Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:39 am GMT

PDB ID	:	6GSN
EMDB ID	:	EMD-0058
Title	:	Structure of a partial yeast 48S preinitiation complex in closed conformation
Authors	:	Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on	:	2018-06-14
Resolution	:	5.75 Å(reported)

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

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

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

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

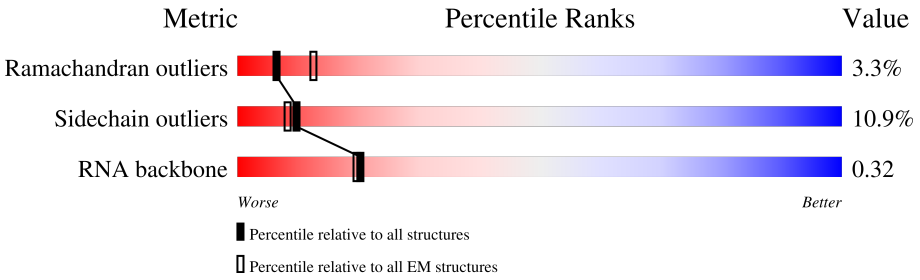
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.75 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	2	1798	53% 47%
2	C	217	85% 14%
3	D	223	78% 22%
4	F	206	79% 19%
5	K	96	77% 23%
6	M	118	12% 80% 19%
7	P	117	78% 20%
8	Q	141	81% 19%

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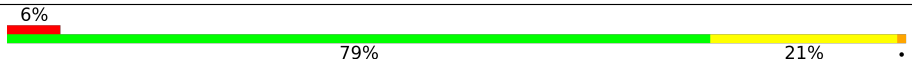
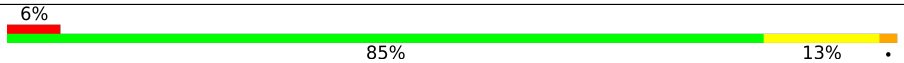
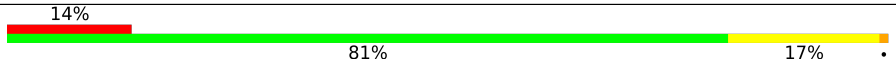
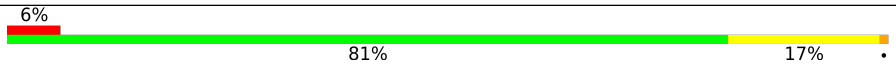
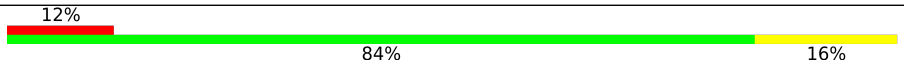
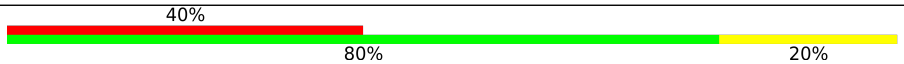
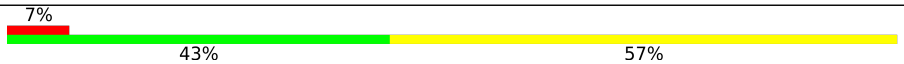
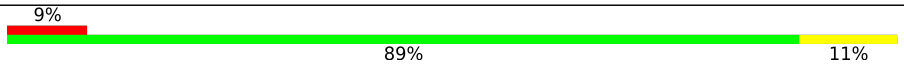
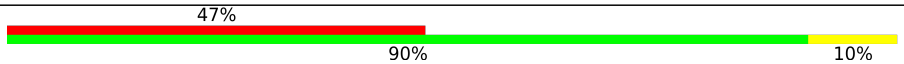
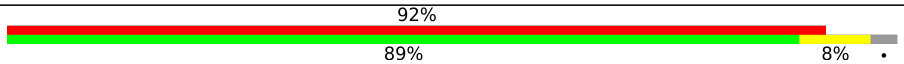
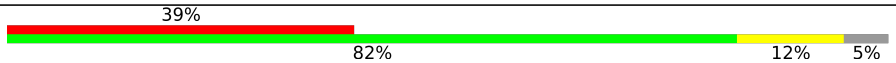
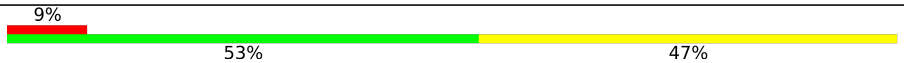
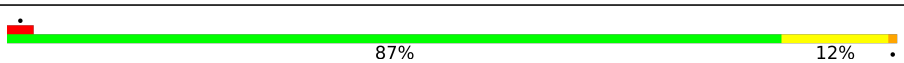
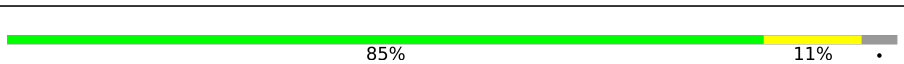
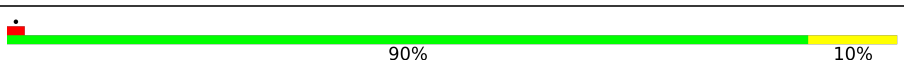
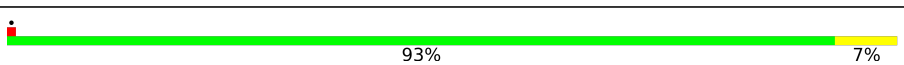
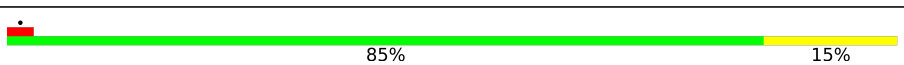
Mol	Chain	Length	Quality of chain
9	R	130	
10	S	145	
11	T	143	
12	U	106	
13	Z	70	
14	c	62	
15	f	69	
16	g	324	
17	d	53	
18	e	58	
19	h	25	
20	3	14	
21	i	111	
22	m	90	
23	o	567	
24	q	699	
25	k	430	
26	l	144	
27	j	263	
28	1	75	
29	A	219	
30	B	231	
31	E	260	
32	G	226	
33	H	184	

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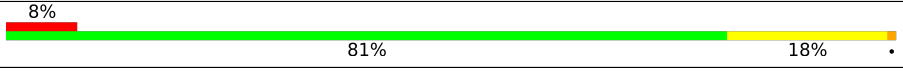
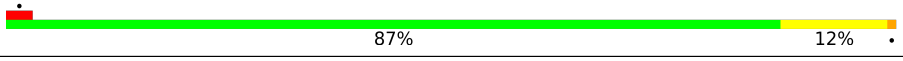
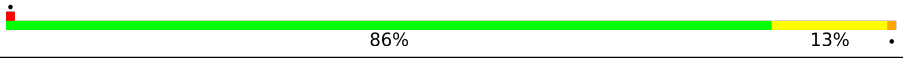
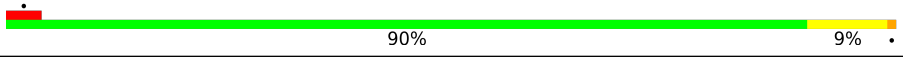
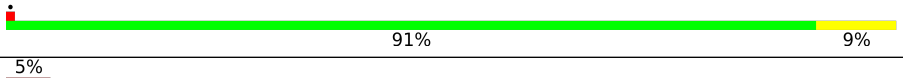
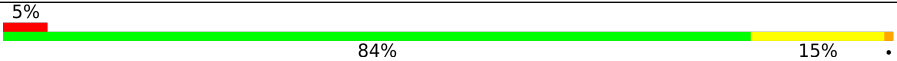
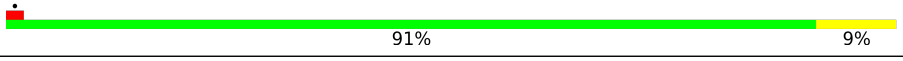
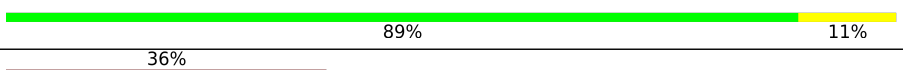
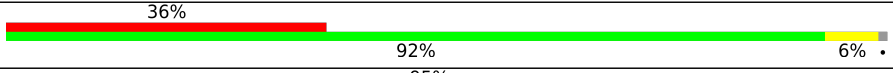
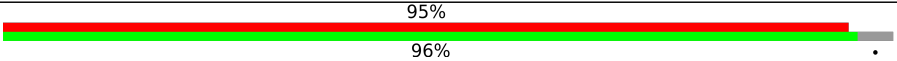
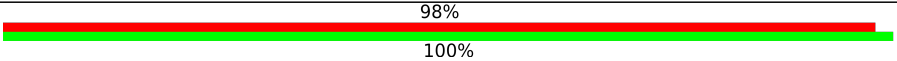
Mol	Chain	Length	Quality of chain
34	I	200	
35	J	182	
36	L	155	
37	N	150	
38	O	127	
39	V	87	
40	W	129	
41	Y	134	
42	X	144	
43	a	98	
44	b	81	
45	p	666	
46	s	342	
47	r	49	

2 Entry composition (i)

There are 51 unique types of molecules in this entry. The entry contains 103798 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 18S rRNA (1798-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1798	38175	17061	6721	12595	1798	0	0

- Molecule 2 is a protein called KLLA0F09812p.

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

- Molecule 3 is a protein called KLLA0D08305p.

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

- Molecule 4 is a protein called KLLA0D10659p.

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

- Molecule 5 is a protein called KLLA0B08173p.

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

- Molecule 6 is a protein called 40S ribosomal protein S12.

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

- Molecule 7 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	117	Total	C	N	O	S	0	0
			927	595	166	161	5		

- Molecule 8 is a protein called 40S ribosomal protein S16.

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

- Molecule 9 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	130	Total	C	N	O	S	0	0
			1027	640	191	193	3		

- Molecule 10 is a protein called KLLA0B01562p.

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

- Molecule 11 is a protein called KLLA0A07194p.

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

- Molecule 12 is a protein called KLLA0F25542p.

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

- Molecule 13 is a protein called KLLA0B06182p.

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

- Molecule 14 is a protein called 40S ribosomal protein S28.

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

- Molecule 15 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	69	Total	C	N	O	S	0	0
			546	351	101	90	4		

- Molecule 16 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 17 is a protein called 40S ribosomal protein S29.

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

- Molecule 18 is a protein called 40S ribosomal protein S30.

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

- Molecule 19 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 20 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3	14	Total	C	N	O	P	0	0
			287	129	42	102	14		

- Molecule 21 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	111	Total	C	N	O	S	0	0
			884	542	170	167	5		

- Molecule 22 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	m	90	Total	C	N	O	S	0	0
			716	452	132	128	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	20	ALA	THR	conflict	UNP P32911
m	23	ALA	SER	conflict	UNP P32911

- Molecule 23 is a protein called Eukaryotic translation initiation factor 3 subunit A,eIF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	521	Total	C	N	O	S	0	0
			3996	2554	685	750	7		

- Molecule 24 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	q	675	Total	C	N	O	S	0	0
			5179	3309	874	984	12		

- Molecule 25 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

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

- Molecule 26 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	126	Total	C	N	O	S	0	0
			1016	646	183	180	7		

- Molecule 27 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

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

- Molecule 28 is a RNA chain called tRNAi (75-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	75	Total	C	N	O	P	0	0
			1607	716	296	520	75		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	31	U	G	conflict	GB 176433
1	39	A	C	conflict	GB 176433

- Molecule 29 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A	219	Total	C	N	O	S	0	0
			1702	1085	299	316	2		

- Molecule 30 is a protein called 40S ribosomal protein S1.

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

- Molecule 31 is a protein called 40S ribosomal protein S4.

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

- Molecule 32 is a protein called 40S ribosomal protein S6.

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

- Molecule 33 is a protein called 40S ribosomal protein S7.

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

- Molecule 34 is a protein called 40S ribosomal protein S8.

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

- Molecule 35 is a protein called KLLA0E23673p.

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

- Molecule 36 is a protein called KLLA0A10483p.

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

- Molecule 37 is a protein called KLLA0F18040p.

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

- Molecule 38 is a protein called 40S ribosomal protein S14.

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

- Molecule 39 is a protein called 40S ribosomal protein S21.

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

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

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

- Molecule 41 is a protein called 40S ribosomal protein S24.

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

- Molecule 42 is a protein called RPS23.

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

- Molecule 43 is a protein called 40S ribosomal protein S26.

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

- Molecule 44 is a protein called 40S ribosomal protein S27.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	658	Total	C	N	O	S	0	0
			5147	3295	889	945	18		

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

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

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

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

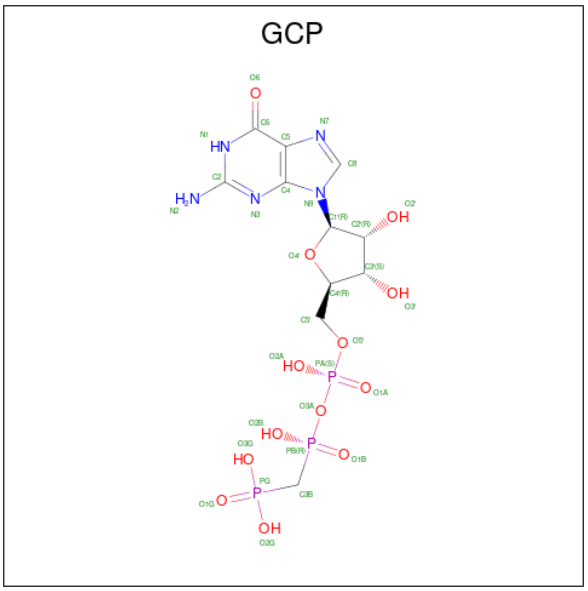
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	76	Total 76	Mg 76	0
48	C	1	Total 1	Mg 1	0
48	h	1	Total 1	Mg 1	0
48	k	1	Total 1	Mg 1	0
48	B	1	Total 1	Mg 1	0
48	a	1	Total 1	Mg 1	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

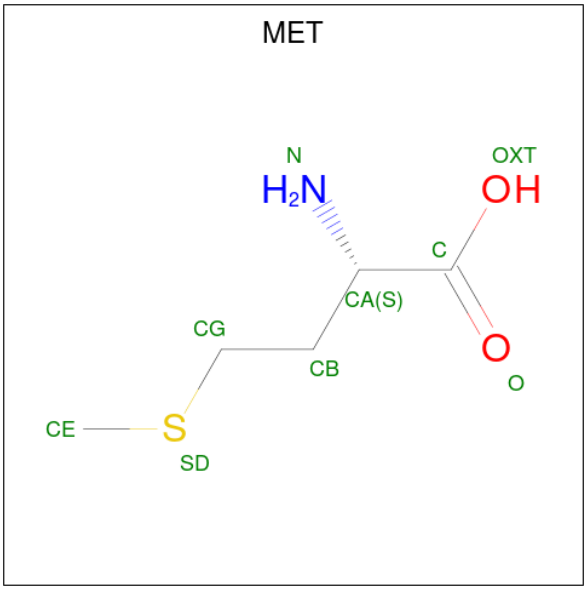
Mol	Chain	Residues	Atoms		AltConf
49	f	1	Total 1	Zn 1	0
49	l	1	Total 1	Zn 1	0
49	a	1	Total 1	Zn 1	0
49	b	1	Total 1	Zn 1	0

- Molecule 50 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



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

- Molecule 51 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



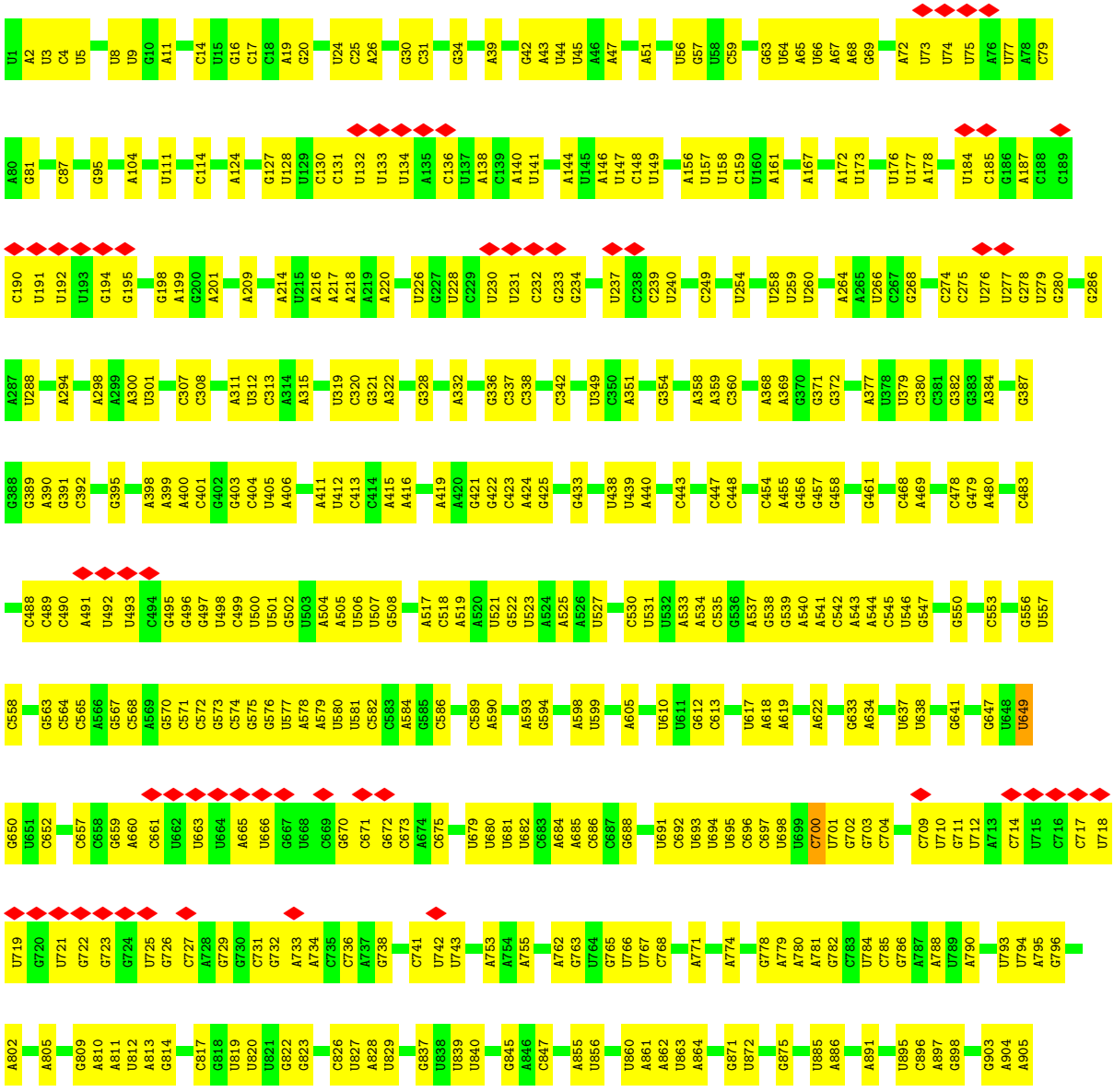
Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

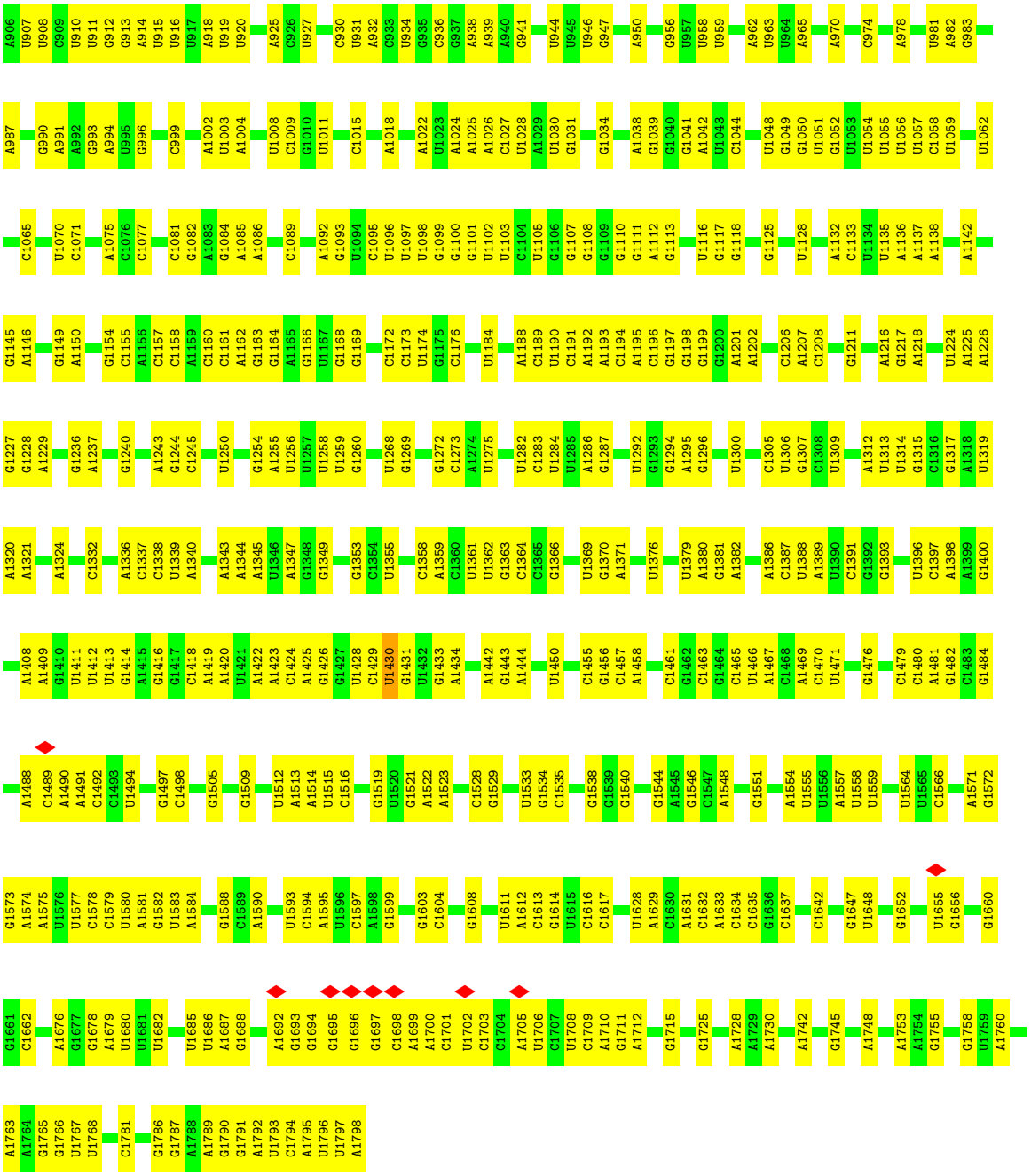
3 Residue-property plots (i)

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: 18S rRNA (1798-MER)

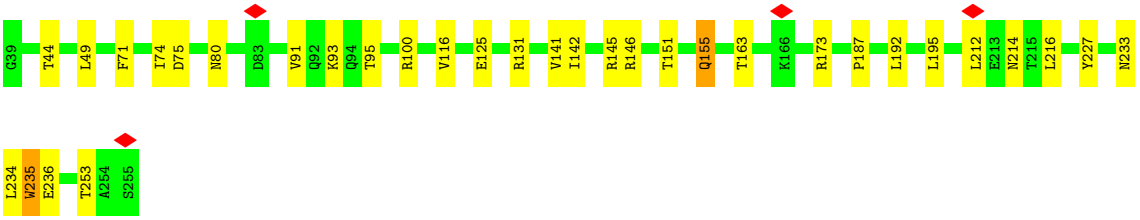
Chain 2:





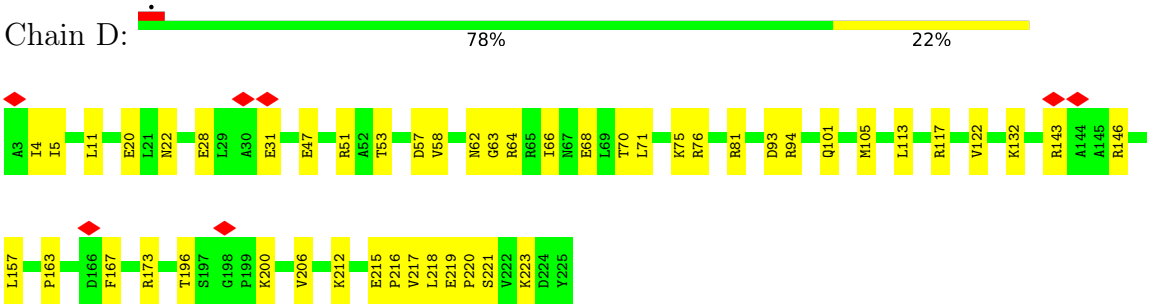
• Molecule 2: KLLA0F09812p

Chain C:



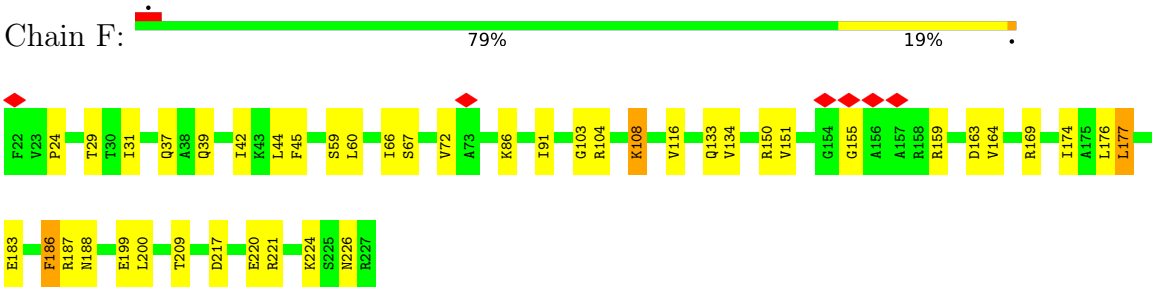
• Molecule 3: KLLA0D08305p

Chain D:



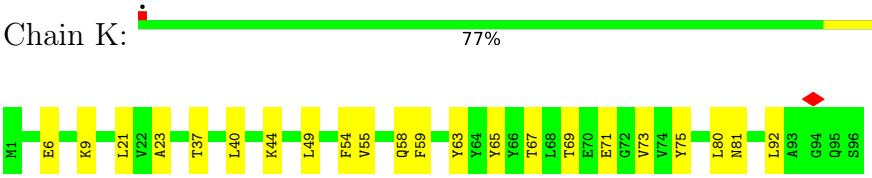
• Molecule 4: KLLA0D10659p

Chain F:



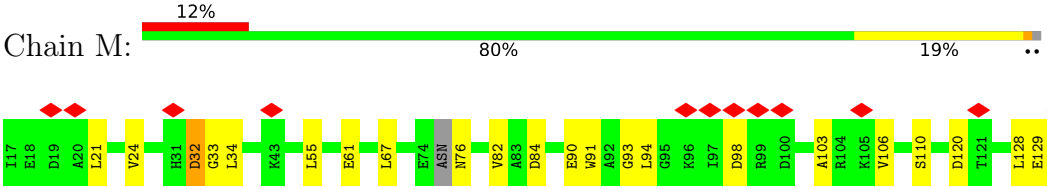
• Molecule 5: KLLA0B08173p

Chain K:



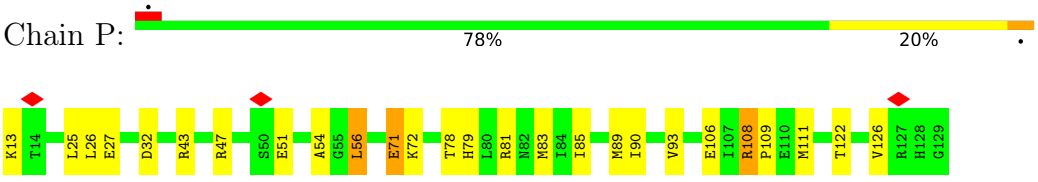
• Molecule 6: 40S ribosomal protein S12

Chain M:



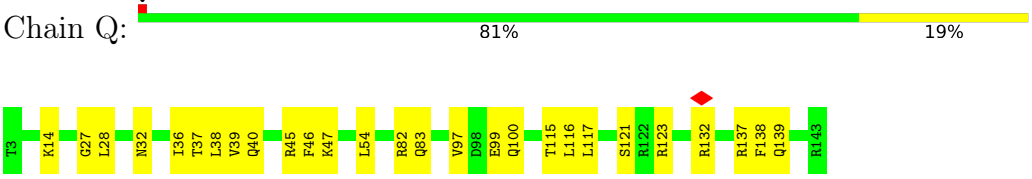
• Molecule 7: KLLA0F07843p

Chain P:



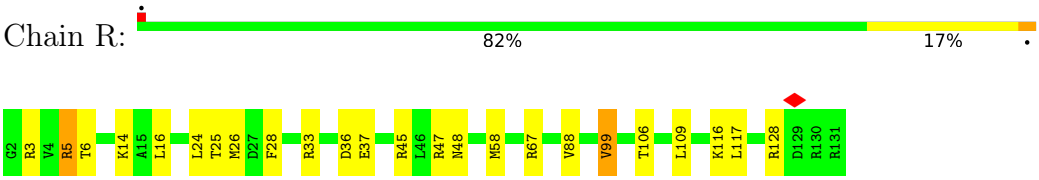
• Molecule 8: 40S ribosomal protein S16

Chain Q:



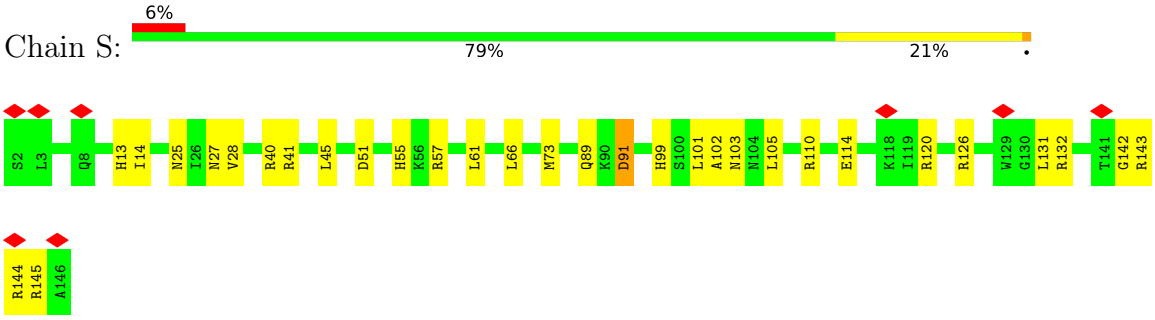
• Molecule 9: KLLA0B01474p

Chain R:



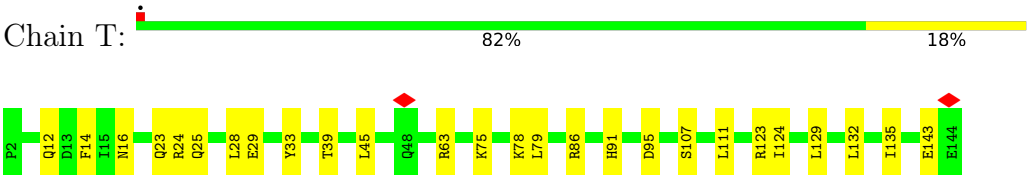
• Molecule 10: KLLA0B01562p

Chain S:



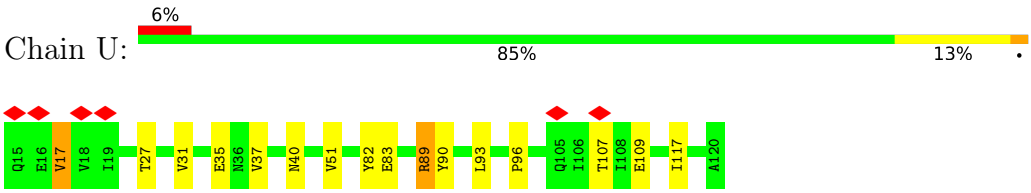
• Molecule 11: KLLA0A07194p

Chain T:



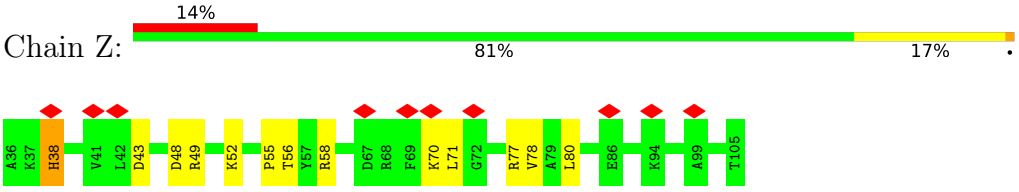
• Molecule 12: KLLA0F25542p

Chain U:



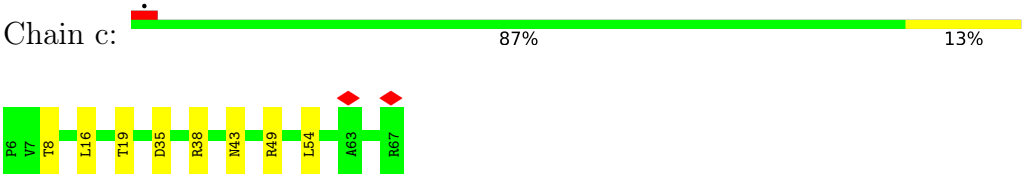
• Molecule 13: KLLA0B06182p

Chain Z:



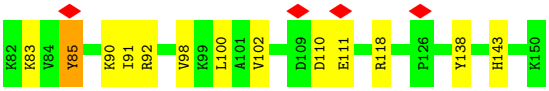
• Molecule 14: 40S ribosomal protein S28

Chain c:



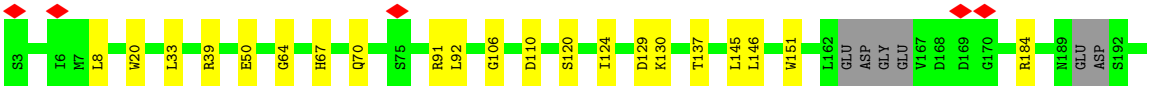
• Molecule 15: Ubiquitin-40S ribosomal protein S27a

Chain f:



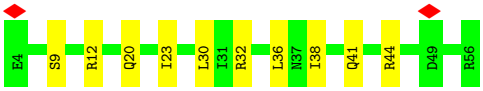
• Molecule 16: KLLA0E12277p

Chain g:



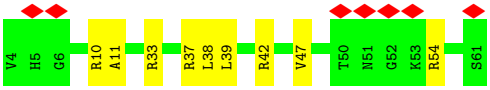
• Molecule 17: 40S ribosomal protein S29

Chain d:



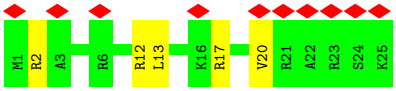
• Molecule 18: 40S ribosomal protein S30

Chain e:



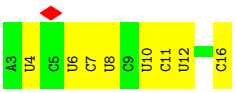
• Molecule 19: 60S ribosomal protein L41-A

Chain h:



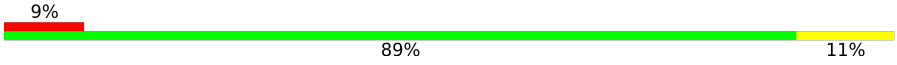
• Molecule 20: mRNA

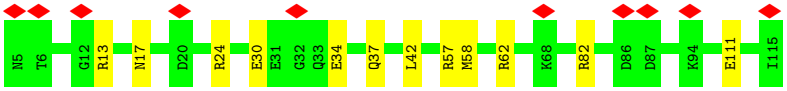
Chain 3:



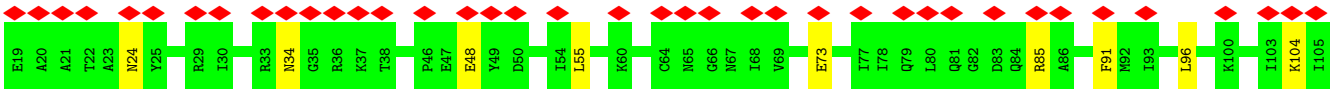
• Molecule 21: Eukaryotic translation initiation factor 1A

Chain i:

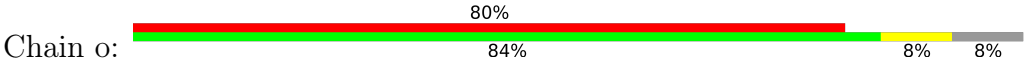


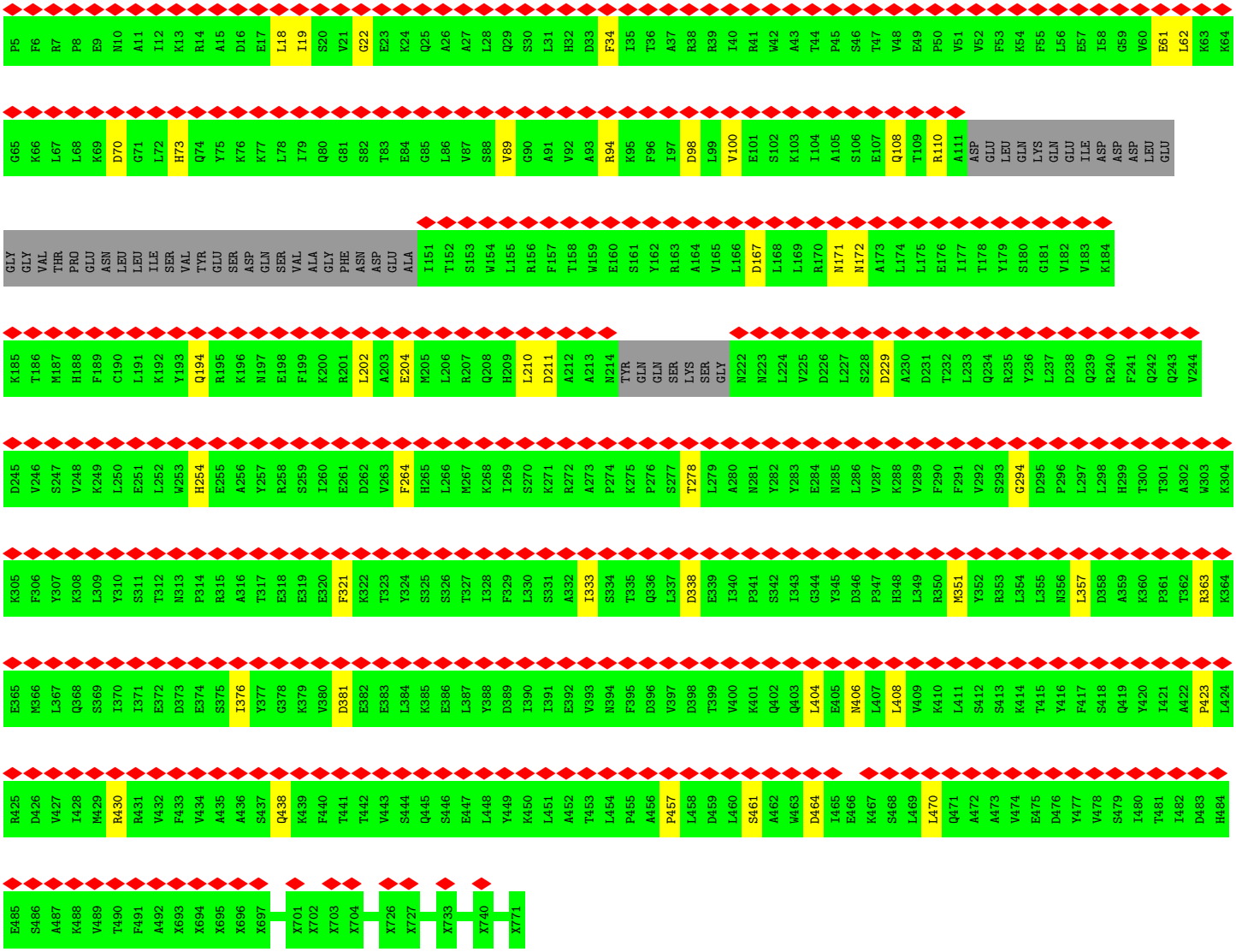


• Molecule 22: Eukaryotic translation initiation factor eIF-1



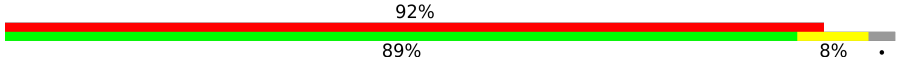
• Molecule 23: Eukaryotic translation initiation factor 3 subunit A,eIF3a

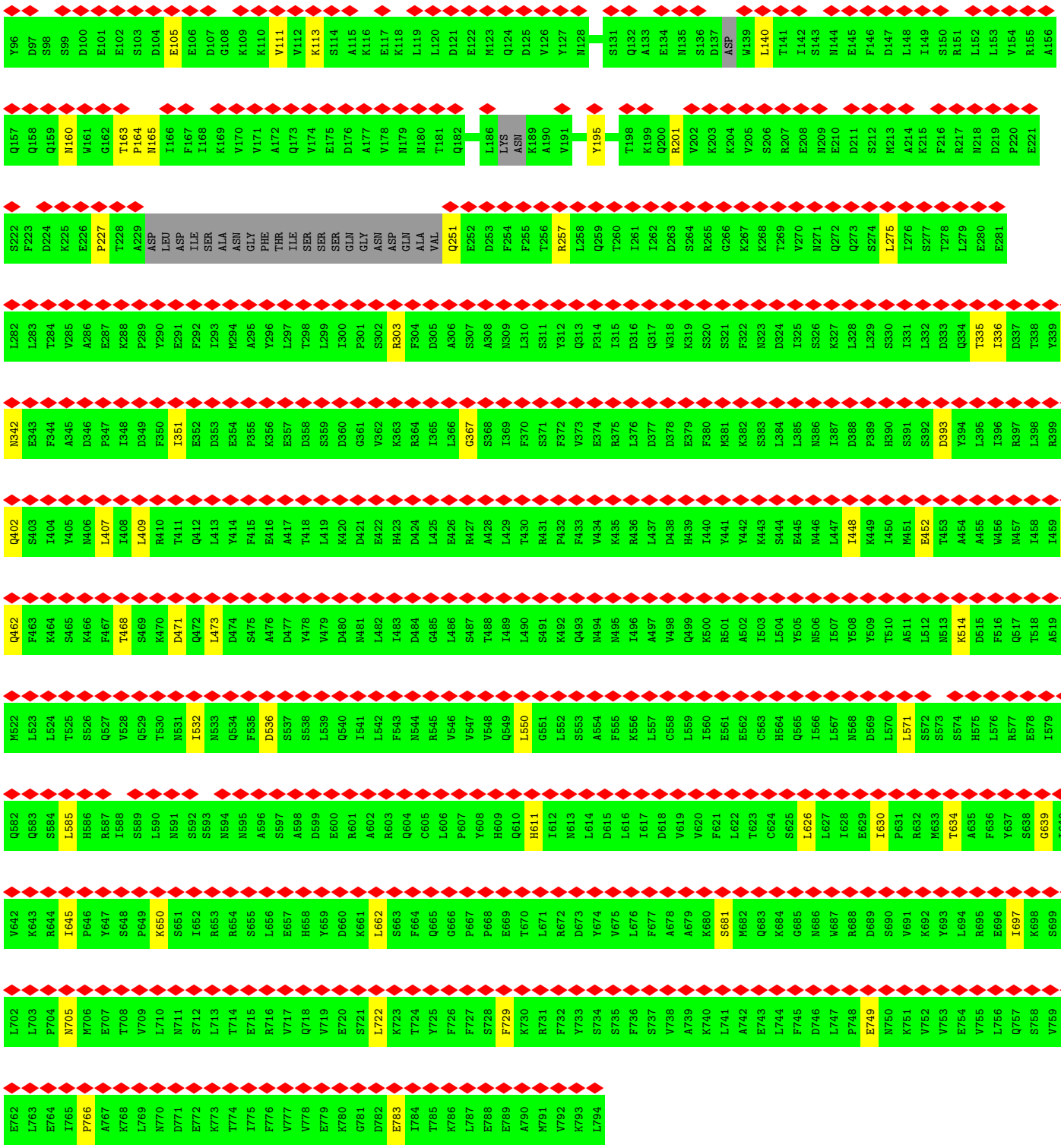




• Molecule 24: Eukaryotic translation initiation factor 3 subunit C

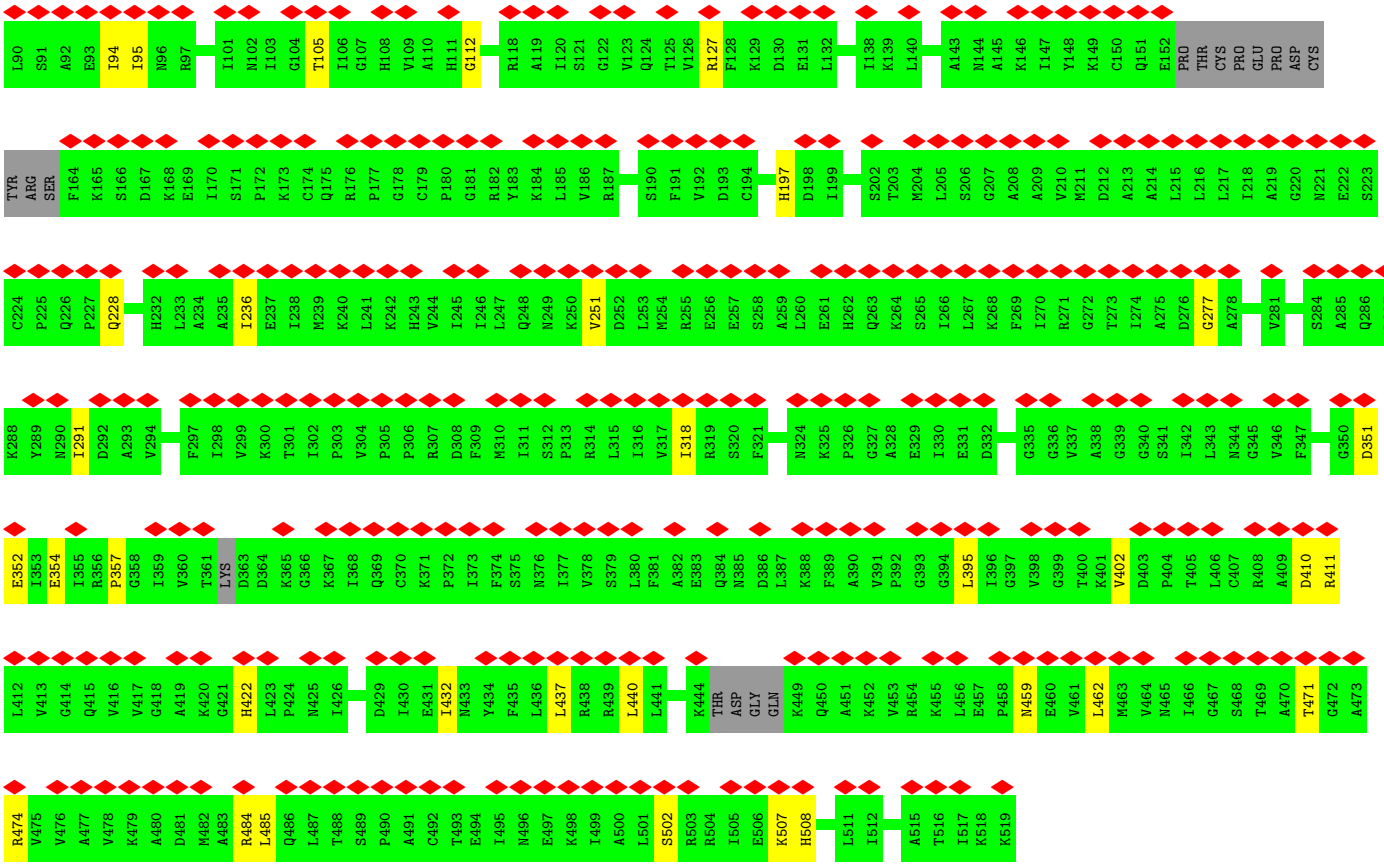
Chain q:





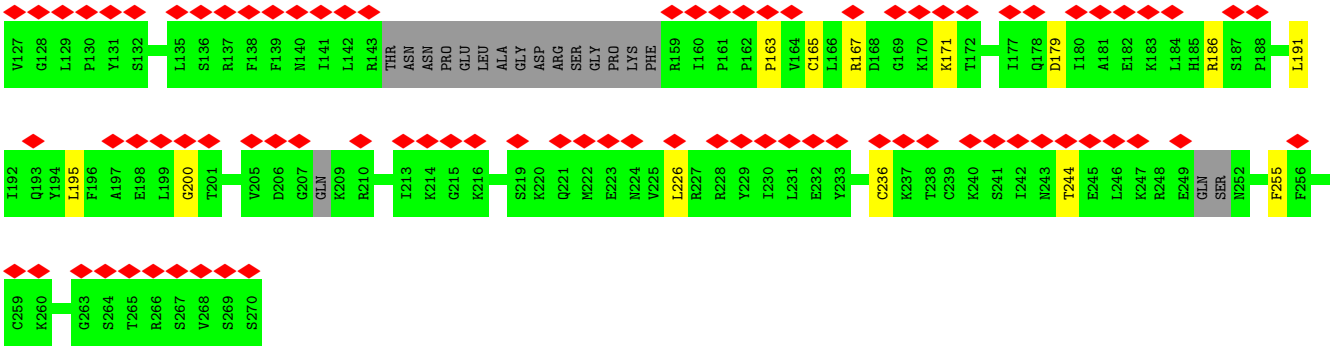
• Molecule 25: Eukaryotic translation initiation factor 2 subunit gamma

Chain k:



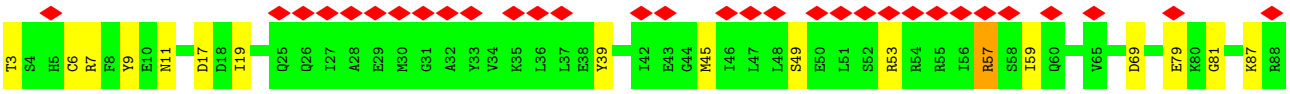
• Molecule 26: Eukaryotic translation initiation factor 2 subunit beta

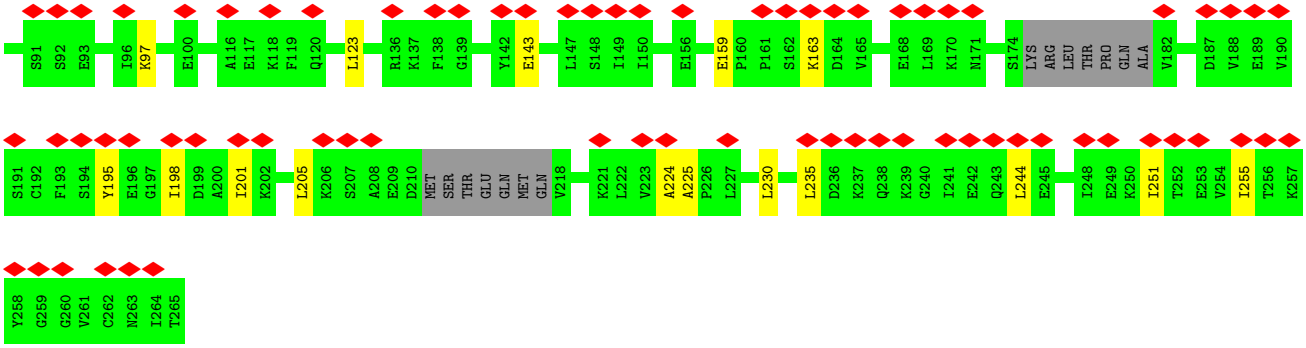
Chain l:



• Molecule 27: Eukaryotic translation initiation factor 2 subunit alpha

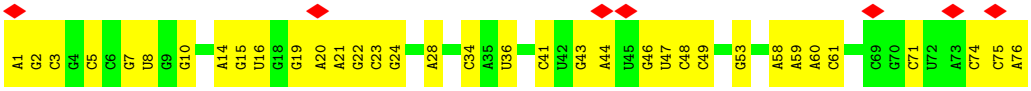
Chain j:





• Molecule 28: tRNAi (75-MER)

Chain 1:

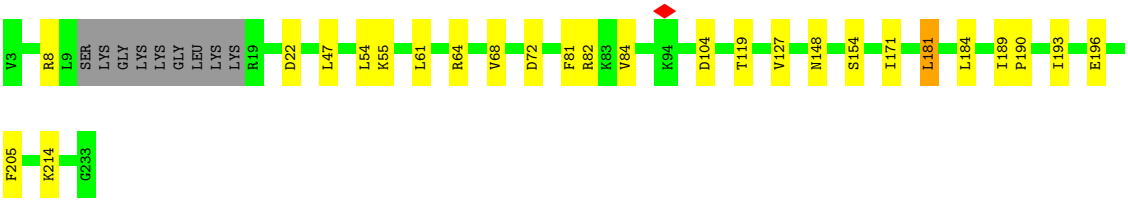


• Molecule 29: 40S ribosomal protein S0

Chain A:

• Molecule 30: 40S ribosomal protein S1

Chain B:

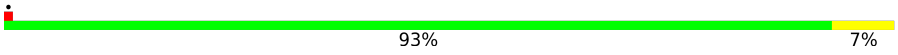


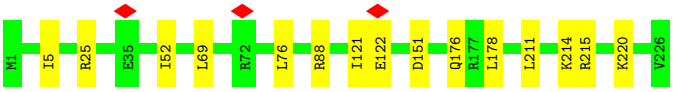
• Molecule 31: 40S ribosomal protein S4

Chain E:

• Molecule 32: 40S ribosomal protein S6

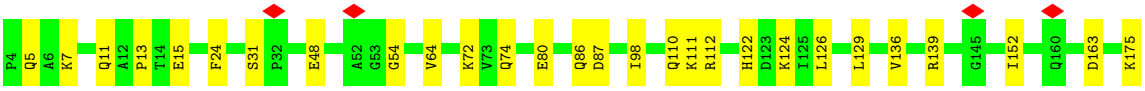
Chain G:





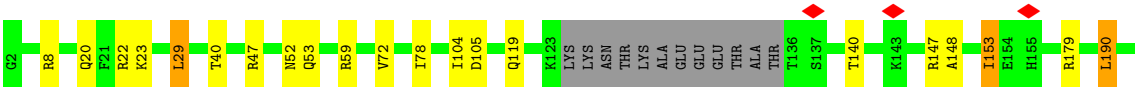
• Molecule 33: 40S ribosomal protein S7

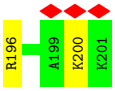
Chain H:



• Molecule 34: 40S ribosomal protein S8

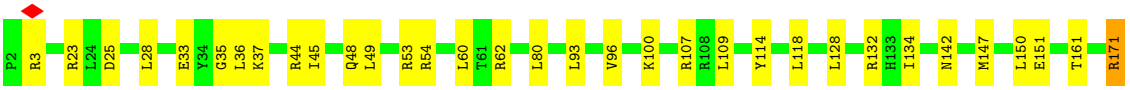
Chain I:

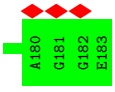




• Molecule 35: KLLA0E23673p

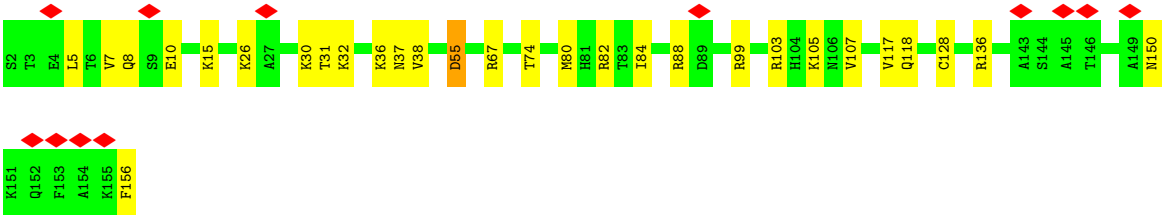
Chain J:



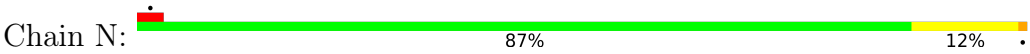


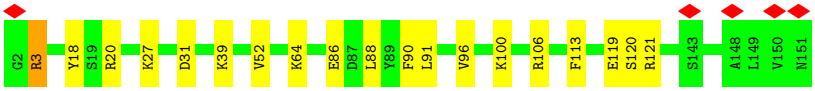
• Molecule 36: KLLA0A10483p

Chain L:

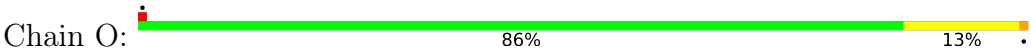


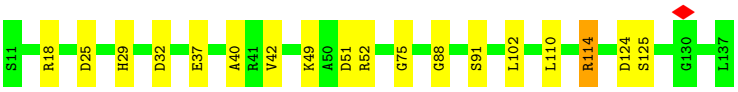
• Molecule 37: KLLA0F18040p



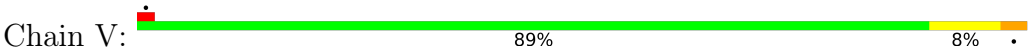


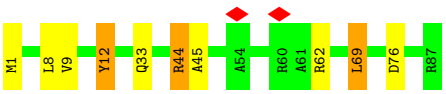
• Molecule 38: 40S ribosomal protein S14



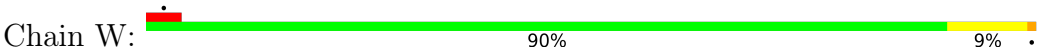


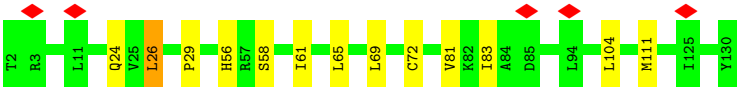
• Molecule 39: 40S ribosomal protein S21



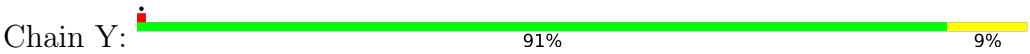


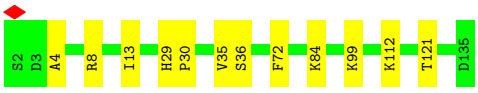
• Molecule 40: 40S ribosomal protein S22



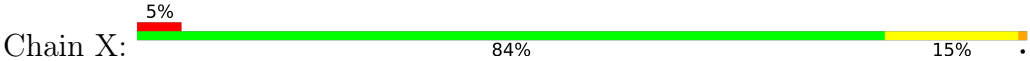


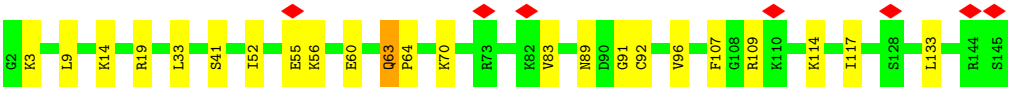
• Molecule 41: 40S ribosomal protein S24





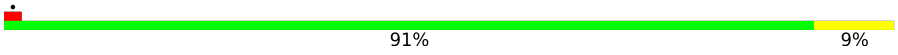
• Molecule 42: RPS23

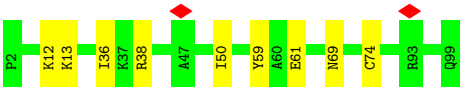




• Molecule 43: 40S ribosomal protein S26

Chain a:



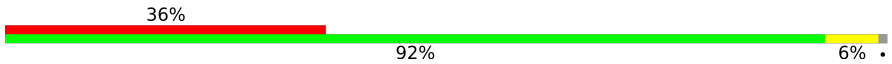


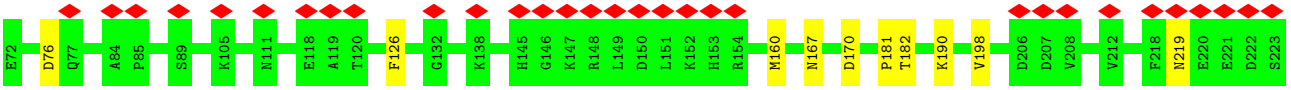
• Molecule 44: 40S ribosomal protein S27

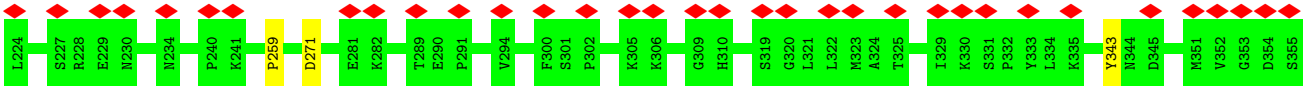
Chain b:

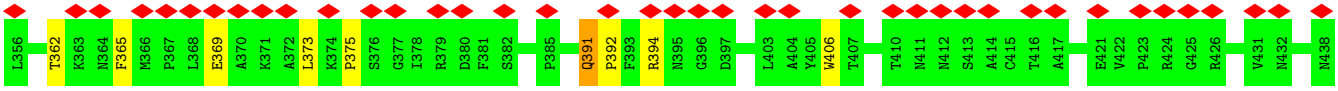
• Molecule 45: Eukaryotic translation initiation factor 3 subunit B

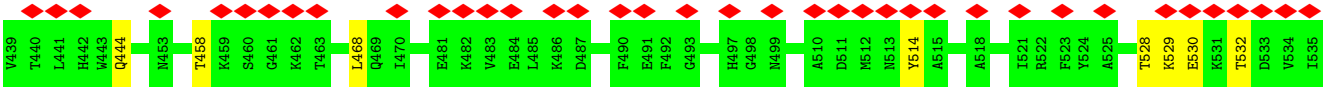
Chain p:

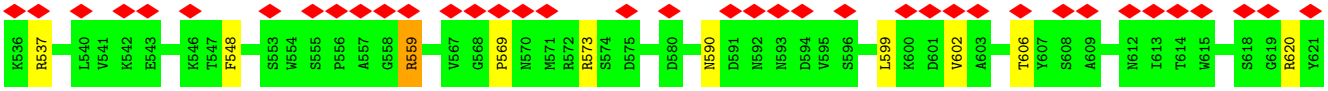


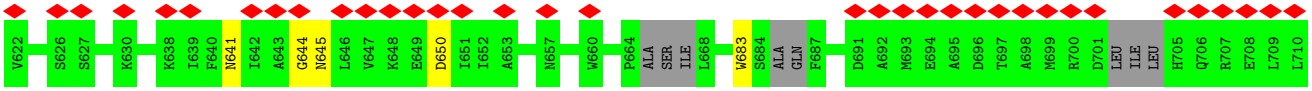


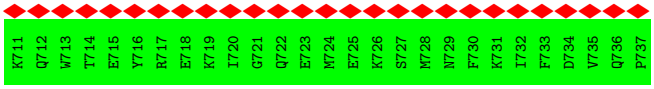






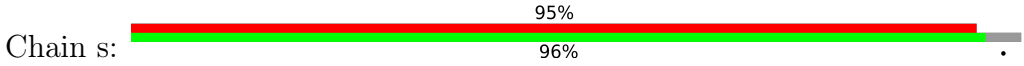


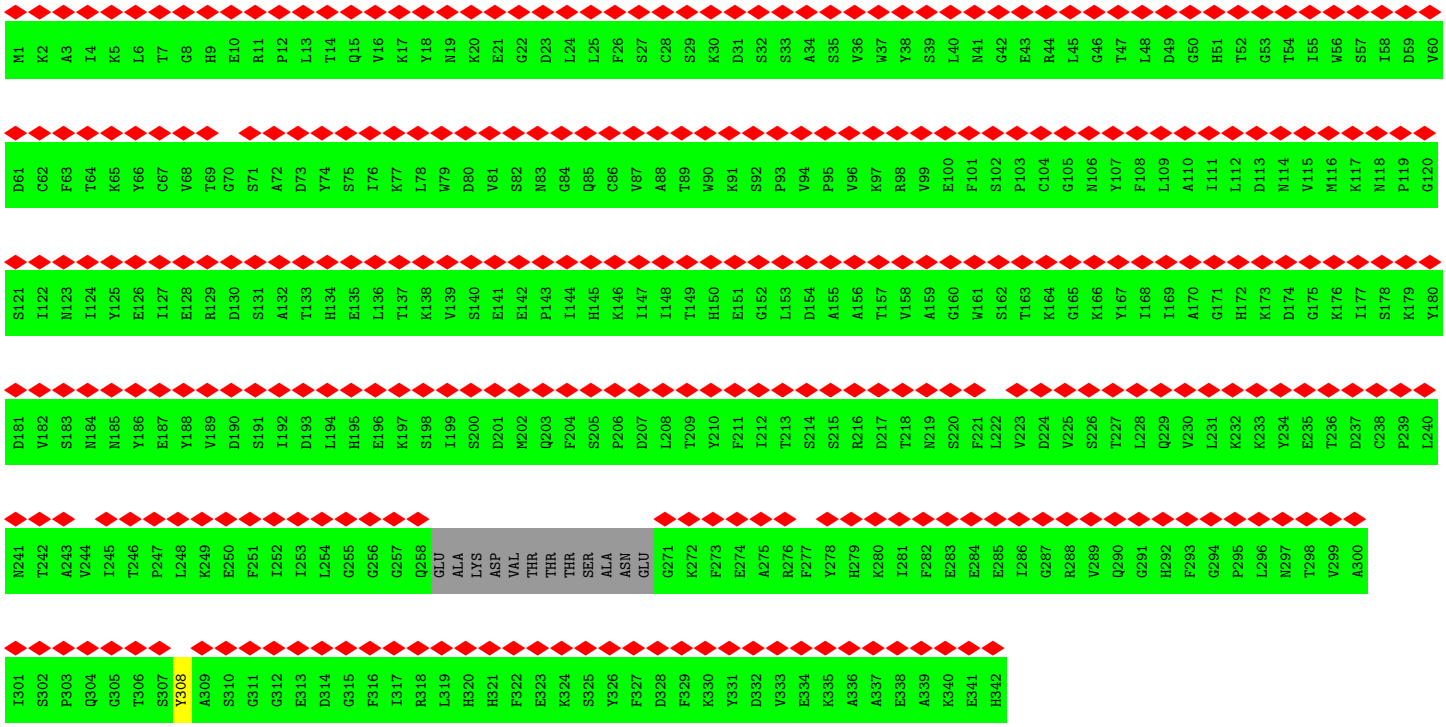




• Molecule 46: Eukaryotic translation initiation factor 3 subunit I

Chain s:





• Molecule 47: Eukaryotic translation initiation factor 3 subunit G

Chain r:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12586	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.275	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.045	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

5.1 Standard geometry

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

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	2	0.23	0/42691	0.65	3/66521 (0.0%)
2	C	0.40	0/1659	0.68	0/2252
3	D	0.41	0/1769	0.71	0/2378
4	F	0.40	0/1628	0.74	1/2198 (0.0%)
5	K	0.45	0/831	0.70	0/1123
6	M	0.44	0/891	0.75	0/1201
7	P	0.43	0/946	0.72	1/1273 (0.1%)
8	Q	0.43	0/1125	0.72	0/1510
9	R	0.42	0/1038	0.80	1/1395 (0.1%)
10	S	0.41	0/1212	0.76	0/1629
11	T	0.39	0/1129	0.71	0/1520
12	U	0.39	0/857	0.68	0/1158
13	Z	0.41	0/567	0.67	0/762
14	c	0.39	0/489	0.71	0/655
15	f	0.48	0/559	0.69	0/747
16	g	0.41	0/2521	0.59	0/3431
17	d	0.42	0/457	0.62	0/607
18	e	0.40	0/471	0.65	0/628
19	h	0.36	0/234	0.64	0/300
20	3	0.26	0/317	0.68	0/489
21	i	0.36	0/894	0.61	0/1188
22	m	0.41	0/723	0.59	0/965
23	o	0.50	0/3671	0.61	0/4961
24	q	0.50	0/5270	0.62	0/7154
25	k	0.44	0/3167	0.63	1/4278 (0.0%)
26	l	0.47	0/1030	0.61	0/1375
27	j	0.44	0/2034	0.63	1/2737 (0.0%)
28	1	0.34	1/1796 (0.1%)	0.64	0/2795
29	A	0.41	0/1742	0.70	1/2383 (0.0%)
30	B	0.40	0/1793	0.69	2/2414 (0.1%)
31	E	0.39	0/2122	0.65	1/2861 (0.0%)
32	G	0.39	0/1835	0.69	1/2451 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	H	0.41	0/1507	0.69	0/2028
34	I	0.40	0/1515	0.70	2/2029 (0.1%)
35	J	0.40	0/1495	0.77	1/2001 (0.0%)
36	L	0.42	0/1276	0.65	0/1718
37	N	0.40	0/1210	0.74	0/1628
38	O	0.40	0/953	0.66	0/1279
39	V	0.37	0/696	0.66	1/938 (0.1%)
40	W	0.38	0/1039	0.70	2/1399 (0.1%)
41	Y	0.39	0/1075	0.67	0/1433
42	X	0.41	0/1137	0.70	1/1516 (0.1%)
43	a	0.37	0/791	0.65	0/1059
44	b	0.39	0/619	0.63	0/837
45	p	0.45	0/5282	0.57	0/7178
46	s	0.35	0/2669	0.53	0/3611
47	r	0.29	0/399	0.45	0/535
All	All	0.36	1/109131 (0.0%)	0.65	20/156528 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
41	Y	0	1
42	X	0	1
45	p	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	1	A	OP3-P	-10.05	1.49	1.61

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	I	190	LEU	CA-CB-CG	7.41	132.35	115.30
7	P	56	LEU	CA-CB-CG	6.99	131.37	115.30
9	R	109	LEU	CA-CB-CG	6.17	129.50	115.30
40	W	26	LEU	CA-CB-CG	6.08	129.29	115.30
1	2	1430	U	C2'-C3'-O3'	6.07	123.41	113.70
1	2	649	U	C2'-C3'-O3'	5.91	123.16	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	184	LEU	CA-CB-CG	5.83	128.70	115.30
35	J	93	LEU	CA-CB-CG	5.81	128.67	115.30
32	G	76	LEU	CA-CB-CG	5.79	128.63	115.30
34	I	29	LEU	CA-CB-CG	5.76	128.56	115.30
39	V	69	LEU	CA-CB-CG	5.64	128.28	115.30
40	W	69	LEU	CA-CB-CG	5.59	128.17	115.30
25	k	462	LEU	CA-CB-CG	5.36	127.63	115.30
42	X	9	LEU	CA-CB-CG	5.35	127.61	115.30
1	2	700	C	C2'-C3'-O3'	5.29	122.16	113.70
27	j	205	LEU	CA-CB-CG	5.21	127.28	115.30
29	A	201	LEU	CA-CB-CG	5.09	127.00	115.30
4	F	177	LEU	CA-CB-CG	5.06	126.93	115.30
31	E	38	LEU	CA-CB-CG	5.05	126.92	115.30
30	B	181	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	X	63	GLN	Peptide
41	Y	29	HIS	Peptide
45	p	391	GLN	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	215/217 (99%)	194 (90%)	14 (6%)	7 (3%)	4 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	221/223 (99%)	196 (89%)	14 (6%)	11 (5%)	2	20
4	F	204/206 (99%)	171 (84%)	22 (11%)	11 (5%)	2	18
5	K	94/96 (98%)	84 (89%)	7 (7%)	3 (3%)	4	26
6	M	113/118 (96%)	86 (76%)	17 (15%)	10 (9%)	1	10
7	P	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	2	19
8	Q	139/141 (99%)	118 (85%)	11 (8%)	10 (7%)	1	13
9	R	128/130 (98%)	107 (84%)	15 (12%)	6 (5%)	2	21
10	S	143/145 (99%)	118 (82%)	17 (12%)	8 (6%)	2	18
11	T	141/143 (99%)	132 (94%)	7 (5%)	2 (1%)	11	46
12	U	104/106 (98%)	91 (88%)	8 (8%)	5 (5%)	2	20
13	Z	68/70 (97%)	56 (82%)	9 (13%)	3 (4%)	2	22
14	c	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	9	42
15	f	67/69 (97%)	51 (76%)	7 (10%)	9 (13%)	0	4
16	g	312/324 (96%)	271 (87%)	33 (11%)	8 (3%)	5	31
17	d	51/53 (96%)	39 (76%)	11 (22%)	1 (2%)	7	37
18	e	56/58 (97%)	45 (80%)	9 (16%)	2 (4%)	3	25
19	h	23/25 (92%)	23 (100%)	0	0	100	100
21	i	109/111 (98%)	90 (83%)	18 (16%)	1 (1%)	17	56
22	m	86/90 (96%)	76 (88%)	7 (8%)	3 (4%)	3	25
23	o	435/567 (77%)	366 (84%)	62 (14%)	7 (2%)	9	43
24	q	667/699 (95%)	577 (86%)	70 (10%)	20 (3%)	4	28
25	k	404/430 (94%)	337 (83%)	60 (15%)	7 (2%)	9	42
26	l	118/144 (82%)	97 (82%)	20 (17%)	1 (1%)	19	60
27	j	243/263 (92%)	210 (86%)	27 (11%)	6 (2%)	5	32
29	A	217/219 (99%)	183 (84%)	24 (11%)	10 (5%)	2	21
30	B	218/231 (94%)	187 (86%)	23 (11%)	8 (4%)	3	24
31	E	258/260 (99%)	240 (93%)	13 (5%)	5 (2%)	8	38
32	G	224/226 (99%)	205 (92%)	18 (8%)	1 (0%)	34	72
33	H	182/184 (99%)	157 (86%)	15 (8%)	10 (6%)	2	18
34	I	184/200 (92%)	166 (90%)	11 (6%)	7 (4%)	3	24
35	J	180/182 (99%)	150 (83%)	25 (14%)	5 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
36	L	153/155 (99%)	132 (86%)	17 (11%)	4 (3%)	5 31
37	N	148/150 (99%)	135 (91%)	12 (8%)	1 (1%)	22 62
38	O	125/127 (98%)	102 (82%)	12 (10%)	11 (9%)	1 10
39	V	85/87 (98%)	75 (88%)	7 (8%)	3 (4%)	3 25
40	W	127/129 (98%)	113 (89%)	9 (7%)	5 (4%)	3 23
41	Y	132/134 (98%)	116 (88%)	13 (10%)	3 (2%)	6 34
42	X	142/144 (99%)	119 (84%)	14 (10%)	9 (6%)	1 16
43	a	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	3 22
44	b	79/81 (98%)	70 (89%)	3 (4%)	6 (8%)	1 13
45	p	650/666 (98%)	538 (83%)	93 (14%)	19 (3%)	4 29
46	s	326/342 (95%)	318 (98%)	8 (2%)	0	100 100
47	r	47/49 (96%)	44 (94%)	3 (6%)	0	100 100
All	All	7889/8271 (95%)	6814 (86%)	816 (10%)	259 (3%)	6 26

All (259) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	141	VAL
2	C	187	PRO
3	D	220	PRO
4	F	67	SER
6	M	82	VAL
6	M	84	ASP
8	Q	39	VAL
8	Q	40	GLN
10	S	27	ASN
10	S	28	VAL
12	U	17	VAL
12	U	96	PRO
15	f	102	VAL
18	e	47	VAL
24	q	111	VAL
29	A	95	ALA
33	H	31	SER
33	H	64	VAL
34	I	147	ARG
34	I	153	ILE
41	Y	30	PRO

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Mol	Chain	Res	Type
42	X	64	PRO
42	X	92	CYS
43	a	59	TYR
44	b	75	GLU
45	p	181	PRO
45	p	392	PRO
3	D	216	PRO
4	F	37	GLN
4	F	59	SER
4	F	60	LEU
4	F	155	GLY
5	K	54	PHE
5	K	92	LEU
7	P	54	ALA
8	Q	97	VAL
8	Q	115	THR
9	R	99	VAL
10	S	51	ASP
10	S	91	ASP
10	S	145	ARG
13	Z	55	PRO
15	f	110	ASP
15	f	143	HIS
16	g	130	LYS
17	d	23	ILE
22	m	73	GLU
23	o	294	GLY
24	q	105	GLU
24	q	160	ASN
24	q	165	ASN
26	l	200	GLY
29	A	166	GLY
29	A	202	TYR
30	B	148	ASN
30	B	214	LYS
31	E	205	PHE
31	E	245	LYS
32	G	122	GLU
33	H	74	GLN
33	H	136	VAL
33	H	163	ASP
34	I	40	THR

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Mol	Chain	Res	Type
34	I	148	ALA
35	J	150	LEU
35	J	171	ARG
36	L	30	LYS
36	L	55	ASP
36	L	105	LYS
38	O	114	ARG
39	V	45	ALA
40	W	58	SER
40	W	83	ILE
41	Y	36	SER
43	a	13	LYS
45	p	167	ASN
45	p	182	THR
45	p	365	PHE
45	p	559	ARG
2	C	155	GLN
3	D	196	THR
3	D	219	GLU
3	D	221	SER
3	D	223	LYS
4	F	24	PRO
4	F	45	PHE
4	F	66	ILE
5	K	23	ALA
6	M	98	ASP
6	M	110	SER
7	P	108	ARG
8	Q	14	LYS
8	Q	27	GLY
8	Q	32	ASN
8	Q	116	LEU
8	Q	121	SER
9	R	5	ARG
9	R	116	LYS
10	S	102	ALA
11	T	29	GLU
13	Z	38	HIS
15	f	111	GLU
16	g	201	GLY
21	i	17	ASN
22	m	85	ARG

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Mol	Chain	Res	Type
23	o	22	GLY
23	o	171	ASN
23	o	194	GLN
23	o	461	SER
24	q	468	THR
24	q	536	ASP
24	q	650	LYS
25	k	127	ARG
27	j	9	TYR
27	j	57	ARG
27	j	225	ALA
30	B	8	ARG
30	B	190	PRO
31	E	195	ILE
33	H	110	GLN
34	I	52	ASN
38	O	18	ARG
38	O	124	ASP
40	W	29	PRO
40	W	72	CYS
42	X	3	LYS
44	b	3	LEU
44	b	51	GLN
45	p	76	ASP
45	p	160	MET
45	p	170	ASP
45	p	219	ASN
45	p	271	ASP
45	p	641	ASN
45	p	644	GLY
2	C	151	THR
2	C	235	TRP
2	C	253	THR
3	D	62	ASN
4	F	186	PHE
6	M	32	ASP
6	M	103	ALA
7	P	89	MET
7	P	90	ILE
7	P	109	PRO
9	R	24	LEU
9	R	88	VAL

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Mol	Chain	Res	Type
10	S	14	ILE
10	S	142	GLY
12	U	89	ARG
14	c	35	ASP
15	f	98	VAL
15	f	100	LEU
15	f	118	ARG
16	g	106	GLY
18	e	11	ALA
22	m	24	ASN
23	o	457	PRO
24	q	113	LYS
24	q	164	PRO
24	q	460	PRO
24	q	514	LYS
24	q	645	ILE
25	k	507	LYS
27	j	49	SER
29	A	21	ARG
29	A	39	LYS
30	B	54	LEU
30	B	55	LYS
31	E	77	ARG
33	H	54	GLY
37	N	3	ARG
38	O	51	ASP
38	O	75	GLY
38	O	125	SER
39	V	12	TYR
41	Y	4	ALA
42	X	63	GLN
42	X	70	LYS
44	b	21	LEU
45	p	259	PRO
45	p	529	LYS
3	D	4	ILE
3	D	217	VAL
6	M	21	LEU
6	M	120	ASP
8	Q	138	PHE
11	T	39	THR
13	Z	56	THR

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Mol	Chain	Res	Type
15	f	90	LYS
16	g	50	GLU
16	g	120	SER
16	g	129	ASP
24	q	140	LEU
24	q	227	PRO
24	q	351	ILE
24	q	639	GLY
25	k	94	ILE
25	k	95	ILE
25	k	357	PRO
27	j	224	ALA
29	A	103	THR
30	B	154	SER
33	H	98	ILE
34	I	59	ARG
35	J	134	ILE
35	J	147	MET
36	L	5	LEU
38	O	25	ASP
38	O	40	ALA
38	O	42	VAL
38	O	91	SER
40	W	56	HIS
42	X	89	ASN
43	a	36	ILE
2	C	44	THR
3	D	163	PRO
4	F	108	LYS
7	P	71	GLU
12	U	107	THR
15	f	85	TYR
25	k	112	GLY
29	A	100	GLY
29	A	158	VAL
29	A	206	ASN
31	E	144	GLY
33	H	13	PRO
33	H	87	ASP
34	I	22	ARG
38	O	88	GLY
39	V	44	ARG

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Mol	Chain	Res	Type
43	a	61	GLU
44	b	62	VAL
45	p	198	VAL
45	p	375	PRO
4	F	103	GLY
16	g	254	PRO
29	A	25	GLY
42	X	91	GLY
45	p	391	GLN
45	p	569	PRO
24	q	163	THR
24	q	367	GLY
35	J	35	GLY
42	X	41	SER
42	X	96	VAL
6	M	33	GLY
9	R	117	LEU
12	U	117	ILE
23	o	423	PRO
24	q	336	ILE
25	k	277	GLY
27	j	81	GLY
3	D	63	GLY
6	M	93	GLY
24	q	766	PRO
44	b	10	PRO
16	g	64	GLY
30	B	22	ASP

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
2	C	176/176 (100%)	148 (84%)	28 (16%)	2 13
3	D	185/185 (100%)	148 (80%)	37 (20%)	1 8
4	F	174/174 (100%)	140 (80%)	34 (20%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	K	88/88 (100%)	69 (78%)	19 (22%)	1 6
6	M	93/94 (99%)	79 (85%)	14 (15%)	3 15
7	P	100/100 (100%)	78 (78%)	22 (22%)	1 6
8	Q	117/117 (100%)	100 (86%)	17 (14%)	3 16
9	R	115/118 (98%)	96 (84%)	19 (16%)	2 12
10	S	128/128 (100%)	104 (81%)	24 (19%)	1 9
11	T	117/117 (100%)	93 (80%)	24 (20%)	1 7
12	U	96/96 (100%)	83 (86%)	13 (14%)	4 17
13	Z	60/60 (100%)	49 (82%)	11 (18%)	1 10
14	c	54/54 (100%)	47 (87%)	7 (13%)	4 18
15	f	57/60 (95%)	52 (91%)	5 (9%)	10 31
16	g	265/270 (98%)	236 (89%)	29 (11%)	6 23
17	d	46/46 (100%)	37 (80%)	9 (20%)	1 8
18	e	51/51 (100%)	44 (86%)	7 (14%)	3 17
19	h	23/23 (100%)	18 (78%)	5 (22%)	1 6
21	i	93/93 (100%)	82 (88%)	11 (12%)	5 20
22	m	77/78 (99%)	71 (92%)	6 (8%)	12 36
23	o	398/438 (91%)	360 (90%)	38 (10%)	8 27
24	q	527/644 (82%)	493 (94%)	34 (6%)	17 42
25	k	332/364 (91%)	307 (92%)	25 (8%)	13 37
26	l	117/132 (89%)	105 (90%)	12 (10%)	7 25
27	j	224/237 (94%)	197 (88%)	27 (12%)	5 20
29	A	180/185 (97%)	160 (89%)	20 (11%)	6 22
30	B	198/210 (94%)	181 (91%)	17 (9%)	10 32
31	E	223/223 (100%)	201 (90%)	22 (10%)	8 26
32	G	192/192 (100%)	179 (93%)	13 (7%)	16 40
33	H	164/164 (100%)	146 (89%)	18 (11%)	6 22
34	I	147/158 (93%)	130 (88%)	17 (12%)	5 21
35	J	153/153 (100%)	125 (82%)	28 (18%)	1 10
36	L	136/136 (100%)	110 (81%)	26 (19%)	1 8
37	N	127/127 (100%)	108 (85%)	19 (15%)	3 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	O	96/96 (100%)	88 (92%)	8 (8%)	11 34
39	V	73/73 (100%)	64 (88%)	9 (12%)	4 19
40	W	110/110 (100%)	103 (94%)	7 (6%)	17 42
41	Y	108/108 (100%)	100 (93%)	8 (7%)	13 38
42	X	119/119 (100%)	106 (89%)	13 (11%)	6 23
43	a	83/83 (100%)	78 (94%)	5 (6%)	19 44
44	b	71/71 (100%)	68 (96%)	3 (4%)	30 54
45	p	537/597 (90%)	510 (95%)	27 (5%)	24 49
46	s	287/297 (97%)	286 (100%)	1 (0%)	92 94
47	r	40/40 (100%)	40 (100%)	0	100 100
All	All	6757/7085 (95%)	6019 (89%)	738 (11%)	10 23

All (738) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	49	LEU
2	C	71	PHE
2	C	74	ILE
2	C	75	ASP
2	C	80	ASN
2	C	91	VAL
2	C	93	LYS
2	C	95	THR
2	C	100	ARG
2	C	116	VAL
2	C	125	GLU
2	C	131	ARG
2	C	142	ILE
2	C	145	ARG
2	C	146	ARG
2	C	155	GLN
2	C	163	THR
2	C	173	ARG
2	C	192	LEU
2	C	195	LEU
2	C	212	LEU
2	C	214	ASN
2	C	216	LEU

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Mol	Chain	Res	Type
2	C	227	TYR
2	C	233	ASN
2	C	234	LEU
2	C	235	TRP
2	C	236	GLU
3	D	5	ILE
3	D	11	LEU
3	D	20	GLU
3	D	22	ASN
3	D	28	GLU
3	D	31	GLU
3	D	47	GLU
3	D	51	ARG
3	D	53	THR
3	D	57	ASP
3	D	58	VAL
3	D	64	ARG
3	D	66	ILE
3	D	68	GLU
3	D	70	THR
3	D	71	LEU
3	D	75	LYS
3	D	76	ARG
3	D	81	ARG
3	D	93	ASP
3	D	94	ARG
3	D	101	GLN
3	D	105	MET
3	D	113	LEU
3	D	117	ARG
3	D	122	VAL
3	D	132	LYS
3	D	143	ARG
3	D	146	ARG
3	D	157	LEU
3	D	167	PHE
3	D	173	ARG
3	D	200	LYS
3	D	206	VAL
3	D	212	LYS
3	D	215	GLU
3	D	218	LEU

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Mol	Chain	Res	Type
4	F	29	THR
4	F	31	ILE
4	F	39	GLN
4	F	42	ILE
4	F	44	LEU
4	F	72	VAL
4	F	86	LYS
4	F	91	ILE
4	F	104	ARG
4	F	108	LYS
4	F	116	VAL
4	F	133	GLN
4	F	134	VAL
4	F	150	ARG
4	F	151	VAL
4	F	159	ARG
4	F	163	ASP
4	F	164	VAL
4	F	169	ARG
4	F	174	ILE
4	F	176	LEU
4	F	177	LEU
4	F	183	GLU
4	F	186	PHE
4	F	187	ARG
4	F	188	ASN
4	F	199	GLU
4	F	200	LEU
4	F	209	THR
4	F	217	ASP
4	F	220	GLU
4	F	221	ARG
4	F	224	LYS
4	F	226	ASN
5	K	6	GLU
5	K	9	LYS
5	K	21	LEU
5	K	37	THR
5	K	40	LEU
5	K	44	LYS
5	K	49	LEU
5	K	55	VAL

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Mol	Chain	Res	Type
5	K	58	GLN
5	K	59	PHE
5	K	63	TYR
5	K	65	TYR
5	K	67	THR
5	K	69	THR
5	K	71	GLU
5	K	73	VAL
5	K	75	TYR
5	K	80	LEU
5	K	81	ASN
6	M	24	VAL
6	M	32	ASP
6	M	34	LEU
6	M	55	LEU
6	M	61	GLU
6	M	67	LEU
6	M	76	ASN
6	M	90	GLU
6	M	91	TRP
6	M	94	LEU
6	M	106	VAL
6	M	128	LEU
6	M	129	GLU
6	M	130	HIS
7	P	13	LYS
7	P	25	LEU
7	P	26	LEU
7	P	27	GLU
7	P	32	ASP
7	P	43	ARG
7	P	47	ARG
7	P	51	GLU
7	P	56	LEU
7	P	71	GLU
7	P	72	LYS
7	P	78	THR
7	P	79	HIS
7	P	81	ARG
7	P	83	MET
7	P	85	ILE
7	P	93	VAL

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Mol	Chain	Res	Type
7	P	106	GLU
7	P	108	ARG
7	P	111	MET
7	P	122	THR
7	P	126	VAL
8	Q	28	LEU
8	Q	36	ILE
8	Q	37	THR
8	Q	38	LEU
8	Q	45	ARG
8	Q	46	PHE
8	Q	47	LYS
8	Q	54	LEU
8	Q	82	ARG
8	Q	83	GLN
8	Q	99	GLU
8	Q	100	GLN
8	Q	117	LEU
8	Q	123	ARG
8	Q	132	ARG
8	Q	137	ARG
8	Q	139	GLN
9	R	3	ARG
9	R	5	ARG
9	R	6	THR
9	R	14	LYS
9	R	16	LEU
9	R	25	THR
9	R	26	MET
9	R	28	PHE
9	R	33	ARG
9	R	36	ASP
9	R	37	GLU
9	R	45	ARG
9	R	47	ARG
9	R	48	ASN
9	R	58	MET
9	R	67	ARG
9	R	99	VAL
9	R	106	THR
9	R	128	ARG
10	S	13	HIS

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Mol	Chain	Res	Type
10	S	25	ASN
10	S	40	ARG
10	S	41	ARG
10	S	45	LEU
10	S	55	HIS
10	S	57	ARG
10	S	61	LEU
10	S	66	LEU
10	S	73	MET
10	S	89	GLN
10	S	91	ASP
10	S	99	HIS
10	S	101	LEU
10	S	103	ASN
10	S	105	LEU
10	S	110	ARG
10	S	114	GLU
10	S	120	ARG
10	S	126	ARG
10	S	131	LEU
10	S	132	ARG
10	S	143	ARG
10	S	144	ARG
11	T	12	GLN
11	T	14	PHE
11	T	16	ASN
11	T	23	GLN
11	T	24	ARG
11	T	25	GLN
11	T	28	LEU
11	T	33	TYR
11	T	45	LEU
11	T	63	ARG
11	T	75	LYS
11	T	78	LYS
11	T	79	LEU
11	T	86	ARG
11	T	91	HIS
11	T	95	ASP
11	T	107	SER
11	T	111	LEU
11	T	123	ARG

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Mol	Chain	Res	Type
11	T	124	ILE
11	T	129	LEU
11	T	132	LEU
11	T	135	ILE
11	T	143	GLU
12	U	17	VAL
12	U	27	THR
12	U	31	VAL
12	U	35	GLU
12	U	37	VAL
12	U	40	ASN
12	U	51	VAL
12	U	82	TYR
12	U	83	GLU
12	U	89	ARG
12	U	90	TYR
12	U	93	LEU
12	U	109	GLU
13	Z	38	HIS
13	Z	43	ASP
13	Z	48	ASP
13	Z	49	ARG
13	Z	52	LYS
13	Z	58	ARG
13	Z	70	LYS
13	Z	71	LEU
13	Z	77	ARG
13	Z	78	VAL
13	Z	80	LEU
14	c	8	THR
14	c	16	LEU
14	c	19	THR
14	c	38	ARG
14	c	43	ASN
14	c	49	ARG
14	c	54	LEU
15	f	83	LYS
15	f	85	TYR
15	f	91	ILE
15	f	92	ARG
15	f	138	TYR
16	g	8	LEU

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Mol	Chain	Res	Type
16	g	20	TRP
16	g	33	LEU
16	g	39	ARG
16	g	67	HIS
16	g	70	GLN
16	g	91	ARG
16	g	92	LEU
16	g	110	ASP
16	g	124	ILE
16	g	137	THR
16	g	145	LEU
16	g	146	LEU
16	g	151	TRP
16	g	184	ARG
16	g	195	ILE
16	g	200	ILE
16	g	205	TYR
16	g	206	ILE
16	g	207	ASN
16	g	210	GLN
16	g	246	GLU
16	g	256	ARG
16	g	263	THR
16	g	272	LEU
16	g	280	GLU
16	g	312	TYR
16	g	313	THR
16	g	318	ARG
17	d	9	SER
17	d	12	ARG
17	d	20	GLN
17	d	30	LEU
17	d	32	ARG
17	d	36	LEU
17	d	38	ILE
17	d	41	GLN
17	d	44	ARG
18	e	10	ARG
18	e	33	ARG
18	e	37	ARG
18	e	38	LEU
18	e	39	LEU

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Mol	Chain	Res	Type
18	e	42	ARG
18	e	54	ARG
19	h	2	ARG
19	h	12	ARG
19	h	13	LEU
19	h	17	ARG
19	h	20	VAL
21	i	13	ARG
21	i	24	ARG
21	i	30	GLU
21	i	34	GLU
21	i	37	GLN
21	i	42	LEU
21	i	57	ARG
21	i	58	MET
21	i	62	ARG
21	i	82	ARG
21	i	111	GLU
22	m	34	ASN
22	m	48	GLU
22	m	55	LEU
22	m	91	PHE
22	m	96	LEU
22	m	104	LYS
23	o	18	LEU
23	o	19	ILE
23	o	34	PHE
23	o	61	GLU
23	o	62	LEU
23	o	70	ASP
23	o	73	HIS
23	o	89	VAL
23	o	94	ARG
23	o	98	ASP
23	o	100	VAL
23	o	108	GLN
23	o	110	ARG
23	o	167	ASP
23	o	172	ASN
23	o	202	LEU
23	o	204	GLU
23	o	210	LEU

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Mol	Chain	Res	Type
23	o	211	ASP
23	o	229	ASP
23	o	254	HIS
23	o	264	PHE
23	o	278	THR
23	o	321	PHE
23	o	333	ILE
23	o	338	ASP
23	o	351	MET
23	o	357	LEU
23	o	363	ARG
23	o	376	ILE
23	o	381	ASP
23	o	404	LEU
23	o	406	ASN
23	o	408	LEU
23	o	430	ARG
23	o	438	GLN
23	o	464	ASP
23	o	470	LEU
24	q	195	TYR
24	q	201	ARG
24	q	251	GLN
24	q	257	ARG
24	q	275	LEU
24	q	303	ARG
24	q	335	THR
24	q	340	GLN
24	q	342	ASN
24	q	393	ASP
24	q	402	GLN
24	q	407	LEU
24	q	409	LEU
24	q	448	ILE
24	q	452	GLU
24	q	462	GLN
24	q	471	ASP
24	q	473	LEU
24	q	532	ILE
24	q	550	LEU
24	q	571	LEU
24	q	585	LEU

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Mol	Chain	Res	Type
24	q	611	HIS
24	q	626	LEU
24	q	630	ILE
24	q	634	THR
24	q	662	LEU
24	q	681	SER
24	q	697	ILE
24	q	705	ASN
24	q	722	LEU
24	q	729	PHE
24	q	749	GLU
24	q	783	GLU
25	k	105	THR
25	k	197	HIS
25	k	228	GLN
25	k	236	ILE
25	k	251	VAL
25	k	291	ILE
25	k	318	ILE
25	k	351	ASP
25	k	352	GLU
25	k	354	GLU
25	k	395	LEU
25	k	402	VAL
25	k	410	ASP
25	k	411	ARG
25	k	422	HIS
25	k	432	ILE
25	k	437	LEU
25	k	440	LEU
25	k	459	ASN
25	k	471	THR
25	k	474	ARG
25	k	484	ARG
25	k	485	LEU
25	k	502	SER
25	k	508	HIS
26	l	163	PRO
26	l	165	CYS
26	l	167	ARG
26	l	171	LYS
26	l	179	ASP

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Mol	Chain	Res	Type
26	l	186	ARG
26	l	191	LEU
26	l	195	LEU
26	l	226	LEU
26	l	236	CYS
26	l	244	THR
26	l	255	PHE
27	j	3	THR
27	j	6	CYS
27	j	7	ARG
27	j	11	ASN
27	j	17	ASP
27	j	19	ILE
27	j	39	TYR
27	j	45	MET
27	j	53	ARG
27	j	57	ARG
27	j	59	ILE
27	j	69	ASP
27	j	79	GLU
27	j	87	LYS
27	j	97	LYS
27	j	123	LEU
27	j	143	GLU
27	j	159	GLU
27	j	163	LYS
27	j	195	TYR
27	j	198	ILE
27	j	201	ILE
27	j	230	LEU
27	j	235	LEU
27	j	244	LEU
27	j	251	ILE
27	j	255	ILE
29	A	3	LEU
29	A	8	ASP
29	A	33	GLN
29	A	39	LYS
29	A	58	VAL
29	A	59	LEU
29	A	72	ASP
29	A	79	ARG

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Mol	Chain	Res	Type
29	A	80	THR
29	A	88	LYS
29	A	93	THR
29	A	101	ARG
29	A	108	THR
29	A	112	THR
29	A	117	GLU
29	A	165	ARG
29	A	170	ILE
29	A	193	GLN
29	A	198	MET
29	A	201	LEU
30	B	47	LEU
30	B	61	LEU
30	B	64	ARG
30	B	68	VAL
30	B	72	ASP
30	B	81	PHE
30	B	82	ARG
30	B	84	VAL
30	B	104	ASP
30	B	119	THR
30	B	127	VAL
30	B	171	ILE
30	B	181	LEU
30	B	189	ILE
30	B	193	ILE
30	B	196	GLU
30	B	205	PHE
31	E	7	LYS
31	E	22	LYS
31	E	42	LEU
31	E	51	ARG
31	E	60	GLU
31	E	65	LEU
31	E	69	HIS
31	E	75	LYS
31	E	77	ARG
31	E	108	ARG
31	E	113	ARG
31	E	123	LEU
31	E	168	THR

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Mol	Chain	Res	Type
31	E	180	LEU
31	E	181	VAL
31	E	189	LEU
31	E	206	ASP
31	E	216	ASN
31	E	225	VAL
31	E	233	ARG
31	E	248	ILE
31	E	259	HIS
32	G	5	ILE
32	G	25	ARG
32	G	52	ILE
32	G	69	LEU
32	G	88	ARG
32	G	121	ILE
32	G	151	ASP
32	G	176	GLN
32	G	178	LEU
32	G	211	LEU
32	G	214	LYS
32	G	215	ARG
32	G	220	LYS
33	H	5	GLN
33	H	7	LYS
33	H	11	GLN
33	H	15	GLU
33	H	24	PHE
33	H	48	GLU
33	H	72	LYS
33	H	80	GLU
33	H	86	GLN
33	H	111	LYS
33	H	112	ARG
33	H	122	HIS
33	H	124	LYS
33	H	126	LEU
33	H	129	LEU
33	H	139	ARG
33	H	152	ILE
33	H	175	LYS
34	I	8	ARG
34	I	20	GLN

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Mol	Chain	Res	Type
34	I	23	LYS
34	I	29	LEU
34	I	47	ARG
34	I	53	GLN
34	I	72	VAL
34	I	78	ILE
34	I	104	ILE
34	I	105	ASP
34	I	119	GLN
34	I	140	THR
34	I	153	ILE
34	I	179	ARG
34	I	190	LEU
34	I	196	ARG
34	I	200	LYS
35	J	3	ARG
35	J	23	ARG
35	J	25	ASP
35	J	28	LEU
35	J	33	GLU
35	J	36	LEU
35	J	37	LYS
35	J	44	ARG
35	J	45	ILE
35	J	48	GLN
35	J	49	LEU
35	J	53	ARG
35	J	54	ARG
35	J	60	LEU
35	J	62	ARG
35	J	80	LEU
35	J	96	VAL
35	J	100	LYS
35	J	107	ARG
35	J	109	LEU
35	J	114	TYR
35	J	118	LEU
35	J	128	LEU
35	J	132	ARG
35	J	142	ASN
35	J	151	GLU
35	J	161	THR

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Mol	Chain	Res	Type
35	J	171	ARG
36	L	7	VAL
36	L	8	GLN
36	L	10	GLU
36	L	15	LYS
36	L	26	LYS
36	L	31	THR
36	L	32	LYS
36	L	36	LYS
36	L	37	ASN
36	L	38	VAL
36	L	55	ASP
36	L	67	ARG
36	L	74	THR
36	L	80	MET
36	L	82	ARG
36	L	84	ILE
36	L	88	ARG
36	L	99	ARG
36	L	103	ARG
36	L	107	VAL
36	L	117	VAL
36	L	118	GLN
36	L	128	CYS
36	L	136	ARG
36	L	150	ASN
36	L	156	PHE
37	N	3	ARG
37	N	18	TYR
37	N	20	ARG
37	N	27	LYS
37	N	31	ASP
37	N	39	LYS
37	N	52	VAL
37	N	64	LYS
37	N	86	GLU
37	N	88	LEU
37	N	90	PHE
37	N	91	LEU
37	N	96	VAL
37	N	100	LYS
37	N	106	ARG

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Mol	Chain	Res	Type
37	N	113	PHE
37	N	119	GLU
37	N	120	SER
37	N	121	ARG
38	O	29	HIS
38	O	32	ASP
38	O	37	GLU
38	O	49	LYS
38	O	52	ARG
38	O	102	LEU
38	O	110	LEU
38	O	114	ARG
39	V	1	MET
39	V	8	LEU
39	V	9	VAL
39	V	12	TYR
39	V	33	GLN
39	V	44	ARG
39	V	62	ARG
39	V	69	LEU
39	V	76	ASP
40	W	24	GLN
40	W	26	LEU
40	W	61	ILE
40	W	65	LEU
40	W	81	VAL
40	W	104	LEU
40	W	111	MET
41	Y	8	ARG
41	Y	13	ILE
41	Y	35	VAL
41	Y	72	PHE
41	Y	84	LYS
41	Y	99	LYS
41	Y	112	LYS
41	Y	121	THR
42	X	14	LYS
42	X	19	ARG
42	X	33	LEU
42	X	52	ILE
42	X	55	GLU
42	X	56	LYS

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Mol	Chain	Res	Type
42	X	60	GLU
42	X	83	VAL
42	X	107	PHE
42	X	109	ARG
42	X	114	LYS
42	X	117	ILE
42	X	133	LEU
43	a	12	LYS
43	a	38	ARG
43	a	50	ILE
43	a	69	ASN
43	a	74	CYS
44	b	20	LYS
44	b	57	GLU
44	b	67	THR
45	p	126	PHE
45	p	190	LYS
45	p	343	TYR
45	p	362	THR
45	p	369	GLU
45	p	373	LEU
45	p	394	ARG
45	p	406	TRP
45	p	444	GLN
45	p	458	THR
45	p	468	LEU
45	p	514	TYR
45	p	528	THR
45	p	530	GLU
45	p	532	THR
45	p	537	ARG
45	p	548	PHE
45	p	559	ARG
45	p	573	ARG
45	p	590	ASN
45	p	599	LEU
45	p	602	VAL
45	p	606	THR
45	p	620	ARG
45	p	645	ASN
45	p	650	ASP
45	p	683	TRP

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Mol	Chain	Res	Type
46	s	308	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	76	GLN
2	C	233	ASN
3	D	56	GLN
4	F	102	ASN
4	F	105	ASN
4	F	106	ASN
4	F	124	ASN
4	F	160	GLN
4	F	188	ASN
5	K	29	GLN
6	M	76	ASN
8	Q	94	GLN
9	R	29	GLN
10	S	78	HIS
10	S	93	ASN
11	T	17	ASN
11	T	43	ASN
11	T	48	GLN
11	T	70	GLN
12	U	36	ASN
12	U	72	ASN
13	Z	38	HIS
13	Z	98	GLN
14	c	27	GLN
16	g	30	GLN
16	g	210	GLN
16	g	292	GLN
17	d	41	GLN
21	i	37	GLN
21	i	44	ASN
21	i	60	HIS
21	i	73	GLN
22	m	65	ASN
22	m	81	GLN
24	q	513	ASN
24	q	564	HIS
24	q	665	GLN

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Mol	Chain	Res	Type
24	q	718	GLN
25	k	422	HIS
27	j	11	ASN
29	A	33	GLN
29	A	131	GLN
29	A	213	GLN
30	B	49	ASN
30	B	56	ASN
30	B	148	ASN
30	B	183	GLN
30	B	208	GLN
31	E	50	ASN
31	E	57	ASN
31	E	69	HIS
31	E	112	HIS
31	E	188	ASN
32	G	4	ASN
32	G	10	ASN
32	G	13	GLN
32	G	89	ASN
32	G	185	GLN
33	H	180	GLN
34	I	84	HIS
34	I	116	HIS
35	J	38	ASN
35	J	123	HIS
35	J	155	HIS
36	L	22	ASN
37	N	49	GLN
37	N	58	HIS
37	N	78	ASN
38	O	29	HIS
38	O	65	GLN
38	O	80	HIS
39	V	3	ASN
39	V	7	GLN
41	Y	22	GLN
42	X	21	ASN
42	X	22	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	828 (46%)	69 (3%)
20	3	13/14 (92%)	8 (61%)	2 (15%)
28	1	73/75 (97%)	32 (43%)	6 (8%)
All	All	1883/1887 (99%)	868 (46%)	77 (4%)

All (868) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	5	U
1	2	8	U
1	2	9	U
1	2	11	A
1	2	14	C
1	2	16	G
1	2	17	C
1	2	19	A
1	2	20	G
1	2	24	U
1	2	25	C
1	2	26	A
1	2	30	G
1	2	31	C
1	2	34	G
1	2	39	A
1	2	42	G
1	2	43	A
1	2	44	U
1	2	45	U
1	2	47	A
1	2	51	A
1	2	56	U
1	2	57	G
1	2	59	C
1	2	63	G
1	2	64	U
1	2	65	A
1	2	66	U
1	2	67	A
1	2	68	A
1	2	69	G

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Mol	Chain	Res	Type
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	79	C
1	2	81	G
1	2	87	C
1	2	95	G
1	2	104	A
1	2	111	U
1	2	114	C
1	2	124	A
1	2	127	G
1	2	128	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	136	C
1	2	138	A
1	2	140	A
1	2	141	U
1	2	144	A
1	2	146	A
1	2	147	U
1	2	148	C
1	2	149	U
1	2	156	A
1	2	157	U
1	2	158	U
1	2	159	C
1	2	161	A
1	2	167	A
1	2	172	A
1	2	173	U
1	2	176	U
1	2	177	U
1	2	178	A
1	2	184	U
1	2	185	C

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Mol	Chain	Res	Type
1	2	187	A
1	2	190	C
1	2	191	U
1	2	192	U
1	2	194	G
1	2	195	G
1	2	198	G
1	2	199	A
1	2	201	A
1	2	209	A
1	2	214	A
1	2	217	A
1	2	218	A
1	2	220	A
1	2	226	U
1	2	228	U
1	2	230	U
1	2	231	U
1	2	232	C
1	2	233	G
1	2	234	G
1	2	237	U
1	2	239	C
1	2	240	U
1	2	249	C
1	2	254	U
1	2	258	U
1	2	259	U
1	2	260	U
1	2	264	A
1	2	266	U
1	2	268	G
1	2	274	C
1	2	275	C
1	2	276	U
1	2	278	G
1	2	279	U
1	2	280	G
1	2	286	G
1	2	288	U
1	2	294	A
1	2	298	A

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Mol	Chain	Res	Type
1	2	300	A
1	2	301	U
1	2	307	C
1	2	308	C
1	2	311	A
1	2	312	U
1	2	313	C
1	2	315	A
1	2	319	U
1	2	320	C
1	2	321	G
1	2	322	A
1	2	328	G
1	2	332	A
1	2	336	G
1	2	337	C
1	2	338	C
1	2	342	C
1	2	349	U
1	2	351	A
1	2	354	G
1	2	358	A
1	2	359	A
1	2	360	C
1	2	368	A
1	2	369	A
1	2	371	G
1	2	372	G
1	2	377	A
1	2	379	U
1	2	380	C
1	2	382	G
1	2	384	A
1	2	387	G
1	2	389	G
1	2	390	A
1	2	391	G
1	2	392	C
1	2	395	G
1	2	398	A
1	2	399	A
1	2	400	A

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Mol	Chain	Res	Type
1	2	401	C
1	2	403	G
1	2	404	C
1	2	405	U
1	2	406	A
1	2	411	A
1	2	412	U
1	2	413	C
1	2	415	A
1	2	416	A
1	2	419	A
1	2	421	G
1	2	422	G
1	2	423	C
1	2	424	A
1	2	425	G
1	2	433	G
1	2	438	U
1	2	439	U
1	2	440	A
1	2	443	C
1	2	447	C
1	2	448	C
1	2	454	C
1	2	455	A
1	2	456	G
1	2	457	G
1	2	458	G
1	2	461	G
1	2	468	C
1	2	469	A
1	2	478	C
1	2	479	G
1	2	480	A
1	2	483	C
1	2	488	C
1	2	489	C
1	2	490	C
1	2	491	A
1	2	492	U
1	2	493	U
1	2	495	G

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Mol	Chain	Res	Type
1	2	496	G
1	2	497	G
1	2	498	U
1	2	499	C
1	2	500	U
1	2	501	U
1	2	502	G
1	2	504	A
1	2	505	A
1	2	506	U
1	2	507	U
1	2	508	G
1	2	517	A
1	2	518	C
1	2	519	A
1	2	521	U
1	2	522	G
1	2	523	U
1	2	525	A
1	2	527	U
1	2	530	C
1	2	531	U
1	2	533	A
1	2	534	A
1	2	535	C
1	2	537	A
1	2	538	G
1	2	539	G
1	2	540	A
1	2	541	A
1	2	542	C
1	2	543	A
1	2	544	A
1	2	545	C
1	2	546	U
1	2	547	G
1	2	550	G
1	2	553	C
1	2	556	G
1	2	557	U
1	2	558	C
1	2	563	G

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Mol	Chain	Res	Type
1	2	564	C
1	2	565	C
1	2	567	G
1	2	568	C
1	2	570	G
1	2	571	C
1	2	572	C
1	2	573	G
1	2	574	C
1	2	575	G
1	2	576	G
1	2	577	U
1	2	578	A
1	2	579	A
1	2	580	U
1	2	581	U
1	2	582	C
1	2	584	A
1	2	586	C
1	2	589	C
1	2	590	A
1	2	593	A
1	2	594	G
1	2	598	A
1	2	599	U
1	2	605	A
1	2	610	U
1	2	612	G
1	2	613	C
1	2	617	U
1	2	618	A
1	2	619	A
1	2	622	A
1	2	633	G
1	2	634	A
1	2	637	U
1	2	638	U
1	2	641	G
1	2	647	G
1	2	650	G
1	2	652	C
1	2	657	C

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Mol	Chain	Res	Type
1	2	659	G
1	2	660	A
1	2	661	C
1	2	663	U
1	2	665	A
1	2	666	U
1	2	671	C
1	2	672	G
1	2	673	C
1	2	675	C
1	2	679	U
1	2	680	U
1	2	681	U
1	2	682	U
1	2	684	A
1	2	685	A
1	2	686	C
1	2	688	G
1	2	691	U
1	2	692	C
1	2	693	U
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	709	C
1	2	710	U
1	2	711	G
1	2	712	U
1	2	714	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	722	G
1	2	723	G

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Mol	Chain	Res	Type
1	2	725	U
1	2	726	G
1	2	727	C
1	2	729	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	738	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	753	A
1	2	755	A
1	2	762	A
1	2	763	G
1	2	765	G
1	2	766	U
1	2	767	U
1	2	768	C
1	2	771	A
1	2	774	A
1	2	778	G
1	2	779	A
1	2	780	A
1	2	781	A
1	2	782	G
1	2	784	U
1	2	785	C
1	2	786	G
1	2	788	A
1	2	790	A
1	2	793	U
1	2	794	U
1	2	795	A
1	2	796	G
1	2	802	A
1	2	805	A
1	2	809	G
1	2	811	A
1	2	812	U

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Mol	Chain	Res	Type
1	2	813	A
1	2	814	G
1	2	817	C
1	2	819	U
1	2	820	U
1	2	822	G
1	2	823	G
1	2	826	C
1	2	827	U
1	2	828	A
1	2	829	U
1	2	837	G
1	2	839	U
1	2	840	U
1	2	845	G
1	2	847	C
1	2	855	A
1	2	856	U
1	2	861	A
1	2	862	A
1	2	863	U
1	2	864	A
1	2	871	G
1	2	872	U
1	2	875	G
1	2	885	U
1	2	886	A
1	2	891	A
1	2	895	U
1	2	897	A
1	2	898	G
1	2	903	G
1	2	904	A
1	2	905	A
1	2	907	U
1	2	908	U
1	2	910	U
1	2	911	U
1	2	912	G
1	2	913	G
1	2	914	A
1	2	915	U

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Mol	Chain	Res	Type
1	2	916	U
1	2	918	A
1	2	919	U
1	2	920	U
1	2	925	A
1	2	927	U
1	2	930	C
1	2	931	U
1	2	932	A
1	2	934	U
1	2	936	C
1	2	939	A
1	2	941	G
1	2	944	U
1	2	946	U
1	2	947	G
1	2	950	A
1	2	956	G
1	2	958	U
1	2	959	U
1	2	962	A
1	2	963	U
1	2	965	A
1	2	970	A
1	2	974	C
1	2	978	A
1	2	981	U
1	2	982	A
1	2	983	G
1	2	987	A
1	2	990	G
1	2	991	A
1	2	993	G
1	2	994	A
1	2	996	G
1	2	999	C
1	2	1002	A
1	2	1003	U
1	2	1004	A
1	2	1008	U
1	2	1009	C
1	2	1011	U

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Mol	Chain	Res	Type
1	2	1015	C
1	2	1018	A
1	2	1022	A
1	2	1024	A
1	2	1025	A
1	2	1026	A
1	2	1027	C
1	2	1028	U
1	2	1030	U
1	2	1031	G
1	2	1034	G
1	2	1038	A
1	2	1039	G
1	2	1041	G
1	2	1042	A
1	2	1044	C
1	2	1048	U
1	2	1049	G
1	2	1050	G
1	2	1051	U
1	2	1052	G
1	2	1054	U
1	2	1055	U
1	2	1056	U
1	2	1057	U
1	2	1058	C
1	2	1059	U
1	2	1062	U
1	2	1065	C
1	2	1070	U
1	2	1071	C
1	2	1075	A
1	2	1077	C
1	2	1081	C
1	2	1082	G
1	2	1084	G
1	2	1085	A
1	2	1086	A
1	2	1089	C
1	2	1092	A
1	2	1093	G
1	2	1095	C

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Mol	Chain	Res	Type
1	2	1096	U
1	2	1097	U
1	2	1098	U
1	2	1099	G
1	2	1100	G
1	2	1101	G
1	2	1102	U
1	2	1103	U
1	2	1105	U
1	2	1108	G
1	2	1111	G
1	2	1112	A
1	2	1113	G
1	2	1116	U
1	2	1117	G
1	2	1118	G
1	2	1125	G
1	2	1128	U
1	2	1132	A
1	2	1133	C
1	2	1135	U
1	2	1136	A
1	2	1137	A
1	2	1138	A
1	2	1142	A
1	2	1145	G
1	2	1146	A
1	2	1149	G
1	2	1150	A
1	2	1154	G
1	2	1155	C
1	2	1157	C
1	2	1158	C
1	2	1160	C
1	2	1161	C
1	2	1162	A
1	2	1163	G
1	2	1164	G
1	2	1166	G
1	2	1168	G
1	2	1169	G
1	2	1172	C

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Mol	Chain	Res	Type
1	2	1173	C
1	2	1174	U
1	2	1176	C
1	2	1184	U
1	2	1188	A
1	2	1189	C
1	2	1190	U
1	2	1191	C
1	2	1192	A
1	2	1193	A
1	2	1195	A
1	2	1196	C
1	2	1197	G
1	2	1198	G
1	2	1199	G
1	2	1201	A
1	2	1202	A
1	2	1206	C
1	2	1207	A
1	2	1208	C
1	2	1211	G
1	2	1216	A
1	2	1217	G
1	2	1218	A
1	2	1224	U
1	2	1225	A
1	2	1226	A
1	2	1227	G
1	2	1228	G
1	2	1229	A
1	2	1236	G
1	2	1237	A
1	2	1240	G
1	2	1243	A
1	2	1244	G
1	2	1245	C
1	2	1250	U
1	2	1254	G
1	2	1255	A
1	2	1256	U
1	2	1258	U
1	2	1259	U

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Mol	Chain	Res	Type
1	2	1260	G
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1273	C
1	2	1275	U
1	2	1282	U
1	2	1283	C
1	2	1284	U
1	2	1286	A
1	2	1287	G
1	2	1292	U
1	2	1294	G
1	2	1295	A
1	2	1296	G
1	2	1300	U
1	2	1305	C
1	2	1306	U
1	2	1307	G
1	2	1309	U
1	2	1312	A
1	2	1313	U
1	2	1314	U
1	2	1315	G
1	2	1317	G
1	2	1319	U
1	2	1320	A
1	2	1321	A
1	2	1324	A
1	2	1332	C
1	2	1336	A
1	2	1337	C
1	2	1338	C
1	2	1339	U
1	2	1340	A
1	2	1343	A
1	2	1344	A
1	2	1345	A
1	2	1347	A
1	2	1349	G
1	2	1353	G
1	2	1355	U

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Mol	Chain	Res	Type
1	2	1358	C
1	2	1359	A
1	2	1361	U
1	2	1362	U
1	2	1363	G
1	2	1364	C
1	2	1366	G
1	2	1369	U
1	2	1370	G
1	2	1371	A
1	2	1376	U
1	2	1379	U
1	2	1380	A
1	2	1381	G
1	2	1382	A
1	2	1386	A
1	2	1387	C
1	2	1388	U
1	2	1391	C
1	2	1393	G
1	2	1396	U
1	2	1397	C
1	2	1398	A
1	2	1400	G
1	2	1408	A
1	2	1409	A
1	2	1411	U
1	2	1412	U
1	2	1413	U
1	2	1414	G
1	2	1416	G
1	2	1418	C
1	2	1419	A
1	2	1420	A
1	2	1422	A
1	2	1423	A
1	2	1424	C
1	2	1425	A
1	2	1426	G
1	2	1428	U
1	2	1429	C
1	2	1430	U

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Mol	Chain	Res	Type
1	2	1431	G
1	2	1433	G
1	2	1434	A
1	2	1442	A
1	2	1443	G
1	2	1444	A
1	2	1450	U
1	2	1455	C
1	2	1456	G
1	2	1457	C
1	2	1458	A
1	2	1461	C
1	2	1463	C
1	2	1465	C
1	2	1466	U
1	2	1467	A
1	2	1469	A
1	2	1470	C
1	2	1471	U
1	2	1476	G
1	2	1479	C
1	2	1480	C
1	2	1481	A
1	2	1482	G
1	2	1484	G
1	2	1488	A
1	2	1489	C
1	2	1490	A
1	2	1491	A
1	2	1492	C
1	2	1494	U
1	2	1497	G
1	2	1498	C
1	2	1505	G
1	2	1509	G
1	2	1512	U
1	2	1513	A
1	2	1514	A
1	2	1515	U
1	2	1516	C
1	2	1519	G
1	2	1521	G

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Mol	Chain	Res	Type
1	2	1522	A
1	2	1523	A
1	2	1528	C
1	2	1529	G
1	2	1533	U
1	2	1534	G
1	2	1535	C
1	2	1538	G
1	2	1540	G
1	2	1544	G
1	2	1546	G
1	2	1548	A
1	2	1551	G
1	2	1554	A
1	2	1555	U
1	2	1557	A
1	2	1558	U
1	2	1559	U
1	2	1564	U
1	2	1566	C
1	2	1571	A
1	2	1572	G
1	2	1573	G
1	2	1574	A
1	2	1575	A
1	2	1577	U
1	2	1578	C
1	2	1579	C
1	2	1580	U
1	2	1581	A
1	2	1582	G
1	2	1583	U
1	2	1584	A
1	2	1588	G
1	2	1590	A
1	2	1593	U
1	2	1594	C
1	2	1595	A
1	2	1597	C
1	2	1599	G
1	2	1603	G
1	2	1604	C

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Mol	Chain	Res	Type
1	2	1608	G
1	2	1611	U
1	2	1612	A
1	2	1613	C
1	2	1614	G
1	2	1616	C
1	2	1617	C
1	2	1628	U
1	2	1629	A
1	2	1631	A
1	2	1632	C
1	2	1633	A
1	2	1634	C
1	2	1635	C
1	2	1637	C
1	2	1642	C
1	2	1647	G
1	2	1648	U
1	2	1652	G
1	2	1655	U
1	2	1656	G
1	2	1660	G
1	2	1662	C
1	2	1676	A
1	2	1678	G
1	2	1679	A
1	2	1680	U
1	2	1682	U
1	2	1685	U
1	2	1686	U
1	2	1687	A
1	2	1688	G
1	2	1692	A
1	2	1693	G
1	2	1694	G
1	2	1695	G
1	2	1696	G
1	2	1697	G
1	2	1698	C
1	2	1699	A
1	2	1700	A
1	2	1701	C

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Mol	Chain	Res	Type
1	2	1702	U
1	2	1703	C
1	2	1705	A
1	2	1706	U
1	2	1708	U
1	2	1709	C
1	2	1710	A
1	2	1711	G
1	2	1712	A
1	2	1715	G
1	2	1725	G
1	2	1728	A
1	2	1730	A
1	2	1742	A
1	2	1745	G
1	2	1748	A
1	2	1753	A
1	2	1755	G
1	2	1758	G
1	2	1760	A
1	2	1763	A
1	2	1766	G
1	2	1767	U
1	2	1768	U
1	2	1781	C
1	2	1786	G
1	2	1787	G
1	2	1789	A
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1793	U
1	2	1794	C
1	2	1795	A
1	2	1796	U
1	2	1797	U
1	2	1798	A
20	3	4	U
20	3	6	U
20	3	7	C
20	3	8	U
20	3	10	U

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Mol	Chain	Res	Type
20	3	11	C
20	3	12	U
20	3	16	C
28	1	2	G
28	1	3	C
28	1	5	C
28	1	8	U
28	1	10	G
28	1	14	A
28	1	15	G
28	1	16	U
28	1	19	G
28	1	20	A
28	1	21	A
28	1	22	G
28	1	23	C
28	1	24	G
28	1	28	A
28	1	34	C
28	1	36	U
28	1	41	C
28	1	43	G
28	1	44	A
28	1	46	G
28	1	47	U
28	1	48	C
28	1	49	C
28	1	53	G
28	1	59	A
28	1	60	A
28	1	61	C
28	1	71	C
28	1	74	C
28	1	75	C
28	1	76	A

All (77) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	66	U
1	2	68	A
1	2	72	A

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Mol	Chain	Res	Type
1	2	74	U
1	2	130	C
1	2	131	C
1	2	157	U
1	2	177	U
1	2	190	C
1	2	216	A
1	2	217	A
1	2	239	C
1	2	258	U
1	2	275	C
1	2	277	U
1	2	279	U
1	2	321	G
1	2	412	U
1	2	439	U
1	2	497	G
1	2	538	G
1	2	542	C
1	2	563	G
1	2	564	C
1	2	593	A
1	2	649	U
1	2	670	G
1	2	673	C
1	2	685	A
1	2	693	U
1	2	695	U
1	2	700	C
1	2	721	U
1	2	736	C
1	2	793	U
1	2	810	A
1	2	812	U
1	2	826	C
1	2	828	A
1	2	860	U
1	2	896	C
1	2	907	U
1	2	938	A
1	2	1092	A
1	2	1107	G

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Mol	Chain	Res	Type
1	2	1110	G
1	2	1132	A
1	2	1157	C
1	2	1194	C
1	2	1195	A
1	2	1198	G
1	2	1199	G
1	2	1206	C
1	2	1226	A
1	2	1283	C
1	2	1343	A
1	2	1389	A
1	2	1411	U
1	2	1430	U
1	2	1455	C
1	2	1465	C
1	2	1491	A
1	2	1534	G
1	2	1571	A
1	2	1599	G
1	2	1613	C
1	2	1655	U
1	2	1678	G
1	2	1765	G
20	3	10	U
20	3	11	C
28	1	7	G
28	1	20	A
28	1	47	U
28	1	58	A
28	1	59	A
28	1	74	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 87 ligands modelled in this entry, 85 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	$\#\|Z\| > 2$
50	GCP	k	602	-	27,34,34	2.16	9 (33%)	34,54,54	1.95	8 (23%)
51	MET	k	603	-	6,7,8	0.46	0	2,7,9	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	GCP	k	602	-	-	3/15/38/38	0/3/3/3
51	MET	k	603	-	-	3/5/6/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	k	602	GCP	PG-O1G	5.41	1.61	1.50
50	k	602	GCP	C5-C6	4.77	1.49	1.41
50	k	602	GCP	PB-O1B	4.16	1.61	1.51
50	k	602	GCP	PB-O2B	-3.39	1.48	1.56
50	k	602	GCP	PB-O3A	3.36	1.62	1.58
50	k	602	GCP	PG-O2G	2.90	1.61	1.54
50	k	602	GCP	PG-O3G	-2.79	1.48	1.54
50	k	602	GCP	C5-C4	2.75	1.48	1.40
50	k	602	GCP	O4'-C1'	2.02	1.43	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	k	602	GCP	C2-N3-C4	5.53	121.67	115.36
50	k	602	GCP	C2-N1-C6	3.97	122.24	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	k	602	GCP	C4-C5-C6	-3.90	117.07	120.80
50	k	602	GCP	C5-C6-N1	-3.64	118.46	123.43
50	k	602	GCP	N3-C2-N1	-3.58	122.45	127.22
50	k	602	GCP	C3'-C2'-C1'	3.24	105.85	100.98
50	k	602	GCP	PB-O3A-PA	-2.92	123.30	132.56
50	k	602	GCP	C4-C5-N7	-2.67	106.62	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

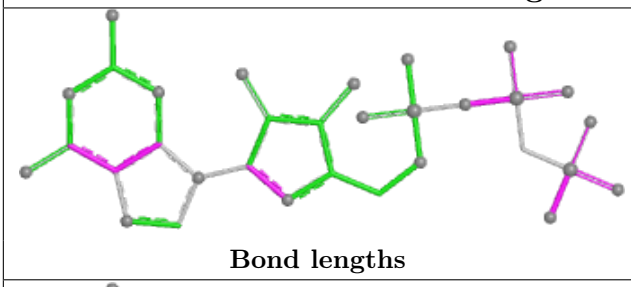
Mol	Chain	Res	Type	Atoms
50	k	602	GCP	O4'-C4'-C5'-O5'
51	k	603	MET	O-C-CA-CB
51	k	603	MET	CA-CB-CG-SD
51	k	603	MET	N-CA-CB-CG
50	k	602	GCP	C4'-C5'-O5'-PA
50	k	602	GCP	PG-C3B-PB-O1B

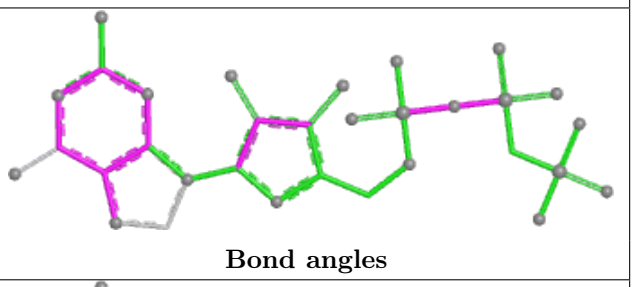
There are no ring outliers.

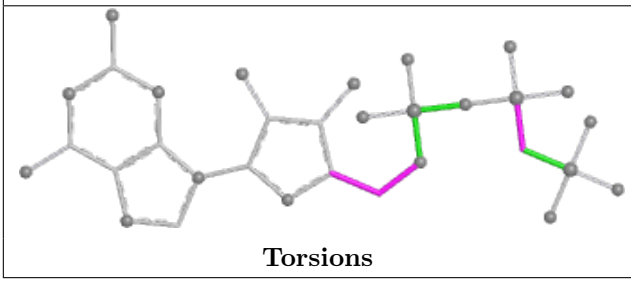
No monomer is involved in short contacts.

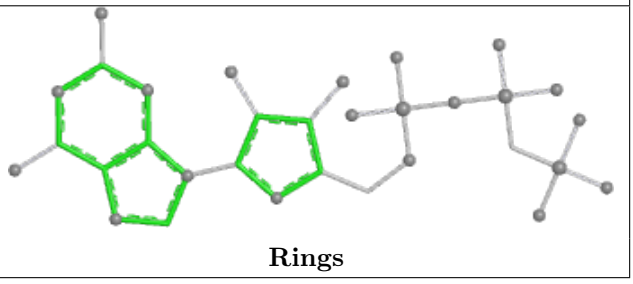
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand GCP k 602


Bond lengths


Bond angles


Torsions


Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	o	2
28	1	1
22	m	1
25	k	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	230.47
1	1	16:U	O3'	18:G	P	5.21
1	m	75:GLY	C	76:GLU	N	4.38
1	k	372:PRO	C	373:ILE	N	3.76
1	o	5:PRO	C	6:PHE	N	3.57

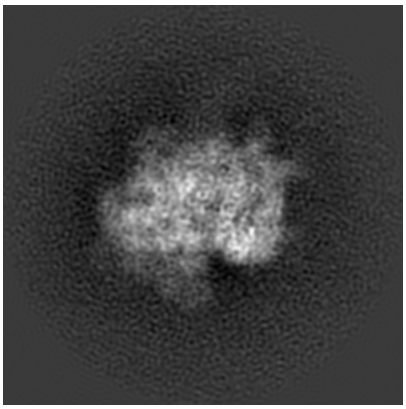
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0058. These allow visual inspection of the internal detail of the map and identification of artifacts.

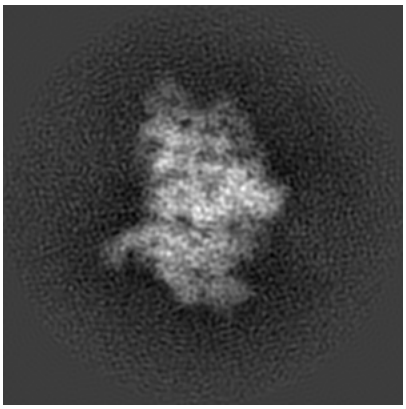
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

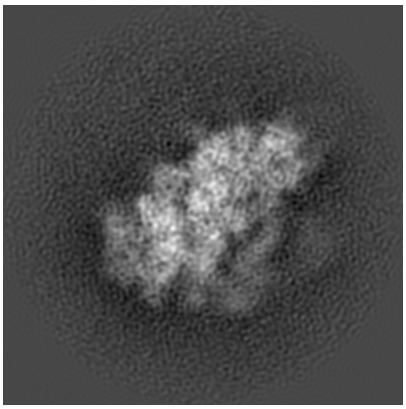
6.1.1 Primary map



X

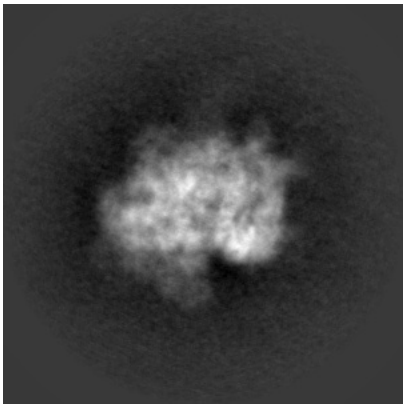


Y

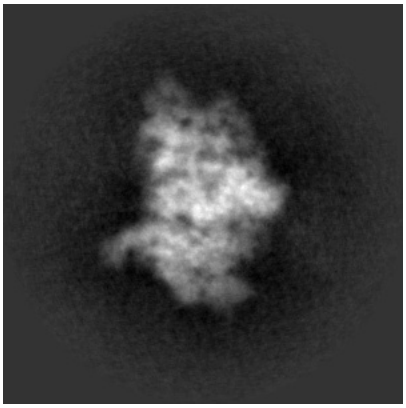


Z

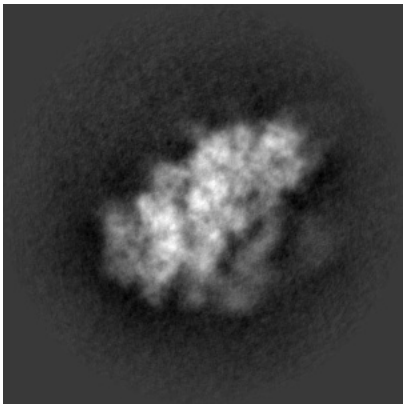
6.1.2 Raw map



X



Y

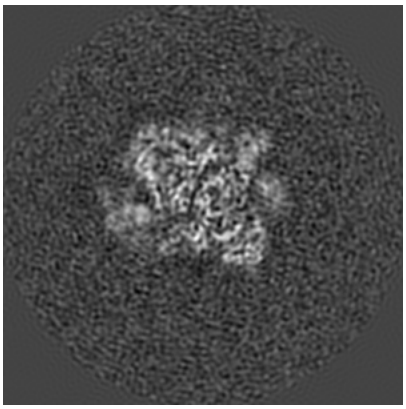


Z

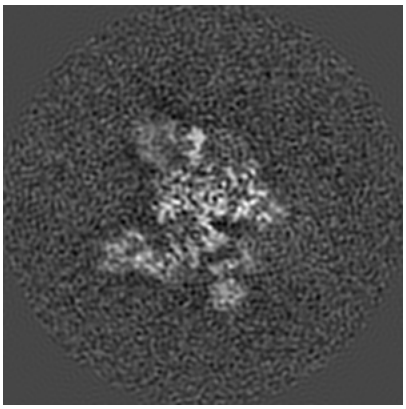
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

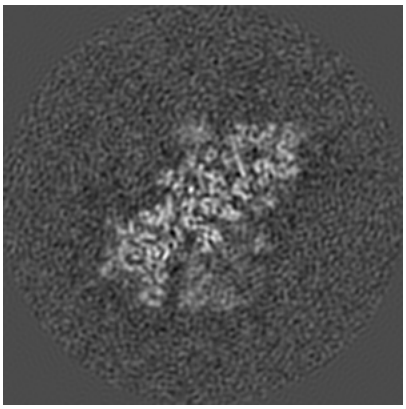
6.2.1 Primary map



X Index: 150

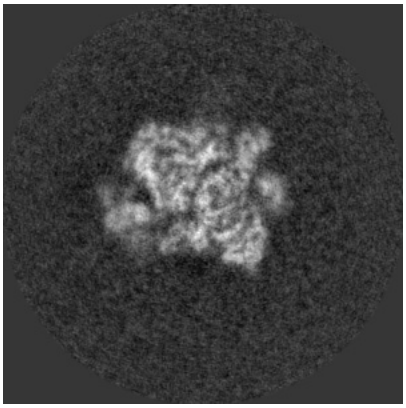


Y Index: 150

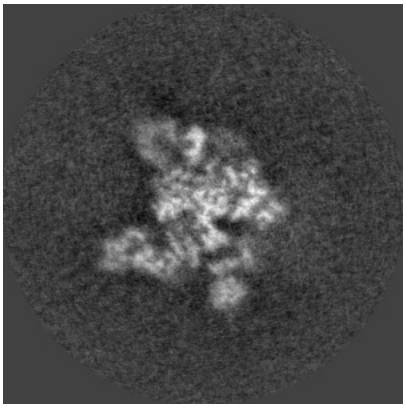


Z Index: 150

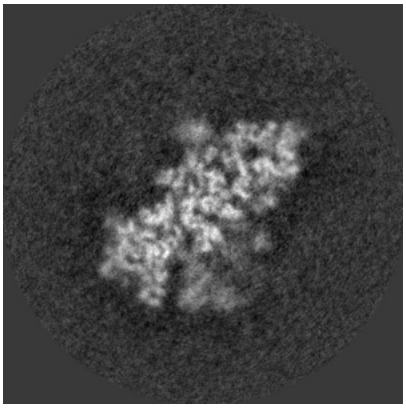
6.2.2 Raw map



X Index: 150



Y Index: 150

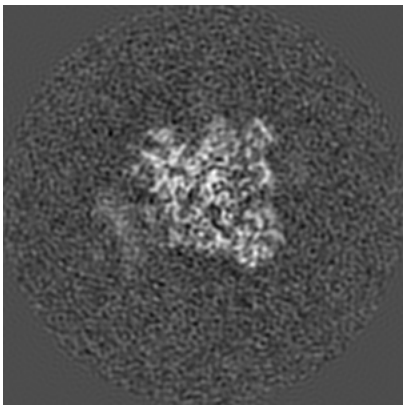


Z Index: 150

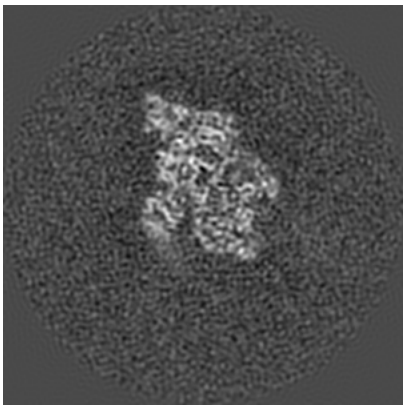
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

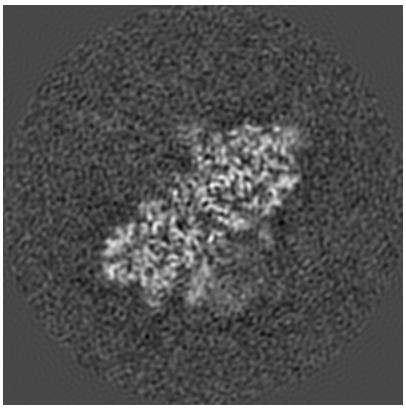
6.3.1 Primary map



X Index: 160

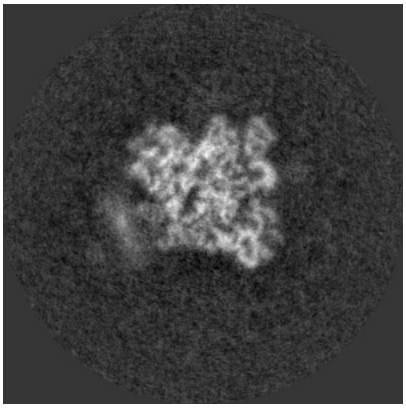


Y Index: 172

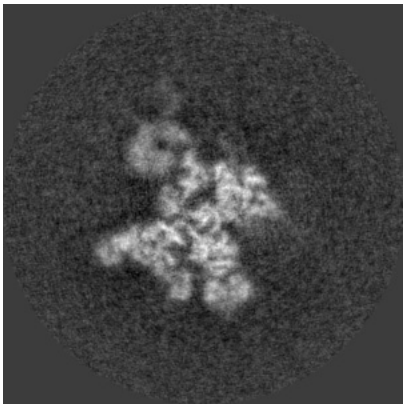


Z Index: 143

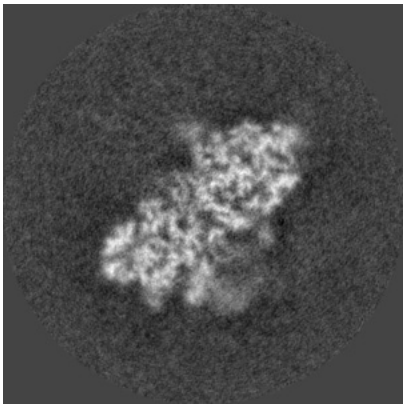
6.3.2 Raw map



X Index: 158



Y Index: 139

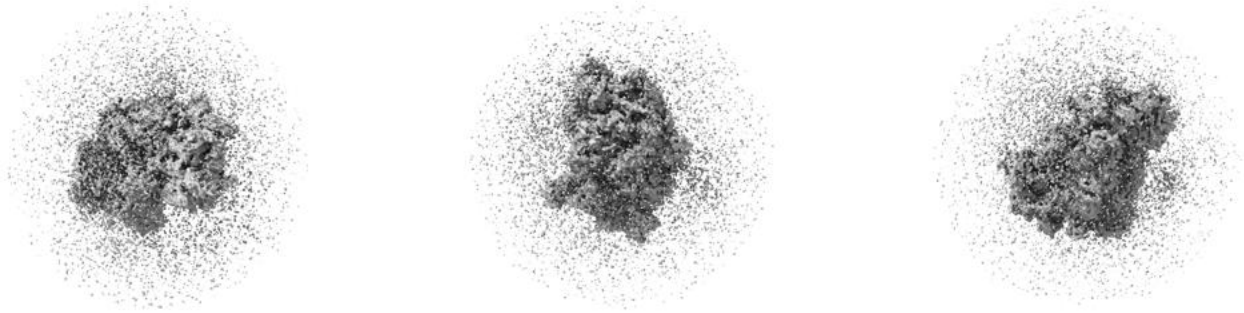


Z Index: 143

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

6.4 Orthogonal surface views (i)

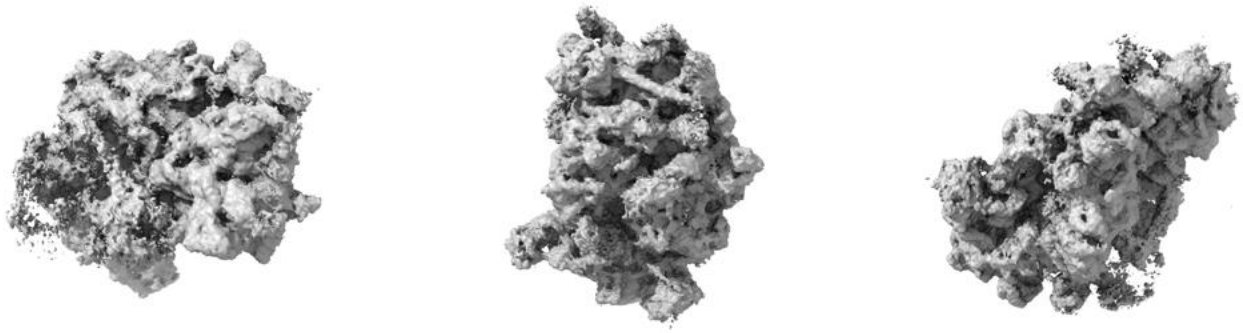
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. 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



X Y Z

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.

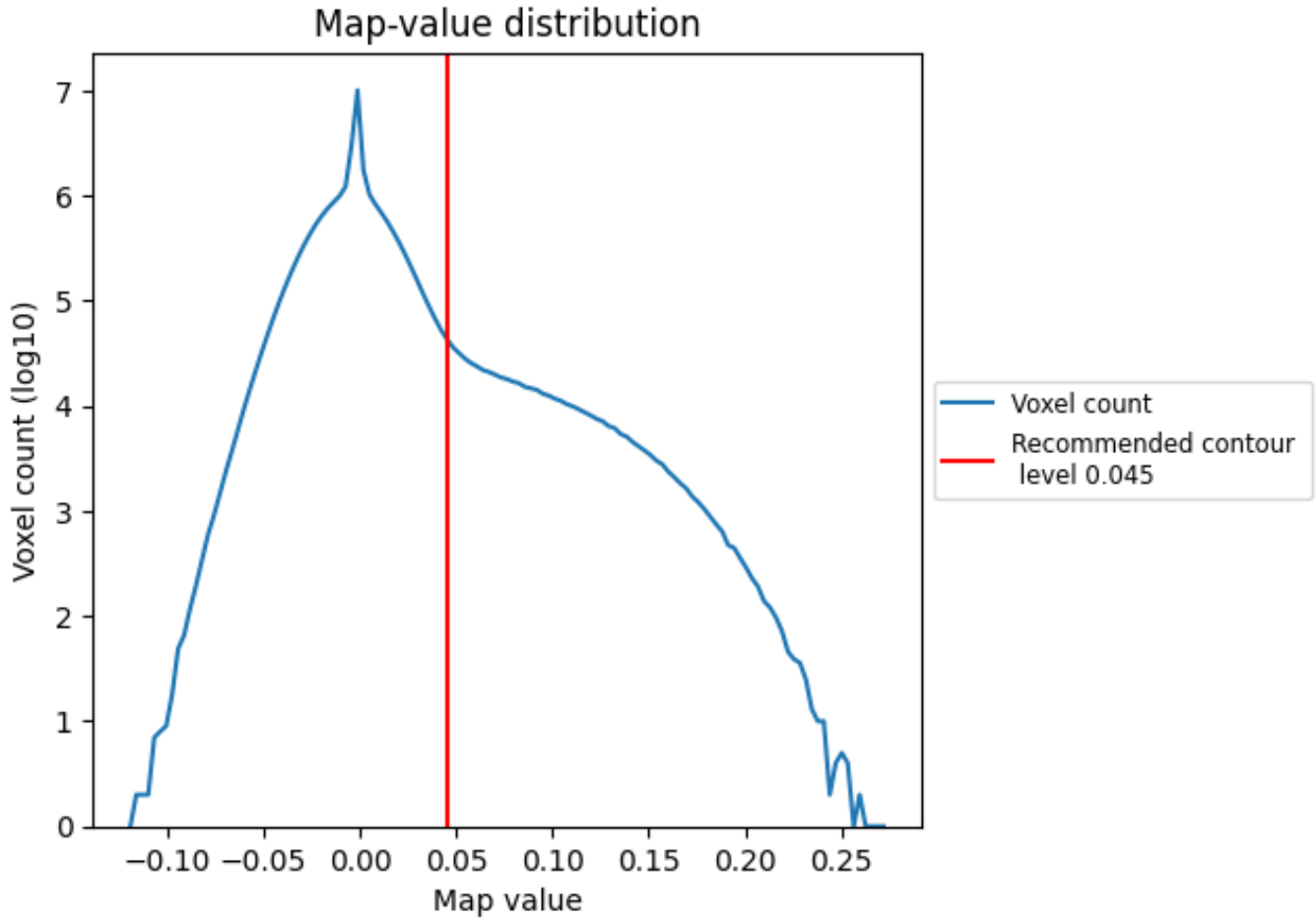
6.5 Mask visualisation (i)

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

7 Map analysis

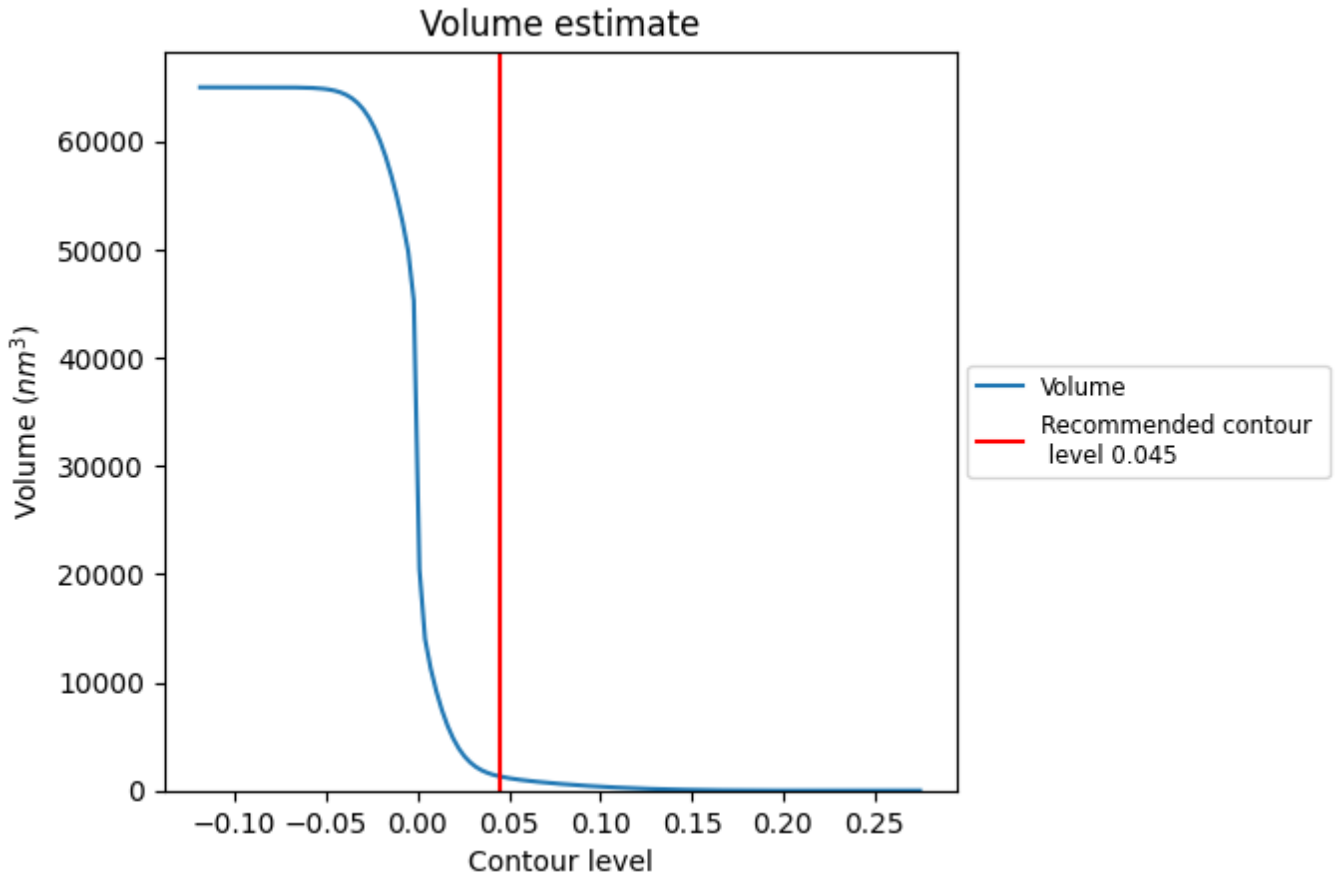
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

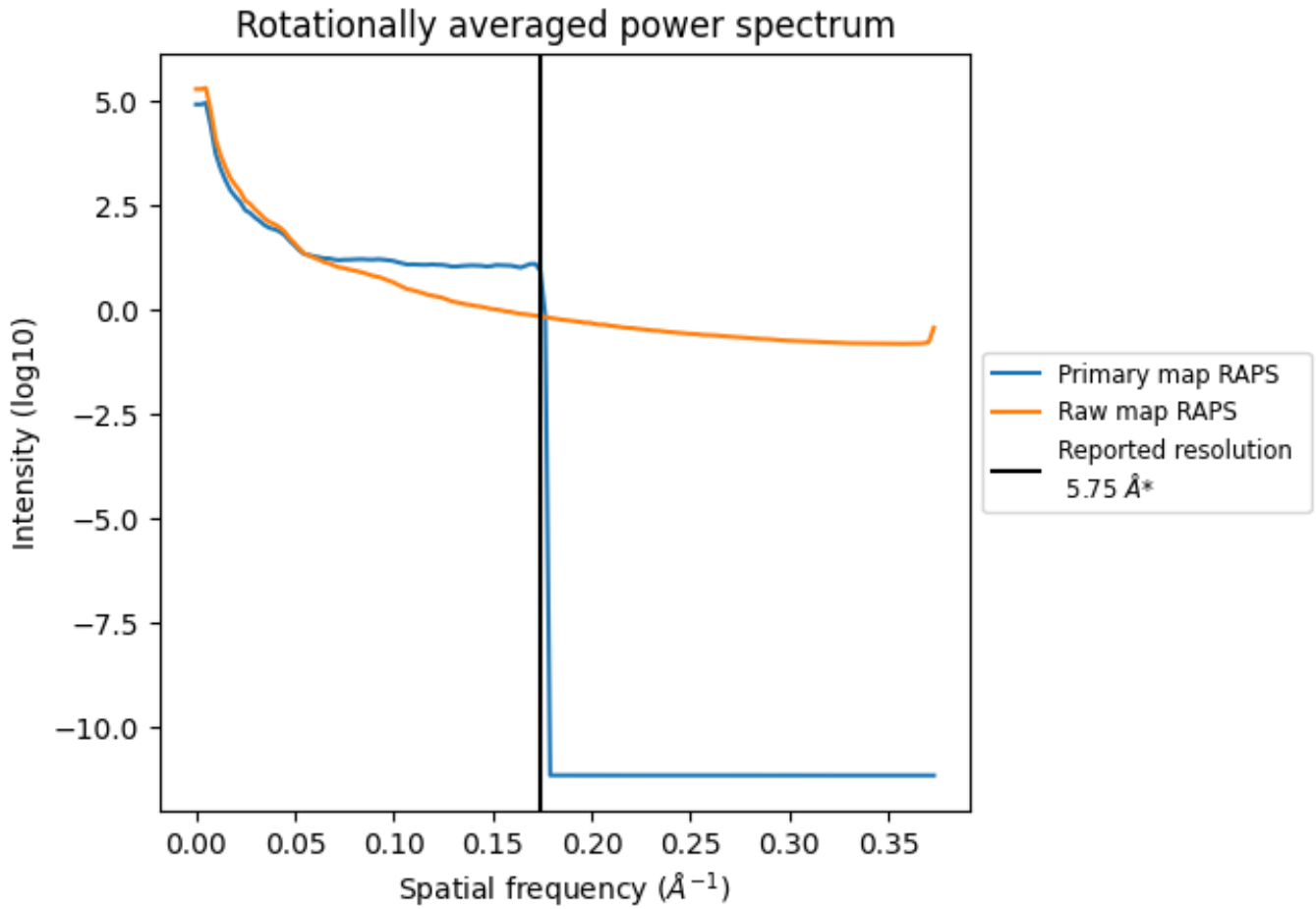
7.2 Volume estimate



The volume at the recommended contour level is 1308 nm^3; this corresponds to an approximate mass of 1181 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)

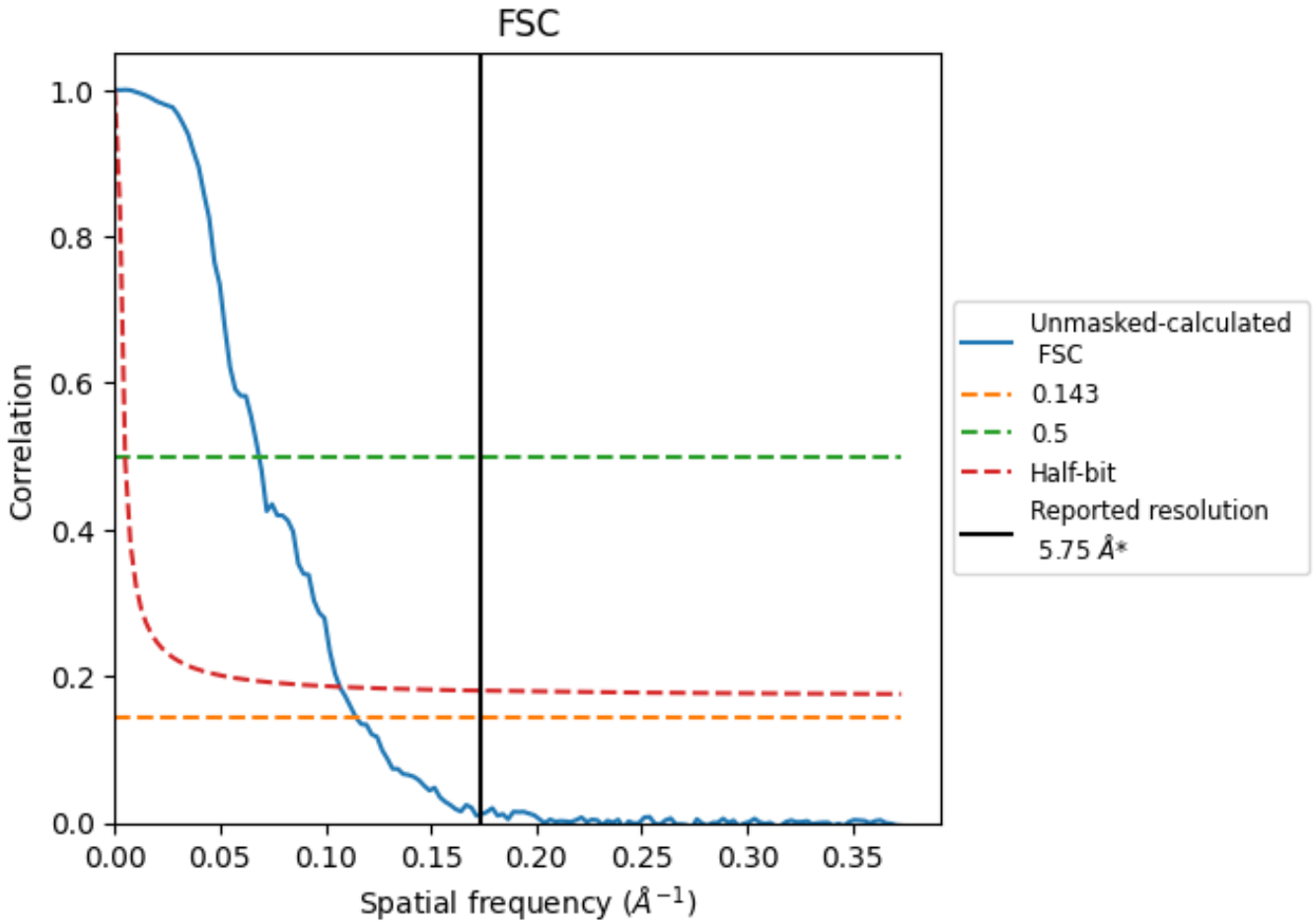


*Reported resolution corresponds to spatial frequency of 0.174 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.174 Å^{-1}

8.2 Resolution estimates (i)

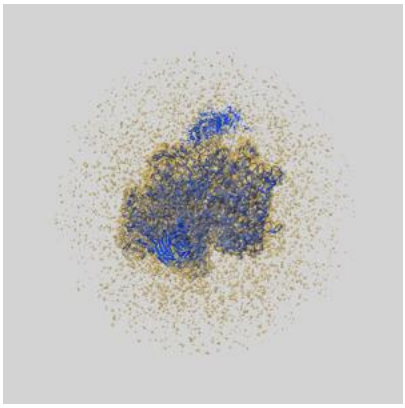
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.73	14.62	9.36

*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 8.73 differs from the reported value 5.75 by more than 10 %

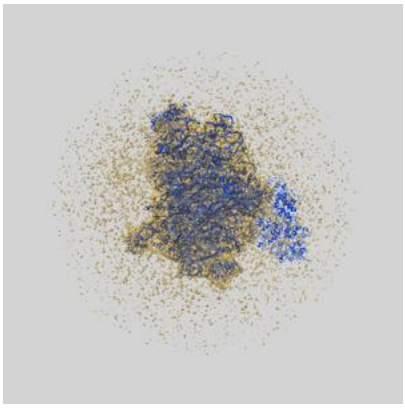
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0058 and PDB model 6GSN. Per-residue inclusion information can be found in section 3 on page 14.

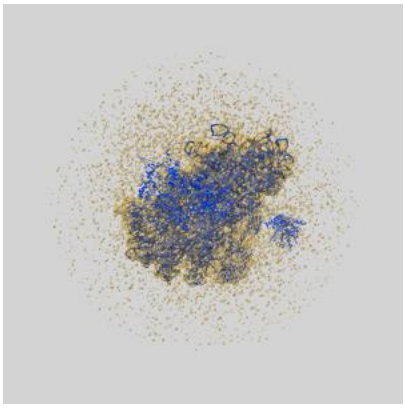
9.1 Map-model overlay



X



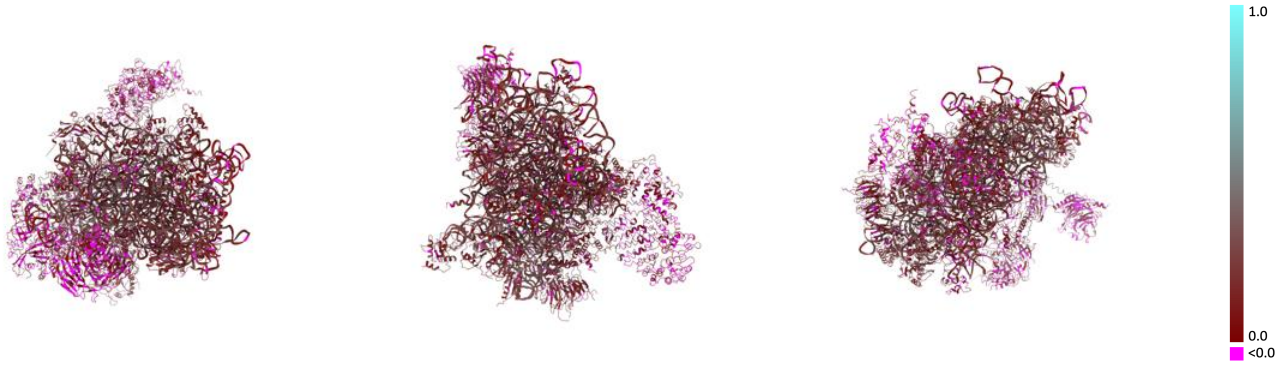
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

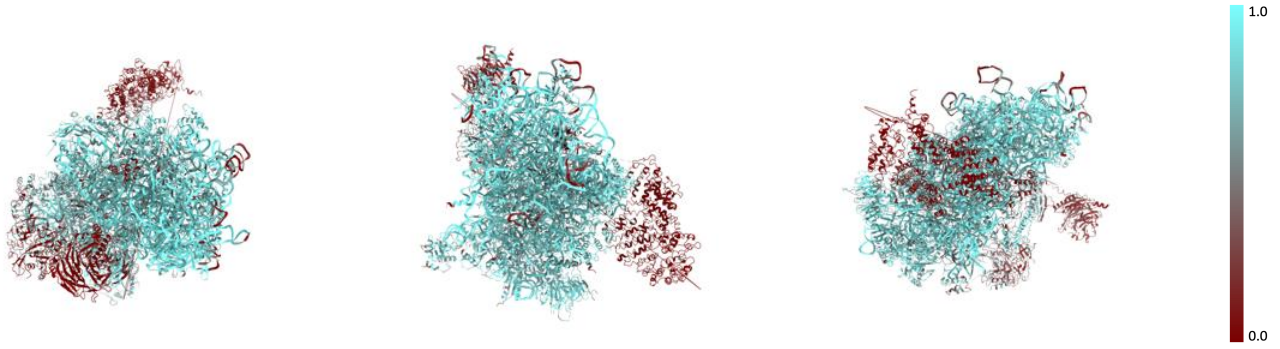
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

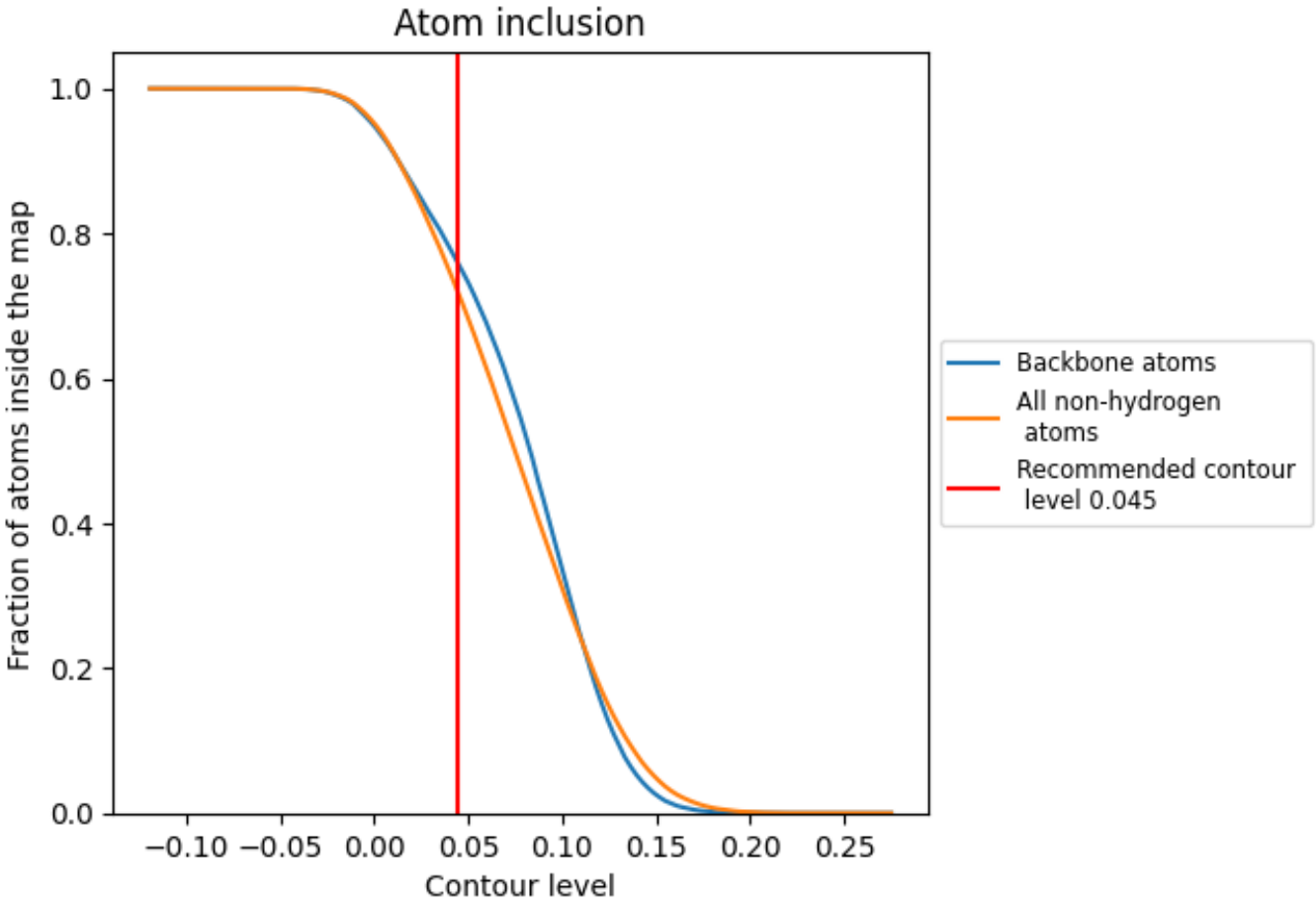
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7167	0.1850
1	0.8133	0.1580
2	0.9261	0.2360
3	0.7352	0.1800
A	0.8204	0.2010
B	0.8444	0.1950
C	0.7728	0.2070
D	0.7760	0.2120
E	0.7917	0.1980
F	0.7869	0.1950
G	0.8346	0.1770
H	0.8226	0.1830
I	0.8020	0.1920
J	0.7917	0.2000
K	0.8254	0.1880
L	0.7671	0.2080
M	0.6962	0.1600
N	0.8170	0.1930
O	0.8551	0.2030
P	0.8396	0.1940
Q	0.8148	0.1760
R	0.7822	0.1940
S	0.7944	0.1800
T	0.8269	0.1810
U	0.7506	0.1810
V	0.8426	0.2120
W	0.7920	0.1980
X	0.7262	0.2060
Y	0.8327	0.2070
Z	0.7348	0.1580
a	0.8327	0.2220
b	0.8405	0.2140
c	0.7944	0.2100
d	0.7845	0.1930
e	0.6927	0.2070

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Chain	Atom inclusion	Q-score
f	0.7896	0.1870
g	0.8280	0.1720
h	0.5399	0.1350
i	0.7158	0.2200
j	0.4784	0.1290
k	0.2493	0.0930
l	0.3017	0.1060
m	0.4460	0.1650
o	0.0946	0.0710
p	0.5484	0.1290
q	0.0459	0.0870
r	0.0211	0.0550
s	0.0234	0.0020