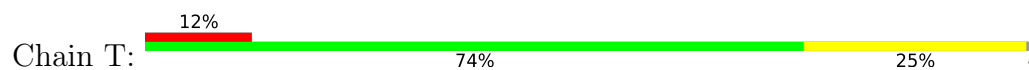


- Molecule 22: eL20

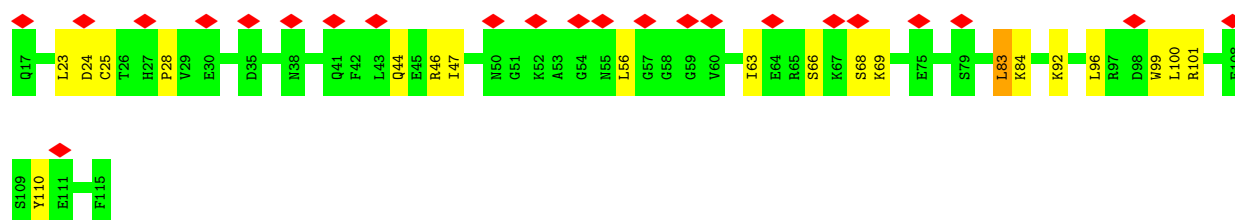
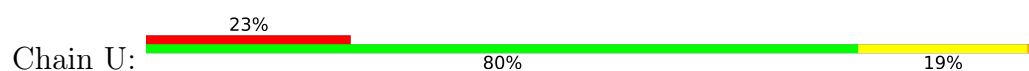
Chain S: 



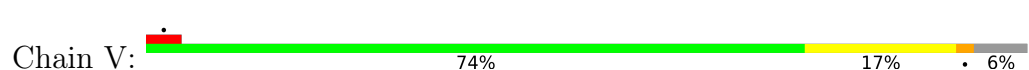
- Molecule 23: eL21



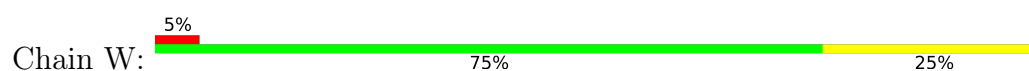
- Molecule 24: Ribosomal protein L22



- Molecule 25: Ribosomal protein L23

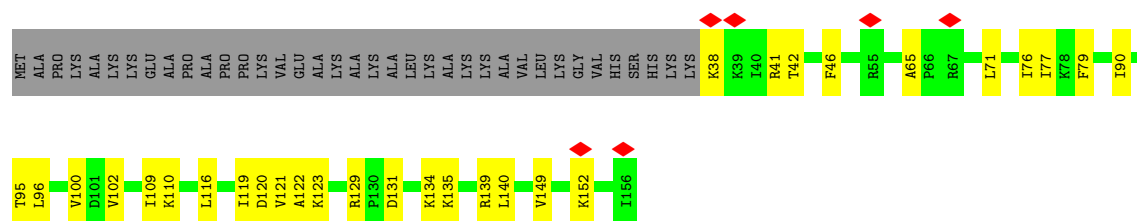


- Molecule 26: Ribosomal protein L24

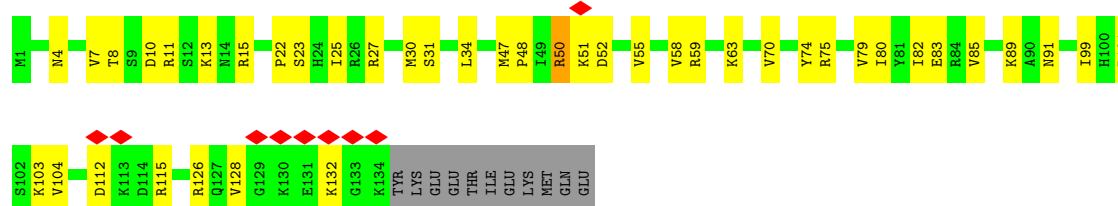


- Molecule 27: uL23

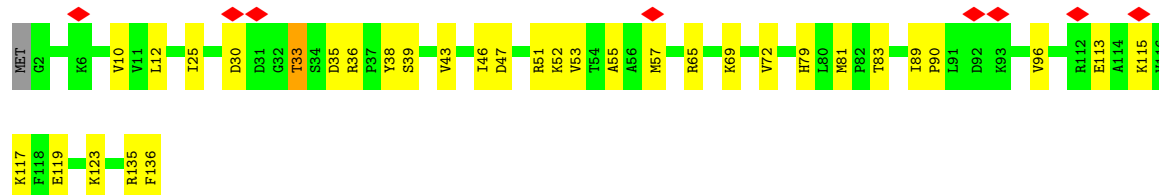
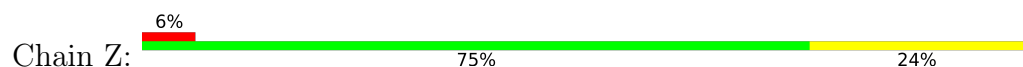




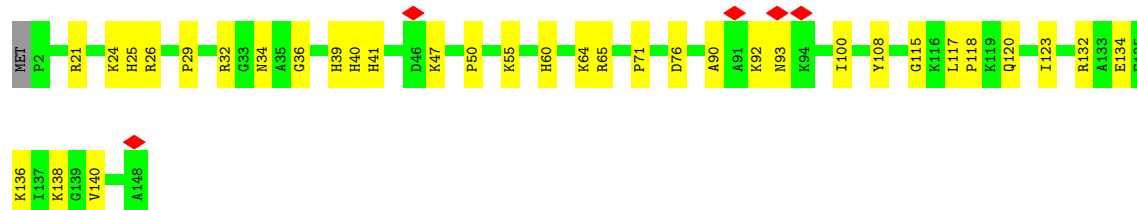
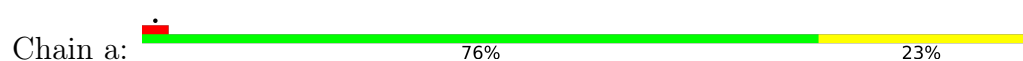
• Molecule 28: Ribosomal protein L26



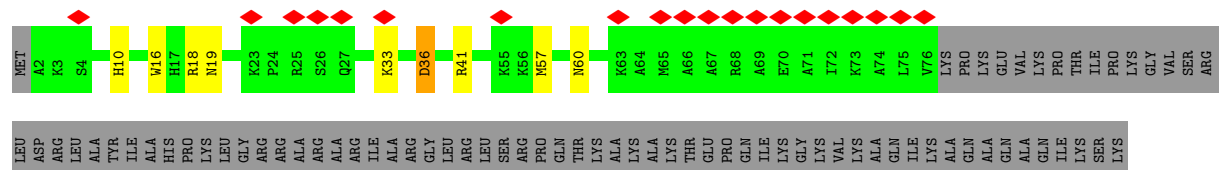
• Molecule 29: 60S ribosomal protein L27

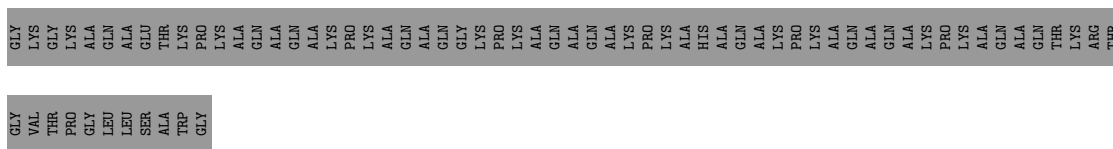


• Molecule 30: uL15

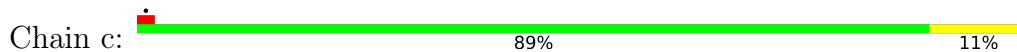


• Molecule 31: 60S ribosomal protein L29

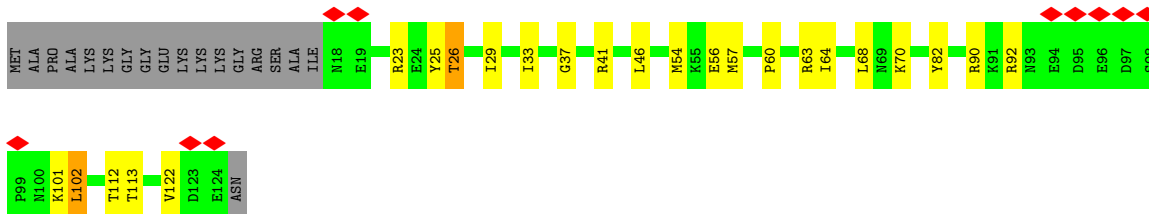




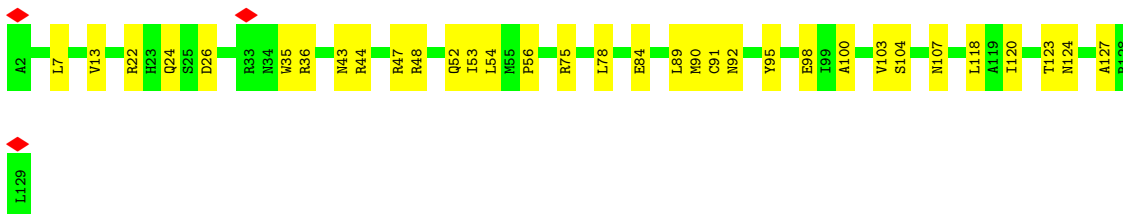
- Molecule 32: eL30



- Molecule 33: eL31



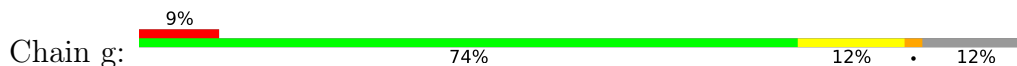
- Molecule 34: eL32



- Molecule 35: eL33

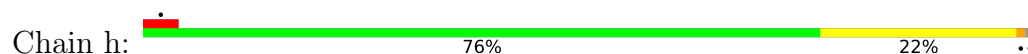


- Molecule 36: 60S ribosomal protein L34

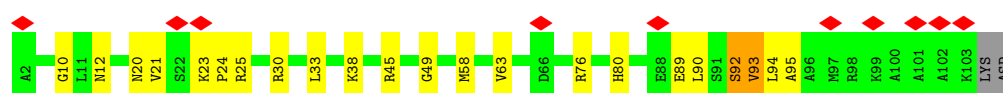
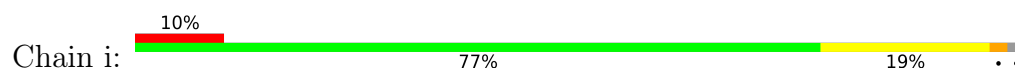




- Molecule 37: uL29



- Molecule 38: eL36



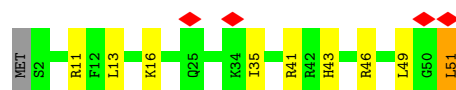
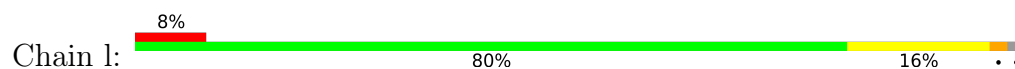
- Molecule 39: Ribosomal protein L37



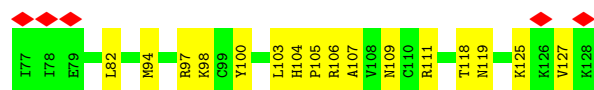
- Molecule 40: eL38



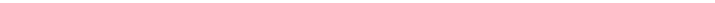
- Molecule 41: eL39



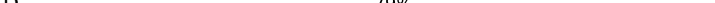
- Molecule 42: 60S RIBOSOMAL PROTEIN EL40



- Molecule 43: 60s ribosomal protein l41

- Chain o: 

Category	Number of Genes
MET	10
N3	9
V2	8
R9	7
C16	6
G16	5
K17	4
H18	3
Q19	2
P20	1
Y26	1
K27	1
K28	1
S32	1
G37	1
K38	1
R39	1
D42	1
R43	1
K44	1
Q45	1
Q51	1
T52	1
K61	1
V67	1
K80	1
H90	1
G95	1
D96	1
K97	1
K98	1
R99	1
K100	1
I104	1
O105	1

- Chain p: 

Category	Value
MET	1
A2	2
K3	3
R4	4
T5	5
K6	6
K7	7
V8	8
G9	9
R17	10
Y18	11
V26	12
T33	13
F41	14
C42	15
T45	16
V52	17
G53	18
B54	19
C57	20
G60	21
G66	22
W69	23
R85	24
E88	25
L89	26
K90	27
D91	28
D92	29

- Chain q: 

Lys	Thr	Gly	Gly	Ala	Asp	Gln	Ser	Ser	Leu	Gln	Gln	Gly	Glu	Gly	Ser		R14	F15	I16	C17	I18	V19	P20	A21	Y22	L23	N24	N25	K26	K27	T28	L29	A30	E31	G32	R33	R34	I35	P36	I37	S38	K39	A40	V41	E42	M43	P44	T45	A46	T47	E48	I49	Q50	D51	V52	C53	S54	A55	V56	G57	L58	M59	V60
F61	L62	E63	K64	N65	K66	H67	V68	S69	R70	E71	H72	M73	R74	D75	V76	Q77	Y78	R79	G80	R81	V82	R83	V84	Q85	L86	K87	Q88	E89	D90	G91	S92	L93	C94	V95	V96	Q97	R98	P99	S100	R101	K102	S103	V104	M105	L106	Y107	A108	A109	E110	M111	I112	P113	K114	L115	K116	T117							
Arg	Thr	Cys	Ala	Ala	Arg	Pro	Ala	Asp	Gln	R14	F15	I16	C17	I18	V19	P20	A21	Y22	L23	N24	N25	K26	K27	T28	L29	A30	E31	G32	R33	R34	I35	P36	I37	S38	K39	A40	V41	E42	M43	P44	T45	A46	T47	E48	I49	Q50	D51	V52	C53	S54	A55	V56	G57	L58	M59	V60							

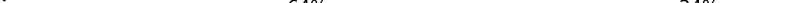
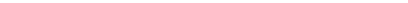
- Chain r: 

Figure 1: Schematic representation of the protein structure of the 120 kDa subunit of the 20S proteasome. The diagram shows a linear sequence of amino acids from Met1 to P104. Residues are color-coded: grey for Met1, yellow for residues 2-10, 11-21, 27-28, 33-35, 40-42, 44-45, 48, 56-57, 63-66, 67, 78-82, 86-89, 94-96, 102-103, and 104. Red diamonds indicate specific residues: Met1, S2, A3, I112, V10, S14, M125, V126, Lys127, D56, R67, and A86. The sequence is divided into two main regions: the N-terminal region (Met1 to Lys127) and the C-terminal region (Lys128 to P104).

- Chain s: 

PRO PRO
LEU LEU
GLU ASP
LYS LYS
LEU LEU
GLN GLN
LYS LYS
THR THR
LYS LYS
SER SER
GLY GLY
LEU LEU
THR THR
GLY GLY
TYR TYR
ILE ILE
LYS LYS
PHE PHE
GLY GLY
PHE PHE
ARG ARG
SER SER

• Molecule 51: Signal recognition particle receptor subunit beta

Chain v: 

MET
ALA
SER
SER
ALA
ASP
SER
SER
ARG
ARG
VAL
ALA
ASP
GLY
GLY
GLY
ALA
GLY
THR
PHE
GLN
PRO
TYR
LEU
ASP
THR
LEU
LEU
SER
VAL
VAL
VAL
VAL
LEU
ALA
VAL
VAL
D98
LEU
LEU
THR
LEU
VAL
VAL
TRP
LYS
ILE
ARG
SER
ARG

ARG
SER
SER
GLN
R65
A66
V67
L68
L69
L70
G71
L72
C73
D74
S75
G76
K77
L78
L79
L80
F81
V82
R83
L84
L85
L86
G87
L88
Y89
R90
D91
T92
Q93
T94
S95
I96
T97
D98
S99
C100
A101
Q102
V103
R104
V105
N106
N107
N108
R109
G110
N111
S112
L113
T114
L115
L116
D117
L118
P119
G120

H121
E122
S123
L124
L125
L126
Q127
F128
L129
E130
R131
F132
S133
S134
S135
A136
R137
A138
I139
V140
F141
V142
V143
D144
S145
A146
A147
F148
Q149
R150
E151
V152
K153
D154
V155
A156
E157
D158
F159
Y160
Q161
V162
L163
I164
D165
S166
M167
G168
L169
K170
M171
T172
P173
S174
F175
L176
I177
C179
N180

K181
Q182
D183
I184
A185
M186
A187
K188
S189
A190
K191
L192
L193
Q194
Q195
Q196
L197
E198
K199
E200
L201
N202
T203
L204
R205
V206
T207
ARG
SER
ALA
ALA
PRO
SER
THR
LEU
ASP
SER
SER
THR
ALA
PRO
ALA
GLN
LEU
GLY
LYS
G229
K230
E231
F232
E233
F234
S235
Q236
L237
P238
L239
K240

V241
E242
F243
L244
E245
C246
S247
A248
D249
G250
G251
G252
G253
D254
V255
G256
S257
A258
D259
I260
Q261
D262
L263
E264
K265
W266
L267
A268
K269
I270
A271

• Molecule 52: Signal recognition particle 9 kDa protein

Chain w: 

MET
P2
Q3
Y4
Q5
T6
W7
E8
E9
F10
S11
R12
A13
A14
E15
K16
L17
Y18
L19
A20
D21
P22
M23
K24
A25
R26
F27
V28
L29
K30
Y31
R32
H33
S34
D35
G36
N37
L38
C39
V40
K41
V42
T43
D44
D45
L46
V47
C48
L49
V50
Y51
K52
T53
D54
Q55
A56
Q57
D58
V59
K60

K61
I62
E63
K64
F65
H66
L72
M73
V74
A75
K76
GLU
ALA
ARG
ASN
VAL
THR
MET
GLU
THR
GLU

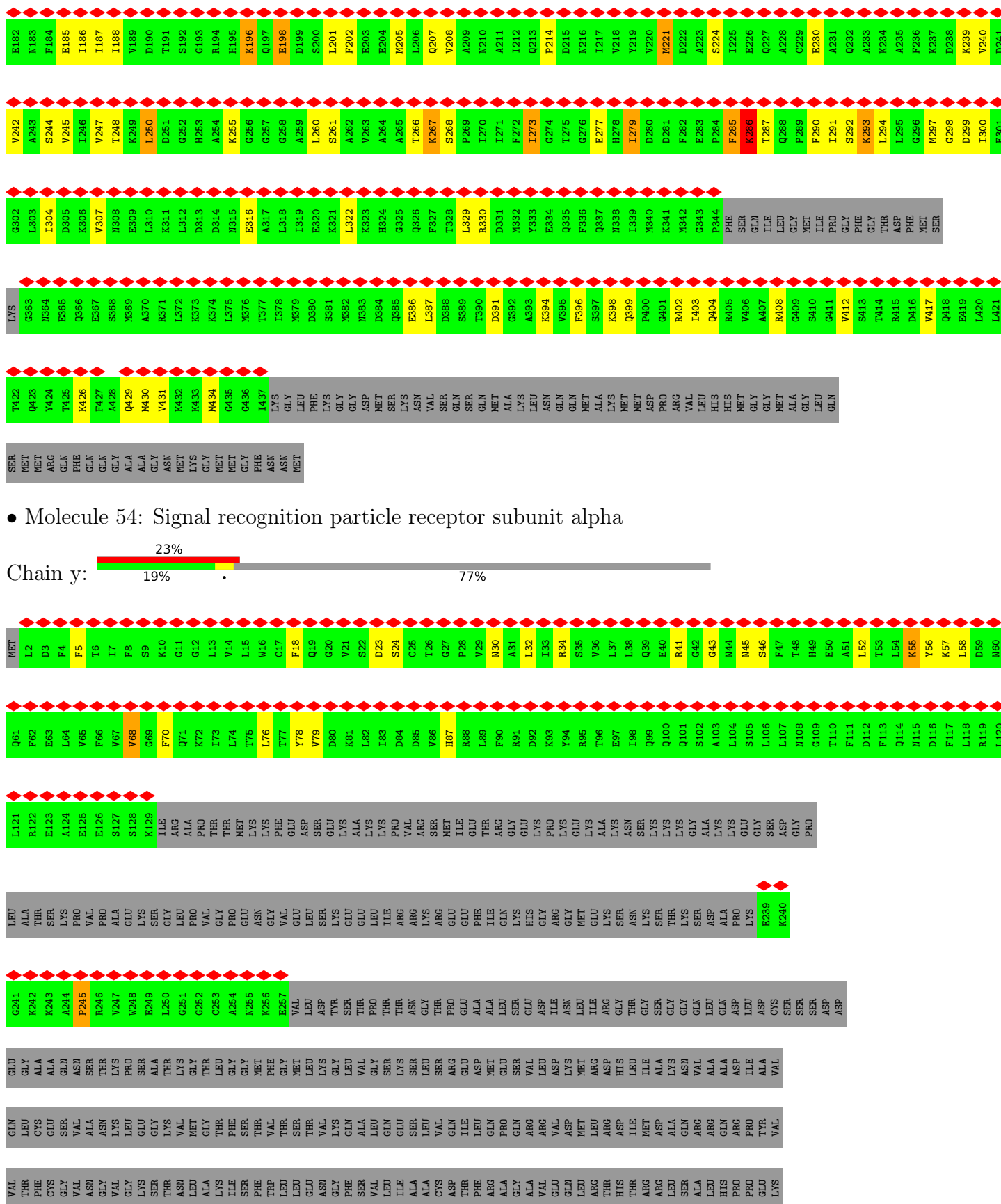
• Molecule 53: Signal recognition particle 54 kDa protein

Chain x: 

MET
VAL
L3
A4
D5
L6
G7
R8
K9
M10
T11
S12
A13
L14
R15
S16
L17
S18
N19
A20
T21
I22
I23
N24
E25
E26
V27
L28
N29
A30
M31
L32
K33
E34
V35
C36
T37
A38
L39
L40
E41
A42
D43
V44
M45
I46
K47
L48
V49
K50
Q51
S52
L53
E54
N55
V56
K57
S58
A59
I60

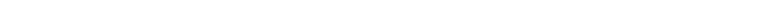
D61
L62
E63
E64
M65
A66
S67
G68
L69
N70
K71
R72
K73
M74
I75
Q76
H77
F80
K81
E82
L83
V84
K85
L86
V87
D88
P89
G90
V91
K92
A93
W94
T95
P96
T97
K98
G99
P100
Q101
N102
V103
I104
M105
F106
V107
G108
L109
Q110
G111
S112
G113
K114
E115
N116
V117
C118
S119
K120
L121

A122
Y123
Y124
Y125
Q126
R127
K128
G129
W130
K131
T132
C133
L134
I135
C136
A137
D138
T139
F140
R141
A142
G143
A144
F145
D146
Q147
L148
K149
Q150
N151
A152
T153
K154
A155
R156
I157
P158
F159
Y160
G161
S162
V163
T164
E165
M166
P168
V169
I170
I171
A172
S173
E174
G175
V176
E177
K178
F179
K180
N181



ILE	SER	MET	THR	THR	ILE	THR	SER	LYS	PRO	ILE	VAL	PHE	VAL	GLY	THR	GLY	GLN	THR	TYR	CYS	ASP	LEU	ARG	SER	LEU	ASN	ALA	LYS	ALA	VAL	VAL	ALA	ALA	LEU	MET	LYS	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 55: Signal recognition particle subunit SRP72

Chain z: 

PHE LYS GLY ALA ASN VAL ILE THR HIS THR LYS VAL LEU ASN SER PHE GLY LYS ALA ASN SER LEU TYR CYS ARG ARG ARG LEU ASN ILE GLY ASN ALA ASN GLN THR THR ASP LYS LEU LYS GLY LEU LEU TYR GLN VAL GLN LEU TYR

ASN	THR	ALA	ALA	CYS	ALA	LEU	ILE	GLY	GLN	GLN	LEU	ASN	ASN	GLN	ALA	MET	LYS	ILE	LEU	LEU	GLN	LYS	ALA	ALA	GLU	ASP	SER	SER	LEU	SER	ASP	THR	GLY	GLU	GLU	GLU	ASP	PRO	GLN	ALA	ALA	GLU	LEU	ALA	ILE	ILE	HIS	GLY	GLN	MET	ALA	ALA	TYR	ILE	LEU	GLN	LEU	GLN	LYS
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LYS	GLN	LEU	GLN	ALA	ILE	GLU	PHE	ASN	LYS	ASN	ALA	LEU	LEU	ALA	MET	TYR	THR	ASN	GLN	ALA	GLU	GLN	CYS	ARG	LYS	SER	ILE	SER	ALA	LEU	GLN	SER	SER	PRO	GLU	HIS	LEU	LEU	PRO	VAL	LEU	ILE	GLN	ALA	ALA	GLN	LEU	CYS	ARG	GLU	LYS	THR	HIS	GLN	ALA	ILE	GLU	GLU
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ASP	ILE	ASP	SER	ALA	ILE	GLU	VAL	PHE	THR	GLN	GLN	ALA	ILE	GLN	TRP	TYR	GLN	ASN	HIS	GLN	PRO	LYS	SER	SER	PRO	ALA	ALA	HIS	LEU	LEU	LEU	ILE	ARG	GLU	ALA	ALA	ASN	PHE	LYS	LYS	LEU	TYR	LYS	ARG	LYS	LYS	GLU	ALA	ALA	ILE	SER	ASP	GLN	GLN	ASN	PRO	LYS	SER
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[illegible]

GLN
LYS
LYS
LYS
LYS
GLY
GLY
LYS
GLY
GLY
TRP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32881	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	475.776, 475.776, 475.776	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.062, 1.062, 1.062	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.09	0/5971	0.24	0/9308
2	5	0.10	0/83726	0.25	1/130593 (0.0%)
3	7	0.07	0/2858	0.18	0/4455
4	8	0.08	0/3701	0.23	0/5766
5	A	0.12	0/1906	0.35	0/2556
6	B	0.10	0/3216	0.30	0/4311
7	C	0.11	0/2937	0.32	0/3946
8	D	0.10	0/2432	0.30	0/3257
9	E	0.13	0/1936	0.40	0/2600
10	F	0.11	0/1905	0.32	0/2539
11	G	0.12	0/1967	0.33	0/2647
12	H	0.11	0/1535	0.33	0/2063
13	I	0.11	0/1693	0.30	0/2260
14	J	0.10	0/1376	0.33	0/1841
15	L	0.12	0/1734	0.36	0/2317
16	M	0.11	0/1158	0.32	0/1547
17	N	0.12	0/1746	0.34	0/2338
18	O	0.11	0/1671	0.31	0/2234
19	P	0.11	0/1268	0.33	0/1700
20	Q	0.11	0/1530	0.33	0/2041
21	R	0.11	0/1524	0.32	0/2013
22	S	0.11	0/1493	0.32	0/2002
23	T	0.11	0/1326	0.31	0/1770
24	U	0.10	0/822	0.32	0/1103
25	V	0.11	0/993	0.30	0/1332
26	W	0.10	0/541	0.29	0/720
27	X	0.10	0/993	0.28	0/1334
28	Y	0.11	0/1132	0.32	0/1504
29	Z	0.11	0/1130	0.34	0/1507
30	a	0.11	0/1191	0.31	0/1590
31	b	0.09	0/619	0.26	0/818
32	c	0.09	0/742	0.24	0/996

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.10	0/903	0.33	0/1216
34	e	0.10	0/1071	0.29	0/1429
35	f	0.11	0/895	0.38	0/1198
36	g	0.10	0/916	0.31	0/1220
37	h	0.10	0/1021	0.29	0/1348
38	i	0.13	0/841	0.41	0/1112
39	j	0.11	0/720	0.32	0/952
40	k	0.12	0/575	0.39	0/761
41	l	0.12	0/454	0.35	0/599
42	m	0.10	0/435	0.32	0/575
43	n	0.11	0/223	0.37	0/284
44	o	0.11	0/864	0.35	0/1140
45	p	0.10	0/718	0.33	0/953
46	q	0.10	0/856	0.30	0/1152
47	r	0.14	0/1017	0.41	0/1364
49	t	0.11	0/699	0.28	0/932
50	u	0.11	0/1665	0.28	0/2229
51	v	0.10	0/1472	0.28	0/1979
52	w	0.09	0/634	0.27	0/851
53	x	0.83	0/3278	1.03	1/4401 (0.0%)
54	y	0.13	0/1151	0.36	1/1553 (0.1%)
55	z	0.15	0/168	0.38	0/231
All	All	0.15	0/159348	0.31	3/234487 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	B	0	1
22	S	0	1
35	f	0	1
53	x	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	y	245	PRO	N-CA-CB	7.23	110.84	103.25
53	x	285	PHE	CA-C-O	-5.17	113.11	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	5061	A	P-O3'-C3'	5.08	127.81	120.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	17	LEU	Peptide
22	S	164	LYS	Peptide
35	f	106	TYR	Peptide
53	x	298	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	5341	0	2701	74	0
2	5	74854	0	37828	1288	0
3	7	2558	0	1296	32	0
4	8	3314	0	1683	56	0
5	A	1868	0	1959	48	0
6	B	3148	0	3267	73	0
7	C	2883	0	3053	63	0
8	D	2386	0	2419	42	0
9	E	1898	0	2035	69	0
10	F	1870	0	1994	38	0
11	G	1934	0	2085	45	0
12	H	1516	0	1597	22	0
13	I	1655	0	1704	27	0
14	J	1353	0	1386	23	0
15	L	1703	0	1820	34	0
16	M	1137	0	1211	24	0
17	N	1701	0	1749	36	0
18	O	1638	0	1777	34	0
19	P	1242	0	1274	21	0
20	Q	1506	0	1623	27	0
21	R	1508	0	1664	26	0
22	S	1454	0	1496	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	T	1298	0	1366	30	0
24	U	808	0	831	12	0
25	V	979	0	1039	19	0
26	W	528	0	541	14	0
27	X	976	0	1053	22	0
28	Y	1115	0	1205	28	0
29	Z	1107	0	1182	20	0
30	a	1162	0	1209	28	0
31	b	609	0	650	8	0
32	c	732	0	769	8	0
33	d	888	0	930	14	0
34	e	1053	0	1147	23	0
35	f	876	0	912	24	0
36	g	906	0	998	16	0
37	h	1013	0	1147	20	0
38	i	830	0	916	17	0
39	j	705	0	737	17	0
40	k	569	0	637	12	0
41	l	444	0	483	7	0
42	m	429	0	465	12	0
43	n	222	0	264	2	0
44	o	851	0	920	15	0
45	p	708	0	756	16	0
46	q	842	0	873	13	0
47	r	1001	0	1060	23	0
48	s	105	0	24	0	0
49	t	693	0	734	14	0
50	u	1637	0	1652	19	0
51	v	1455	0	1496	19	0
52	w	623	0	636	8	0
53	x	3236	0	3308	50	0
54	y	1133	0	1081	14	0
55	z	161	0	159	2	0
56	g	1	0	0	0	0
56	j	1	0	0	0	0
56	m	1	0	0	0	0
56	o	1	0	0	0	0
56	p	1	0	0	0	0
57	v	1	0	0	0	0
57	x	1	0	0	0	0
58	v	32	0	12	1	0
59	x	32	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	148232	0	108826	2233	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 2233 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:1444:G:N2	2:5:2100:A:H62	1.48	1.12
2:5:1444:G:H21	2:5:2100:A:N6	1.52	1.06
2:5:2845:A:H61	2:5:3843:C:N4	1.52	1.05
2:5:2845:A:N6	2:5:3843:C:H42	1.55	1.03
2:5:4421:C:H42	2:5:4475:G:N2	1.67	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	242/245 (99%)	225 (93%)	17 (7%)	0	100	100
6	B	392/403 (97%)	379 (97%)	13 (3%)	0	100	100
7	C	360/413 (87%)	345 (96%)	15 (4%)	0	100	100
8	D	290/297 (98%)	278 (96%)	12 (4%)	0	100	100
9	E	232/291 (80%)	198 (85%)	34 (15%)	0	100	100
10	F	223/225 (99%)	217 (97%)	6 (3%)	0	100	100
11	G	239/319 (75%)	225 (94%)	14 (6%)	0	100	100
12	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
13	I	200/214 (94%)	194 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	J	167/178 (94%)	155 (93%)	12 (7%)	0	100	100
15	L	208/210 (99%)	191 (92%)	16 (8%)	1 (0%)	24	59
16	M	136/218 (62%)	132 (97%)	4 (3%)	0	100	100
17	N	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
18	O	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
19	P	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
20	Q	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
21	R	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
22	S	173/175 (99%)	166 (96%)	7 (4%)	0	100	100
23	T	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
24	U	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
25	V	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
26	W	61/63 (97%)	61 (100%)	0	0	100	100
27	X	117/156 (75%)	114 (97%)	3 (3%)	0	100	100
28	Y	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
29	Z	133/136 (98%)	122 (92%)	11 (8%)	0	100	100
30	a	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
31	b	73/223 (33%)	70 (96%)	3 (4%)	0	100	100
32	c	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
33	d	105/125 (84%)	101 (96%)	4 (4%)	0	100	100
34	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
35	f	107/110 (97%)	100 (94%)	7 (6%)	0	100	100
36	g	112/129 (87%)	112 (100%)	0	0	100	100
37	h	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
38	i	100/104 (96%)	94 (94%)	4 (4%)	2 (2%)	6	31
39	j	84/97 (87%)	84 (100%)	0	0	100	100
40	k	67/69 (97%)	58 (87%)	9 (13%)	0	100	100
41	l	48/51 (94%)	42 (88%)	6 (12%)	0	100	100
42	m	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
43	n	21/25 (84%)	21 (100%)	0	0	100	100
44	o	102/105 (97%)	94 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	p	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
46	q	102/144 (71%)	97 (95%)	5 (5%)	0	100	100
47	r	123/137 (90%)	111 (90%)	11 (9%)	1 (1%)	16	50
49	t	84/136 (62%)	83 (99%)	1 (1%)	0	100	100
50	u	194/627 (31%)	188 (97%)	6 (3%)	0	100	100
51	v	182/271 (67%)	180 (99%)	2 (1%)	0	100	100
52	w	74/86 (86%)	74 (100%)	0	0	100	100
53	x	413/504 (82%)	377 (91%)	30 (7%)	6 (2%)	8	37
54	y	143/638 (22%)	126 (88%)	16 (11%)	1 (1%)	18	52
55	z	17/671 (2%)	13 (76%)	4 (24%)	0	100	100
All	All	7561/10091 (75%)	7180 (95%)	370 (5%)	11 (0%)	49	79

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	i	92	SER
53	x	96	PRO
53	x	286	LYS
54	y	245	PRO
38	i	93	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	187/188 (100%)	181 (97%)	6 (3%)	34	65
6	B	336/348 (97%)	328 (98%)	8 (2%)	43	70
7	C	302/337 (90%)	299 (99%)	3 (1%)	68	80
8	D	247/250 (99%)	241 (98%)	6 (2%)	43	70
9	E	208/251 (83%)	198 (95%)	10 (5%)	23	56
10	F	194/195 (100%)	188 (97%)	6 (3%)	35	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	G	206/273 (76%)	197 (96%)	9 (4%)	25	59
12	H	169/171 (99%)	160 (95%)	9 (5%)	20	53
13	I	174/181 (96%)	168 (97%)	6 (3%)	32	64
14	J	142/149 (95%)	141 (99%)	1 (1%)	76	83
15	L	176/176 (100%)	171 (97%)	5 (3%)	38	68
16	M	117/160 (73%)	110 (94%)	7 (6%)	17	50
17	N	171/172 (99%)	164 (96%)	7 (4%)	27	60
18	O	171/171 (100%)	165 (96%)	6 (4%)	32	64
19	P	134/134 (100%)	132 (98%)	2 (2%)	57	76
20	Q	163/163 (100%)	158 (97%)	5 (3%)	35	66
21	R	159/159 (100%)	156 (98%)	3 (2%)	50	73
22	S	156/156 (100%)	153 (98%)	3 (2%)	50	73
23	T	139/140 (99%)	136 (98%)	3 (2%)	45	71
24	U	89/89 (100%)	87 (98%)	2 (2%)	45	71
25	V	101/107 (94%)	97 (96%)	4 (4%)	28	61
26	W	55/55 (100%)	55 (100%)	0	100	100
27	X	107/134 (80%)	105 (98%)	2 (2%)	50	73
28	Y	124/135 (92%)	120 (97%)	4 (3%)	34	65
29	Z	117/118 (99%)	112 (96%)	5 (4%)	26	59
30	a	119/120 (99%)	119 (100%)	0	100	100
31	b	62/170 (36%)	60 (97%)	2 (3%)	34	65
32	c	79/79 (100%)	78 (99%)	1 (1%)	61	78
33	d	98/110 (89%)	93 (95%)	5 (5%)	21	54
34	e	114/114 (100%)	111 (97%)	3 (3%)	40	69
35	f	88/89 (99%)	85 (97%)	3 (3%)	32	64
36	g	98/109 (90%)	94 (96%)	4 (4%)	27	60
37	h	109/110 (99%)	104 (95%)	5 (5%)	24	58
38	i	86/88 (98%)	84 (98%)	2 (2%)	44	70
39	j	73/80 (91%)	71 (97%)	2 (3%)	39	68
40	k	64/64 (100%)	59 (92%)	5 (8%)	11	41
41	l	47/48 (98%)	45 (96%)	2 (4%)	26	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	m	48/48 (100%)	47 (98%)	1 (2%)	47	71
43	n	22/24 (92%)	21 (96%)	1 (4%)	24	58
44	o	92/93 (99%)	91 (99%)	1 (1%)	65	79
45	p	74/75 (99%)	71 (96%)	3 (4%)	27	60
46	q	93/121 (77%)	91 (98%)	2 (2%)	45	71
47	r	109/121 (90%)	102 (94%)	7 (6%)	16	48
49	t	78/106 (74%)	77 (99%)	1 (1%)	61	78
50	u	172/529 (32%)	169 (98%)	3 (2%)	53	75
51	v	160/229 (70%)	158 (99%)	2 (1%)	61	78
52	w	69/78 (88%)	68 (99%)	1 (1%)	59	77
53	x	352/421 (84%)	270 (77%)	82 (23%)	1	5
54	y	116/533 (22%)	114 (98%)	2 (2%)	53	75
55	z	19/572 (3%)	19 (100%)	0	100	100
All	All	6585/8543 (77%)	6323 (96%)	262 (4%)	29	61

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	x	202	PHE
53	x	244	SER
54	y	55	LYS
21	R	50	ILE
20	Q	95	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
28	Y	72	GLN
54	y	49	HIS
34	e	117	GLN
54	y	45	ASN
52	w	66	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	245/299 (81%)	50 (20%)	6 (2%)
2	5	3478/3493 (99%)	738 (21%)	87 (2%)
3	7	119/120 (99%)	14 (11%)	0
4	8	155/156 (99%)	34 (21%)	1 (0%)
All	All	3997/4068 (98%)	836 (20%)	94 (2%)

5 of 836 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	G
1	1	17	C
1	1	29	C
1	1	32	A
1	1	33	G

5 of 94 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	2256	C
2	5	3904	G
2	5	2260	C
2	5	2661	U
2	5	4232	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	$\# Z > 2$
59	GNP	x	601	57	34,34,34	1.29	5 (14%)	47,54,54	0.57	0
58	GTP	v	301	57	33,34,34	0.91	1 (3%)	50,54,54	1.69	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GNP	x	601	57	-	6/18/38/38	0/3/3/3
58	GTP	v	301	57	-	3/22/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	x	601	GNP	PB-O3A	4.19	1.64	1.59
59	x	601	GNP	PB-O1B	3.18	1.51	1.46
59	x	601	GNP	PG-N3B	3.08	1.71	1.63
59	x	601	GNP	PG-O1G	2.92	1.50	1.46
59	x	601	GNP	PB-O2B	-2.24	1.50	1.56

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	v	301	GTP	C5-C4-N3	-5.56	119.54	128.39
58	v	301	GTP	C2-N3-C4	4.93	120.79	112.30
58	v	301	GTP	N9-C4-N3	3.64	133.23	125.95
58	v	301	GTP	C2-N1-C6	-2.98	119.70	125.11
58	v	301	GTP	C5-C6-N1	2.53	119.69	113.25

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	x	601	GNP	PG-N3B-PB-O1B
59	x	601	GNP	PG-N3B-PB-O3A
59	x	601	GNP	C5'-O5'-PA-O1A
59	x	601	GNP	O4'-C4'-C5'-O5'

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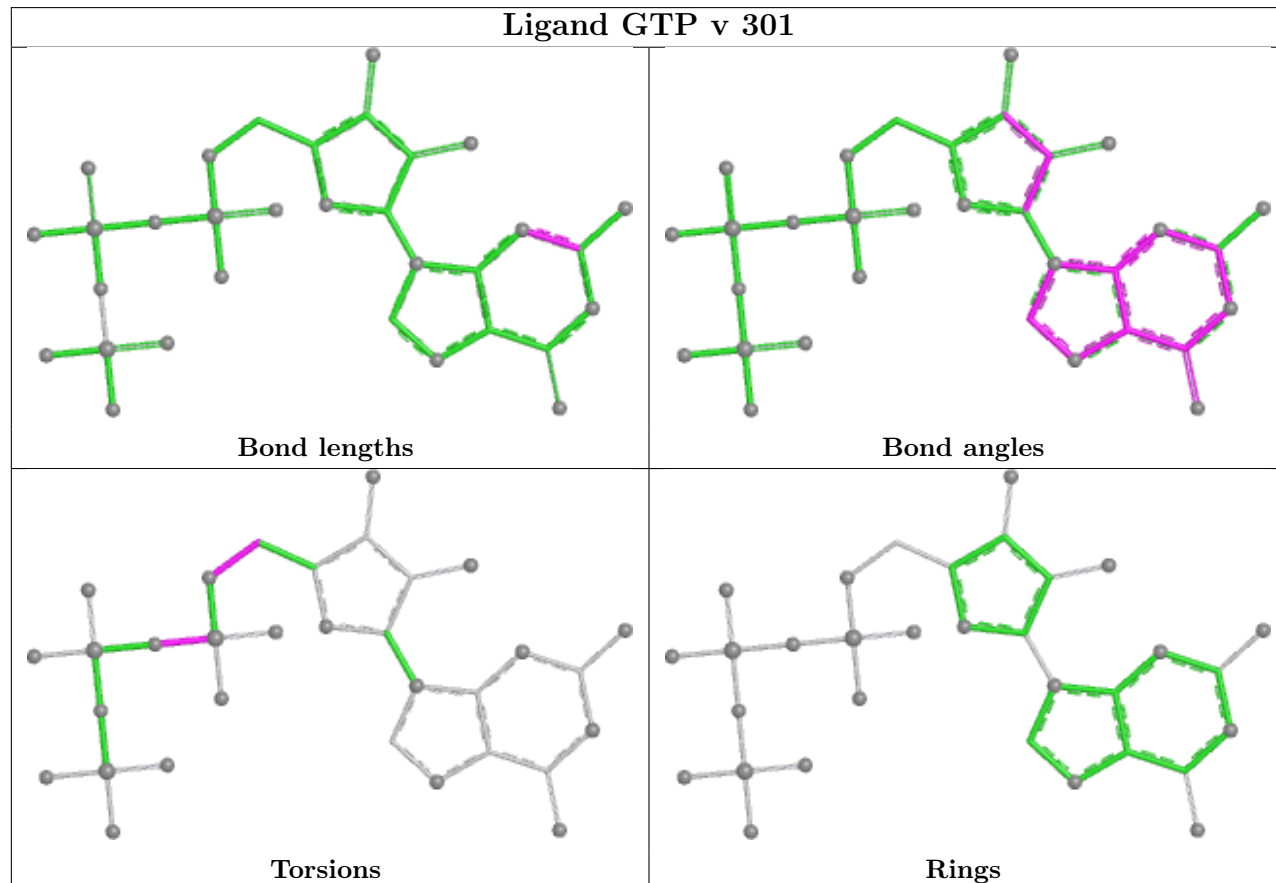
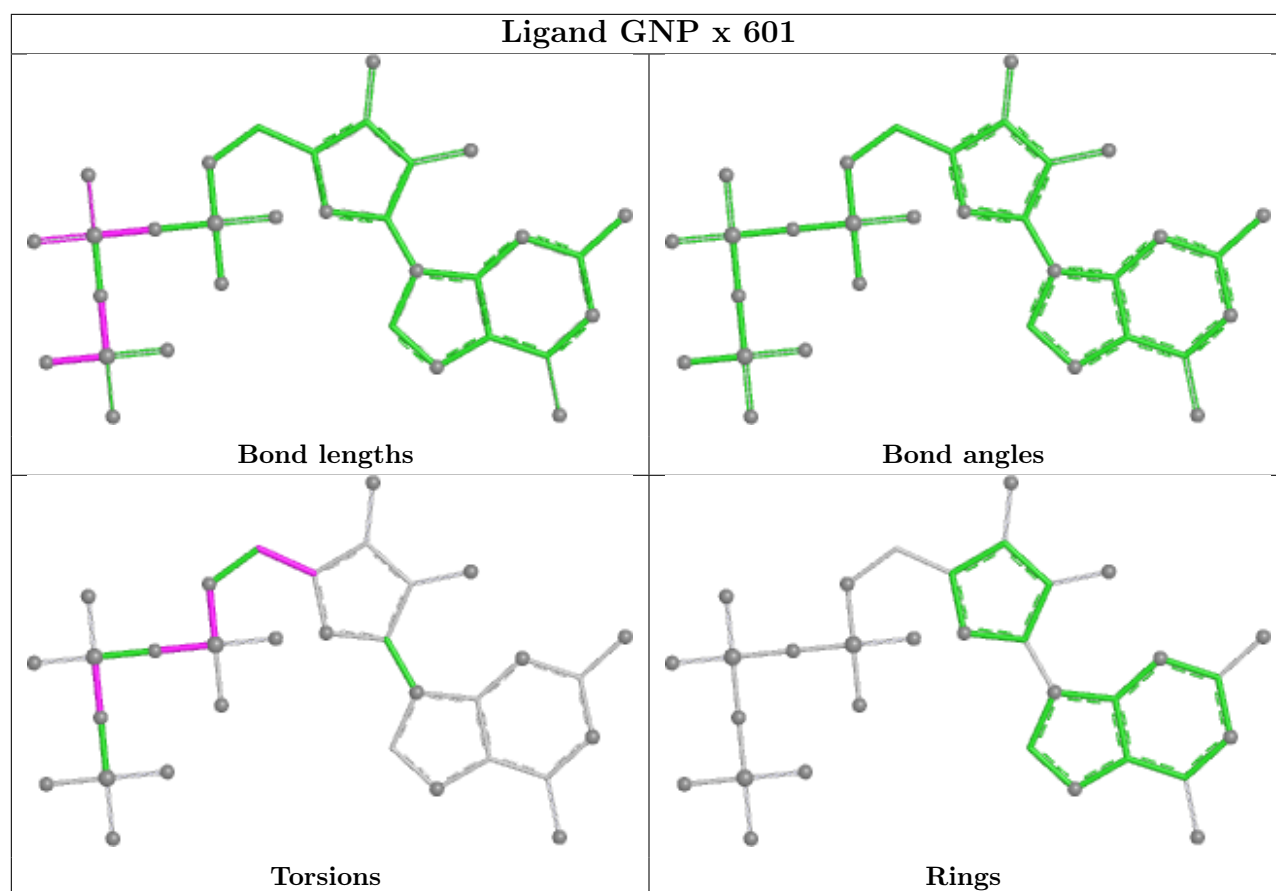
Mol	Chain	Res	Type	Atoms
58	v	301	GTP	PB-O3A-PA-O1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	x	601	GNP	1	0
58	v	301	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	5	15
1	1	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	462:G	O3'	467:U	P	20.97
1	5	4776:G	O3'	4859:C	P	17.65
1	5	4097:G	O3'	4112:C	P	17.38
1	5	2910:G	O3'	3583:U	P	17.30
1	5	757:G	O3'	906:C	P	17.29

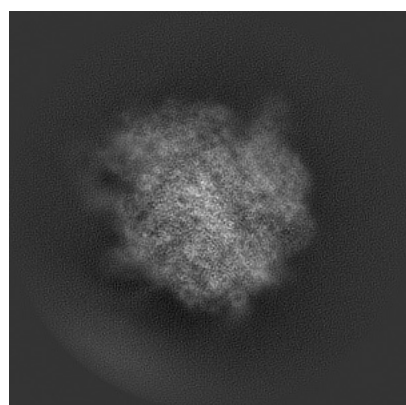
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12303. These allow visual inspection of the internal detail of the map and identification of artifacts.

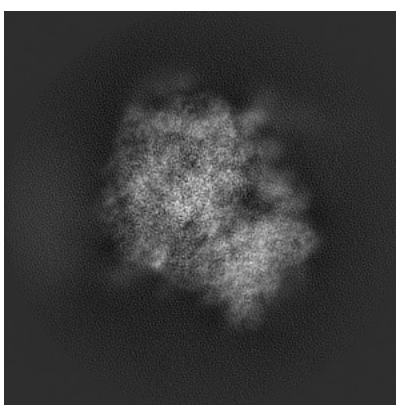
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

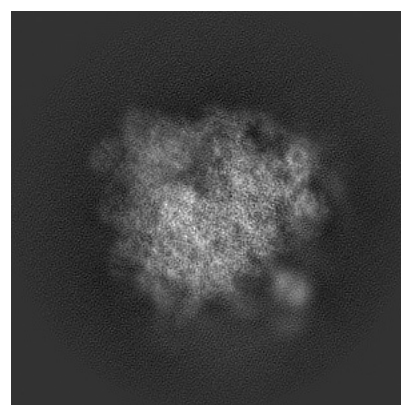
6.1.1 Primary map



X



Y

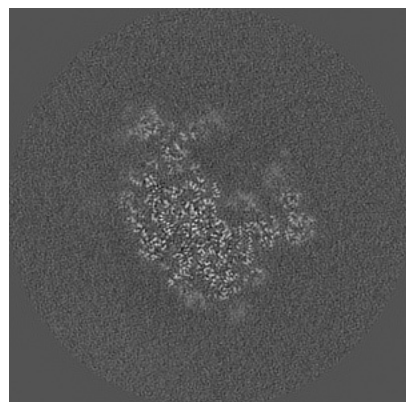


Z

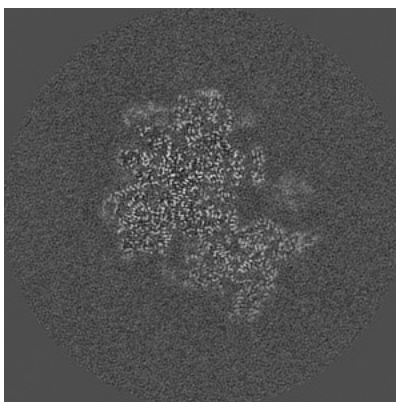
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

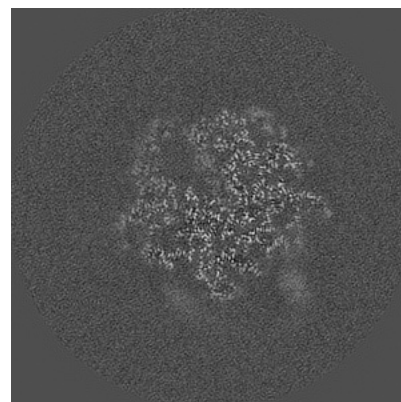
6.2.1 Primary map



X Index: 224



Y Index: 224

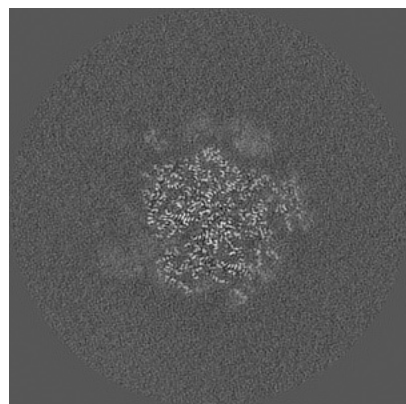


Z Index: 224

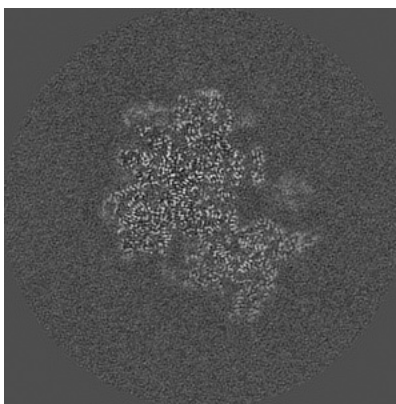
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

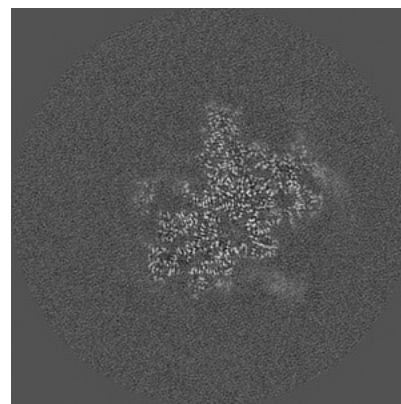
6.3.1 Primary map



X Index: 259



Y Index: 224

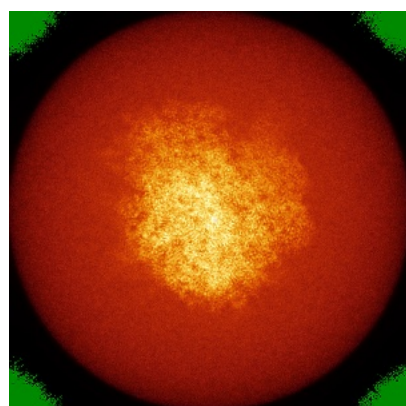


Z Index: 195

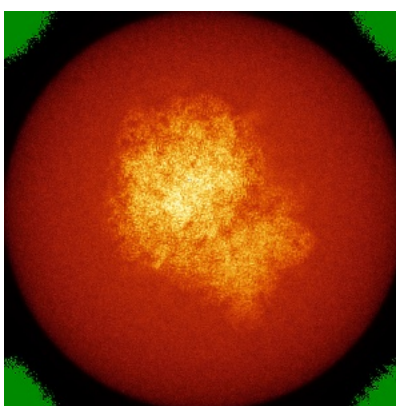
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

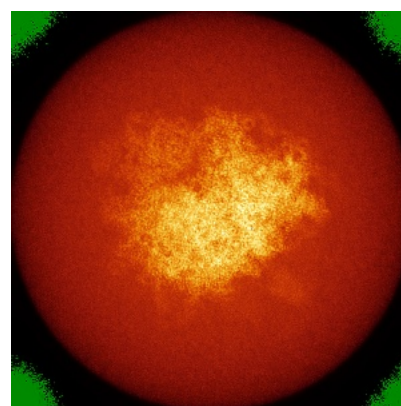
6.4.1 Primary map



X



Y

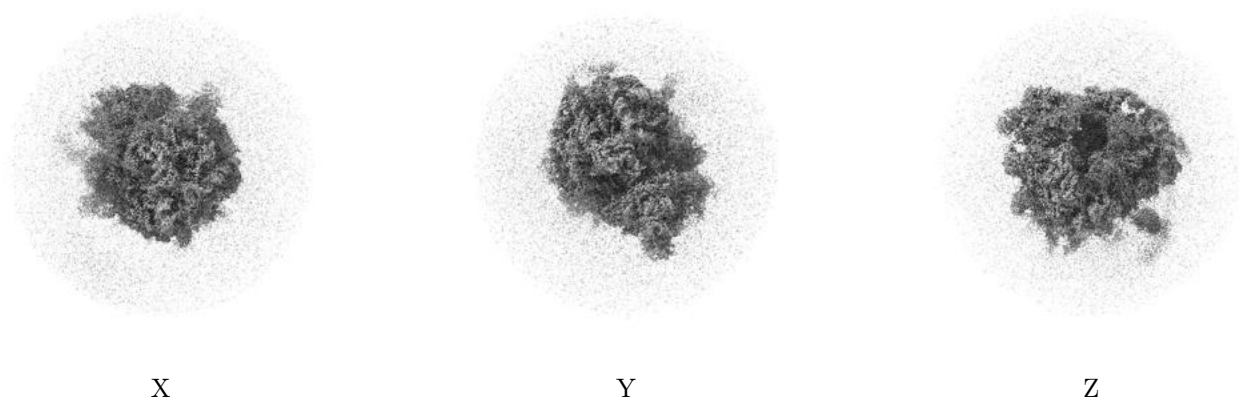


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

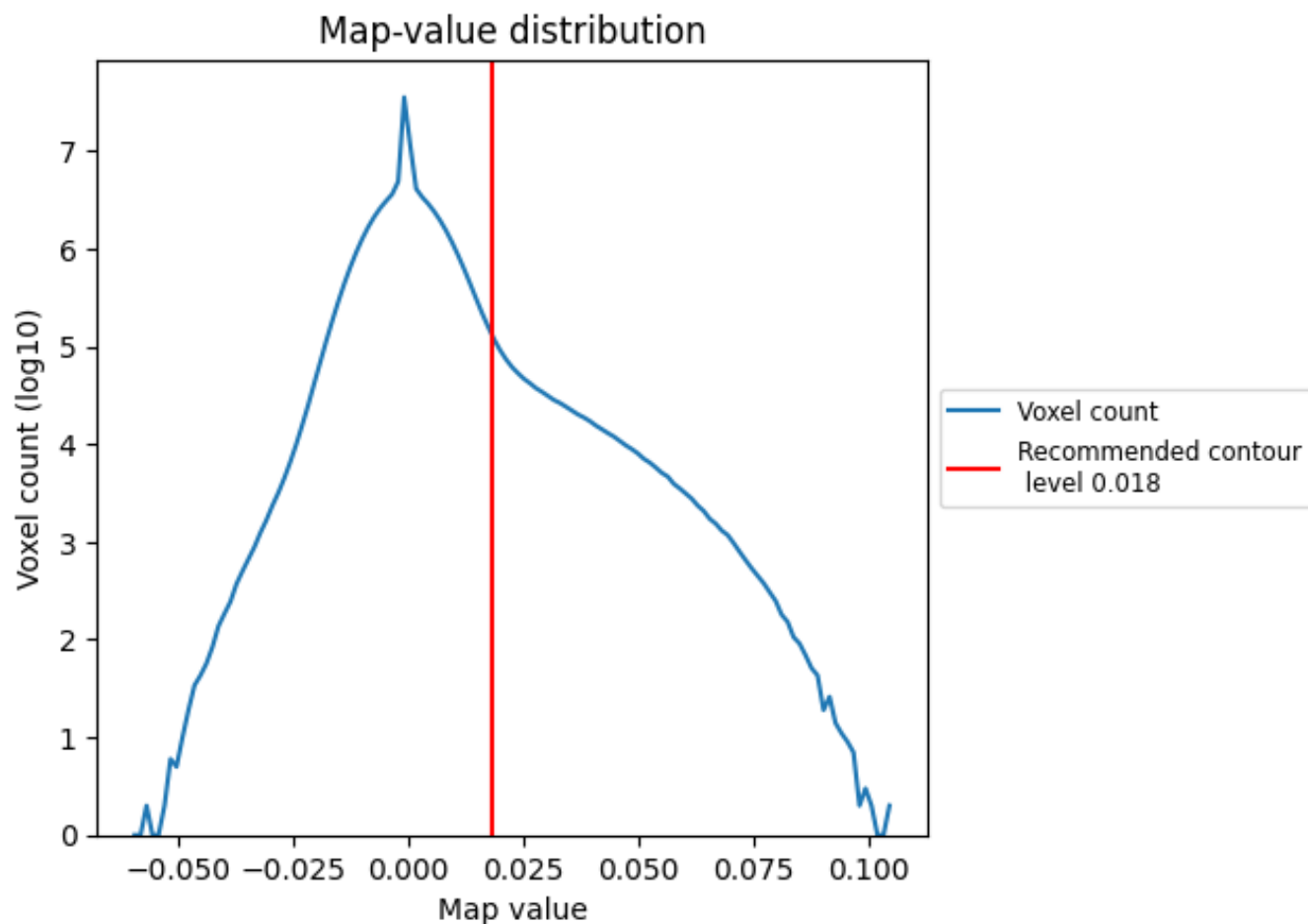
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

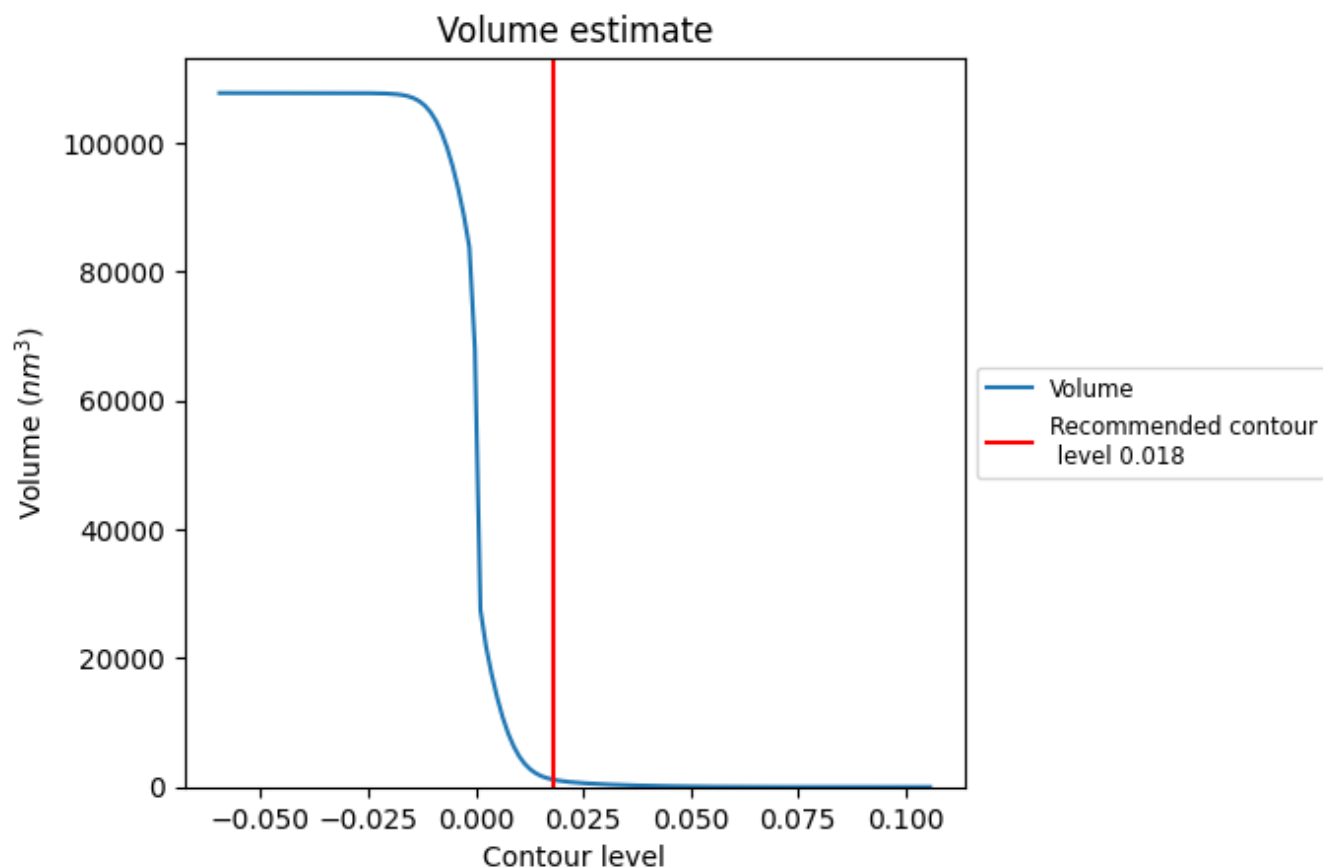
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

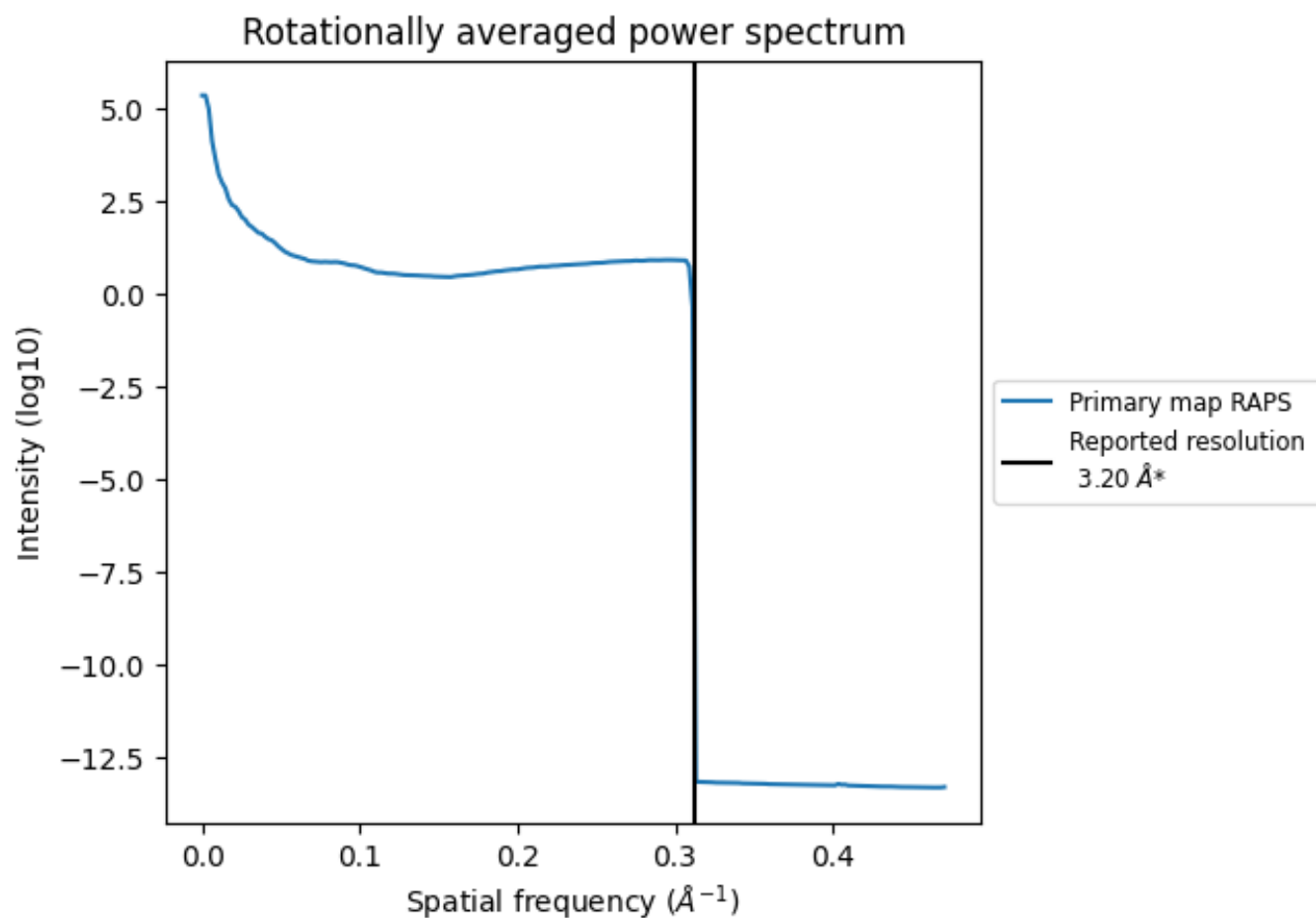
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1146 nm³; this corresponds to an approximate mass of 1035 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation

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

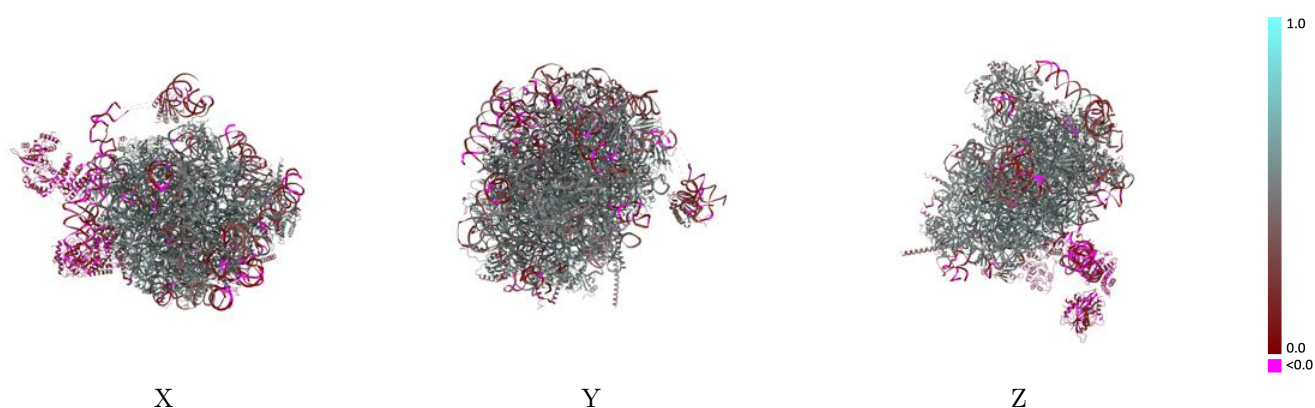
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12303 and PDB model 7NFX. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)

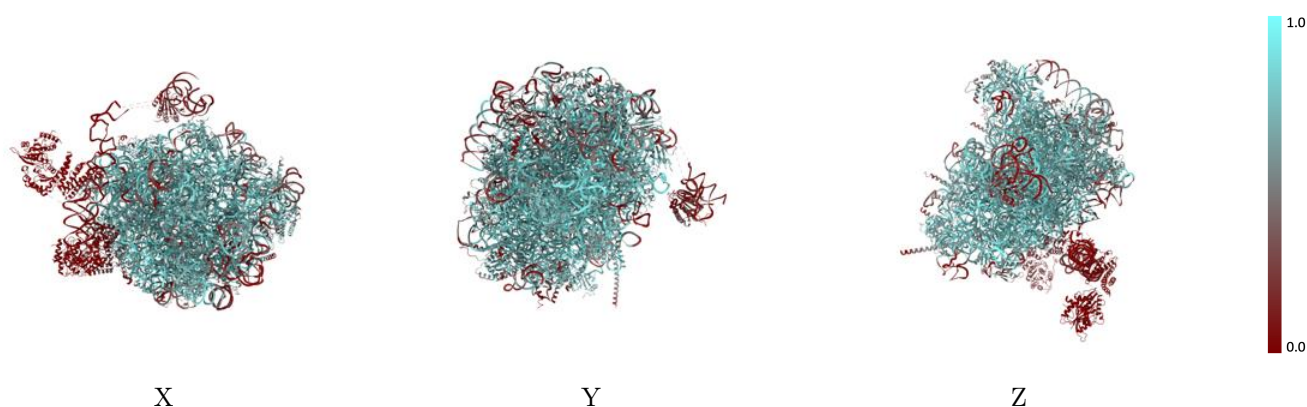
This section was not generated.

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



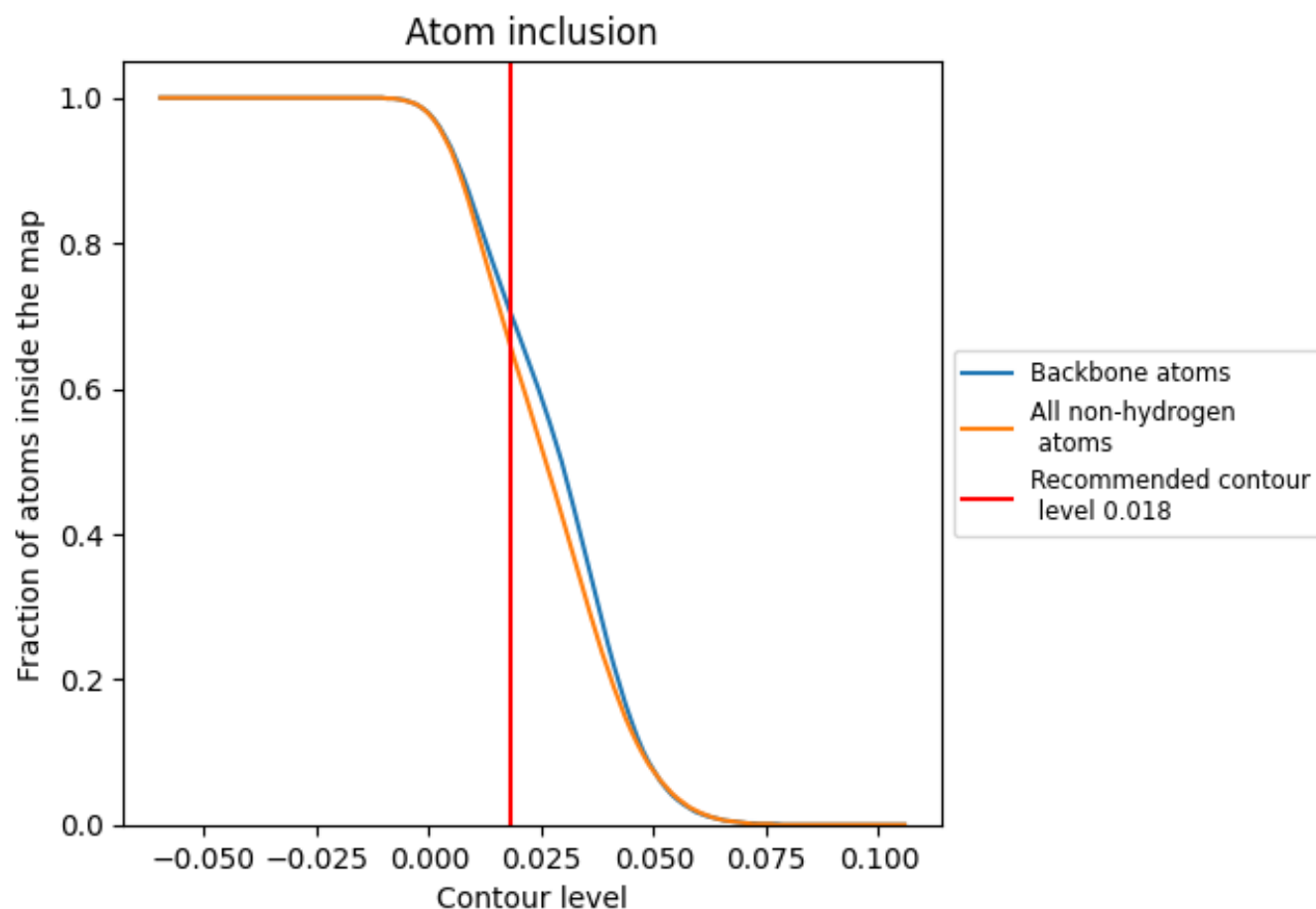
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 66% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6620	 0.4320
1	 0.0850	 0.0720
5	 0.7430	 0.4430
7	 0.8460	 0.4990
8	 0.7720	 0.4660
A	 0.7610	 0.5380
B	 0.7500	 0.5330
C	 0.7390	 0.5180
D	 0.6490	 0.4730
E	 0.6030	 0.4290
F	 0.7460	 0.5160
G	 0.5920	 0.4500
H	 0.6620	 0.4970
I	 0.7070	 0.4970
J	 0.5620	 0.4360
L	 0.6530	 0.4810
M	 0.7190	 0.5120
N	 0.7880	 0.5400
O	 0.7470	 0.5210
P	 0.7500	 0.5410
Q	 0.7630	 0.5250
R	 0.6810	 0.4920
S	 0.7440	 0.5180
T	 0.6830	 0.4940
U	 0.5580	 0.4470
V	 0.7340	 0.5280
W	 0.7150	 0.5250
X	 0.6920	 0.4980
Y	 0.7290	 0.5210
Z	 0.6990	 0.4930
a	 0.7710	 0.5330
b	 0.6040	 0.4410
c	 0.7060	 0.5000
d	 0.6870	 0.5070
e	 0.7760	 0.5450



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Chain	Atom inclusion	Q-score
f	 0.7740	 0.5370
g	 0.7170	 0.5110
h	 0.6810	 0.4990
i	 0.6340	 0.4600
j	 0.8010	 0.5320
k	 0.5910	 0.4400
l	 0.7350	 0.5220
m	 0.7120	 0.4930
n	 0.7070	 0.4920
o	 0.6750	 0.4910
p	 0.7160	 0.5190
q	 0.0280	 0.1090
r	 0.7260	 0.5140
s	 0.0290	 0.0640
t	 0.2060	 0.3110
u	 0.0310	 0.0940
v	 0.0030	 0.1180
w	 0.1740	 0.2720
x	 0.0670	 0.1390
y	 0.0100	 0.0960
z	 0.0130	 0.0740