



## Full wwPDB EM Validation Report ⓘ

Feb 16, 2023 – 04:12 pm GMT

PDB ID : 6GSM  
EMDB ID : EMD-0057  
Title : Structure of a partial yeast 48S preinitiation complex in open conformation  
Authors : Llacer, J.L.; Hussain, T.; Gordiyenko, Y.; Ramakrishnan, V.  
Deposited on : 2018-06-14  
Resolution : 5.20 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

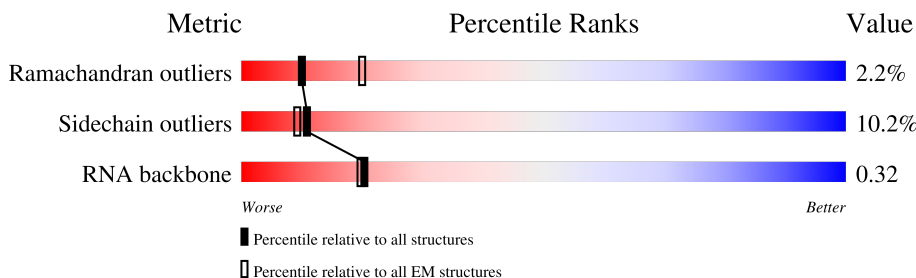
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.20 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)
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	1	76	
2	2	1798	
3	A	208	
4	3	3	
5	B	231	
6	C	217	
7	D	223	
8	E	260	

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Mol	Chain	Length	Quality of chain
9	F	206	47% 84% 16%
10	G	226	38% 86% 14%
11	H	184	43% 77% 22%
12	I	200	38% 84% 10% 6%
13	J	182	27% 86% 14%
14	K	96	58% 92% 8%
15	L	155	39% 90% 10%
16	M	118	86% 88% 11%
17	N	150	25% 90% 10%
18	O	127	28% 93% 6%
19	P	119	69% 85% 15%
20	Q	141	38% 87% 13%
21	R	125	46% 74% 14% 11%
22	S	145	51% 86% 14%
23	T	143	36% 91% 9%
24	U	106	64% 94% 6%
25	V	87	38% 90% 9%
26	W	129	28% 90% 9%
27	X	144	41% 86% 13%
28	Y	134	25% 89% 11%
29	Z	70	80% 94% 6%
30	a	98	38% 92% 8%
31	b	81	46% 89% 11%
32	c	62	61% 87% 13%
33	d	53	43% 96%

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Mol	Chain	Length	Quality of chain
34	e	58	
35	f	69	
36	g	324	
37	h	25	
38	i	95	
39	j	263	
40	k	430	
41	l	144	
42	m	96	
43	o	567	
44	p	651	
45	q	665	
46	s	342	
47	r	49	

## 2 Entry composition [i](#)

There are 51 unique types of molecules in this entry. The entry contains 103158 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 Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	74	1617	724	293	525	75	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1798	38175	17061	6721	12595	1798	0	0

- Molecule 3 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	208	1626	1040	286	298	2	0	0

- Molecule 4 is a RNA chain called mRNA (5'-R(P\*AP\*AP\*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	3	64	29	12	20	3	0	0

- Molecule 5 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	222	1769	1117	324	325	3	0	0

- Molecule 6 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	217	1629	1041	287	297	4	0	0

- Molecule 7 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 8 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 9 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 10 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 11 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	184	Total	C	N	O	S	0	0
			1483	950	270	263			

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 14 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	K	96	809	533	129	146	1	0	0

- Molecule 15 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	L	155	1248	798	237	210	3	0	0

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	M	117	885	553	161	171		0	0

- Molecule 17 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	N	150	1187	756	223	206	2	0	0

- Molecule 18 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	O	127	942	578	188	173	3	0	0

- Molecule 19 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	119	943	604	171	163	5	0	0

- Molecule 20 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Q	141	1105	709	204	192		0	0

- Molecule 21 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	111	Total	C	N	O	S	0	0
			892	554	165	170	3		

- Molecule 22 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 23 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 24 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 25 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 26 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 27 is a protein called KLLA0B11231p.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 28 is a protein called 40S ribosomal protein S24.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 29 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 30 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	98	Total	C	N	O	S	0	0
			779	480	165	129	5		

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	62	Total	C	N	O	S	0	0
			487	301	97	88	1		

- Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	58	Total	C	N	O	S	0	0
			463	290	94	78	1		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 36 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	309	Total	C	N	O	S	0	0
			2403	1526	419	453	5		

- Molecule 37 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 38 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	95	Total	C	N	O	S	0	0
			765	475	142	143	5		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	414	Total	C	N	O	S	0	0
			3123	1985	560	562	16		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	130	Total	C	N	O	S	0	0
			1048	669	188	184	7		

- Molecule 42 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	m	96	736	464	134	134	4	0	0

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit A, Eukaryotic translation initiation factor 3 subunit A, eIF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	528	4051	2587	695	762	7	0	0

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	651	5092	3259	881	935	17	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	?	-	ALA	deletion	UNP P06103
p	?	-	SER	deletion	UNP P06103
p	?	-	ILE	deletion	UNP P06103
p	?	-	ALA	deletion	UNP P06103
p	?	-	GLN	deletion	UNP P06103
p	?	-	PHE	deletion	UNP P06103
p	?	-	ASP	deletion	UNP P06103
p	?	-	LEU	deletion	UNP P06103
p	?	-	ILE	deletion	UNP P06103
p	?	-	LEU	deletion	UNP P06103

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	q	665	5051	3212	857	970	12	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	?	-	ASP	deletion	UNP P32497
q	?	-	LYS	deletion	UNP P32497
q	?	-	ASN	deletion	UNP P32497

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Chain	Residue	Modelled	Actual	Comment	Reference
q	?	-	PRO	deletion	UNP P32497
q	?	-	GLU	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	PHE	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	LYS	deletion	UNP P32497
q	?	-	GLU	deletion	UNP P32497
q	?	-	PRO	deletion	UNP P32497
q	?	-	THR	deletion	UNP P32497
q	?	-	ALA	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	LEU	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	ILE	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	ALA	deletion	UNP P32497
q	?	-	ASN	deletion	UNP P32497
q	?	-	GLY	deletion	UNP P32497
q	?	-	PHE	deletion	UNP P32497
q	?	-	THR	deletion	UNP P32497
q	?	-	ILE	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	GLN	deletion	UNP P32497
q	?	-	GLY	deletion	UNP P32497
q	?	-	ASN	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	GLN	deletion	UNP P32497
q	?	-	ALA	deletion	UNP P32497
q	?	-	VAL	deletion	UNP P32497

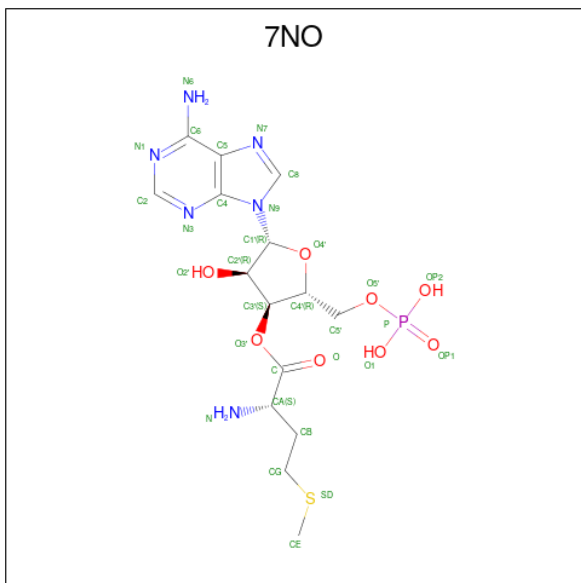
- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	s	330	2606	1661	429	507	9	0	0

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	r	49	392	240	76	76	0	0

- Molecule 48 is [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-2-(phosphonooxymethyl)oxolan-3-yl] (2 {S})-2-azanyl-4-methylsulfanyl-butanoate (three-letter code: 7NO) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>6</sub>O<sub>8</sub>PS).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
48	1	1	30	15	6	7	1	1	0

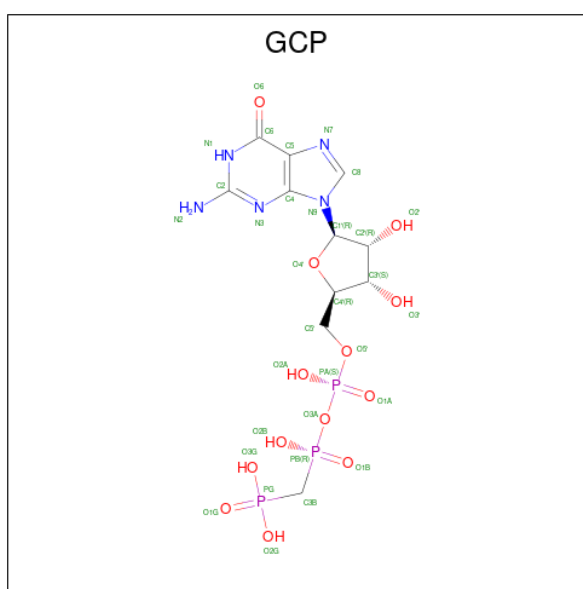
- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	2	76	Total	Mg	0
			76	76	
49	C	3	Total	Mg	0
			3	3	
49	O	1	Total	Mg	0
			1	1	
49	Q	1	Total	Mg	0
			1	1	
49	k	1	Total	Mg	0
			1	1	

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
50	O	1	Total Zn 1 1	0
50	b	1	Total Zn 1 1	0
50	f	1	Total Zn 1 1	0
50	l	1	Total Zn 1 1	0

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

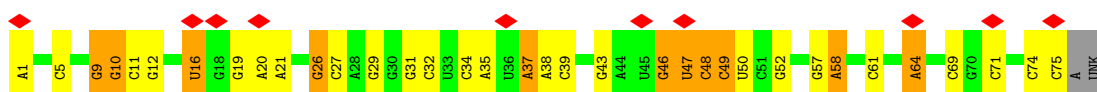


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	k	1	32	11	5	13	3	0

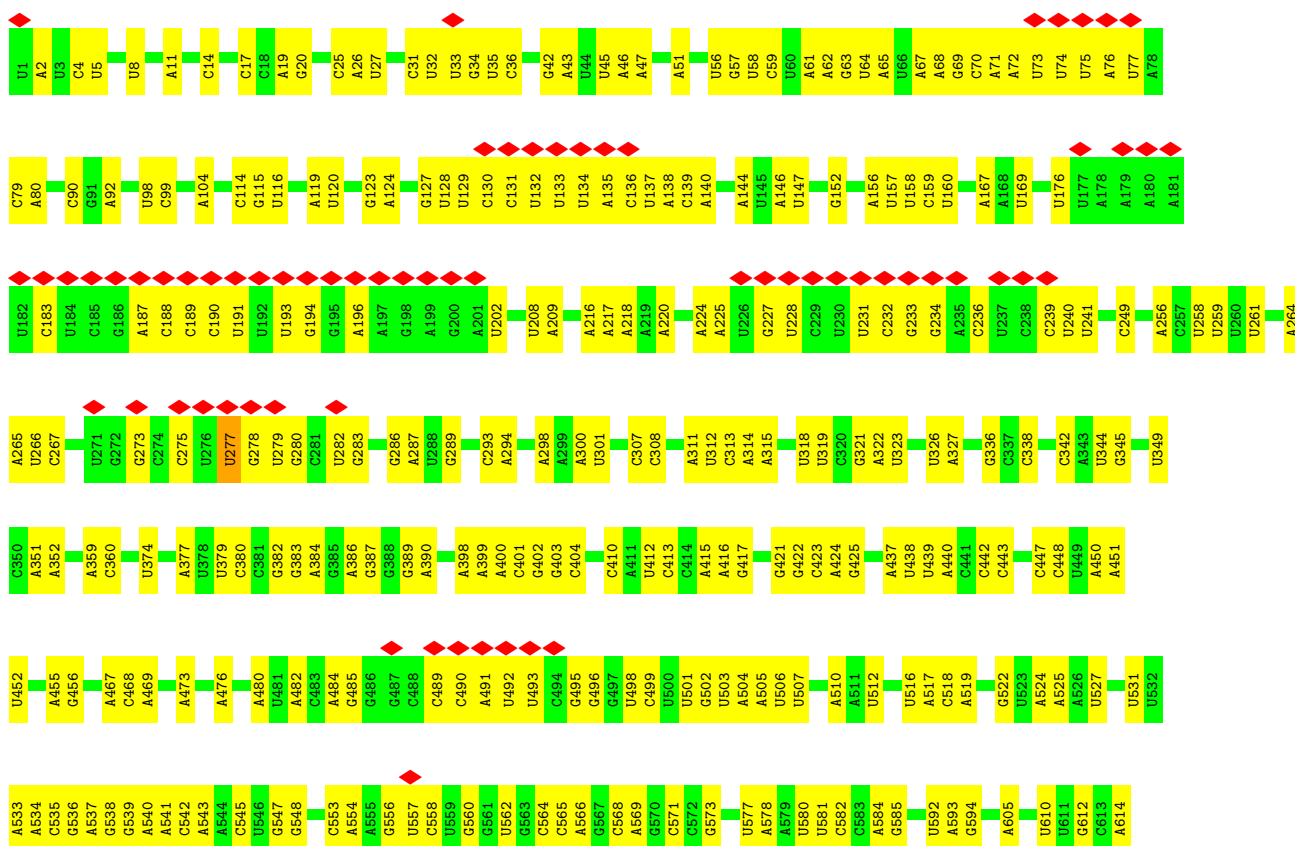
### 3 Residue-property plots [i](#)

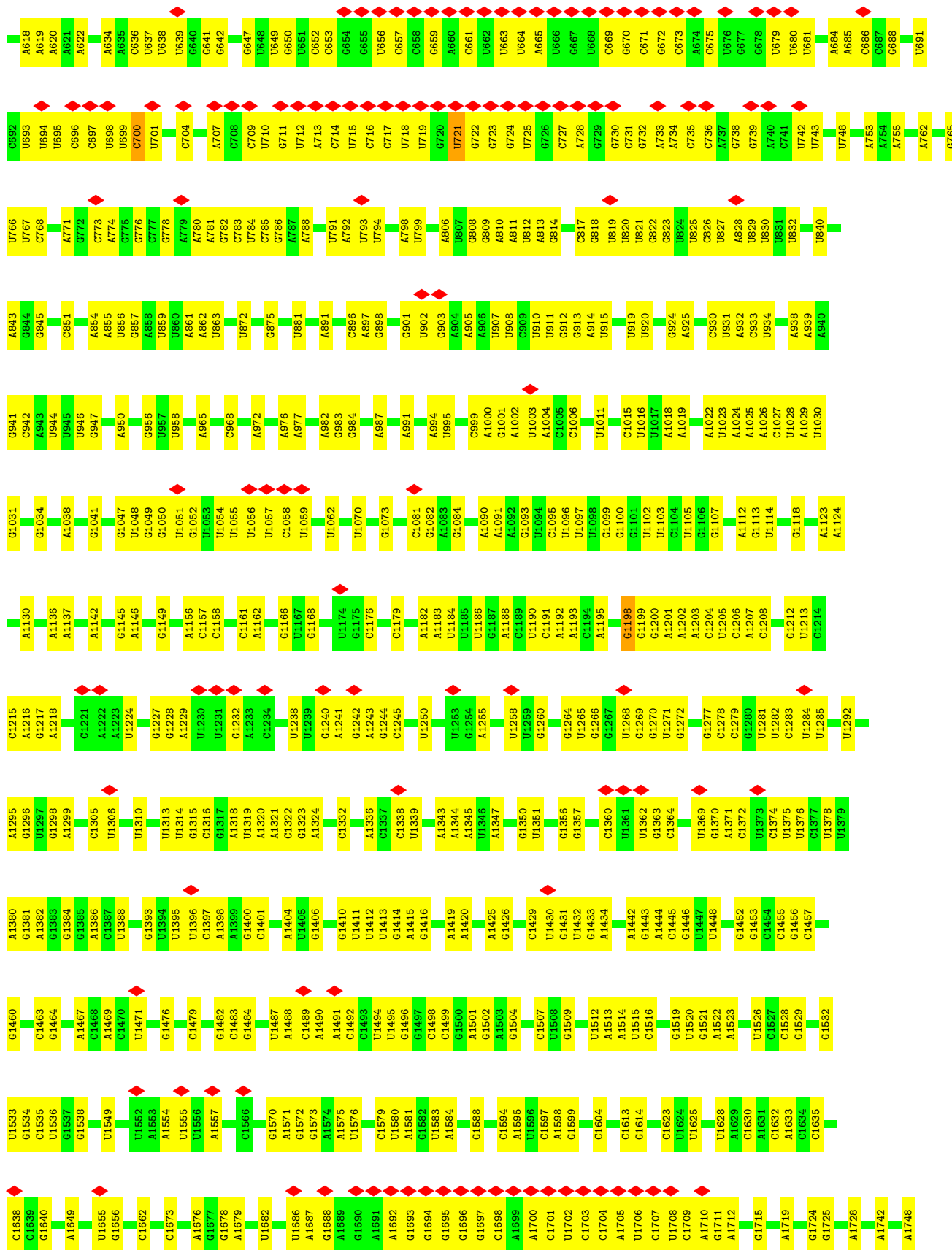
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Met-tRNAi



#### • Molecule 2: 18S ribosomal RNA

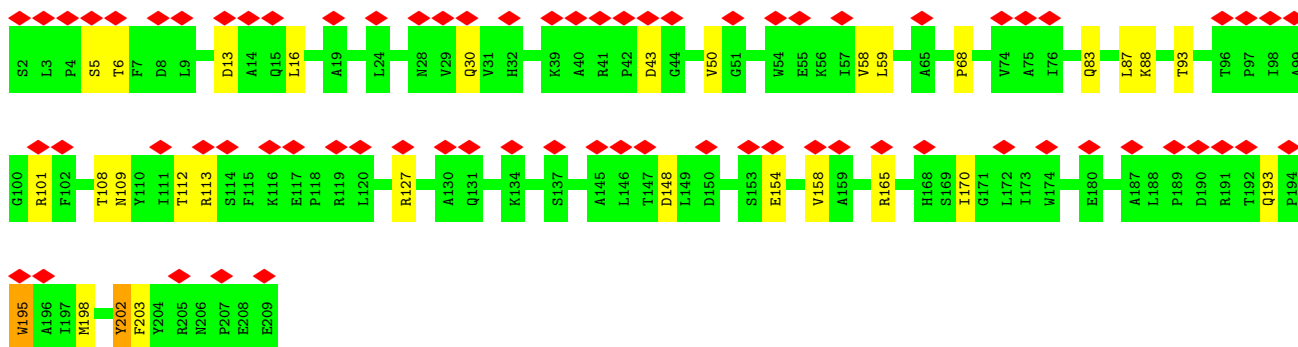
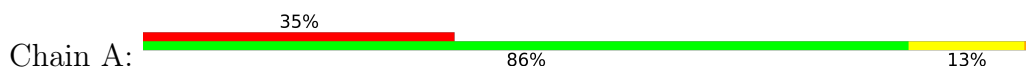








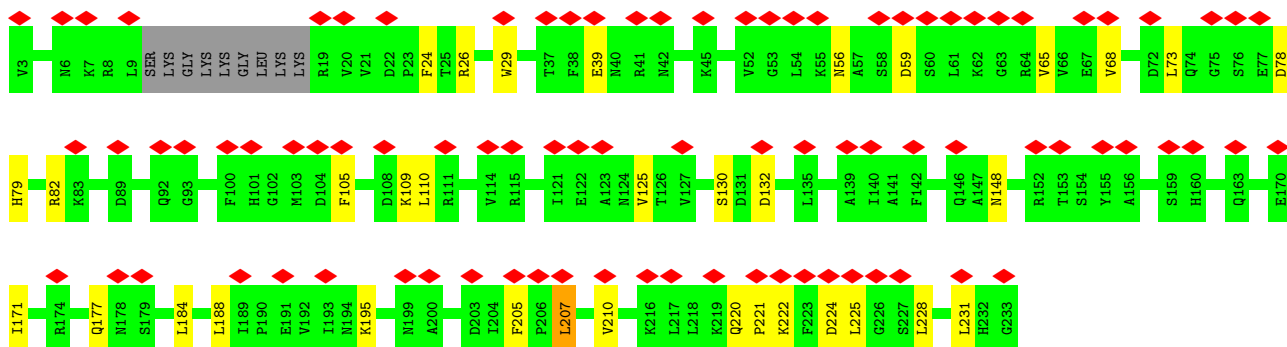
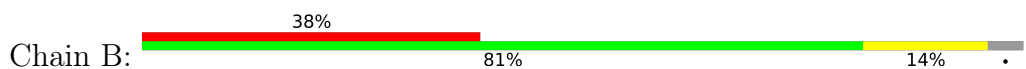
- Molecule 3: 40S ribosomal protein S0



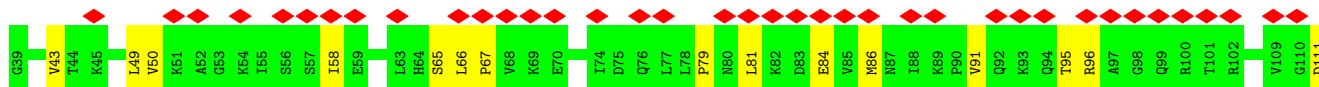
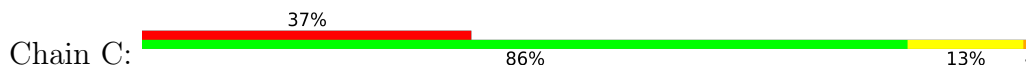
- Molecule 4: mRNA (5'-R(P\*AP\*AP\*U)-3')

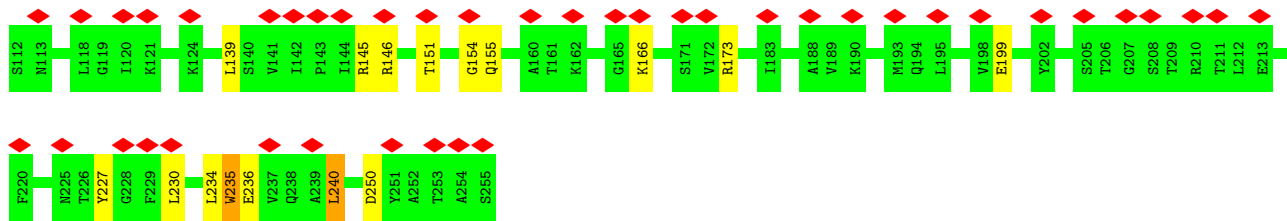


- Molecule 5: 40S ribosomal protein S1

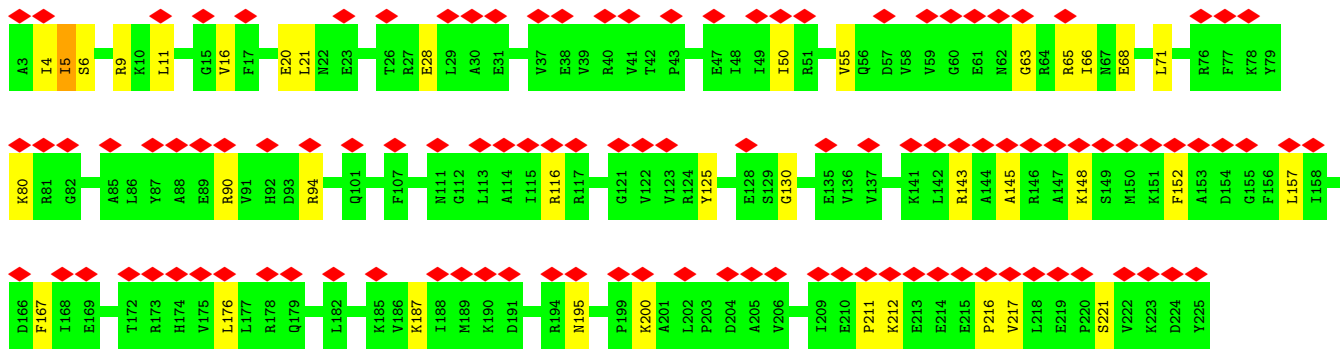
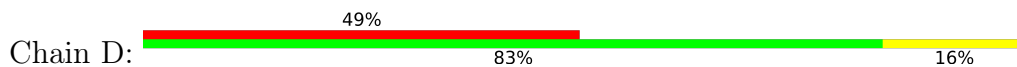


- Molecule 6: KLLA0F09812p

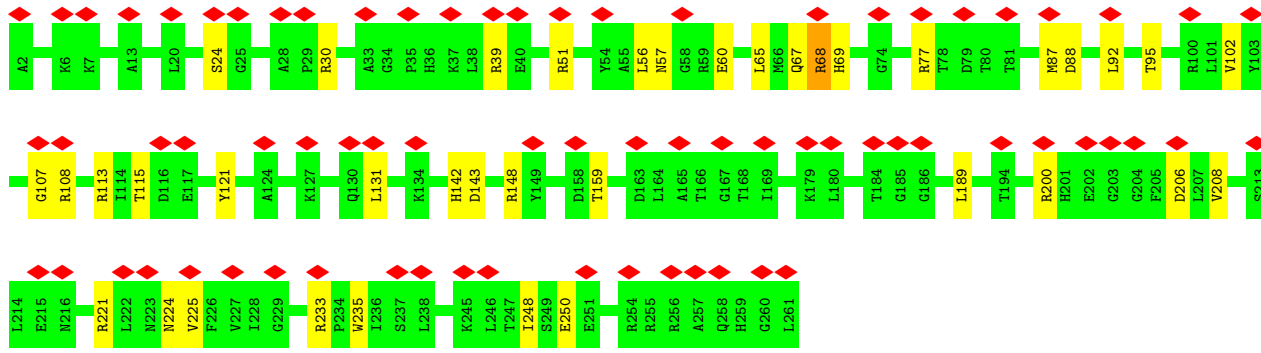
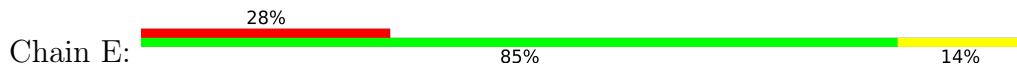




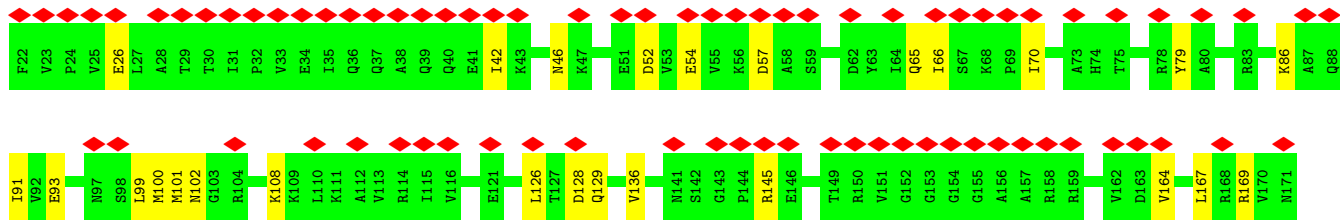
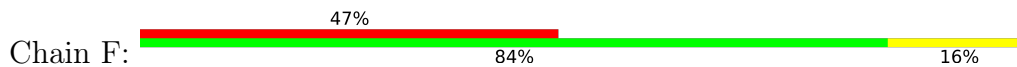
• Molecule 7: KLLA0D08305p



• Molecule 8: 40S ribosomal protein S4

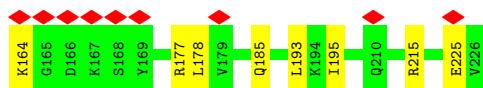
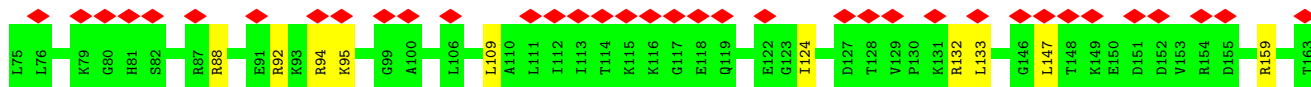
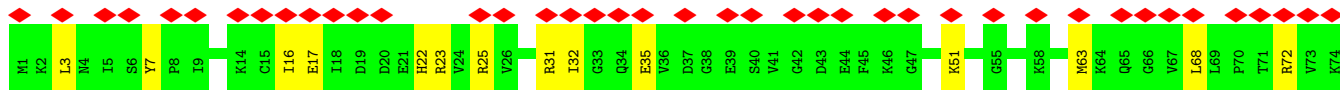
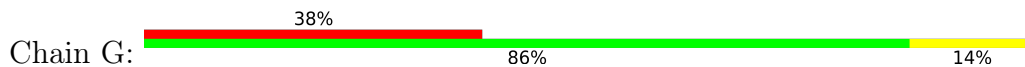


• Molecule 9: KLLA0D10659p

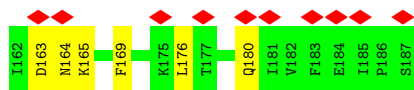
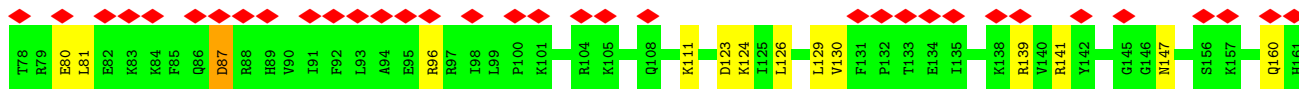
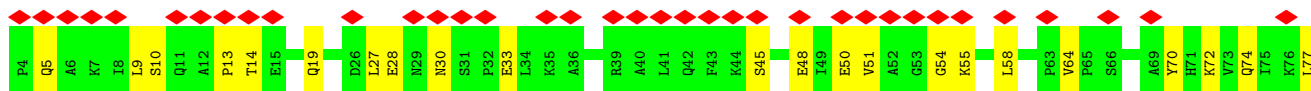
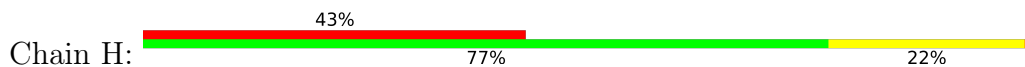




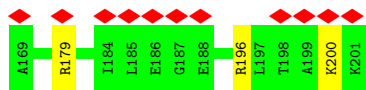
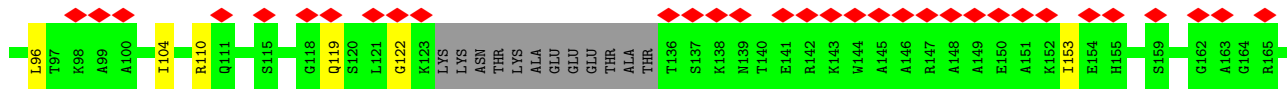
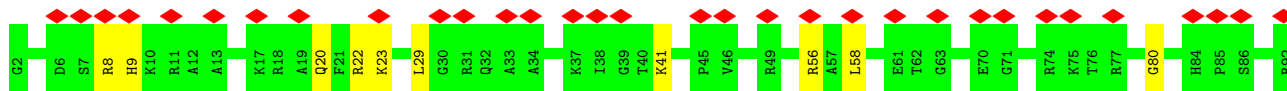
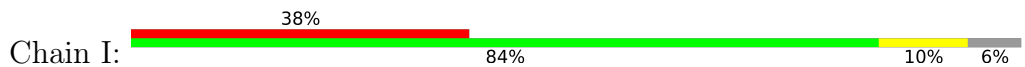
• Molecule 10: 40S ribosomal protein S6



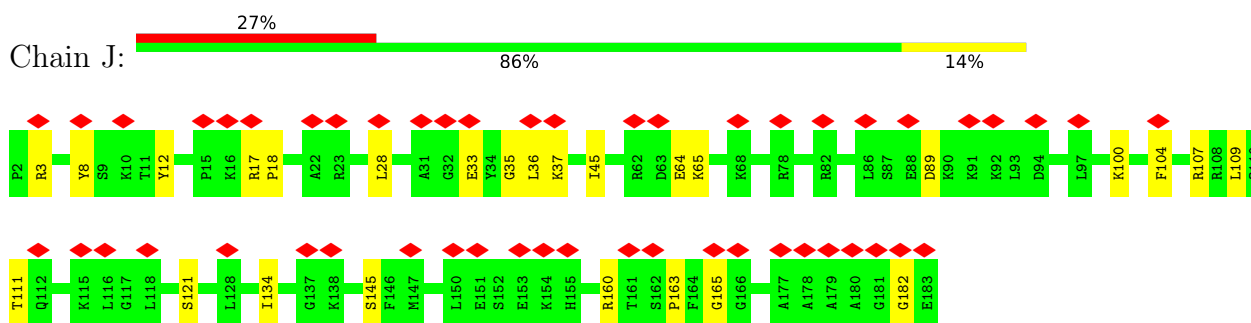
• Molecule 11: 40S ribosomal protein S7



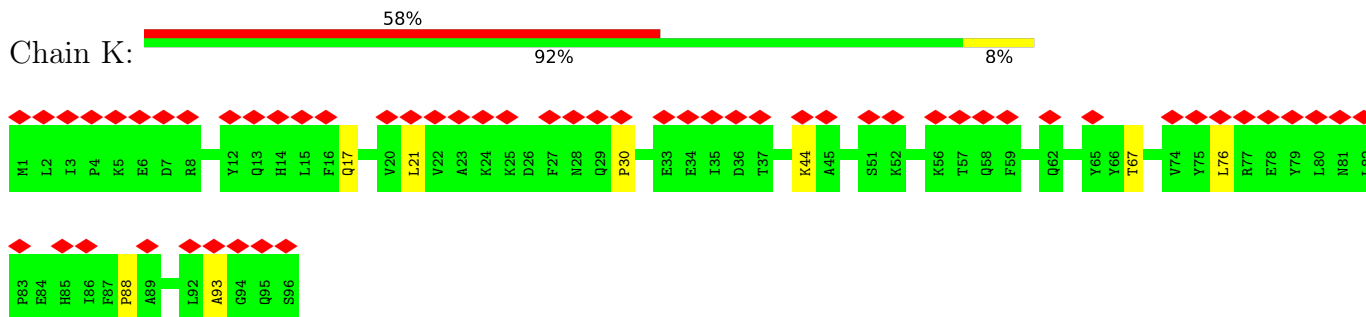
• Molecule 12: 40S ribosomal protein S8



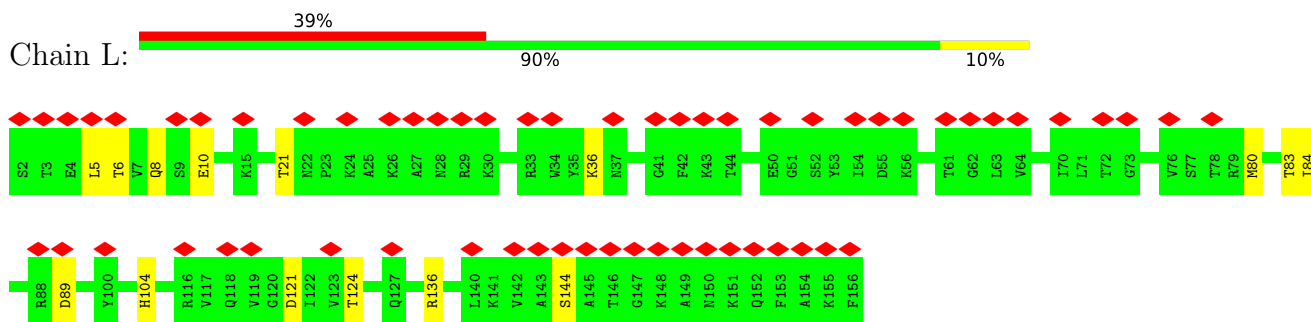
• Molecule 13: KLLA0E23673p



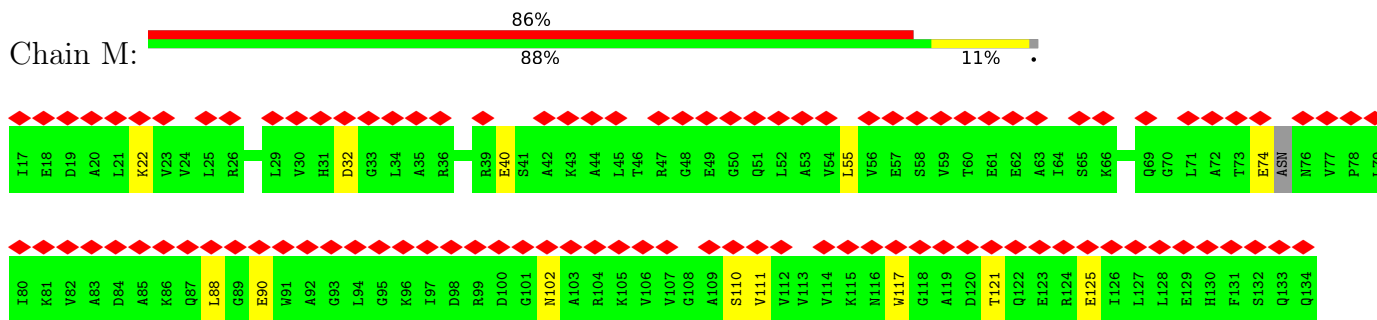
• Molecule 14: KLLA0B08173p



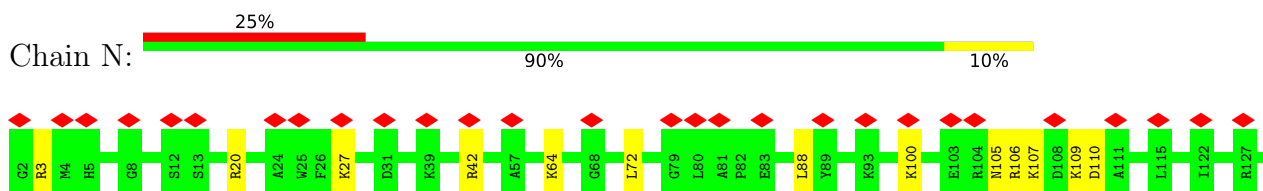
• Molecule 15: KLLA0A10483p

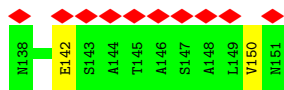


• Molecule 16: 40S ribosomal protein S12



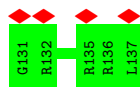
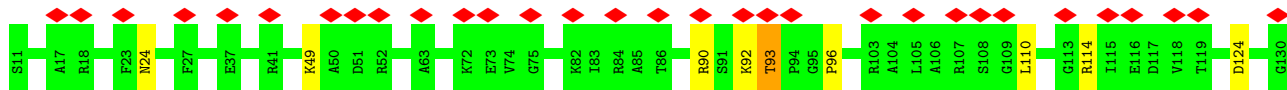
• Molecule 17: KLLA0F18040p





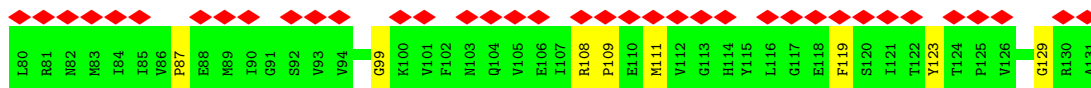
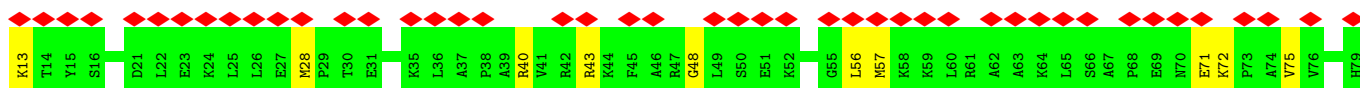
- Molecule 18: 40S ribosomal protein S14

Chain O: 28% 93% 6%



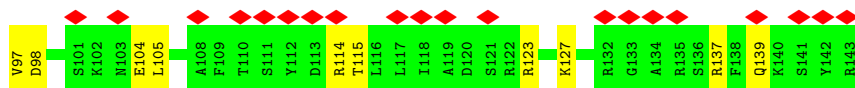
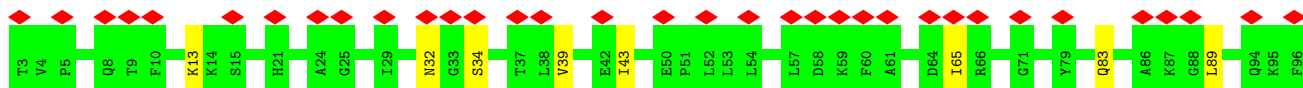
- Molecule 19: KLLA0F07843p

Chain P: 69% 85% 15%



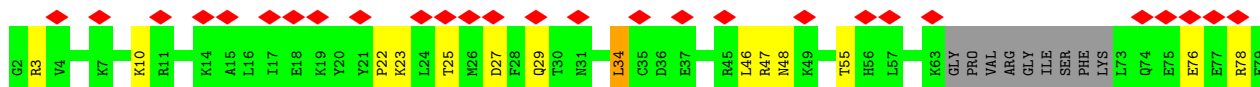
- Molecule 20: 40S ribosomal protein S16

Chain Q: 38% 87% 13%

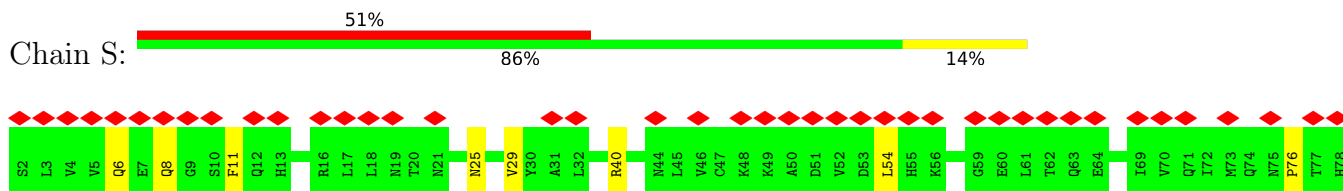


- Molecule 21: KLLA0B01474p

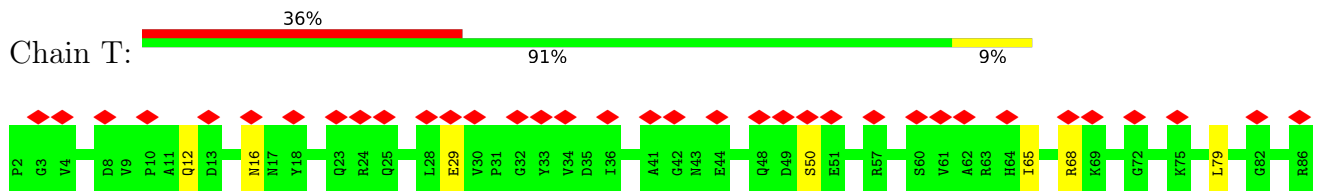
Chain R: 46% 74% 14% 11%



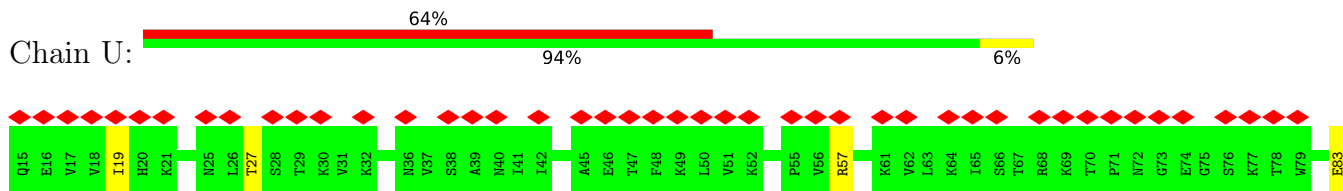
- Molecule 22: KLLA0B01562p



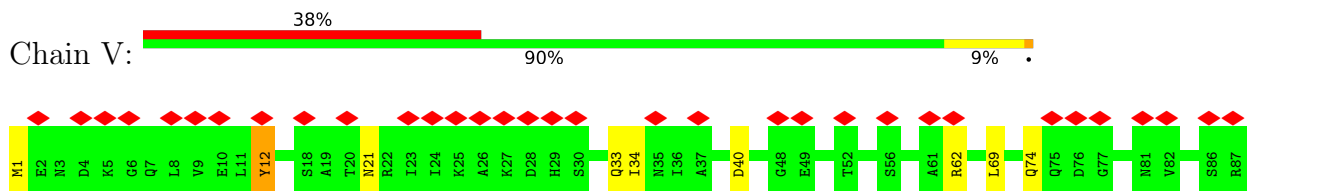
• Molecule 23: KLLA0A07194p



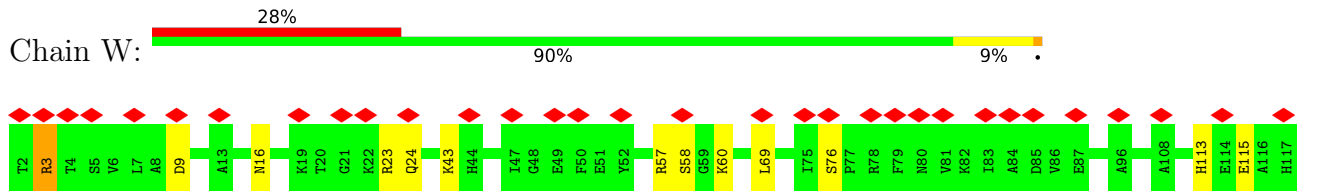
• Molecule 24: KLLA0F25542p



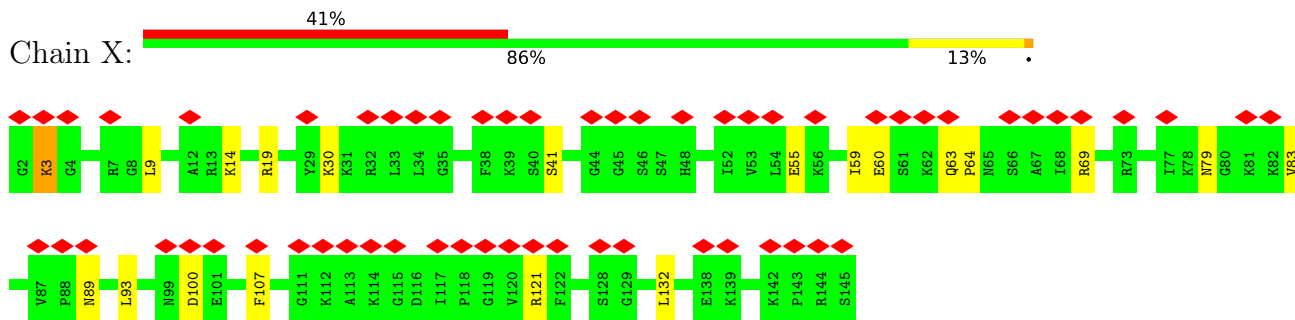
• Molecule 25: 40S ribosomal protein S21



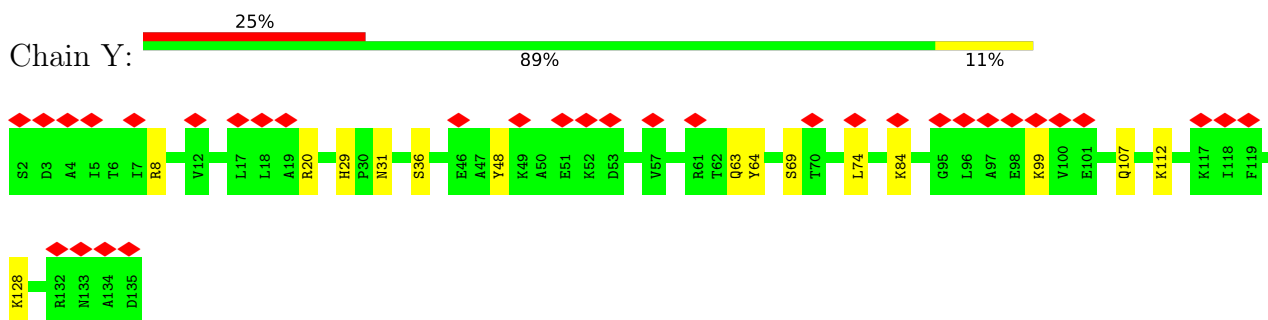
• Molecule 26: 40S ribosomal protein S22



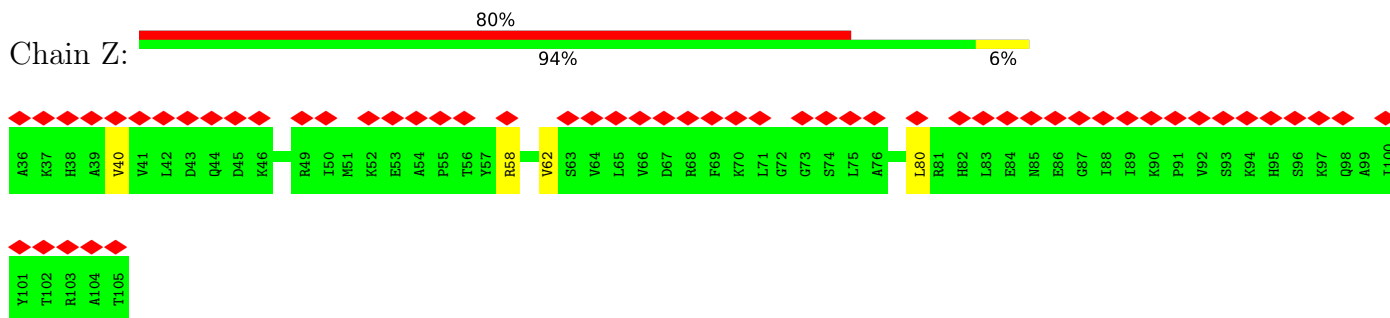
- Molecule 27: KLLA0B11231p



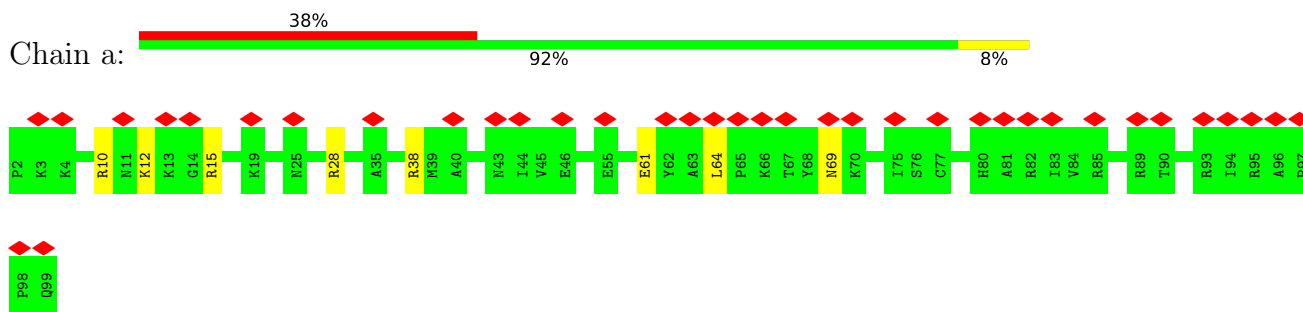
- Molecule 28: 40S ribosomal protein S24



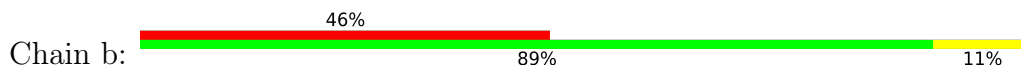
- Molecule 29: KLLA0B06182p

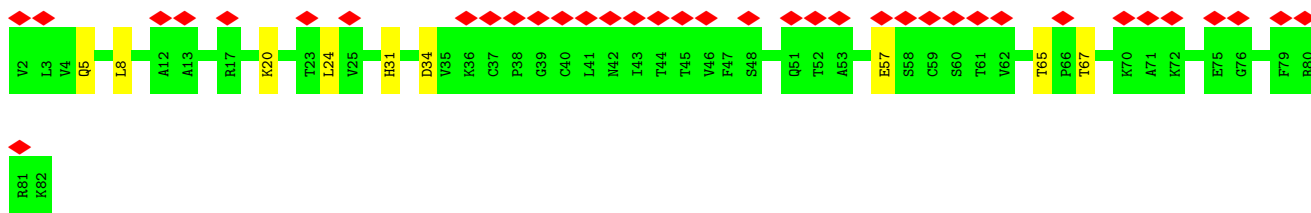


- Molecule 30: 40S ribosomal protein S26

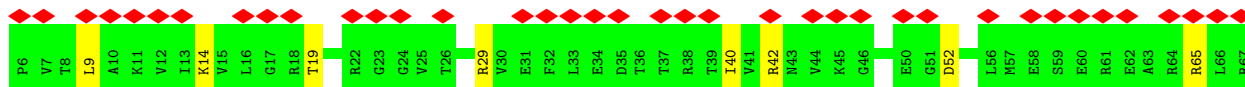
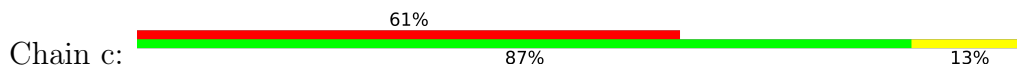


- Molecule 31: 40S ribosomal protein S27

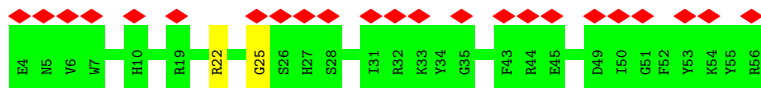
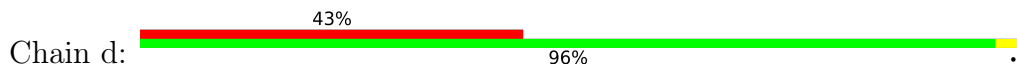




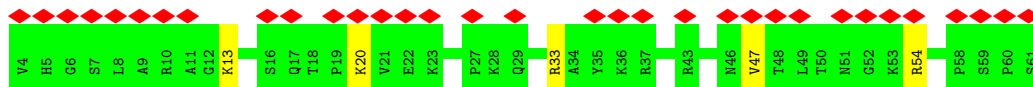
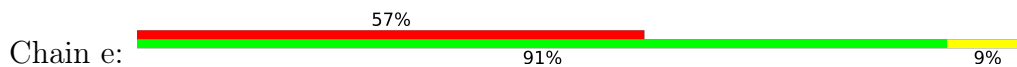
• Molecule 32: 40S ribosomal protein S28



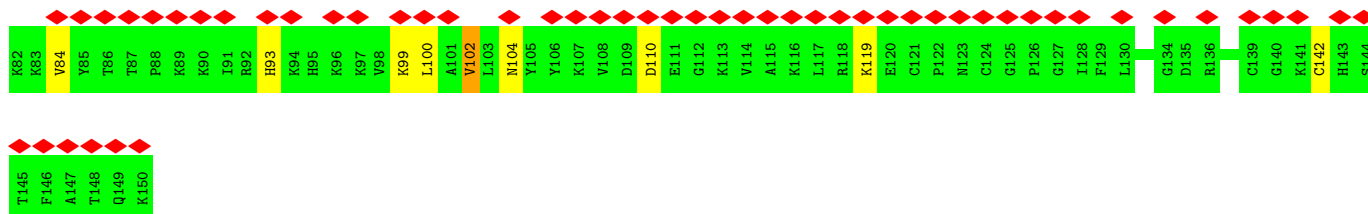
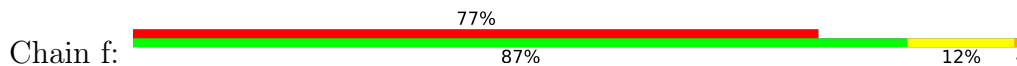
• Molecule 33: 40S ribosomal protein S29



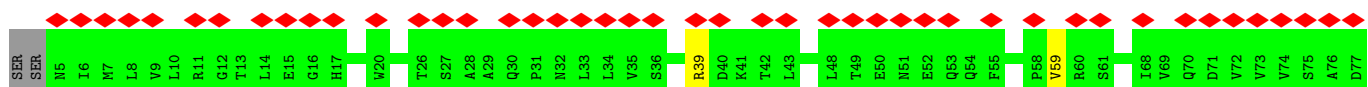
• Molecule 34: 40S ribosomal protein S30



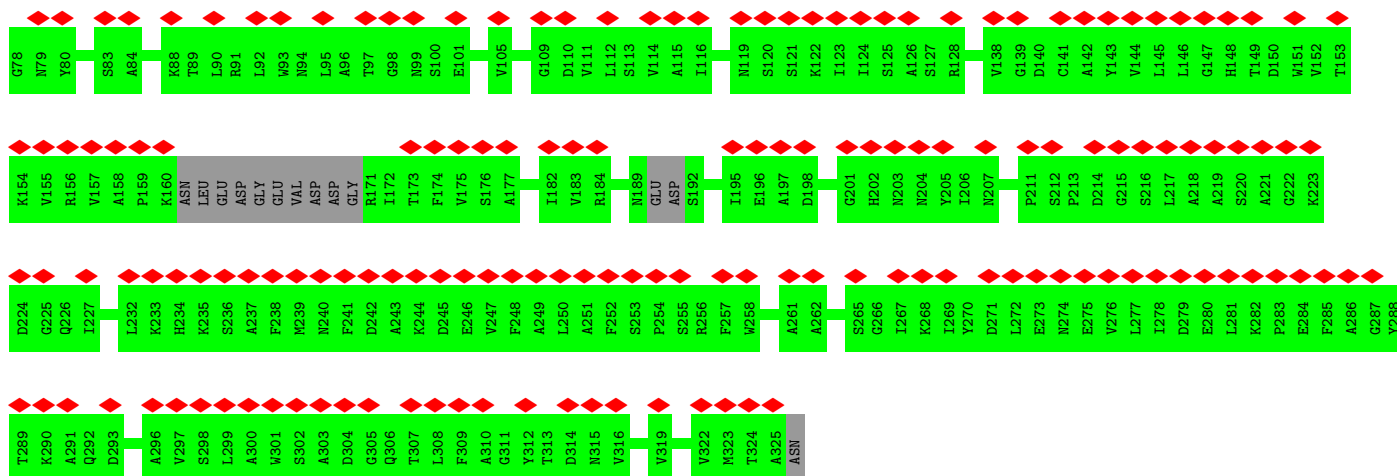
• Molecule 35: Ubiquitin-40S ribosomal protein S27a



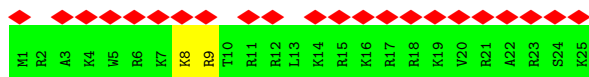
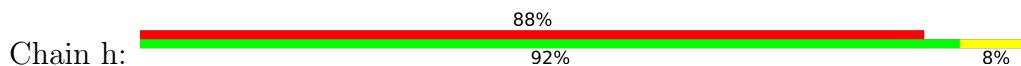
• Molecule 36: KLLA0E12277p



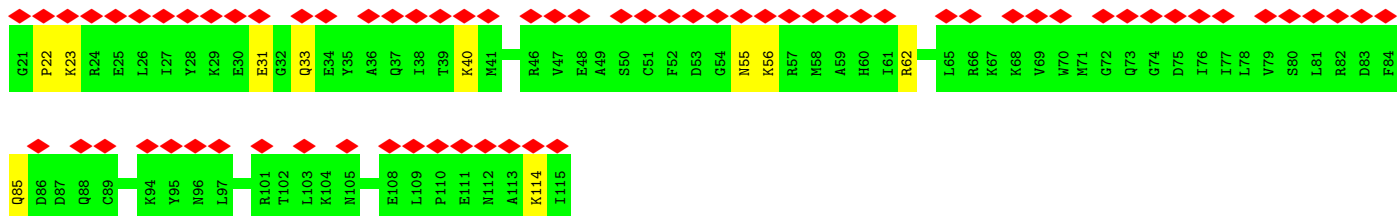
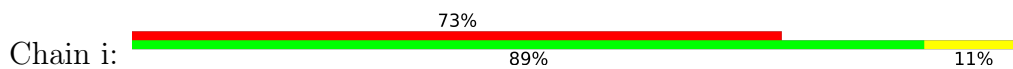




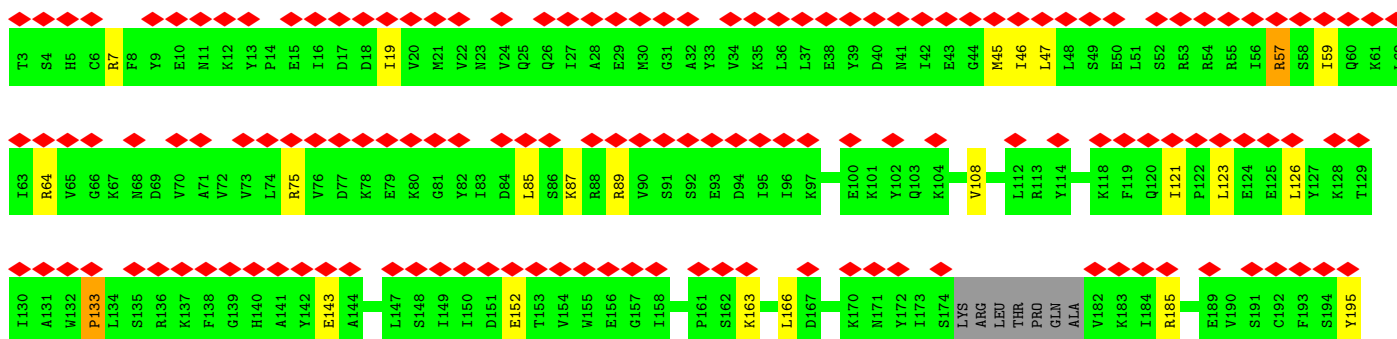
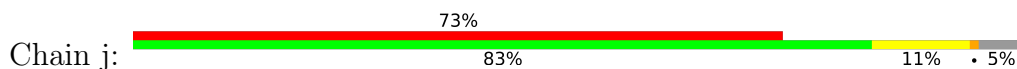
• Molecule 37: 60S ribosomal protein L41-A

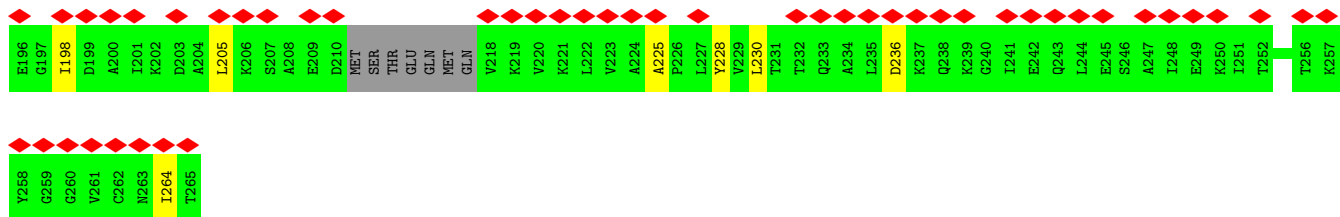


• Molecule 38: Eukaryotic translation initiation factor 1A

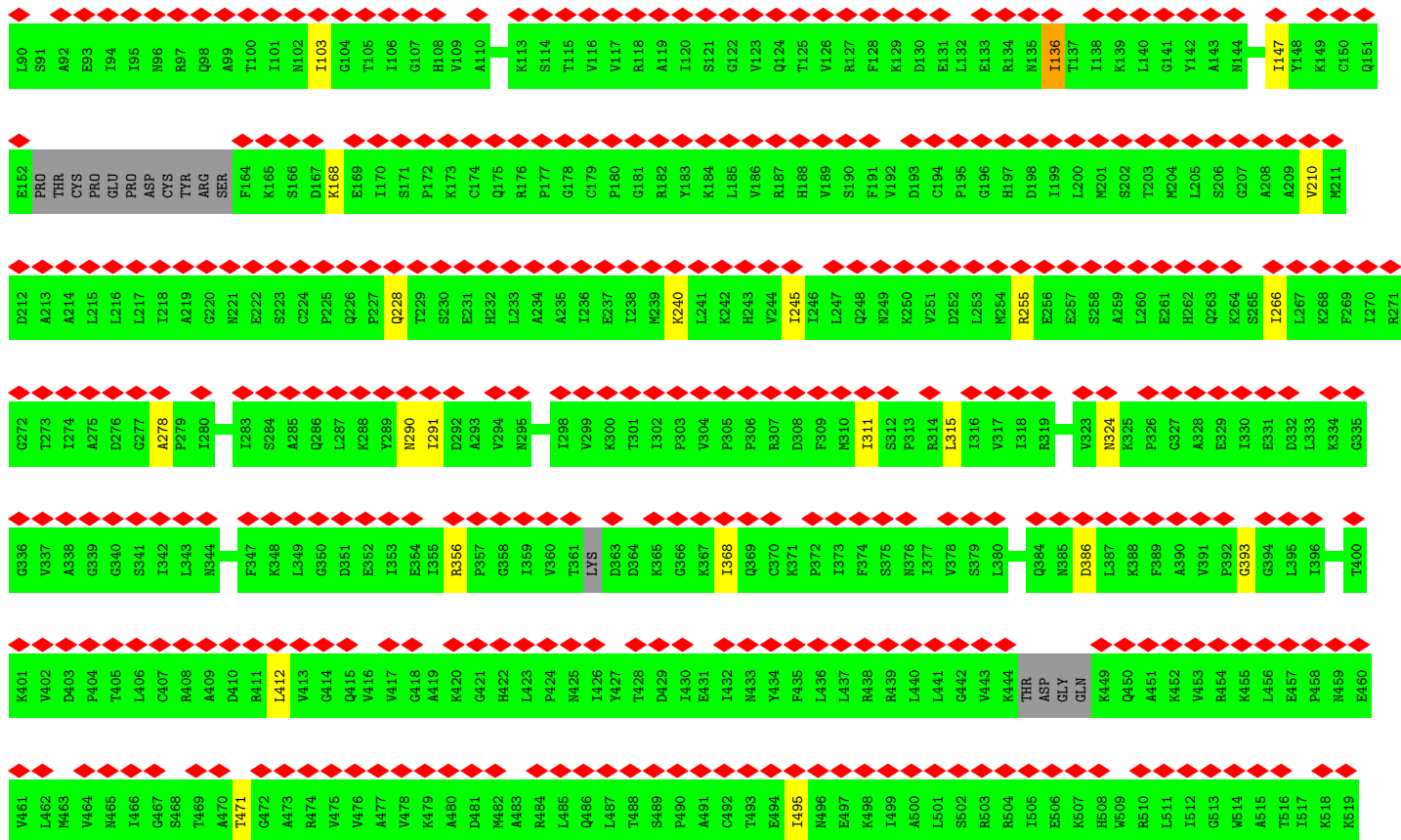
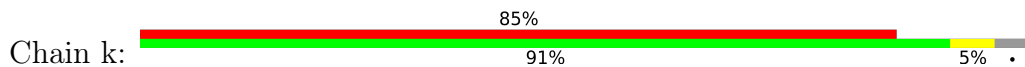


• Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha

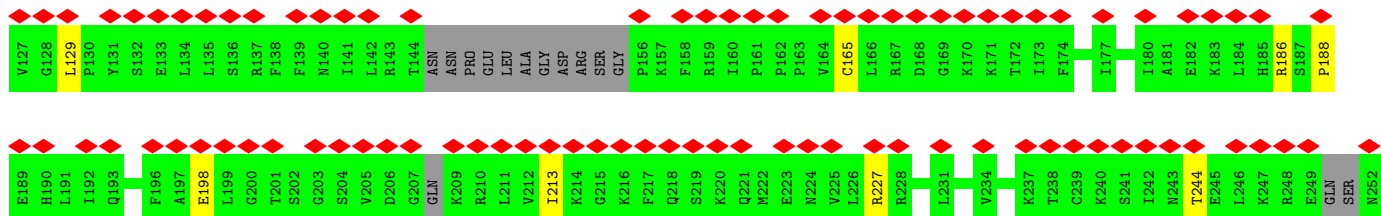
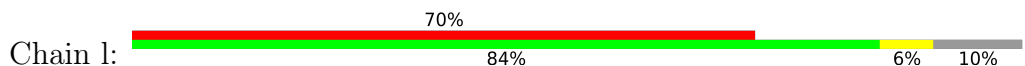


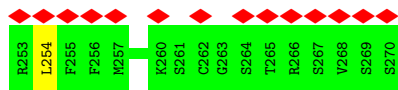


• Molecule 40: Eukaryotic translation initiation factor 2 subunit gamma

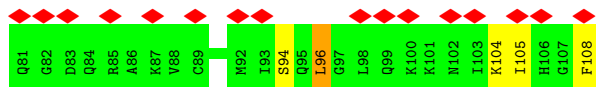
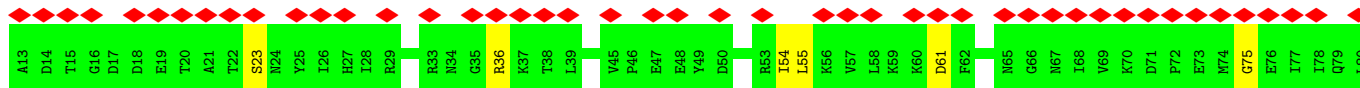
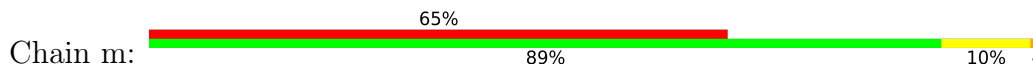


• Molecule 41: Eukaryotic translation initiation factor 2 subunit beta

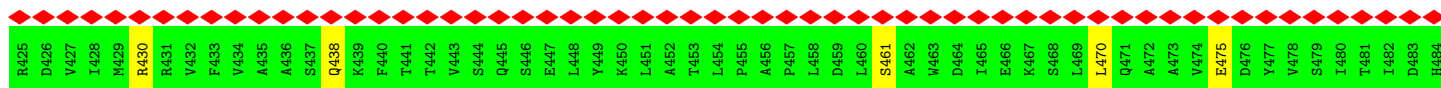
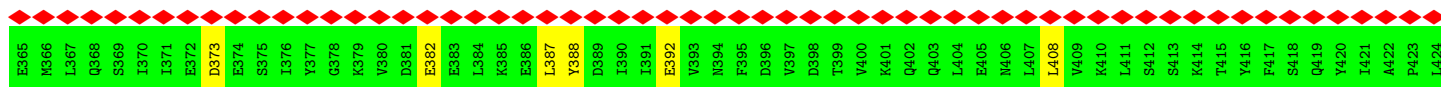
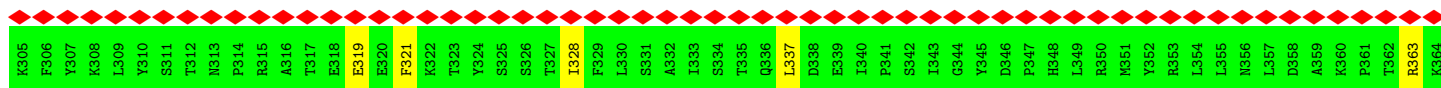
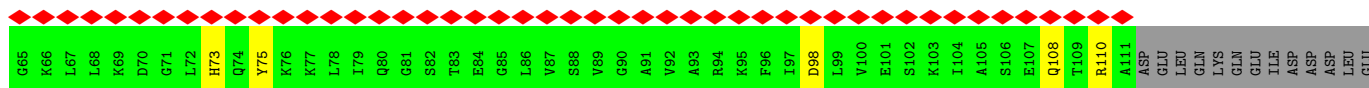
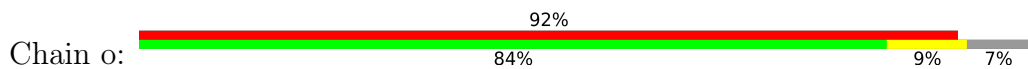


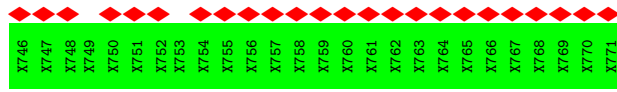
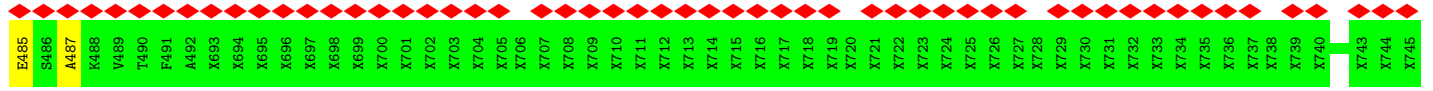


• Molecule 42: Eukaryotic translation initiation factor eIF-1

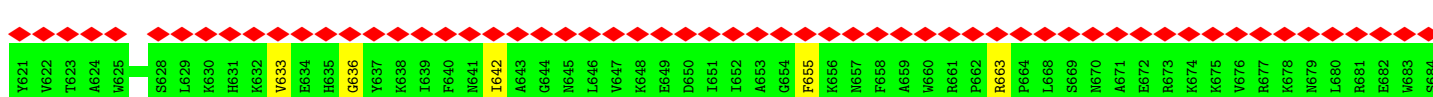
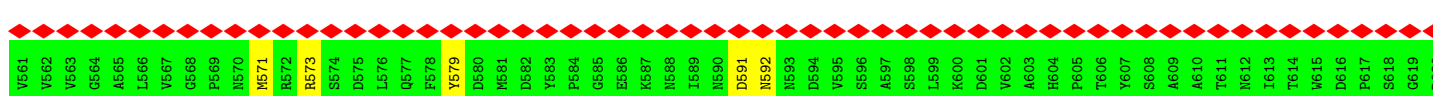
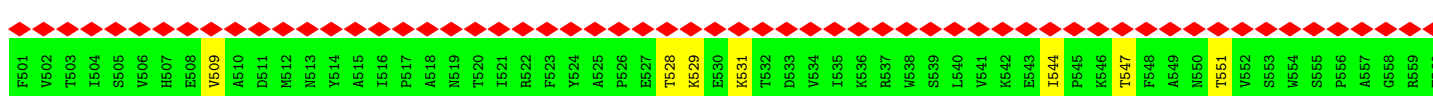
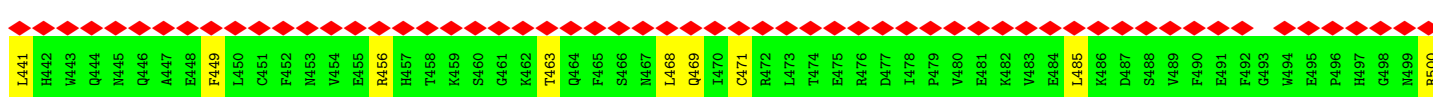
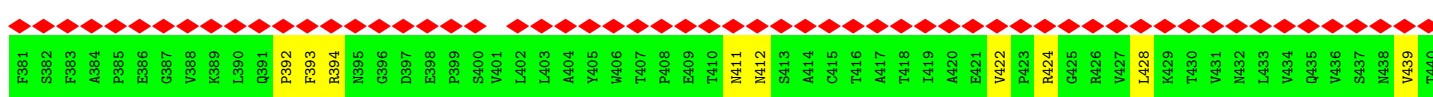
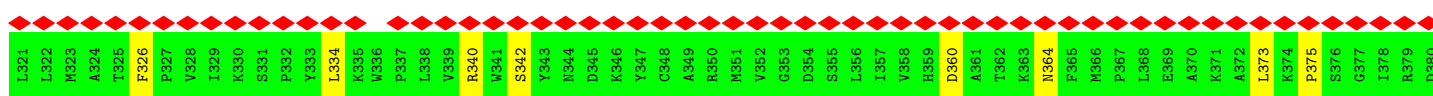
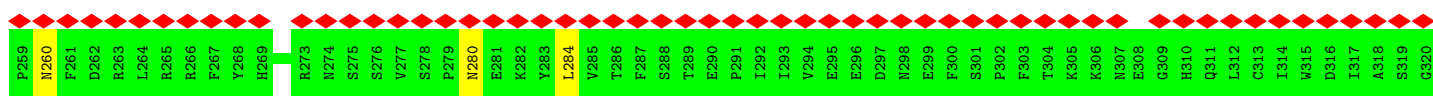
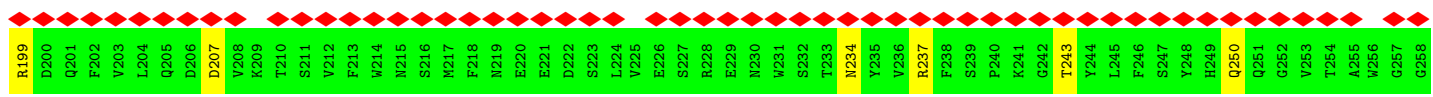
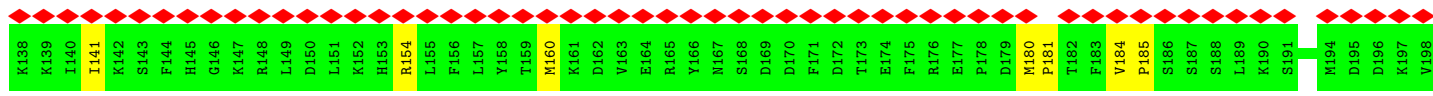
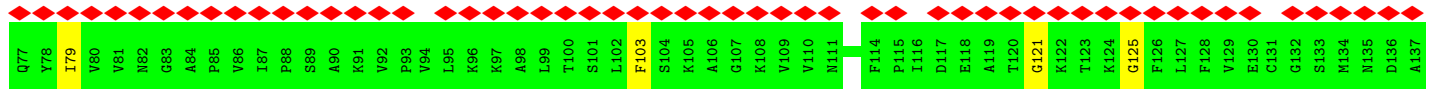
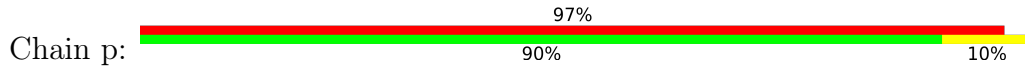


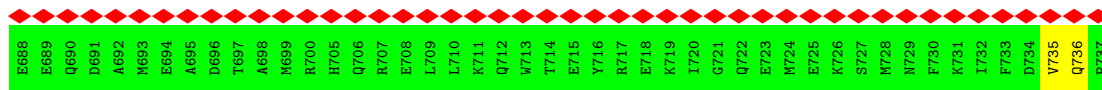
• Molecule 43: Eukaryotic translation initiation factor 3 subunit A, Eukaryotic translation initiation factor 3 subunit A, eIF3a



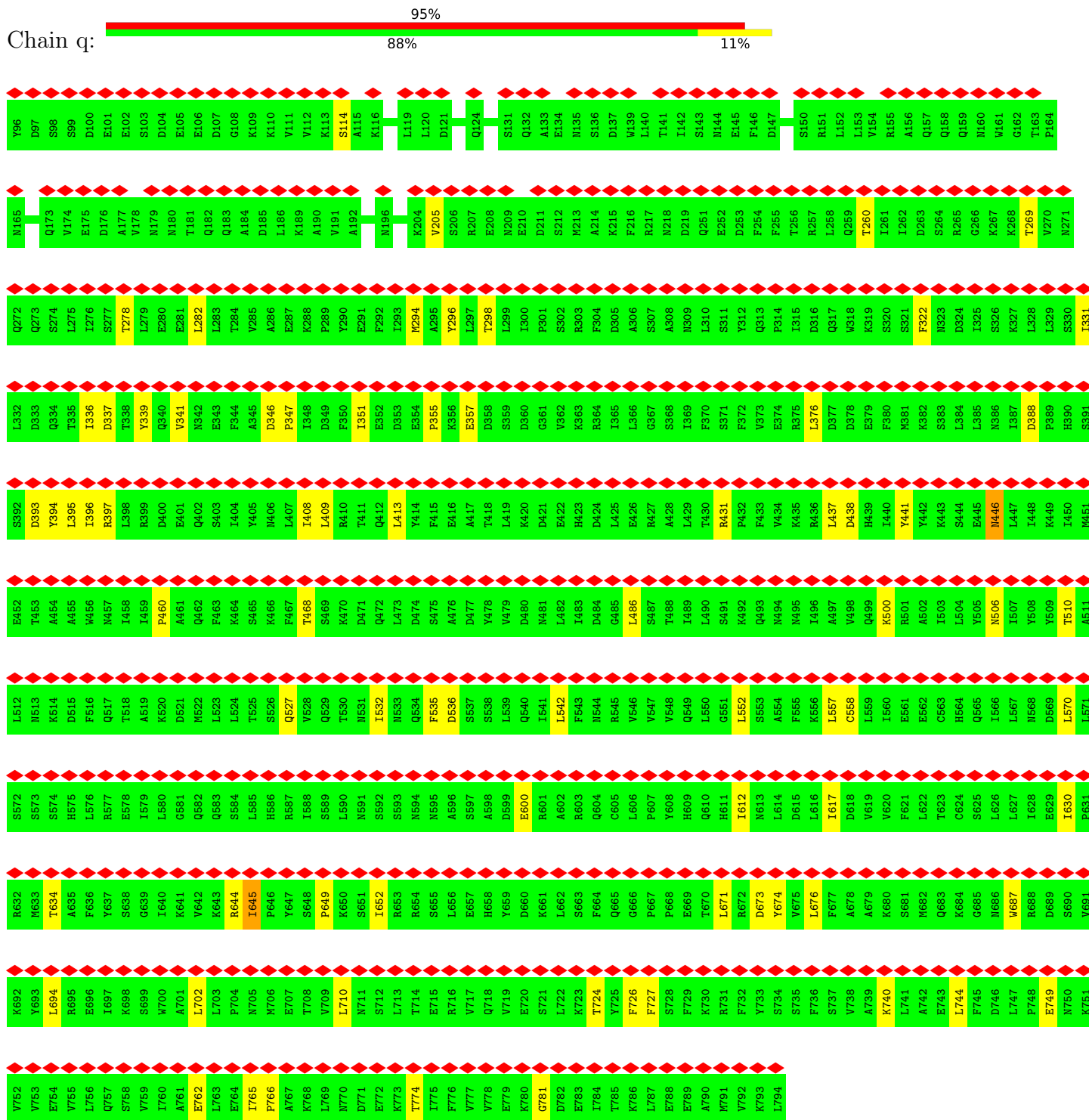


• Molecule 44: Eukaryotic translation initiation factor 3 subunit B

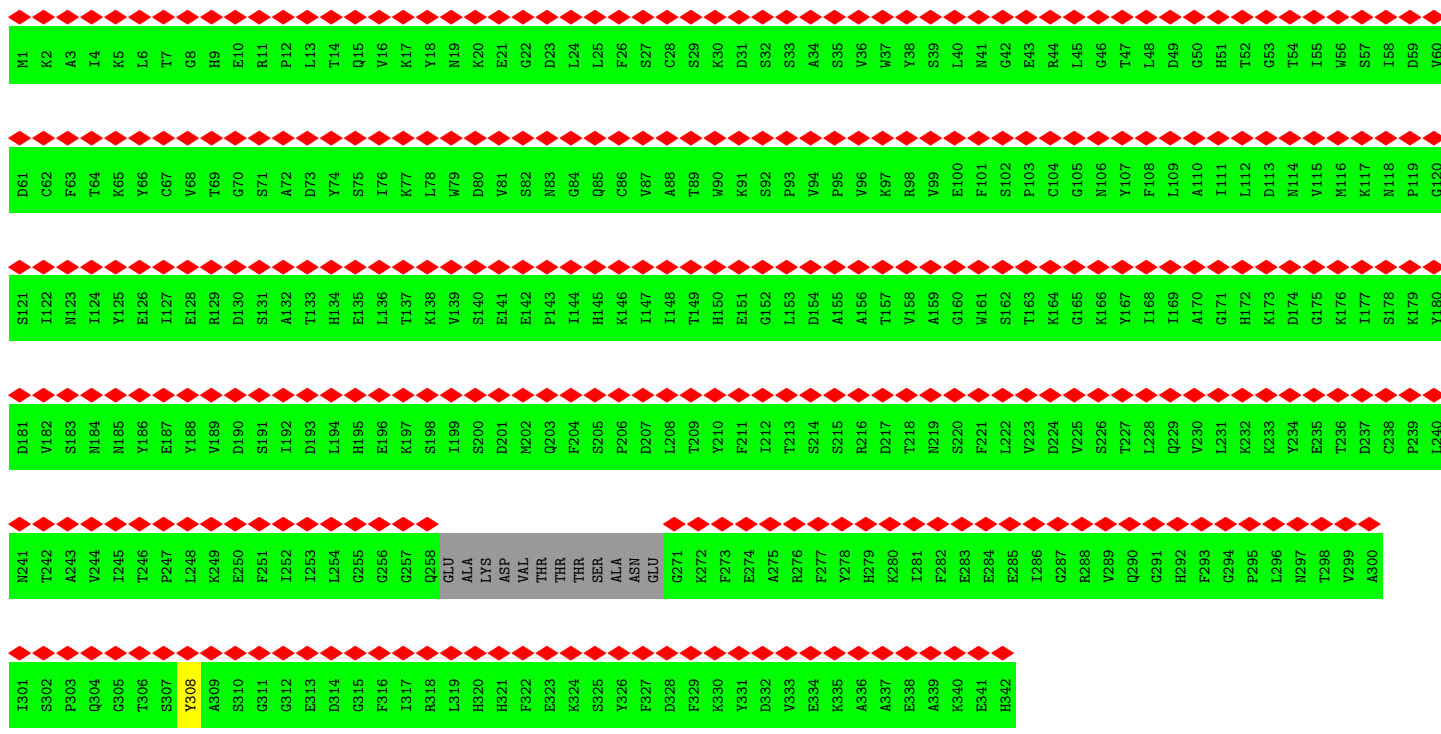




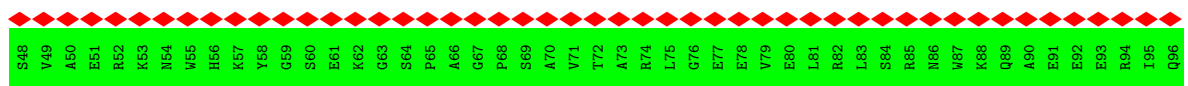
• Molecule 45: Eukaryotic translation initiation factor 3 subunit C



• Molecule 46: Eukaryotic translation initiation factor 3 subunit I



• Molecule 47: Eukaryotic translation initiation factor 3 subunit G



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5750	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.249	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: M2G, 1MA, 1MG, ZN, 5MC, H2U, GCP, T6A, 7NO, 2MG, RIA, 7MG, MG

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	0.38	1/1504 (0.1%)	0.67	0/2337
2	2	0.23	0/42691	0.66	4/66521 (0.0%)
3	A	0.45	1/1666 (0.1%)	0.69	0/2279
4	3	0.25	0/71	0.65	0/108
5	B	0.42	0/1793	0.71	2/2414 (0.1%)
6	C	0.40	0/1659	0.66	0/2252
7	D	0.44	0/1769	0.72	0/2378
8	E	0.41	0/2122	0.72	2/2861 (0.1%)
9	F	0.42	0/1628	0.70	0/2198
10	G	0.39	0/1835	0.71	1/2451 (0.0%)
11	H	0.41	0/1507	0.70	0/2028
12	I	0.41	0/1515	0.72	1/2029 (0.0%)
13	J	0.39	0/1495	0.76	0/2001
14	K	0.49	0/831	0.68	0/1123
15	L	0.41	0/1276	0.64	0/1718
16	M	0.43	0/891	0.69	0/1201
17	N	0.38	0/1210	0.66	0/1628
18	O	0.41	0/953	0.74	1/1279 (0.1%)
19	P	0.46	0/962	0.71	0/1294
20	Q	0.42	0/1125	0.71	0/1510
21	R	0.45	0/899	0.82	2/1204 (0.2%)
22	S	0.46	0/1212	0.75	0/1629
23	T	0.43	0/1129	0.71	0/1520
24	U	0.40	0/857	0.69	0/1158
25	V	0.39	0/696	0.69	0/938
26	W	0.41	0/1039	0.75	2/1399 (0.1%)
27	X	0.46	0/1137	0.80	2/1516 (0.1%)
28	Y	0.40	0/1075	0.66	0/1433
29	Z	0.47	0/567	0.71	0/762
30	a	0.47	0/791	0.79	1/1059 (0.1%)
31	b	0.41	0/619	0.66	0/837
32	c	0.44	0/489	0.75	0/655



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	d	0.51	0/457	0.66	1/607 (0.2%)
34	e	0.44	0/471	0.72	0/628
35	f	0.55	0/562	0.80	0/751
36	g	0.35	0/2459	0.56	2/3348 (0.1%)
37	h	0.43	0/234	0.85	0/300
38	i	0.47	0/775	0.68	0/1034
39	j	0.48	0/2034	0.69	2/2737 (0.1%)
40	k	0.51	0/3168	0.68	0/4281
41	l	0.49	0/1064	0.65	0/1420
42	m	0.44	0/744	0.68	0/997
43	o	0.55	0/3729	0.66	0/5041
44	p	0.52	0/5225	0.66	1/7101 (0.0%)
45	q	0.54	0/5132	0.67	0/6965
46	s	0.42	0/2669	0.53	0/3611
47	r	0.36	0/399	0.42	0/535
All	All	0.38	2/108135 (0.0%)	0.67	24/155076 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	A	OP3-P	-10.19	1.49	1.61
3	A	202	TYR	CE1-CZ	-5.67	1.31	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	34	LEU	CB-CG-CD2	-11.76	91.00	111.00
36	g	39	ARG	NE-CZ-NH2	-10.95	114.82	120.30
26	W	3	ARG	NE-CZ-NH1	8.02	124.31	120.30
27	X	3	LYS	N-CA-C	7.51	131.28	111.00
44	p	280	ASN	N-CA-C	-7.35	91.17	111.00
10	G	68	LEU	CA-CB-CG	6.23	129.63	115.30
39	j	57	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	2	721	U	C2'-C3'-O3'	6.02	123.33	113.70
2	2	1198	G	C2'-C3'-O3'	5.88	123.11	113.70
36	g	39	ARG	NH1-CZ-NH2	5.70	125.67	119.40
30	a	10	ARG	NE-CZ-NH1	5.63	123.12	120.30
18	O	93	THR	N-CA-CB	5.62	120.97	110.30
2	2	700	C	C2'-C3'-O3'	5.56	122.59	113.70
12	I	96	LEU	CA-CB-CG	5.47	127.89	115.30
2	2	277	U	C2'-C3'-O3'	5.30	122.17	113.70
39	j	89	ARG	NE-CZ-NH1	5.21	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	221	ARG	NE-CZ-NH1	5.19	122.89	120.30
33	d	22	ARG	NE-CZ-NH1	5.12	122.86	120.30
5	B	188	LEU	CA-CB-CG	5.09	127.01	115.30
8	E	68	ARG	NE-CZ-NH2	-5.09	117.76	120.30
26	W	69	LEU	CA-CB-CG	5.07	126.95	115.30
5	B	220	GLN	C-N-CD	-5.04	109.51	120.60
21	R	27	ASP	CB-CG-OD2	-5.04	113.77	118.30
27	X	69	ARG	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	206/208 (99%)	185 (90%)	16 (8%)	5 (2%)	6	35
5	B	218/231 (94%)	190 (87%)	20 (9%)	8 (4%)	3	27
6	C	215/217 (99%)	196 (91%)	12 (6%)	7 (3%)	4	29
7	D	221/223 (99%)	193 (87%)	19 (9%)	9 (4%)	3	24
8	E	258/260 (99%)	231 (90%)	26 (10%)	1 (0%)	34	72
9	F	204/206 (99%)	182 (89%)	17 (8%)	5 (2%)	5	34
10	G	224/226 (99%)	204 (91%)	19 (8%)	1 (0%)	34	72
11	H	182/184 (99%)	158 (87%)	16 (9%)	8 (4%)	2	24
12	I	184/200 (92%)	165 (90%)	16 (9%)	3 (2%)	9	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	J	180/182 (99%)	161 (89%)	12 (7%)	7 (4%)	3	25
14	K	94/96 (98%)	82 (87%)	9 (10%)	3 (3%)	4	29
15	L	153/155 (99%)	140 (92%)	13 (8%)	0	100	100
16	M	113/118 (96%)	88 (78%)	22 (20%)	3 (3%)	5	33
17	N	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
18	O	125/127 (98%)	112 (90%)	11 (9%)	2 (2%)	9	44
19	P	117/119 (98%)	86 (74%)	24 (20%)	7 (6%)	1	18
20	Q	139/141 (99%)	120 (86%)	16 (12%)	3 (2%)	6	36
21	R	105/125 (84%)	87 (83%)	11 (10%)	7 (7%)	1	17
22	S	143/145 (99%)	125 (87%)	16 (11%)	2 (1%)	11	46
23	T	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	11	46
24	U	104/106 (98%)	94 (90%)	9 (9%)	1 (1%)	15	54
25	V	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	13	50
26	W	127/129 (98%)	115 (91%)	9 (7%)	3 (2%)	6	35
27	X	142/144 (99%)	124 (87%)	13 (9%)	5 (4%)	3	28
28	Y	132/134 (98%)	118 (89%)	11 (8%)	3 (2%)	6	35
29	Z	68/70 (97%)	62 (91%)	5 (7%)	1 (2%)	10	46
30	a	96/98 (98%)	82 (85%)	11 (12%)	3 (3%)	4	30
31	b	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
32	c	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
33	d	51/53 (96%)	41 (80%)	9 (18%)	1 (2%)	7	39
34	e	56/58 (97%)	45 (80%)	10 (18%)	1 (2%)	8	41
35	f	67/69 (97%)	46 (69%)	17 (25%)	4 (6%)	1	18
36	g	305/324 (94%)	289 (95%)	16 (5%)	0	100	100
37	h	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
38	i	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	14	51
39	j	243/263 (92%)	207 (85%)	32 (13%)	4 (2%)	9	44
40	k	406/430 (94%)	345 (85%)	52 (13%)	9 (2%)	6	36
41	l	122/144 (85%)	100 (82%)	20 (16%)	2 (2%)	9	44
42	m	94/96 (98%)	74 (79%)	16 (17%)	4 (4%)	2	24
43	o	445/567 (78%)	371 (83%)	68 (15%)	6 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	p	643/651 (99%)	537 (84%)	86 (13%)	20 (3%)	4	30
45	q	657/665 (99%)	537 (82%)	98 (15%)	22 (3%)	4	29
46	s	326/342 (95%)	318 (98%)	8 (2%)	0	100	100
47	r	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
All	All	7841/8198 (96%)	6836 (87%)	831 (11%)	174 (2%)	10	36

All (174) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	26	ARG
5	B	210	VAL
6	C	235	TRP
7	D	195	ASN
9	F	46	ASN
10	G	32	ILE
11	H	64	VAL
11	H	74	GLN
11	H	87	ASP
12	I	153	ILE
16	M	102	ASN
16	M	111	VAL
18	O	93	THR
20	Q	32	ASN
20	Q	39	VAL
22	S	29	VAL
23	T	50	SER
26	W	76	SER
27	X	3	LYS
29	Z	40	VAL
35	f	102	VAL
35	f	104	ASN
39	j	225	ALA
40	k	136	ILE
40	k	240	LYS
40	k	290	ASN
40	k	324	ASN
42	m	23	SER
42	m	75	GLY
42	m	94	SER
42	m	96	LEU
44	p	160	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
44	p	736	GLN
45	q	357	GLU
5	B	207	LEU
5	B	221	PRO
6	C	43	VAL
7	D	130	GLY
7	D	145	ALA
9	F	65	GLN
9	F	100	MET
11	H	28	GLU
13	J	121	SER
13	J	163	PRO
13	J	182	GLY
19	P	109	PRO
21	R	76	GLU
21	R	98	ASP
35	f	84	VAL
38	i	22	PRO
39	j	198	ILE
44	p	185	PRO
44	p	411	ASN
44	p	529	LYS
45	q	336	ILE
45	q	460	PRO
45	q	652	ILE
3	A	5	SER
3	A	195	TRP
6	C	79	PRO
6	C	240	LEU
7	D	5	ILE
9	F	102	ASN
13	J	35	GLY
16	M	32	ASP
19	P	108	ARG
21	R	22	PRO
21	R	23	LYS
21	R	114	GLY
25	V	12	TYR
26	W	57	ARG
28	Y	64	TYR
30	a	61	GLU
30	a	64	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	d	25	GLY
35	f	93	HIS
40	k	255	ARG
41	l	129	LEU
43	o	194	GLN
43	o	461	SER
44	p	125	GLY
45	q	114	SER
45	q	337	ASP
45	q	346	ASP
45	q	527	GLN
3	A	109	ASN
5	B	132	ASP
8	E	107	GLY
11	H	14	THR
11	H	45	SER
11	H	54	GLY
18	O	96	PRO
19	P	48	GLY
21	R	25	THR
21	R	115	LEU
23	T	96	ALA
24	U	19	ILE
26	W	58	SER
27	X	64	PRO
30	a	28	ARG
34	e	13	LYS
39	j	75	ARG
40	k	278	ALA
40	k	495	ILE
41	l	188	PRO
43	o	392	GLU
43	o	487	ALA
44	p	180	MET
44	p	181	PRO
44	p	342	SER
44	p	364	ASN
45	q	341	VAL
45	q	468	THR
45	q	536	ASP
45	q	645	ILE
3	A	158	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	B	56	ASN
5	B	148	ASN
5	B	224	ASP
11	H	13	PRO
13	J	18	PRO
13	J	134	ILE
14	K	30	PRO
20	Q	34	SER
27	X	63	GLN
28	Y	36	SER
40	k	168	LYS
43	o	294	GLY
44	p	184	VAL
44	p	375	PRO
44	p	531	LYS
44	p	633	VAL
44	p	735	VAL
45	q	347	PRO
45	q	351	ILE
45	q	446	ASN
45	q	630	ILE
45	q	762	GLU
45	q	766	PRO
45	q	781	GLY
6	C	66	LEU
6	C	154	GLY
7	D	217	VAL
9	F	66	ILE
14	K	93	ALA
19	P	75	VAL
27	X	89	ASN
13	J	165	GLY
14	K	88	PRO
40	k	393	GLY
44	p	121	GLY
44	p	422	VAL
44	p	509	VAL
45	q	205	VAL
7	D	216	PRO
12	I	80	GLY
19	P	99	GLY
19	P	129	GLY

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Mol	Chain	Res	Type
22	S	76	PRO
7	D	4	ILE
12	I	122	GLY
19	P	87	PRO
28	Y	29	HIS
39	j	133	PRO
43	o	49	GLU
44	p	392	PRO
45	q	649	PRO
6	C	67	PRO
7	D	63	GLY
7	D	211	PRO
44	p	636	GLY
45	q	355	PRO
3	A	68	PRO
27	X	41	SER

### 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	
3	A	174/176 (99%)	148 (85%)	26 (15%)	3	16
5	B	198/210 (94%)	173 (87%)	25 (13%)	4	20
6	C	176/176 (100%)	150 (85%)	26 (15%)	3	16
7	D	185/185 (100%)	156 (84%)	29 (16%)	2	15
8	E	223/223 (100%)	187 (84%)	36 (16%)	2	14
9	F	174/174 (100%)	146 (84%)	28 (16%)	2	14
10	G	192/192 (100%)	162 (84%)	30 (16%)	2	15
11	H	164/164 (100%)	129 (79%)	35 (21%)	1	6
12	I	147/158 (93%)	132 (90%)	15 (10%)	7	26
13	J	153/153 (100%)	134 (88%)	19 (12%)	4	21
14	K	88/88 (100%)	83 (94%)	5 (6%)	20	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	L	136/136 (100%)	121 (89%)	15 (11%)	6	24
16	M	93/94 (99%)	83 (89%)	10 (11%)	6	25
17	N	127/127 (100%)	112 (88%)	15 (12%)	5	22
18	O	96/96 (100%)	89 (93%)	7 (7%)	14	40
19	P	101/101 (100%)	90 (89%)	11 (11%)	6	25
20	Q	117/117 (100%)	102 (87%)	15 (13%)	4	20
21	R	102/113 (90%)	91 (89%)	11 (11%)	6	25
22	S	128/128 (100%)	109 (85%)	19 (15%)	3	16
23	T	117/117 (100%)	106 (91%)	11 (9%)	8	29
24	U	96/96 (100%)	91 (95%)	5 (5%)	23	49
25	V	73/73 (100%)	64 (88%)	9 (12%)	4	21
26	W	110/110 (100%)	101 (92%)	9 (8%)	11	36
27	X	119/119 (100%)	105 (88%)	14 (12%)	5	22
28	Y	108/108 (100%)	96 (89%)	12 (11%)	6	24
29	Z	60/60 (100%)	57 (95%)	3 (5%)	24	50
30	a	83/83 (100%)	79 (95%)	4 (5%)	25	51
31	b	71/71 (100%)	62 (87%)	9 (13%)	4	20
32	c	54/54 (100%)	46 (85%)	8 (15%)	3	16
33	d	46/46 (100%)	46 (100%)	0	100	100
34	e	51/51 (100%)	47 (92%)	4 (8%)	12	38
35	f	58/60 (97%)	52 (90%)	6 (10%)	7	26
36	g	257/270 (95%)	256 (100%)	1 (0%)	91	94
37	h	23/23 (100%)	21 (91%)	2 (9%)	10	33
38	i	81/81 (100%)	72 (89%)	9 (11%)	6	24
39	j	224/237 (94%)	198 (88%)	26 (12%)	5	22
40	k	332/364 (91%)	317 (96%)	15 (4%)	27	53
41	l	120/132 (91%)	113 (94%)	7 (6%)	20	46
42	m	76/84 (90%)	68 (90%)	8 (10%)	7	26
43	o	404/438 (92%)	361 (89%)	43 (11%)	6	25
44	p	533/584 (91%)	489 (92%)	44 (8%)	11	36
45	q	509/615 (83%)	451 (89%)	58 (11%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	s	287/297 (97%)	286 (100%)	1 (0%)	92	95
47	r	40/40 (100%)	40 (100%)	0	100	100
All	All	6706/7024 (96%)	6021 (90%)	685 (10%)	11	26

All (685) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	THR
3	A	13	ASP
3	A	16	LEU
3	A	30	GLN
3	A	43	ASP
3	A	50	VAL
3	A	58	VAL
3	A	59	LEU
3	A	83	GLN
3	A	87	LEU
3	A	88	LYS
3	A	93	THR
3	A	101	ARG
3	A	108	THR
3	A	112	THR
3	A	113	ARG
3	A	127	ARG
3	A	148	ASP
3	A	154	GLU
3	A	165	ARG
3	A	170	ILE
3	A	193	GLN
3	A	195	TRP
3	A	198	MET
3	A	202	TYR
3	A	203	PHE
5	B	24	PHE
5	B	29	TRP
5	B	39	GLU
5	B	59	ASP
5	B	65	VAL
5	B	68	VAL
5	B	73	LEU
5	B	78	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	B	79	HIS
5	B	82	ARG
5	B	105	PHE
5	B	109	LYS
5	B	110	LEU
5	B	125	VAL
5	B	130	SER
5	B	171	ILE
5	B	177	GLN
5	B	184	LEU
5	B	195	LYS
5	B	205	PHE
5	B	207	LEU
5	B	222	LYS
5	B	225	LEU
5	B	228	LEU
5	B	231	LEU
6	C	49	LEU
6	C	50	VAL
6	C	58	ILE
6	C	65	SER
6	C	81	LEU
6	C	84	GLU
6	C	86	MET
6	C	91	VAL
6	C	95	THR
6	C	96	ARG
6	C	111	ASP
6	C	139	LEU
6	C	145	ARG
6	C	146	ARG
6	C	151	THR
6	C	155	GLN
6	C	166	LYS
6	C	173	ARG
6	C	199	GLU
6	C	227	TYR
6	C	230	LEU
6	C	234	LEU
6	C	235	TRP
6	C	236	GLU
6	C	240	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	C	250	ASP
7	D	5	ILE
7	D	6	SER
7	D	9	ARG
7	D	11	LEU
7	D	16	VAL
7	D	20	GLU
7	D	21	LEU
7	D	28	GLU
7	D	50	ILE
7	D	55	VAL
7	D	65	ARG
7	D	66	ILE
7	D	68	GLU
7	D	71	LEU
7	D	80	LYS
7	D	90	ARG
7	D	94	ARG
7	D	116	ARG
7	D	125	TYR
7	D	143	ARG
7	D	148	LYS
7	D	152	PHE
7	D	157	LEU
7	D	167	PHE
7	D	176	LEU
7	D	187	LYS
7	D	200	LYS
7	D	212	LYS
7	D	221	SER
8	E	24	SER
8	E	30	ARG
8	E	39	ARG
8	E	51	ARG
8	E	56	LEU
8	E	57	ASN
8	E	60	GLU
8	E	65	LEU
8	E	67	GLN
8	E	68	ARG
8	E	69	HIS
8	E	77	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	E	87	MET
8	E	88	ASP
8	E	92	LEU
8	E	95	THR
8	E	102	VAL
8	E	108	ARG
8	E	113	ARG
8	E	115	THR
8	E	121	TYR
8	E	131	LEU
8	E	142	HIS
8	E	143	ASP
8	E	148	ARG
8	E	159	THR
8	E	189	LEU
8	E	200	ARG
8	E	206	ASP
8	E	208	VAL
8	E	224	ASN
8	E	225	VAL
8	E	233	ARG
8	E	235	TRP
8	E	248	ILE
8	E	250	GLU
9	F	26	GLU
9	F	42	ILE
9	F	52	ASP
9	F	54	GLU
9	F	57	ASP
9	F	70	ILE
9	F	79	TYR
9	F	86	LYS
9	F	91	ILE
9	F	93	GLU
9	F	99	LEU
9	F	101	MET
9	F	108	LYS
9	F	126	LEU
9	F	128	ASP
9	F	129	GLN
9	F	136	VAL
9	F	145	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	F	164	VAL
9	F	167	LEU
9	F	169	ARG
9	F	187	ARG
9	F	188	ASN
9	F	211	TYR
9	F	216	LYS
9	F	219	LEU
9	F	221	ARG
9	F	224	LYS
10	G	3	LEU
10	G	7	TYR
10	G	16	ILE
10	G	17	GLU
10	G	22	HIS
10	G	23	ARG
10	G	25	ARG
10	G	31	ARG
10	G	35	GLU
10	G	51	LYS
10	G	63	MET
10	G	72	ARG
10	G	88	ARG
10	G	92	ARG
10	G	94	ARG
10	G	95	LYS
10	G	109	LEU
10	G	124	ILE
10	G	132	ARG
10	G	133	LEU
10	G	147	LEU
10	G	159	ARG
10	G	164	LYS
10	G	177	ARG
10	G	178	LEU
10	G	185	GLN
10	G	193	LEU
10	G	195	ILE
10	G	215	ARG
10	G	225	GLU
11	H	5	GLN
11	H	9	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	H	10	SER
11	H	19	GLN
11	H	27	LEU
11	H	30	ASN
11	H	33	GLU
11	H	48	GLU
11	H	50	GLU
11	H	51	VAL
11	H	55	LYS
11	H	58	LEU
11	H	70	TYR
11	H	72	LYS
11	H	77	LEU
11	H	80	GLU
11	H	81	LEU
11	H	87	ASP
11	H	96	ARG
11	H	111	LYS
11	H	123	ASP
11	H	124	LYS
11	H	126	LEU
11	H	129	LEU
11	H	130	VAL
11	H	139	ARG
11	H	141	ARG
11	H	147	ASN
11	H	160	GLN
11	H	163	ASP
11	H	164	ASN
11	H	165	LYS
11	H	169	PHE
11	H	176	LEU
11	H	180	GLN
12	I	8	ARG
12	I	9	HIS
12	I	20	GLN
12	I	22	ARG
12	I	23	LYS
12	I	29	LEU
12	I	41	LYS
12	I	56	ARG
12	I	58	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	I	104	ILE
12	I	110	ARG
12	I	119	GLN
12	I	179	ARG
12	I	196	ARG
12	I	200	LYS
13	J	3	ARG
13	J	8	TYR
13	J	12	TYR
13	J	17	ARG
13	J	28	LEU
13	J	33	GLU
13	J	36	LEU
13	J	37	LYS
13	J	45	ILE
13	J	64	GLU
13	J	65	LYS
13	J	89	ASP
13	J	100	LYS
13	J	104	PHE
13	J	107	ARG
13	J	109	LEU
13	J	111	THR
13	J	145	SER
13	J	160	ARG
14	K	17	GLN
14	K	21	LEU
14	K	44	LYS
14	K	67	THR
14	K	76	LEU
15	L	5	LEU
15	L	6	THR
15	L	8	GLN
15	L	10	GLU
15	L	21	THR
15	L	36	LYS
15	L	80	MET
15	L	83	THR
15	L	84	ILE
15	L	89	ASP
15	L	104	HIS
15	L	121	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	L	124	THR
15	L	136	ARG
15	L	144	SER
16	M	22	LYS
16	M	40	GLU
16	M	55	LEU
16	M	74	GLU
16	M	88	LEU
16	M	90	GLU
16	M	110	SER
16	M	117	TRP
16	M	121	THR
16	M	125	GLU
17	N	3	ARG
17	N	20	ARG
17	N	27	LYS
17	N	42	ARG
17	N	64	LYS
17	N	72	LEU
17	N	88	LEU
17	N	100	LYS
17	N	105	ASN
17	N	106	ARG
17	N	107	LYS
17	N	109	LYS
17	N	110	ASP
17	N	142	GLU
17	N	150	VAL
18	O	24	ASN
18	O	49	LYS
18	O	90	ARG
18	O	92	LYS
18	O	110	LEU
18	O	114	ARG
18	O	124	ASP
19	P	13	LYS
19	P	28	MET
19	P	40	ARG
19	P	43	ARG
19	P	56	LEU
19	P	57	MET
19	P	71	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	P	72	LYS
19	P	111	MET
19	P	119	PHE
19	P	123	TYR
20	Q	13	LYS
20	Q	43	ILE
20	Q	65	ILE
20	Q	83	GLN
20	Q	89	LEU
20	Q	97	VAL
20	Q	98	ASP
20	Q	104	GLU
20	Q	105	LEU
20	Q	114	ARG
20	Q	115	THR
20	Q	123	ARG
20	Q	127	LYS
20	Q	137	ARG
20	Q	139	GLN
21	R	3	ARG
21	R	10	LYS
21	R	29	GLN
21	R	34	LEU
21	R	46	LEU
21	R	47	ARG
21	R	48	ASN
21	R	55	THR
21	R	78	ARG
21	R	80	ARG
21	R	100	LEU
22	S	6	GLN
22	S	8	GLN
22	S	11	PHE
22	S	25	ASN
22	S	40	ARG
22	S	54	LEU
22	S	86	LEU
22	S	88	ARG
22	S	96	LYS
22	S	97	ASP
22	S	103	ASN
22	S	105	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	S	109	LEU
22	S	110	ARG
22	S	114	GLU
22	S	126	ARG
22	S	128	PHE
22	S	141	THR
22	S	144	ARG
23	T	12	GLN
23	T	16	ASN
23	T	29	GLU
23	T	65	ILE
23	T	68	ARG
23	T	79	LEU
23	T	91	HIS
23	T	103	LYS
23	T	124	ILE
23	T	129	LEU
23	T	135	ILE
24	U	27	THR
24	U	57	ARG
24	U	83	GLU
24	U	89	ARG
24	U	93	LEU
25	V	1	MET
25	V	12	TYR
25	V	21	ASN
25	V	33	GLN
25	V	34	ILE
25	V	40	ASP
25	V	62	ARG
25	V	69	LEU
25	V	74	GLN
26	W	3	ARG
26	W	9	ASP
26	W	16	ASN
26	W	23	ARG
26	W	24	GLN
26	W	43	LYS
26	W	60	LYS
26	W	113	HIS
26	W	115	GLU
27	X	9	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	X	14	LYS
27	X	19	ARG
27	X	30	LYS
27	X	55	GLU
27	X	59	ILE
27	X	60	GLU
27	X	79	ASN
27	X	83	VAL
27	X	93	LEU
27	X	100	ASP
27	X	107	PHE
27	X	121	ARG
27	X	132	LEU
28	Y	8	ARG
28	Y	20	ARG
28	Y	31	ASN
28	Y	48	TYR
28	Y	63	GLN
28	Y	69	SER
28	Y	74	LEU
28	Y	84	LYS
28	Y	99	LYS
28	Y	107	GLN
28	Y	112	LYS
28	Y	128	LYS
29	Z	58	ARG
29	Z	62	VAL
29	Z	80	LEU
30	a	12	LYS
30	a	15	ARG
30	a	38	ARG
30	a	69	ASN
31	b	5	GLN
31	b	8	LEU
31	b	20	LYS
31	b	24	LEU
31	b	31	HIS
31	b	34	ASP
31	b	57	GLU
31	b	65	THR
31	b	67	THR
32	c	9	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	c	14	LYS
32	c	19	THR
32	c	29	ARG
32	c	40	ILE
32	c	42	ARG
32	c	52	ASP
32	c	65	ARG
34	e	20	LYS
34	e	33	ARG
34	e	47	VAL
34	e	54	ARG
35	f	99	LYS
35	f	100	LEU
35	f	102	VAL
35	f	110	ASP
35	f	119	LYS
35	f	142	CYS
36	g	59	VAL
37	h	8	LYS
37	h	9	ARG
38	i	23	LYS
38	i	31	GLU
38	i	33	GLN
38	i	40	LYS
38	i	55	ASN
38	i	56	LYS
38	i	62	ARG
38	i	85	GLN
38	i	114	LYS
39	j	7	ARG
39	j	19	ILE
39	j	45	MET
39	j	46	ILE
39	j	47	LEU
39	j	57	ARG
39	j	59	ILE
39	j	64	ARG
39	j	85	LEU
39	j	87	LYS
39	j	108	VAL
39	j	121	ILE
39	j	123	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	j	126	LEU
39	j	133	PRO
39	j	143	GLU
39	j	152	GLU
39	j	163	LYS
39	j	166	LEU
39	j	185	ARG
39	j	195	TYR
39	j	205	LEU
39	j	228	TYR
39	j	230	LEU
39	j	236	ASP
39	j	264	ILE
40	k	103	ILE
40	k	136	ILE
40	k	147	ILE
40	k	210	VAL
40	k	228	GLN
40	k	245	ILE
40	k	266	ILE
40	k	291	ILE
40	k	311	ILE
40	k	315	LEU
40	k	356	ARG
40	k	368	ILE
40	k	386	ASP
40	k	412	LEU
40	k	471	THR
41	l	165	CYS
41	l	186	ARG
41	l	198	GLU
41	l	213	ILE
41	l	227	ARG
41	l	244	THR
41	l	254	LEU
42	m	36	ARG
42	m	54	ILE
42	m	55	LEU
42	m	61	ASP
42	m	96	LEU
42	m	104	LYS
42	m	105	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
42	m	108	PHE
43	o	18	LEU
43	o	33	ASP
43	o	38	ARG
43	o	41	ARG
43	o	42	TRP
43	o	52	VAL
43	o	62	LEU
43	o	73	HIS
43	o	75	TYR
43	o	98	ASP
43	o	108	GLN
43	o	110	ARG
43	o	152	THR
43	o	167	ASP
43	o	199	PHE
43	o	202	LEU
43	o	206	LEU
43	o	214	ASN
43	o	229	ASP
43	o	231	ASP
43	o	232	THR
43	o	252	LEU
43	o	254	HIS
43	o	257	TYR
43	o	265	HIS
43	o	266	LEU
43	o	290	PHE
43	o	303	TRP
43	o	319	GLU
43	o	321	PHE
43	o	328	ILE
43	o	337	LEU
43	o	363	ARG
43	o	373	ASP
43	o	382	GLU
43	o	387	LEU
43	o	388	TYR
43	o	408	LEU
43	o	430	ARG
43	o	438	GLN
43	o	470	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
43	o	475	GLU
43	o	485	GLU
44	p	79	ILE
44	p	103	PHE
44	p	141	ILE
44	p	154	ARG
44	p	199	ARG
44	p	207	ASP
44	p	234	ASN
44	p	237	ARG
44	p	243	THR
44	p	250	GLN
44	p	260	ASN
44	p	284	LEU
44	p	326	PHE
44	p	334	LEU
44	p	340	ARG
44	p	360	ASP
44	p	373	LEU
44	p	393	PHE
44	p	394	ARG
44	p	412	ASN
44	p	424	ARG
44	p	428	LEU
44	p	439	VAL
44	p	441	LEU
44	p	449	PHE
44	p	456	ARG
44	p	463	THR
44	p	468	LEU
44	p	469	GLN
44	p	471	CYS
44	p	485	LEU
44	p	500	ARG
44	p	528	THR
44	p	544	ILE
44	p	547	THR
44	p	551	THR
44	p	571	MET
44	p	573	ARG
44	p	579	TYR
44	p	591	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
44	p	592	ASN
44	p	642	ILE
44	p	655	PHE
44	p	663	ARG
45	q	260	THR
45	q	269	THR
45	q	278	THR
45	q	282	LEU
45	q	294	MET
45	q	296	TYR
45	q	298	THR
45	q	322	PHE
45	q	331	ILE
45	q	339	TYR
45	q	376	LEU
45	q	388	ASP
45	q	393	ASP
45	q	394	TYR
45	q	395	LEU
45	q	396	ILE
45	q	397	ARG
45	q	408	ILE
45	q	409	LEU
45	q	413	LEU
45	q	431	ARG
45	q	437	LEU
45	q	438	ASP
45	q	441	TYR
45	q	446	ASN
45	q	486	LEU
45	q	500	LYS
45	q	506	ASN
45	q	510	THR
45	q	532	ILE
45	q	535	PHE
45	q	542	LEU
45	q	552	LEU
45	q	557	LEU
45	q	558	CYS
45	q	570	LEU
45	q	600	GLU
45	q	612	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	q	617	ILE
45	q	634	THR
45	q	644	ARG
45	q	645	ILE
45	q	671	LEU
45	q	673	ASP
45	q	674	TYR
45	q	676	LEU
45	q	687	TRP
45	q	694	LEU
45	q	702	LEU
45	q	710	LEU
45	q	724	THR
45	q	726	PHE
45	q	727	PHE
45	q	740	LYS
45	q	744	LEU
45	q	749	GLU
45	q	765	ILE
45	q	774	THR
46	s	308	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	30	GLN
3	A	92	HIS
5	B	148	ASN
5	B	177	GLN
5	B	178	ASN
5	B	183	GLN
5	B	232	HIS
6	C	72	GLN
6	C	152	ASN
6	C	155	GLN
7	D	162	GLN
8	E	130	GLN
8	E	224	ASN
9	F	36	GLN
9	F	129	GLN
9	F	188	ASN
10	G	10	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	G	199	GLN
11	H	19	GLN
11	H	30	ASN
11	H	71	HIS
11	H	108	GLN
11	H	110	GLN
11	H	147	ASN
11	H	164	ASN
12	I	53	GLN
12	I	139	ASN
16	M	130	HIS
17	N	49	GLN
17	N	58	HIS
17	N	78	ASN
18	O	24	ASN
19	P	128	HIS
20	Q	62	ASN
20	Q	83	GLN
20	Q	94	GLN
20	Q	100	GLN
21	R	31	ASN
22	S	44	ASN
22	S	136	GLN
23	T	17	ASN
23	T	23	GLN
23	T	43	ASN
25	V	33	GLN
26	W	64	GLN
26	W	80	ASN
26	W	98	GLN
27	X	22	ASN
27	X	79	ASN
28	Y	22	GLN
28	Y	106	GLN
29	Z	98	GLN
30	a	25	ASN
32	c	27	GLN
33	d	20	GLN
33	d	41	GLN
35	f	104	ASN
36	g	204	ASN
36	g	210	GLN

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Mol	Chain	Res	Type
36	g	234	HIS
36	g	292	GLN
38	i	60	HIS
38	i	73	GLN
39	j	23	ASN
39	j	25	GLN
39	j	103	GLN
40	k	98	GLN
40	k	108	HIS
40	k	144	ASN
42	m	67	ASN
42	m	99	GLN
43	o	73	HIS
43	o	216	GLN
44	p	145	HIS
44	p	219	ASN
44	p	359	HIS
44	p	411	ASN
44	p	412	ASN
44	p	467	ASN
44	p	513	ASN
44	p	588	ASN
44	p	592	ASN
45	q	402	GLN
45	q	406	ASN
45	q	595	ASN
45	q	610	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	71/76 (93%)	33 (46%)	9 (12%)
2	2	1797/1798 (99%)	814 (45%)	70 (3%)
4	3	2/3 (66%)	0	0
All	All	1870/1877 (99%)	847 (45%)	79 (4%)

All (847) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	5	C
1	1	9	1MG

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Mol	Chain	Res	Type
1	1	10	2MG
1	1	11	C
1	1	12	G
1	1	16	H2U
1	1	19	G
1	1	21	A
1	1	26	M2G
1	1	27	C
1	1	29	G
1	1	31	G
1	1	32	C
1	1	34	C
1	1	35	A
1	1	37	T6A
1	1	38	A
1	1	39	C
1	1	43	G
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	49	5MC
1	1	50	U
1	1	52	G
1	1	57	G
1	1	58	1MA
1	1	61	C
1	1	64	RIA
1	1	69	C
1	1	71	C
1	1	74	C
1	1	75	C
2	2	2	A
2	2	4	C
2	2	5	U
2	2	8	U
2	2	11	A
2	2	14	C
2	2	17	C
2	2	19	A
2	2	20	G
2	2	25	C
2	2	26	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	27	U
2	2	31	C
2	2	32	U
2	2	33	U
2	2	34	G
2	2	35	U
2	2	36	C
2	2	42	G
2	2	43	A
2	2	45	U
2	2	46	A
2	2	47	A
2	2	51	A
2	2	56	U
2	2	57	G
2	2	58	U
2	2	59	C
2	2	61	A
2	2	62	A
2	2	63	G
2	2	64	U
2	2	65	A
2	2	67	A
2	2	68	A
2	2	69	G
2	2	70	C
2	2	71	A
2	2	72	A
2	2	73	U
2	2	74	U
2	2	75	U
2	2	76	A
2	2	77	U
2	2	79	C
2	2	80	A
2	2	90	C
2	2	92	A
2	2	98	U
2	2	99	C
2	2	104	A
2	2	114	C
2	2	116	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	119	A
2	2	120	U
2	2	123	G
2	2	124	A
2	2	127	G
2	2	128	U
2	2	129	U
2	2	130	C
2	2	131	C
2	2	132	U
2	2	133	U
2	2	134	U
2	2	135	A
2	2	136	C
2	2	137	U
2	2	138	A
2	2	139	C
2	2	140	A
2	2	144	A
2	2	146	A
2	2	147	U
2	2	152	G
2	2	156	A
2	2	157	U
2	2	158	U
2	2	159	C
2	2	160	U
2	2	167	A
2	2	169	U
2	2	176	U
2	2	183	C
2	2	187	A
2	2	188	C
2	2	189	C
2	2	190	C
2	2	191	U
2	2	193	U
2	2	194	G
2	2	196	A
2	2	202	U
2	2	208	U
2	2	209	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	217	A
2	2	218	A
2	2	220	A
2	2	224	A
2	2	225	A
2	2	227	G
2	2	228	U
2	2	231	U
2	2	232	C
2	2	233	G
2	2	234	G
2	2	236	C
2	2	239	C
2	2	240	U
2	2	241	U
2	2	249	C
2	2	256	A
2	2	259	U
2	2	261	U
2	2	264	A
2	2	265	A
2	2	266	U
2	2	267	C
2	2	273	G
2	2	275	C
2	2	277	U
2	2	278	G
2	2	279	U
2	2	280	G
2	2	282	U
2	2	283	G
2	2	286	G
2	2	287	A
2	2	289	G
2	2	293	C
2	2	294	A
2	2	298	A
2	2	300	A
2	2	301	U
2	2	307	C
2	2	308	C
2	2	311	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	312	U
2	2	313	C
2	2	314	A
2	2	315	A
2	2	318	U
2	2	319	U
2	2	321	G
2	2	322	A
2	2	323	U
2	2	326	U
2	2	327	A
2	2	336	G
2	2	338	C
2	2	342	C
2	2	345	G
2	2	349	U
2	2	351	A
2	2	352	A
2	2	359	A
2	2	360	C
2	2	374	U
2	2	377	A
2	2	379	U
2	2	380	C
2	2	382	G
2	2	383	G
2	2	384	A
2	2	386	A
2	2	387	G
2	2	389	G
2	2	390	A
2	2	398	A
2	2	399	A
2	2	400	A
2	2	401	C
2	2	402	G
2	2	403	G
2	2	404	C
2	2	410	C
2	2	412	U
2	2	413	C
2	2	415	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	416	A
2	2	417	G
2	2	421	G
2	2	422	G
2	2	423	C
2	2	424	A
2	2	425	G
2	2	437	A
2	2	438	U
2	2	439	U
2	2	440	A
2	2	442	C
2	2	443	C
2	2	447	C
2	2	448	C
2	2	450	A
2	2	451	A
2	2	452	U
2	2	455	A
2	2	456	G
2	2	467	A
2	2	468	C
2	2	469	A
2	2	473	A
2	2	476	A
2	2	480	A
2	2	482	A
2	2	484	A
2	2	485	G
2	2	489	C
2	2	490	C
2	2	491	A
2	2	492	U
2	2	493	U
2	2	495	G
2	2	496	G
2	2	498	U
2	2	499	C
2	2	501	U
2	2	502	G
2	2	503	U
2	2	504	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	505	A
2	2	506	U
2	2	507	U
2	2	510	A
2	2	512	U
2	2	516	U
2	2	517	A
2	2	518	C
2	2	519	A
2	2	522	G
2	2	524	A
2	2	525	A
2	2	527	U
2	2	531	U
2	2	533	A
2	2	534	A
2	2	535	C
2	2	536	G
2	2	537	A
2	2	538	G
2	2	539	G
2	2	540	A
2	2	541	A
2	2	542	C
2	2	543	A
2	2	545	C
2	2	547	G
2	2	548	G
2	2	553	C
2	2	554	A
2	2	556	G
2	2	557	U
2	2	558	C
2	2	560	G
2	2	562	U
2	2	564	C
2	2	565	C
2	2	566	A
2	2	568	C
2	2	569	A
2	2	571	C
2	2	573	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	577	U
2	2	578	A
2	2	580	U
2	2	581	U
2	2	582	C
2	2	584	A
2	2	585	G
2	2	592	U
2	2	593	A
2	2	594	G
2	2	605	A
2	2	610	U
2	2	612	G
2	2	614	A
2	2	618	A
2	2	619	A
2	2	620	A
2	2	622	A
2	2	634	A
2	2	636	C
2	2	637	U
2	2	638	U
2	2	639	U
2	2	641	G
2	2	642	G
2	2	647	G
2	2	650	G
2	2	652	C
2	2	653	C
2	2	656	U
2	2	657	C
2	2	659	G
2	2	661	C
2	2	663	U
2	2	664	U
2	2	665	A
2	2	669	C
2	2	671	C
2	2	672	G
2	2	673	C
2	2	675	C
2	2	679	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	680	U
2	2	681	U
2	2	684	A
2	2	685	A
2	2	686	C
2	2	688	G
2	2	691	U
2	2	693	U
2	2	694	U
2	2	696	C
2	2	697	C
2	2	698	U
2	2	699	U
2	2	700	C
2	2	701	U
2	2	704	C
2	2	707	A
2	2	709	C
2	2	710	U
2	2	711	G
2	2	712	U
2	2	713	A
2	2	714	C
2	2	715	U
2	2	716	C
2	2	717	C
2	2	718	U
2	2	719	U
2	2	721	U
2	2	722	G
2	2	723	G
2	2	724	G
2	2	725	U
2	2	727	C
2	2	728	A
2	2	730	G
2	2	731	C
2	2	732	G
2	2	733	A
2	2	734	A
2	2	736	C
2	2	738	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	739	G
2	2	742	U
2	2	743	U
2	2	748	U
2	2	753	A
2	2	755	A
2	2	762	A
2	2	765	G
2	2	766	U
2	2	767	U
2	2	768	C
2	2	771	A
2	2	773	C
2	2	774	A
2	2	776	G
2	2	778	G
2	2	780	A
2	2	781	A
2	2	782	G
2	2	783	C
2	2	784	U
2	2	785	C
2	2	786	G
2	2	788	A
2	2	791	U
2	2	792	A
2	2	793	U
2	2	794	U
2	2	798	A
2	2	799	U
2	2	806	A
2	2	808	G
2	2	809	G
2	2	810	A
2	2	811	A
2	2	813	A
2	2	814	G
2	2	817	C
2	2	818	G
2	2	819	U
2	2	820	U
2	2	821	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	822	G
2	2	823	G
2	2	825	U
2	2	826	C
2	2	827	U
2	2	828	A
2	2	829	U
2	2	830	U
2	2	832	U
2	2	840	U
2	2	843	A
2	2	845	G
2	2	851	C
2	2	855	A
2	2	856	U
2	2	857	G
2	2	859	U
2	2	861	A
2	2	862	A
2	2	863	U
2	2	872	U
2	2	875	G
2	2	881	U
2	2	891	A
2	2	897	A
2	2	898	G
2	2	901	G
2	2	902	U
2	2	903	G
2	2	905	A
2	2	907	U
2	2	908	U
2	2	910	U
2	2	911	U
2	2	912	G
2	2	913	G
2	2	914	A
2	2	915	U
2	2	919	U
2	2	920	U
2	2	924	G
2	2	925	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	930	C
2	2	931	U
2	2	932	A
2	2	933	C
2	2	934	U
2	2	939	A
2	2	941	G
2	2	942	C
2	2	944	U
2	2	946	U
2	2	947	G
2	2	950	A
2	2	956	G
2	2	958	U
2	2	965	A
2	2	968	C
2	2	972	A
2	2	976	A
2	2	977	A
2	2	982	A
2	2	983	G
2	2	984	G
2	2	987	A
2	2	991	A
2	2	994	A
2	2	995	U
2	2	999	C
2	2	1000	A
2	2	1001	G
2	2	1002	A
2	2	1003	U
2	2	1004	A
2	2	1006	C
2	2	1011	U
2	2	1015	C
2	2	1016	U
2	2	1018	A
2	2	1019	A
2	2	1022	A
2	2	1023	U
2	2	1024	A
2	2	1025	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	1026	A
2	2	1027	C
2	2	1028	U
2	2	1029	A
2	2	1030	U
2	2	1031	G
2	2	1034	G
2	2	1038	A
2	2	1041	G
2	2	1047	G
2	2	1048	U
2	2	1049	G
2	2	1050	G
2	2	1051	U
2	2	1052	G
2	2	1054	U
2	2	1055	U
2	2	1056	U
2	2	1057	U
2	2	1058	C
2	2	1059	U
2	2	1062	U
2	2	1070	U
2	2	1073	G
2	2	1081	C
2	2	1082	G
2	2	1084	G
2	2	1090	A
2	2	1091	A
2	2	1093	G
2	2	1095	C
2	2	1096	U
2	2	1097	U
2	2	1099	G
2	2	1100	G
2	2	1102	U
2	2	1103	U
2	2	1105	U
2	2	1112	A
2	2	1113	G
2	2	1114	U
2	2	1118	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	1123	A
2	2	1124	A
2	2	1130	A
2	2	1136	A
2	2	1137	A
2	2	1142	A
2	2	1145	G
2	2	1146	A
2	2	1149	G
2	2	1156	A
2	2	1157	C
2	2	1158	C
2	2	1161	C
2	2	1162	A
2	2	1166	G
2	2	1168	G
2	2	1176	C
2	2	1179	C
2	2	1182	A
2	2	1183	A
2	2	1184	U
2	2	1186	U
2	2	1188	A
2	2	1190	U
2	2	1191	C
2	2	1192	A
2	2	1193	A
2	2	1195	A
2	2	1198	G
2	2	1199	G
2	2	1200	G
2	2	1201	A
2	2	1202	A
2	2	1203	A
2	2	1204	C
2	2	1205	U
2	2	1207	A
2	2	1208	C
2	2	1212	G
2	2	1213	U
2	2	1215	C
2	2	1216	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	1217	G
2	2	1218	A
2	2	1224	U
2	2	1227	G
2	2	1228	G
2	2	1229	A
2	2	1232	G
2	2	1238	U
2	2	1240	G
2	2	1241	A
2	2	1242	G
2	2	1243	A
2	2	1244	G
2	2	1245	C
2	2	1250	U
2	2	1255	A
2	2	1258	U
2	2	1260	G
2	2	1264	G
2	2	1265	U
2	2	1266	G
2	2	1268	U
2	2	1269	G
2	2	1270	G
2	2	1271	U
2	2	1272	G
2	2	1277	G
2	2	1278	C
2	2	1279	C
2	2	1281	U
2	2	1282	U
2	2	1283	C
2	2	1284	U
2	2	1285	U
2	2	1292	U
2	2	1295	A
2	2	1296	G
2	2	1298	G
2	2	1299	A
2	2	1305	C
2	2	1306	U
2	2	1310	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	1313	U
2	2	1314	U
2	2	1315	G
2	2	1316	C
2	2	1318	A
2	2	1319	U
2	2	1320	A
2	2	1321	A
2	2	1322	C
2	2	1323	G
2	2	1324	A
2	2	1332	C
2	2	1336	A
2	2	1338	C
2	2	1339	U
2	2	1343	A
2	2	1344	A
2	2	1345	A
2	2	1347	A
2	2	1350	G
2	2	1351	U
2	2	1356	G
2	2	1357	G
2	2	1360	C
2	2	1362	U
2	2	1363	G
2	2	1364	C
2	2	1369	U
2	2	1370	G
2	2	1371	A
2	2	1372	C
2	2	1374	C
2	2	1375	U
2	2	1376	U
2	2	1378	U
2	2	1380	A
2	2	1381	G
2	2	1382	A
2	2	1384	G
2	2	1386	A
2	2	1388	U
2	2	1393	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	1395	U
2	2	1396	U
2	2	1397	C
2	2	1398	A
2	2	1400	G
2	2	1401	C
2	2	1404	A
2	2	1406	G
2	2	1410	G
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1414	G
2	2	1415	A
2	2	1416	G
2	2	1419	A
2	2	1420	A
2	2	1425	A
2	2	1426	G
2	2	1429	C
2	2	1430	U
2	2	1431	G
2	2	1432	U
2	2	1433	G
2	2	1434	A
2	2	1442	A
2	2	1443	G
2	2	1444	A
2	2	1445	C
2	2	1446	G
2	2	1448	U
2	2	1452	G
2	2	1453	G
2	2	1455	C
2	2	1456	G
2	2	1457	C
2	2	1460	G
2	2	1463	C
2	2	1464	G
2	2	1467	A
2	2	1469	A
2	2	1471	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	1476	G
2	2	1479	C
2	2	1482	G
2	2	1483	C
2	2	1484	G
2	2	1488	A
2	2	1489	C
2	2	1490	A
2	2	1491	A
2	2	1492	C
2	2	1494	U
2	2	1495	U
2	2	1496	G
2	2	1498	C
2	2	1499	C
2	2	1501	A
2	2	1502	G
2	2	1504	G
2	2	1507	C
2	2	1509	G
2	2	1512	U
2	2	1513	A
2	2	1514	A
2	2	1515	U
2	2	1516	C
2	2	1519	G
2	2	1520	U
2	2	1521	G
2	2	1522	A
2	2	1523	A
2	2	1526	U
2	2	1528	C
2	2	1529	G
2	2	1532	G
2	2	1533	U
2	2	1534	G
2	2	1535	C
2	2	1536	U
2	2	1538	G
2	2	1549	U
2	2	1554	A
2	2	1555	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	1557	A
2	2	1570	G
2	2	1571	A
2	2	1572	G
2	2	1573	G
2	2	1575	A
2	2	1576	U
2	2	1579	C
2	2	1581	A
2	2	1583	U
2	2	1584	A
2	2	1588	G
2	2	1594	C
2	2	1595	A
2	2	1597	C
2	2	1598	A
2	2	1599	G
2	2	1604	C
2	2	1613	C
2	2	1614	G
2	2	1623	C
2	2	1625	U
2	2	1628	U
2	2	1630	C
2	2	1632	C
2	2	1633	A
2	2	1635	C
2	2	1638	C
2	2	1640	G
2	2	1649	A
2	2	1655	U
2	2	1656	G
2	2	1662	C
2	2	1673	C
2	2	1676	A
2	2	1678	G
2	2	1679	A
2	2	1682	U
2	2	1686	U
2	2	1687	A
2	2	1688	G
2	2	1692	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	1693	G
2	2	1694	G
2	2	1695	G
2	2	1696	G
2	2	1697	G
2	2	1698	C
2	2	1700	A
2	2	1701	C
2	2	1702	U
2	2	1703	C
2	2	1704	C
2	2	1705	A
2	2	1706	U
2	2	1707	C
2	2	1708	U
2	2	1709	C
2	2	1710	A
2	2	1711	G
2	2	1712	A
2	2	1715	G
2	2	1719	A
2	2	1724	G
2	2	1725	G
2	2	1728	A
2	2	1742	A
2	2	1748	A
2	2	1752	A
2	2	1753	A
2	2	1754	A
2	2	1758	G
2	2	1763	A
2	2	1764	A
2	2	1767	U
2	2	1768	U
2	2	1777	U
2	2	1778	G
2	2	1781	C
2	2	1787	G
2	2	1789	A
2	2	1790	G
2	2	1791	G
2	2	1792	A

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Mol	Chain	Res	Type
2	2	1793	U
2	2	1794	C
2	2	1796	U
2	2	1797	U
2	2	1798	A

All (79) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	9	1MG
1	1	10	2MG
1	1	20	A
1	1	26	M2G
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	49	5MC
1	1	74	C
2	2	25	C
2	2	58	U
2	2	61	A
2	2	68	A
2	2	74	U
2	2	115	G
2	2	130	C
2	2	140	A
2	2	191	U
2	2	216	A
2	2	217	A
2	2	239	C
2	2	258	U
2	2	265	A
2	2	277	U
2	2	279	U
2	2	318	U
2	2	321	G
2	2	344	U
2	2	437	A
2	2	524	A
2	2	538	G
2	2	542	C
2	2	557	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	564	C
2	2	637	U
2	2	649	U
2	2	670	G
2	2	685	A
2	2	695	U
2	2	700	C
2	2	721	U
2	2	735	C
2	2	742	U
2	2	765	G
2	2	812	U
2	2	822	G
2	2	828	A
2	2	854	A
2	2	896	C
2	2	907	U
2	2	912	G
2	2	938	A
2	2	946	U
2	2	1001	G
2	2	1030	U
2	2	1051	U
2	2	1107	G
2	2	1123	A
2	2	1149	G
2	2	1198	G
2	2	1206	C
2	2	1314	U
2	2	1343	A
2	2	1386	A
2	2	1410	G
2	2	1411	U
2	2	1430	U
2	2	1445	C
2	2	1455	C
2	2	1487	U
2	2	1491	A
2	2	1534	G
2	2	1571	A
2	2	1580	U
2	2	1613	C

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Mol	Chain	Res	Type
2	2	1678	G
2	2	1789	A
2	2	1792	A
2	2	1795	A

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

11 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
1	2MG	1	10	1	18,26,27	1.04	2 (11%)	16,38,41	1.38	3 (18%)
1	RIA	1	64	1	31,38,39	1.09	3 (9%)	39,57,60	1.40	5 (12%)
1	7MG	1	46	1	22,26,27	1.49	4 (18%)	29,39,42	2.55	8 (27%)
1	T6A	1	37	1	27,34,35	1.16	3 (11%)	29,49,52	2.32	6 (20%)
1	H2U	1	47	1	18,21,22	0.72	0	21,30,33	1.41	3 (14%)
1	1MG	1	9	1	18,26,27	1.04	1 (5%)	19,39,42	1.69	5 (26%)
1	5MC	1	49	1	18,22,23	1.40	3 (16%)	26,32,35	1.49	2 (7%)
1	H2U	1	16	1	18,21,22	0.80	0	21,30,33	1.54	5 (23%)
1	M2G	1	26	1	20,27,28	1.68	2 (10%)	22,40,43	1.30	4 (18%)
1	5MC	1	48	1	18,22,23	1.04	0	26,32,35	1.51	6 (23%)
1	1MA	1	58	1	16,25,26	1.83	3 (18%)	18,37,40	1.36	4 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	1	10	1	-	2/5/27/28	0/3/3/3
1	RIA	1	64	1	-	7/13/51/52	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	7MG	1	46	1	-	2/7/37/38	0/3/3/3
1	T6A	1	37	1	-	10/19/41/42	0/3/3/3
1	H2U	1	47	1	-	5/7/38/39	0/2/2/2
1	1MG	1	9	1	-	3/3/25/26	0/3/3/3
1	5MC	1	49	1	-	1/7/25/26	0/2/2/2
1	H2U	1	16	1	-	2/7/38/39	0/2/2/2
1	M2G	1	26	1	-	5/7/29/30	0/3/3/3
1	5MC	1	48	1	-	0/7/25/26	0/2/2/2
1	1MA	1	58	1	-	2/3/25/26	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	58	1MA	C2-N3	5.54	1.35	1.29
1	1	26	M2G	C2-N3	5.48	1.37	1.30
1	1	26	M2G	C2-N2	3.59	1.42	1.35
1	1	58	1MA	C6-N6	3.56	1.36	1.27
1	1	46	7MG	C5-C4	3.36	1.49	1.38
1	1	64	RIA	O4'-C1A	3.20	1.45	1.41
1	1	49	5MC	C6-C5	3.12	1.39	1.34
1	1	37	T6A	C5-C4	3.00	1.48	1.40
1	1	46	7MG	C8-N9	2.92	1.47	1.46
1	1	64	RIA	C5-C4	2.79	1.48	1.40
1	1	37	T6A	O4'-C1'	2.51	1.44	1.41
1	1	64	RIA	C2-N3	2.45	1.36	1.32
1	1	46	7MG	C1'-N9	2.35	1.51	1.46
1	1	46	7MG	C5-C6	2.23	1.49	1.43
1	1	37	T6A	C2-N3	2.15	1.35	1.32
1	1	10	2MG	O4'-C1'	2.14	1.44	1.41
1	1	10	2MG	C5-C4	2.11	1.48	1.43
1	1	58	1MA	C5-C4	2.11	1.48	1.43
1	1	9	1MG	C5-C4	2.11	1.48	1.43
1	1	49	5MC	O2-C2	2.09	1.27	1.23
1	1	49	5MC	O4'-C1'	-2.01	1.37	1.42

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	46	7MG	N9-C4-N3	8.59	138.32	125.47
1	1	37	T6A	C2-N1-C6	7.70	123.19	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	37	T6A	N6-C10-N11	5.88	121.97	113.76
1	1	46	7MG	C5-C4-N3	-5.76	117.15	128.13
1	1	46	7MG	C2-N3-C4	4.83	120.91	112.30
1	1	49	5MC	O2-C2-N3	-4.25	115.42	122.33
1	1	37	T6A	O10-C10-N6	-4.22	116.48	123.62
1	1	9	1MG	C3'-C2'-C1'	4.20	107.30	100.98
1	1	46	7MG	N9-C8-N7	-4.10	97.52	103.38
1	1	37	T6A	N3-C2-N1	-3.55	123.12	128.68
1	1	48	5MC	C3'-C2'-C1'	3.55	108.18	101.43
1	1	16	H2U	O4'-C1'-N1	3.48	114.05	109.30
1	1	64	RIA	N3-C2-N1	-3.42	123.33	128.68
1	1	37	T6A	C4-C5-N7	-3.32	105.94	109.40
1	1	26	M2G	C3'-C2'-C1'	3.26	105.88	100.98
1	1	48	5MC	C5-C4-N3	-3.17	118.25	121.67
1	1	10	2MG	C3'-C2'-C1'	3.17	105.75	100.98
1	1	64	RIA	C1'-C2'-C3'	3.15	106.29	102.30
1	1	47	H2U	O4'-C1'-N1	3.07	113.48	109.30
1	1	16	H2U	C4-N3-C2	-2.94	123.36	125.79
1	1	46	7MG	C5-C6-N1	2.91	116.12	110.99
1	1	9	1MG	C5-C6-N1	2.83	118.15	113.90
1	1	58	1MA	C3'-C2'-C1'	2.74	105.11	100.98
1	1	9	1MG	O6-C6-C5	-2.69	119.42	124.19
1	1	47	H2U	C4-N3-C2	-2.67	123.58	125.79
1	1	47	H2U	C5-C4-N3	2.61	119.58	116.65
1	1	48	5MC	O2-C2-N3	-2.54	118.20	122.33
1	1	26	M2G	N1-C2-N2	2.53	120.19	118.04
1	1	16	H2U	C5-C4-N3	2.52	119.48	116.65
1	1	37	T6A	C12-N11-C10	2.46	126.04	121.94
1	1	58	1MA	C5-C6-N1	2.46	117.57	113.90
1	1	9	1MG	C8-N7-C5	2.44	107.64	102.99
1	1	10	2MG	C8-N7-C5	2.37	107.51	102.99
1	1	48	5MC	C4'-O4'-C1'	2.37	114.69	109.47
1	1	16	H2U	C3'-C2'-C1'	2.36	105.92	101.43
1	1	10	2MG	C5-C6-N1	2.34	118.09	113.95
1	1	26	M2G	C8-N7-C5	2.33	107.42	102.99
1	1	46	7MG	C3'-C2'-C1'	2.32	105.83	101.43
1	1	26	M2G	C5-C6-N1	2.26	117.95	113.95
1	1	48	5MC	CM5-C5-C6	-2.23	119.87	122.85
1	1	64	RIA	C4-C5-N7	-2.22	107.09	109.40
1	1	64	RIA	C2A-C3A-C4A	2.20	106.78	101.99
1	1	46	7MG	CM7-N7-C5	2.13	131.89	126.40
1	1	58	1MA	C8-N7-C5	2.12	107.03	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	49	5MC	N1-C2-N3	2.11	122.64	118.81
1	1	46	7MG	O4'-C1'-N9	2.08	112.13	109.30
1	1	48	5MC	C2'-C3'-C4'	2.06	106.65	102.64
1	1	64	RIA	O1'-C1'-C2'	2.05	107.62	104.98
1	1	16	H2U	C5-C6-N1	-2.04	104.88	111.61
1	1	58	1MA	N1-C2-N3	-2.01	123.67	126.02
1	1	9	1MG	C2-N1-C6	-2.01	119.31	120.95

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	16	H2U	O4'-C4'-C5'-O5'
1	1	26	M2G	N1-C2-N2-CM1
1	1	26	M2G	N3-C2-N2-CM1
1	1	26	M2G	N3-C2-N2-CM2
1	1	37	T6A	O4'-C4'-C5'-O5'
1	1	37	T6A	C3'-C4'-C5'-O5'
1	1	37	T6A	C5-C6-N6-C10
1	1	37	T6A	C13-C12-C14-O14
1	1	37	T6A	C13-C12-C14-C15
1	1	46	7MG	C3'-C4'-C5'-O5'
1	1	47	H2U	O4'-C1'-N1-C2
1	1	47	H2U	O4'-C1'-N1-C6
1	1	58	1MA	O4'-C4'-C5'-O5'
1	1	58	1MA	C3'-C4'-C5'-O5'
1	1	64	RIA	O1'-C1'-O2A-C2A
1	1	64	RIA	C2'-C1'-O2A-C2A
1	1	64	RIA	C4'-C5'-O5'-P'
1	1	9	1MG	O4'-C4'-C5'-O5'
1	1	9	1MG	C3'-C4'-C5'-O5'
1	1	10	2MG	O4'-C4'-C5'-O5'
1	1	10	2MG	C3'-C4'-C5'-O5'
1	1	16	H2U	C3'-C4'-C5'-O5'
1	1	47	H2U	O4'-C4'-C5'-O5'
1	1	47	H2U	C3'-C4'-C5'-O5'
1	1	46	7MG	O4'-C4'-C5'-O5'
1	1	47	H2U	C4'-C5'-O5'-P
1	1	37	T6A	N11-C12-C14-O14
1	1	64	RIA	C3'-C4'-C5'-O5'
1	1	26	M2G	C3'-C4'-C5'-O5'
1	1	37	T6A	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	1	26	M2G	N1-C2-N2-CM2
1	1	9	1MG	C4'-C5'-O5'-P
1	1	37	T6A	N11-C12-C14-C15
1	1	37	T6A	N1-C6-N6-C10
1	1	49	5MC	C4'-C5'-O5'-P
1	1	37	T6A	N11-C12-C13-ODB
1	1	64	RIA	C4A-C5A-O5A-P
1	1	64	RIA	O1'-C4'-C5'-O5'
1	1	64	RIA	C3A-C2A-O2A-C1'

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 88 ligands modelled in this entry, 86 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
48	7NO	1	101	1	26,32,33	1.55	1 (3%)	26,45,48	6.11	4 (15%)
51	GCP	k	602	49	27,34,34	1.63	6 (22%)	34,54,54	1.90	8 (23%)

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
48	7NO	1	101	1	-	7/15/37/38	0/3/3/3
51	GCP	k	602	49	-	7/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	1	101	7NO	O3'-C	7.20	1.51	1.34
51	k	602	GCP	C5-C6	4.70	1.49	1.41
51	k	602	GCP	PG-O2G	3.21	1.62	1.54
51	k	602	GCP	PB-O3A	2.86	1.61	1.58
51	k	602	GCP	C5-C4	2.77	1.48	1.40
51	k	602	GCP	PG-O3G	2.53	1.60	1.54
51	k	602	GCP	PB-O2B	2.18	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	1	101	7NO	C3'-O3'-C	24.44	159.74	117.78
48	1	101	7NO	O3'-C-O	-15.88	94.30	123.94
48	1	101	7NO	O3'-C-CA	10.30	135.89	111.35
51	k	602	GCP	C2-N3-C4	5.59	121.74	115.36
51	k	602	GCP	C2-N1-C6	3.89	122.11	115.93
51	k	602	GCP	C5-C6-N1	-3.75	118.31	123.43
51	k	602	GCP	C4-C5-C6	-3.53	117.43	120.80
51	k	602	GCP	N3-C2-N1	-3.44	122.63	127.22
51	k	602	GCP	C3'-C2'-C1'	3.11	105.66	100.98
51	k	602	GCP	C4-C5-N7	-2.73	106.55	109.40
48	1	101	7NO	C5-C6-N6	2.17	123.64	120.35
51	k	602	GCP	PB-O3A-PA	-2.05	126.07	132.56

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	1	101	7NO	O4'-C4'-C5'-O5'
48	1	101	7NO	C4'-C3'-O3'-C
48	1	101	7NO	CA-C-O3'-C3'
48	1	101	7NO	O-C-O3'-C3'
48	1	101	7NO	O3'-C-CA-N
51	k	602	GCP	PG-C3B-PB-O2B
51	k	602	GCP	C5'-O5'-PA-O1A
51	k	602	GCP	O4'-C4'-C5'-O5'

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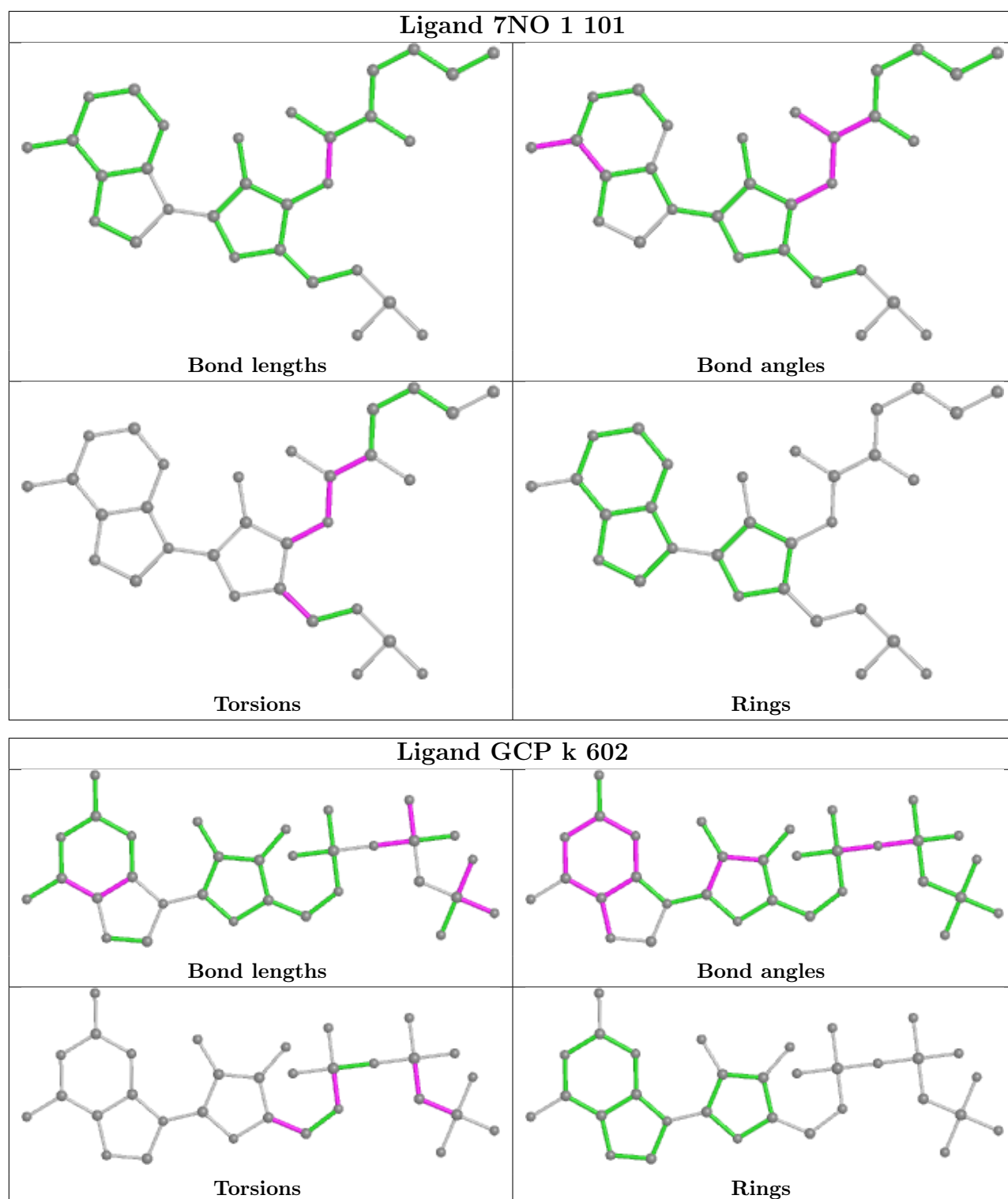
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Mol	Chain	Res	Type	Atoms
51	k	602	GCP	C3'-C4'-C5'-O5'
48	1	101	7NO	C3'-C4'-C5'-O5'
51	k	602	GCP	C5'-O5'-PA-O3A
48	1	101	7NO	O-C-CA-N
51	k	602	GCP	PG-C3B-PB-O1B
51	k	602	GCP	PB-C3B-PG-O1G

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
45	q	3
44	p	3
1	1	2
43	o	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	492:ALA	C	693:UNK	N	236.15
1	q	219:ASP	C	251:GLN	N	49.57
1	q	186:LEU	C	189:LYS	N	9.27
1	p	700:ARG	C	705:HIS	N	8.32
1	1	64:RIA	O3'	65:G	P	6.22
1	p	684:SER	C	688:GLU	N	5.94
1	1	16:H2U	O3'	18:G	P	5.10
1	p	664:PRO	C	668:LEU	N	5.10
1	q	137:ASP	C	139:TRP	N	3.87

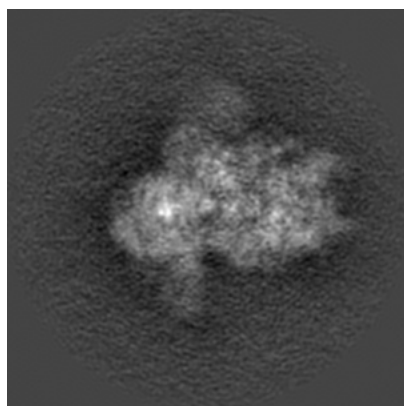
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0057. These allow visual inspection of the internal detail of the map and identification of artifacts.

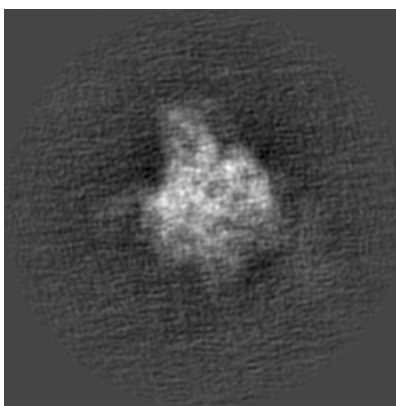
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

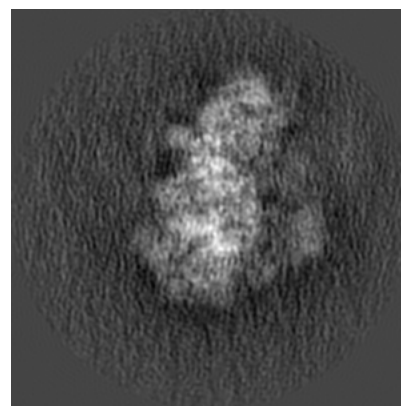
#### 6.1.1 Primary map



X

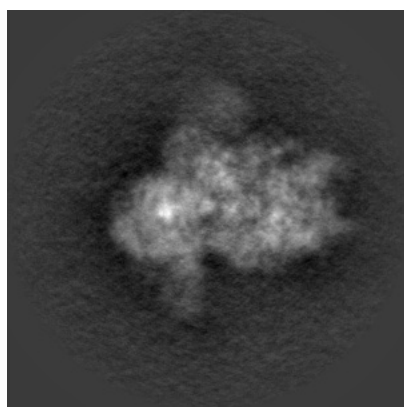


Y

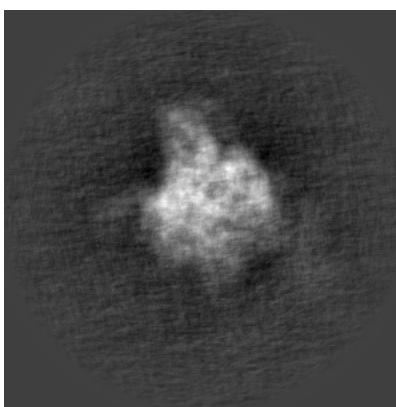


Z

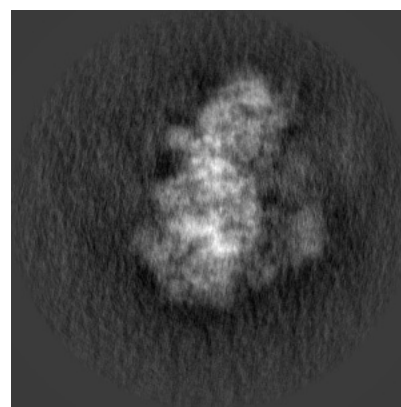
#### 6.1.2 Raw map



X



Y

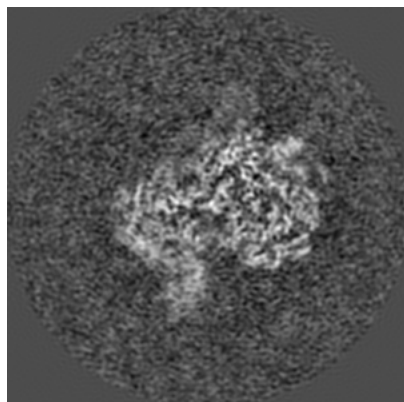


Z

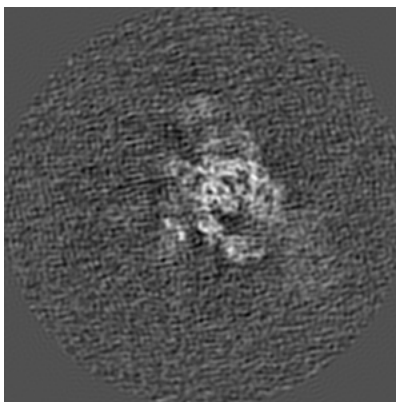
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

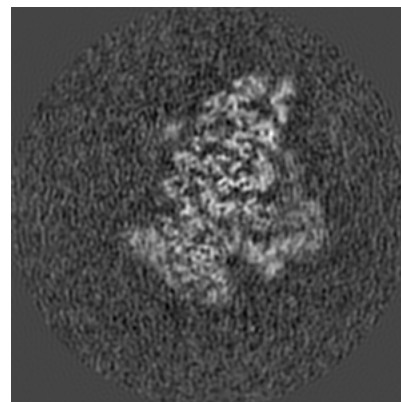
### 6.2.1 Primary map



X Index: 150

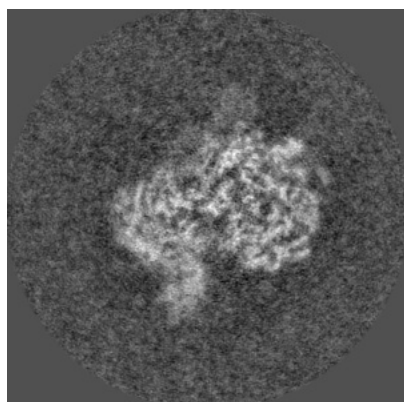


Y Index: 150

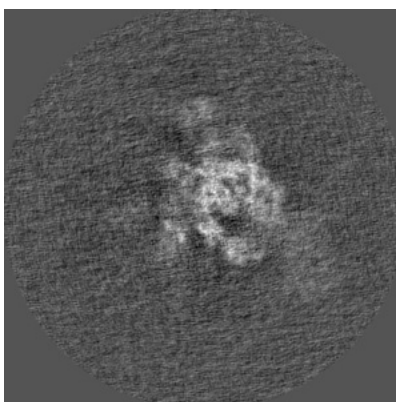


Z Index: 150

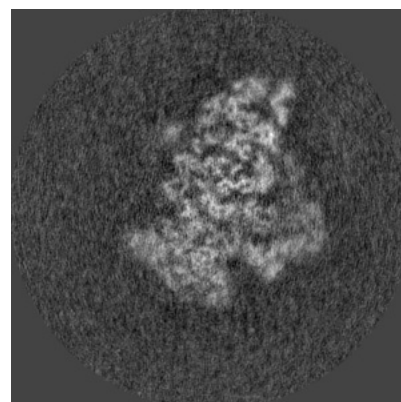
### 6.2.2 Raw map



X Index: 150



Y Index: 150

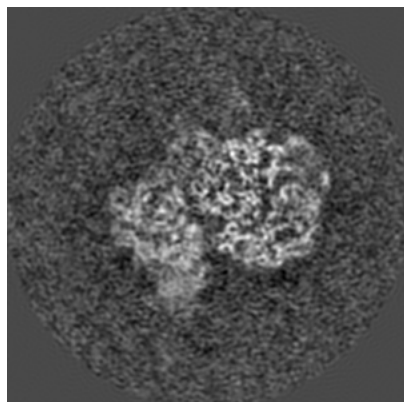


Z Index: 150

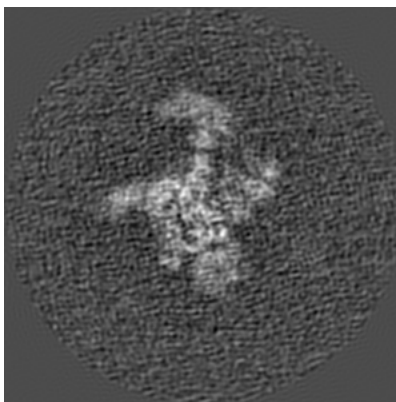
The images above show central slices of the map in three orthogonal directions.

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

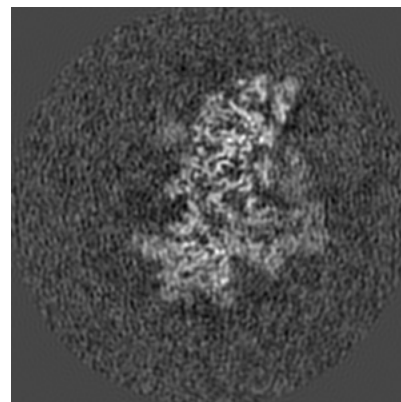
### 6.3.1 Primary map



X Index: 153

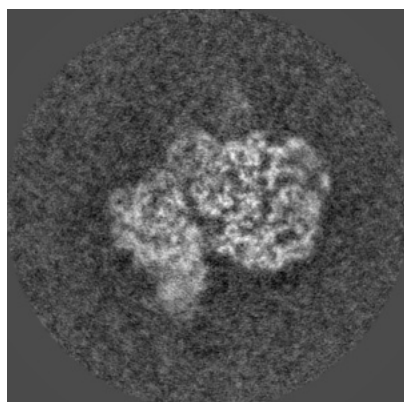


Y Index: 120

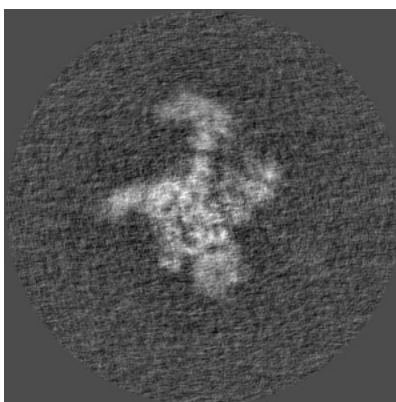


Z Index: 146

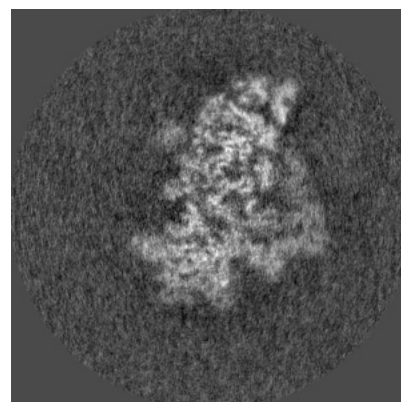
### 6.3.2 Raw map



X Index: 153



Y Index: 120

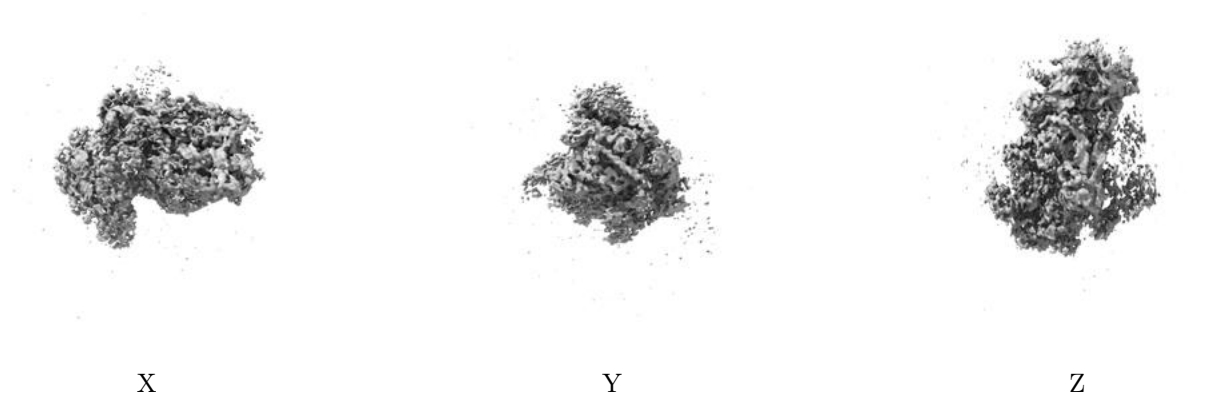


Z Index: 147

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

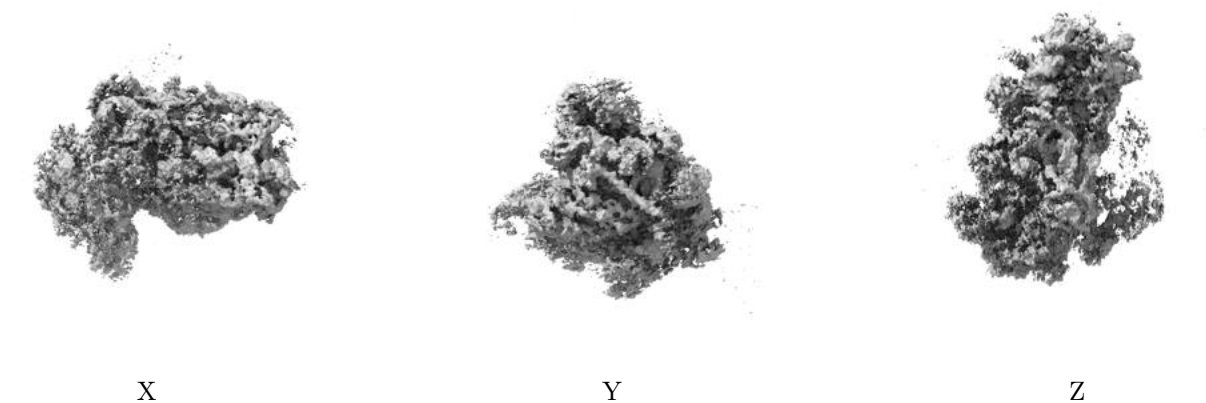
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

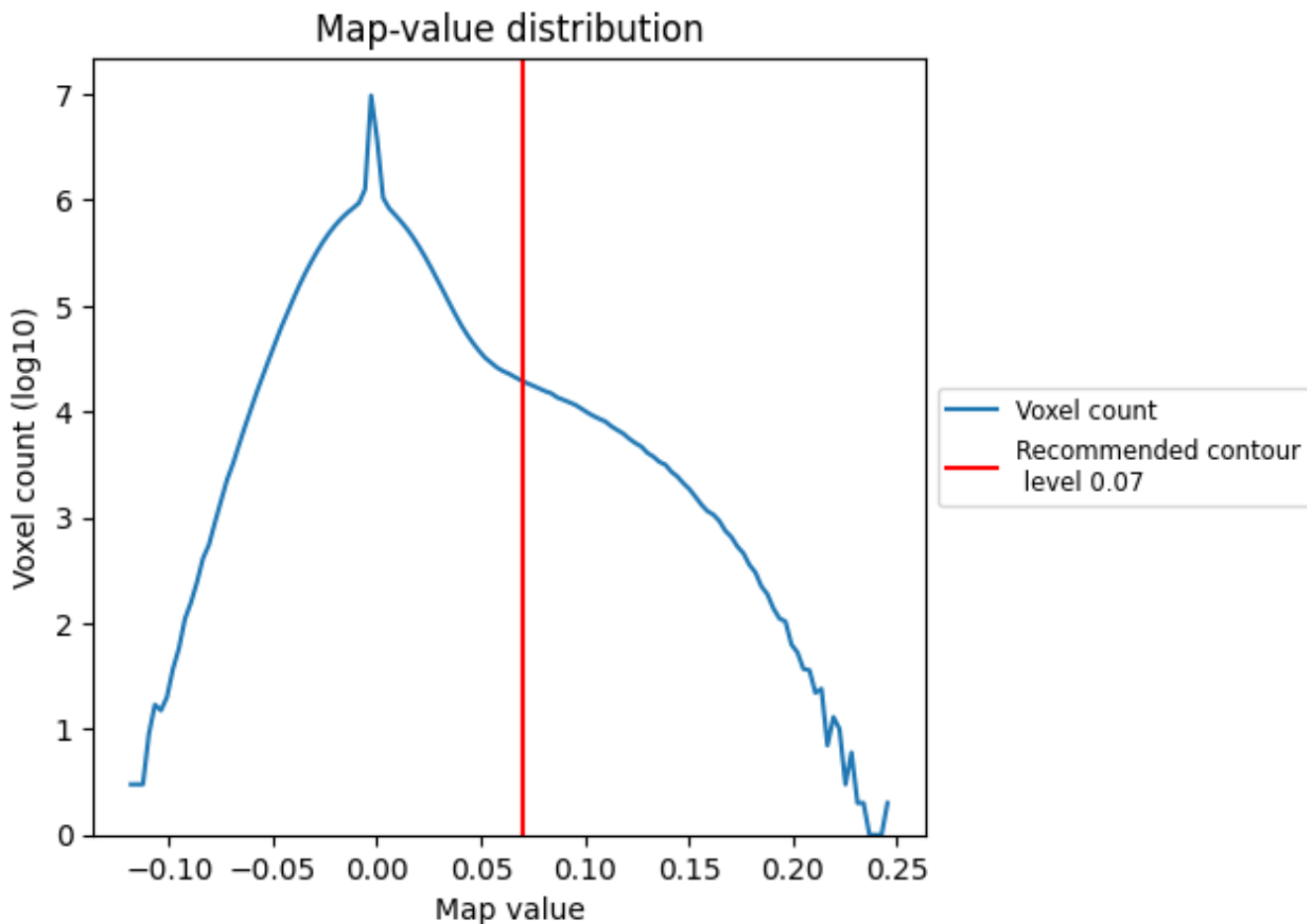
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

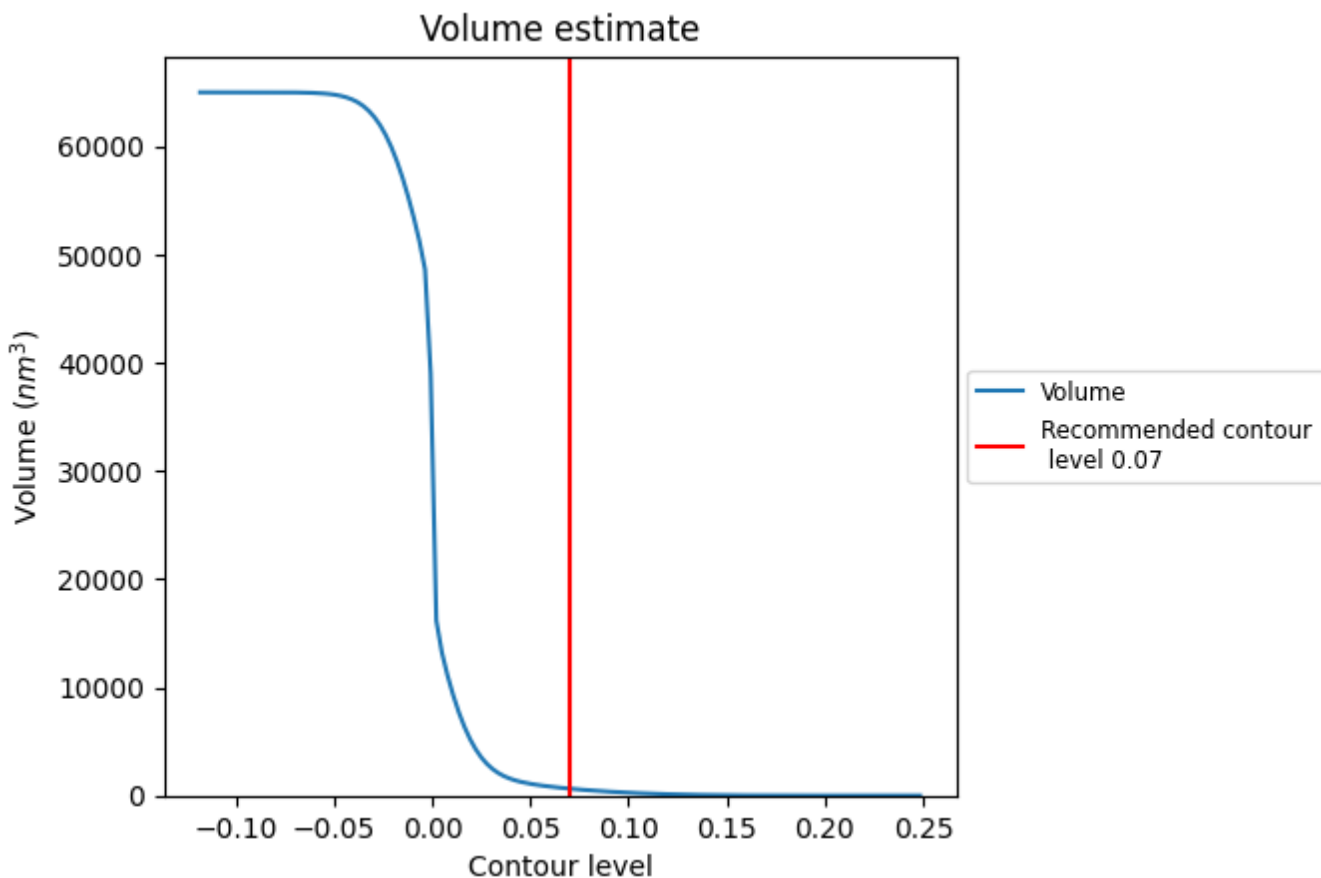
### 7.1 Map-value distribution [i](#)



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



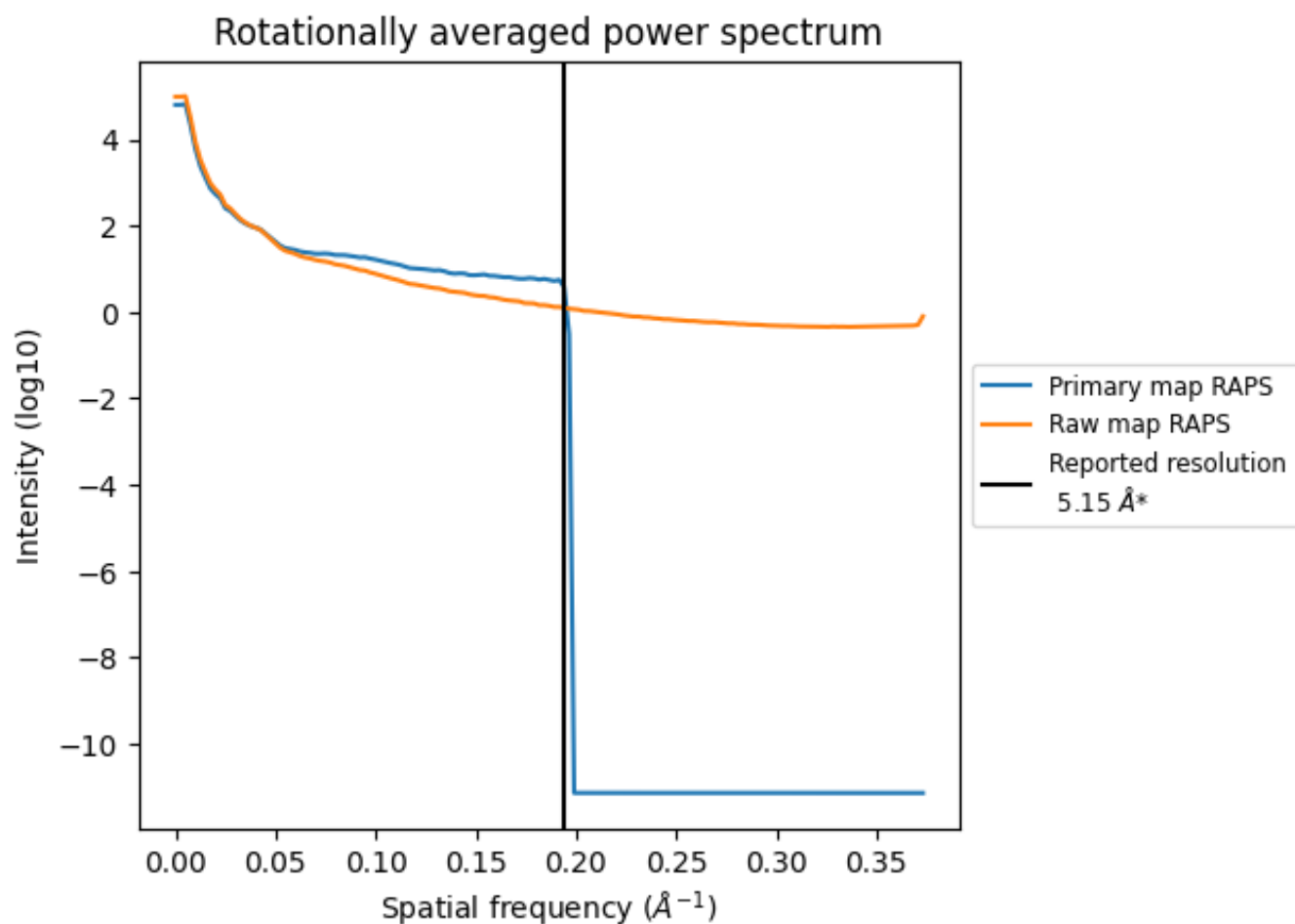
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638  $\text{nm}^3$ ; this corresponds to an approximate mass of 576 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](#)

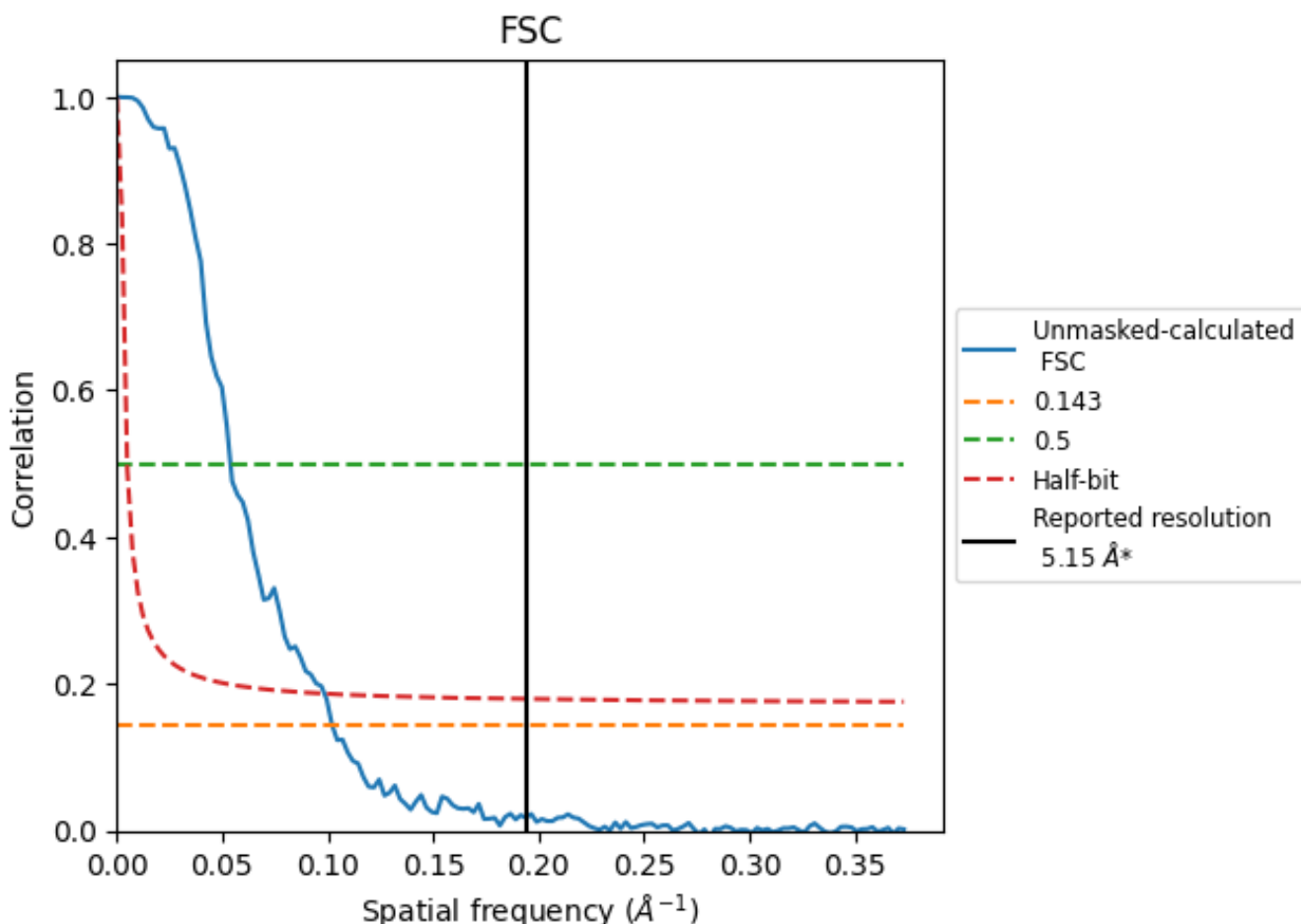


\*Reported resolution corresponds to spatial frequency of 0.194 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.194  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

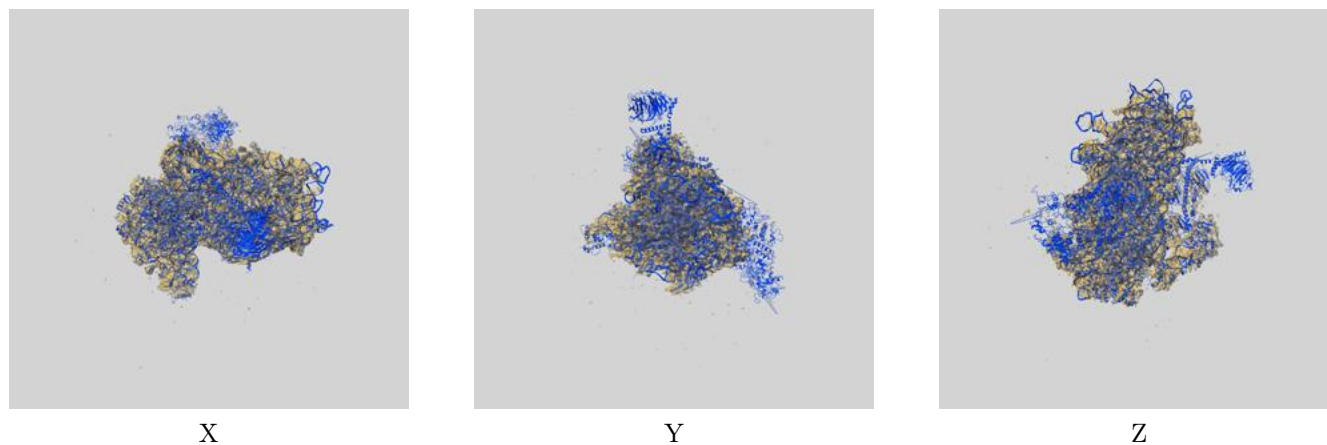
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.79	18.55	10.16

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.79 differs from the reported value 5.15 by more than 10 %

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

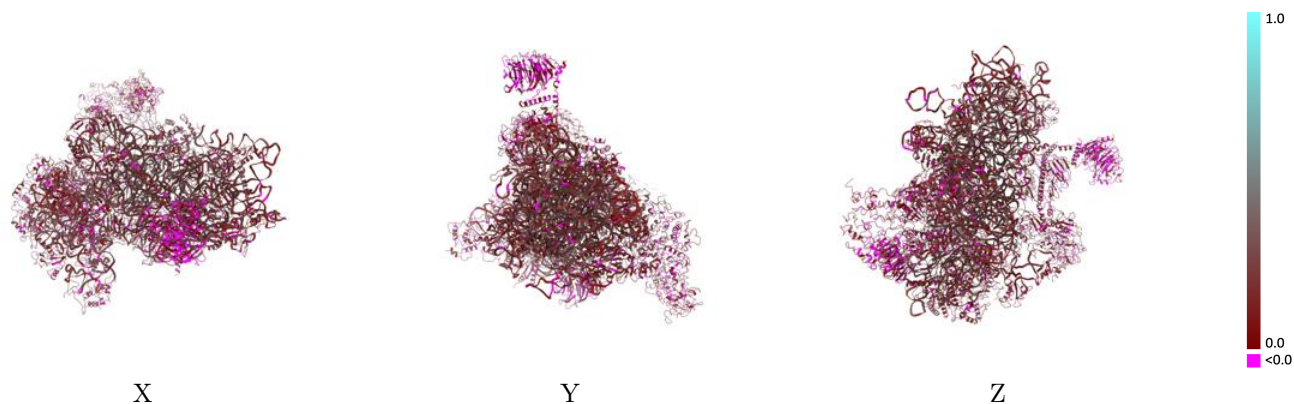
This section contains information regarding the fit between EMDB map EMD-0057 and PDB model 6GSM. Per-residue inclusion information can be found in section 3 on page 15.

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



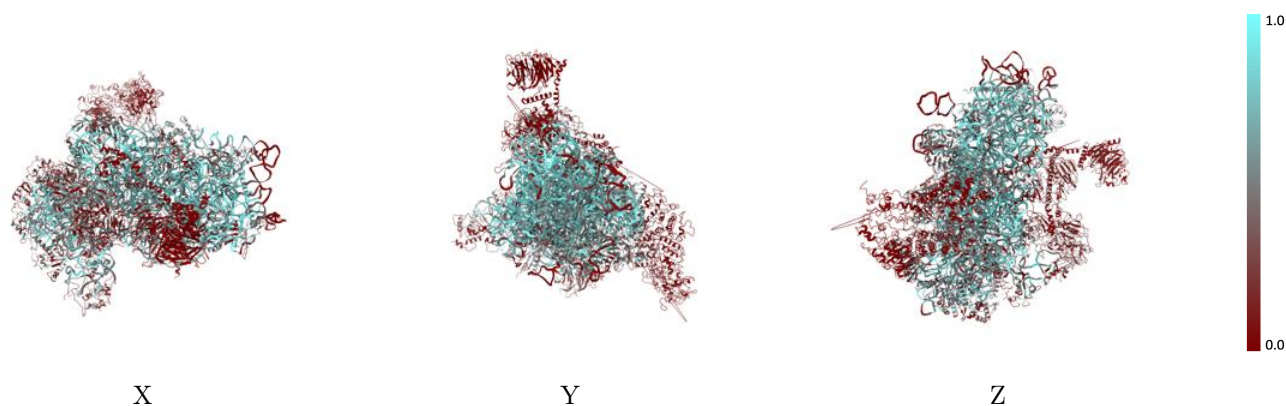
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



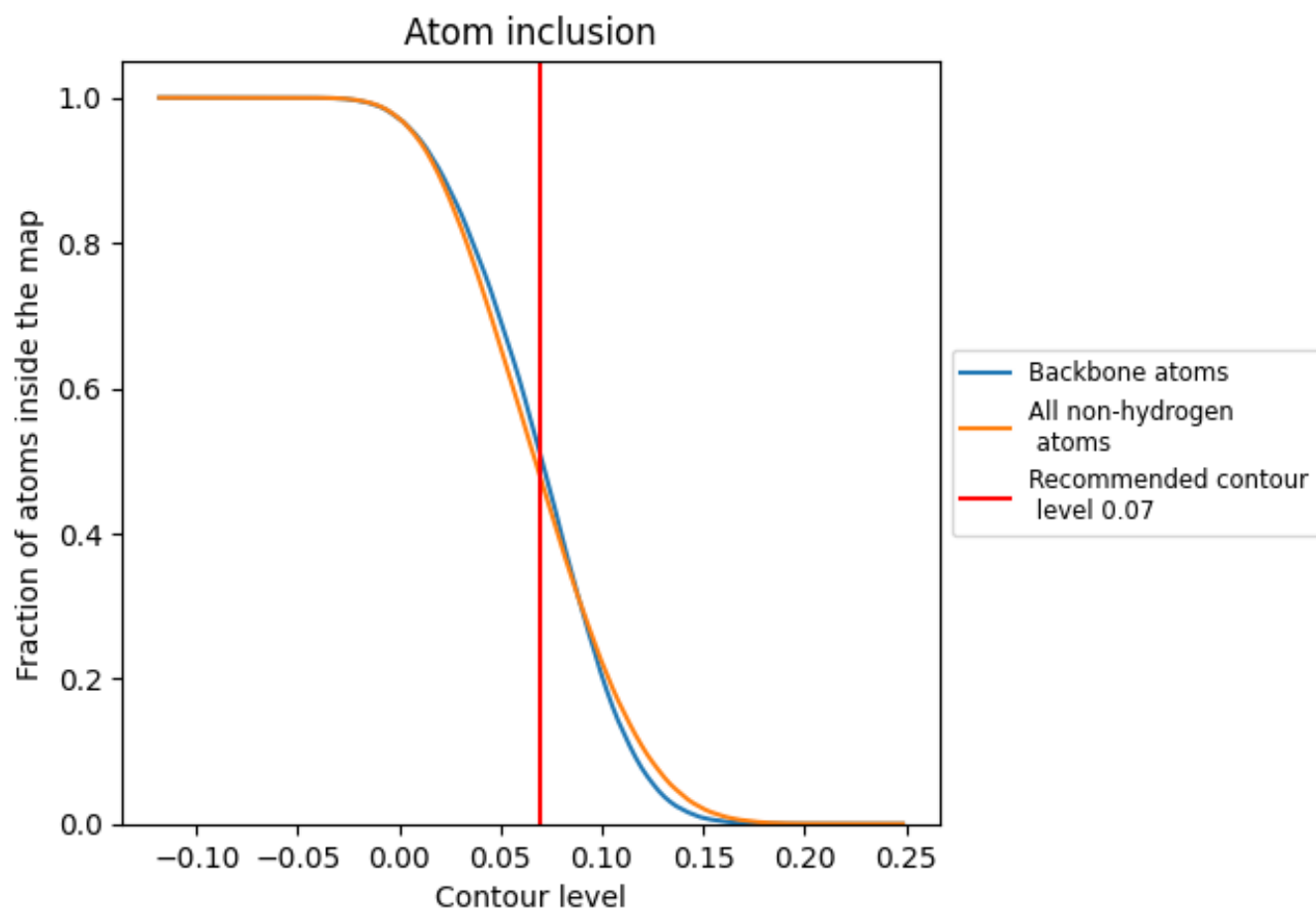
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 47% 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 (0.07) and Q-score for the entire model and for each chain.



























Chain	Atom inclusion	Q-score
All	 0.4743	 0.1970
1	 0.6084	 0.1980
2	 0.7538	 0.2370
3	 0.2500	 0.1880
A	 0.4902	 0.2070
B	 0.4833	 0.2200
C	 0.4794	 0.2350
D	 0.3851	 0.2040
E	 0.5388	 0.2180
F	 0.4288	 0.1890
G	 0.4827	 0.1860
H	 0.4360	 0.1970
I	 0.4833	 0.2010
J	 0.5487	 0.2300
K	 0.3606	 0.1570
L	 0.4650	 0.2250
M	 0.1162	 0.1290
N	 0.5542	 0.2160
O	 0.5422	 0.1940
P	 0.3061	 0.1580
Q	 0.4644	 0.1840
R	 0.3885	 0.1990
S	 0.3990	 0.1750
T	 0.5269	 0.1740
U	 0.3337	 0.1690
V	 0.5127	 0.2130
W	 0.5260	 0.2270
X	 0.4332	 0.2240
Y	 0.5623	 0.2130
Z	 0.2247	 0.1680
a	 0.4886	 0.2410
b	 0.4435	 0.2110
c	 0.3298	 0.2070
d	 0.4496	 0.1660
e	 0.3586	 0.2060



*Continued on next page...*



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Chain	Atom inclusion	Q-score
f	 0.2296	 0.1300
g	 0.3121	 0.0840
h	 0.1887	 0.1960
i	 0.2450	 0.2080
j	 0.2222	 0.1810
k	 0.1411	 0.1520
l	 0.2151	 0.1960
m	 0.3209	 0.2410
o	 0.0186	 0.1410
p	 0.0492	 0.1440
q	 0.0434	 0.1570
r	 0.0000	 0.0030
s	 0.0000	 0.0140