Full wwPDB EM Validation Report

Dec 1, 2021 – 04:48 pm GMT

PDB ID	:	7OHW
EMDB ID	:	EMD-12911
Title	:	Nog1-TAP associated immature ribosomal particles from S. cerevisiae after rpL25 expression shut down, population B
Authors	:	Milkereit, P.; Poell, G.
Deposited on	:	2021-05-11
Resolution	:	3.50 Å(reported)
Based on initial model	:	6EM1

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

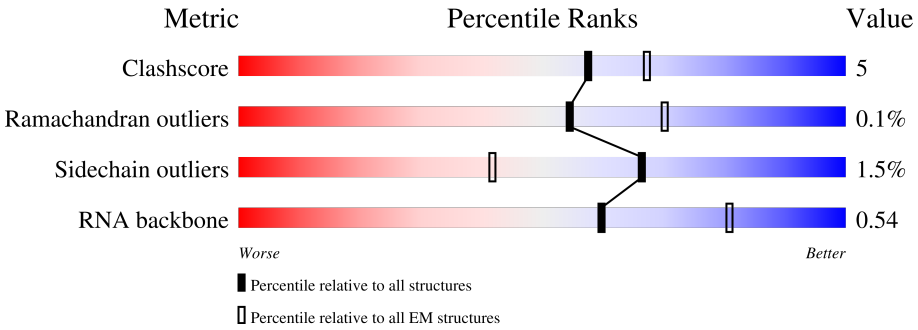
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1	3396	29% 15% 52%
2	2	158	58% 34% 6%
3	3	306	50% 7% 43%
4	4	278	67% 11% 22%
5	5	463	78% 6% 17%
6	6	232	12% 9% 6% 72%
7	A	291	9% 43% 6% 51%

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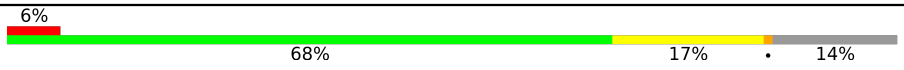
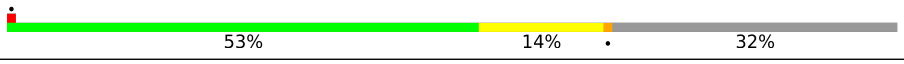
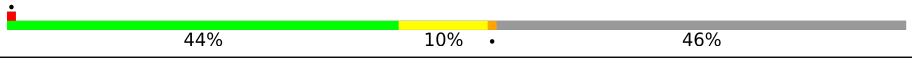
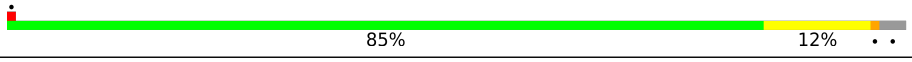
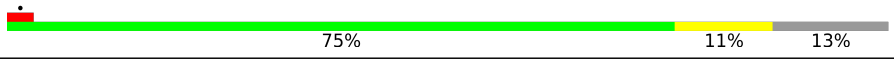
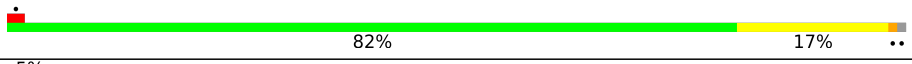
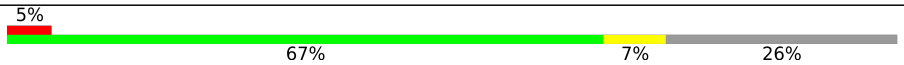
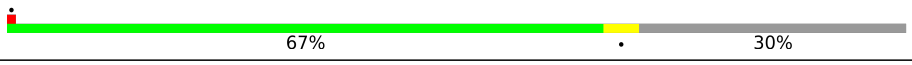
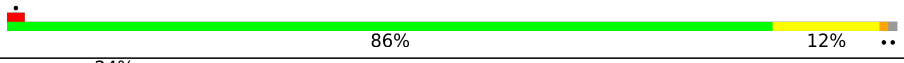
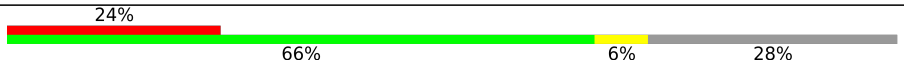
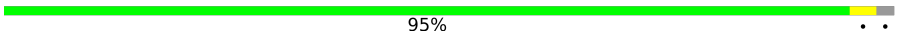
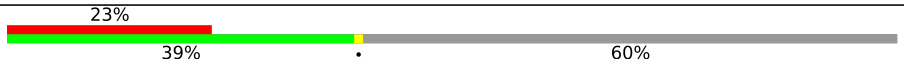
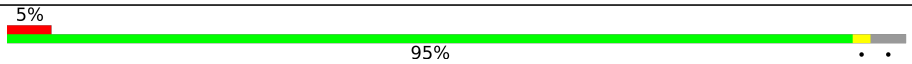
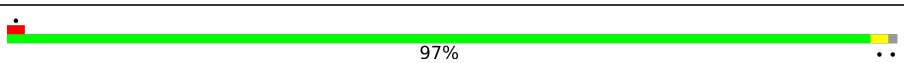
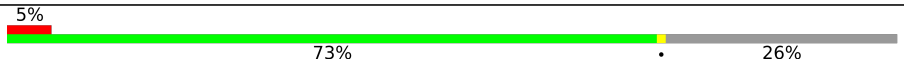
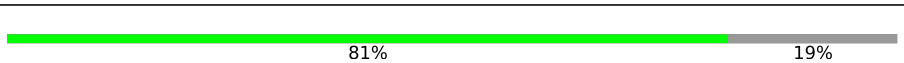
Mol	Chain	Length	Quality of chain
8	B	387	
9	C	362	
10	D	505	
11	E	176	
12	F	244	
13	G	256	
14	H	191	
15	J	427	
16	K	376	
17	L	199	
18	M	138	
19	N	204	
20	O	199	
21	P	184	
22	Q	186	
23	S	172	
24	V	137	
25	W	236	
26	Y	127	
27	b	647	
28	e	130	
29	f	107	
30	h	120	
31	i	100	
32	j	88	

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Mol	Chain	Length	Quality of chain
33	m	807	19% 81%
34	n	605	55% 45%
35	o	220	60% 40%
36	r	261	11% 21% 79%
37	t	322	73% 25%
38	v	231	56% 44%
39	x	295	89% 9%
40	y	245	22% 89% 11%

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 171568 atoms, of which 76920 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 25S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	1	1639	52739	15672	17632	6362	11434	1639	0	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	2	149	4767	1416	1601	558	1043	149	0	0

- Molecule 3 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	3	173	2908	901	1474	274	250	9	0	0

- Molecule 4 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	4	217	3744	1208	1891	319	323	3	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein NSA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	5	385	6170	1957	3115	514	573	11	0	0

- Molecule 6 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	6	65	2061	614	691	228	463	65	0	0

- Molecule 7 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	144	Total	C	H	N	O	S	0	0
			2411	775	1208	217	209	2		

- Molecule 8 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	333	Total	C	H	N	O	S	0	0
			5374	1680	2728	490	470	6		

- Molecule 9 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	343	Total	C	H	N	O	S	0	0
			5336	1643	2725	499	466	3		

- Molecule 10 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	D	437	Total	C	H	N	O	S	0	0
			7106	2247	3620	600	627	12		

- Molecule 11 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	151	Total	C	H	N	O	S	0	0
			2497	780	1292	215	209	1		

- Molecule 12 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	F	241	Total	C	H	N	O	S	0	0
			3969	1246	2033	351	338	1		

- Molecule 13 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	G	159	Total	C	H	N	O	S	0	0
			2520	794	1289	209	226	2		

- Molecule 14 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	H	174	Total	C	H	N	O	S	0	0
			2862	890	1468	254	247	3		

- Molecule 15 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	J	63	Total	C	H	N	O	S	0	0
			1035	329	506	94	105	1		

- Molecule 16 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	K	257	Total	C	H	N	O	S	0	0
			4230	1337	2157	341	392	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	108	Total	C	H	N	O	0	0
			1782	541	918	180	143		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	M	134	Total	C	H	N	O	S	0	0
			2179	668	1138	197	174	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	N	177	Total	C	H	N	O	S	0	0
			3079	948	1566	320	244	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	O	197	Total	C	H	N	O	S	0	0
			3215	1003	1660	289	262	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	137	Total	C	H	N	O	0	0
			2139	666	1077	198	198		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Q	131	Total	C	H	N	O	S	0	0
			2101	645	1092	190	173	1		

- Molecule 23 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	S	170	Total	C	H	N	O	S	0	0
			2904	922	1472	265	242	3		

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	V	98	Total	C	H	N	O	S	0	0
			1498	462	760	136	133	7		

- Molecule 25 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	W	185	Total	C	H	N	O	S	0	0
			3049	963	1527	263	292	4		

- Molecule 26 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	125	Total	C	H	N	O	0	0
			2060	620	1076	191	173		

- Molecule 27 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	b	259	Total	C	H	N	O	S	0	0
			4221	1344	2116	355	395	11		

- Molecule 28 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	e	125	Total	C	H	N	O	S	0	0
			2090	641	1081	203	164	1		

- Molecule 29 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	f	106	Total	C	H	N	O	S	0	0
			1731	540	881	165	144	1		

- Molecule 30 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	h	119	Total	C	H	N	O	S	0	0
			2048	615	1079	186	167	1		

- Molecule 31 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	i	74	Total	C	H	N	O	S	0	0
			1236	367	642	125	101	1		

- Molecule 32 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	j	71	Total	C	H	N	O	S	0	0
			1137	344	571	123	94	5		

- Molecule 33 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	m	156	Total	C	H	N	O	S	0	0
			2643	847	1318	233	241	4		

- Molecule 34 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	n	334	Total	C	H	N	O	S	0	0
			5516	1787	2782	457	482	8		

- Molecule 35 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	o	133	Total	C	H	N	O	S	0	0
			2267	716	1160	198	189	4		

- Molecule 36 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	r	54	Total	C	H	N	O	0	0
			962	294	485	102	81		

- Molecule 37 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	t	240	Total	C	H	N	O	S	0	0
			3923	1217	2018	340	345	3		

- Molecule 38 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	v	130	Total	C	H	N	O	S	0	0
			2223	678	1136	211	195	3		

- Molecule 39 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	x	267	Total	C	H	N	O	S	0	0
			4573	1444	2305	413	407	4		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	y	217	Total	C	H	N	O	S	0	0
			3262	1016	1630	280	329	7		

- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

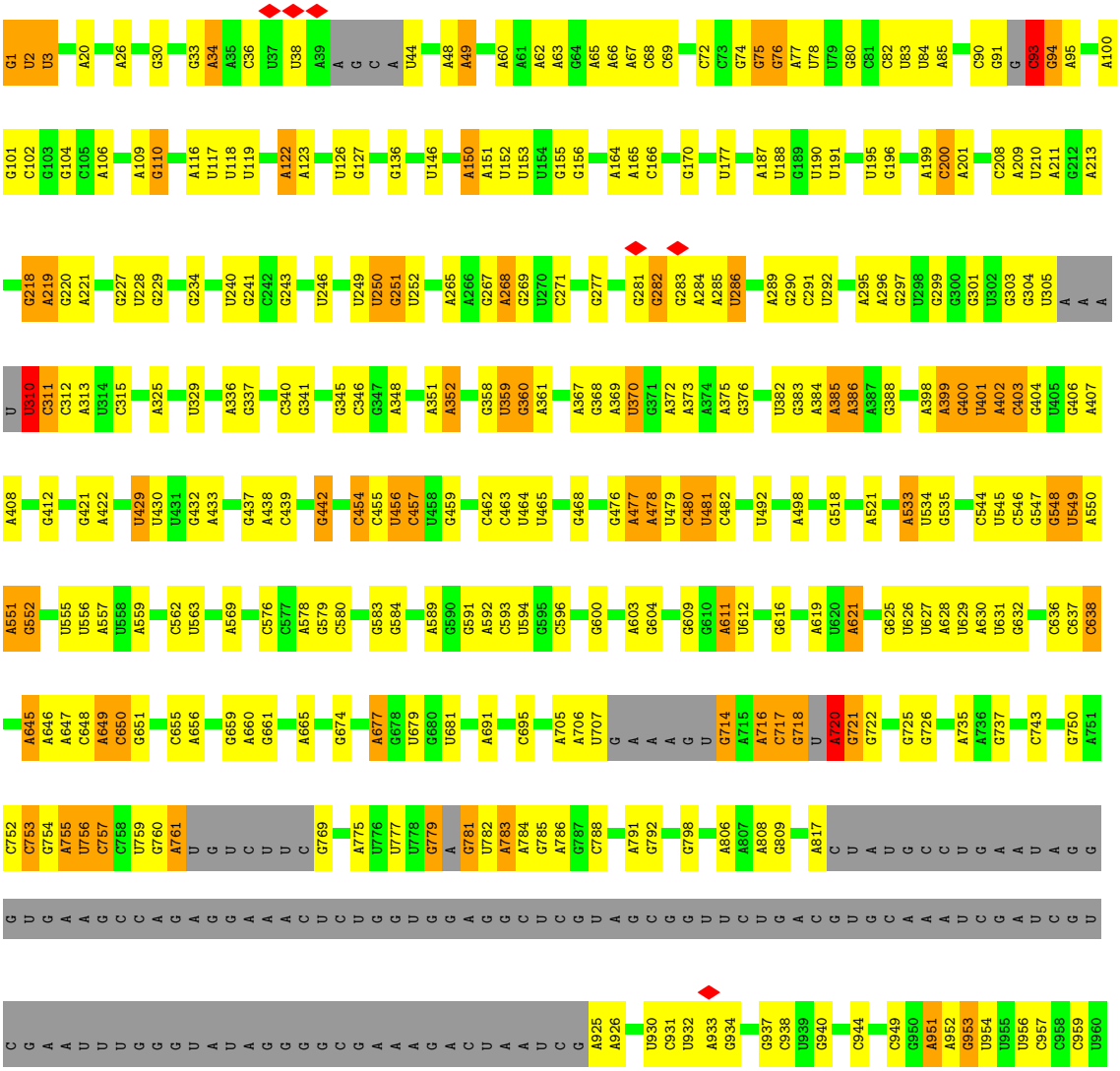
Mol	Chain	Residues	Atoms		AltConf
41	j	1	Total	Zn	0
			1	1	

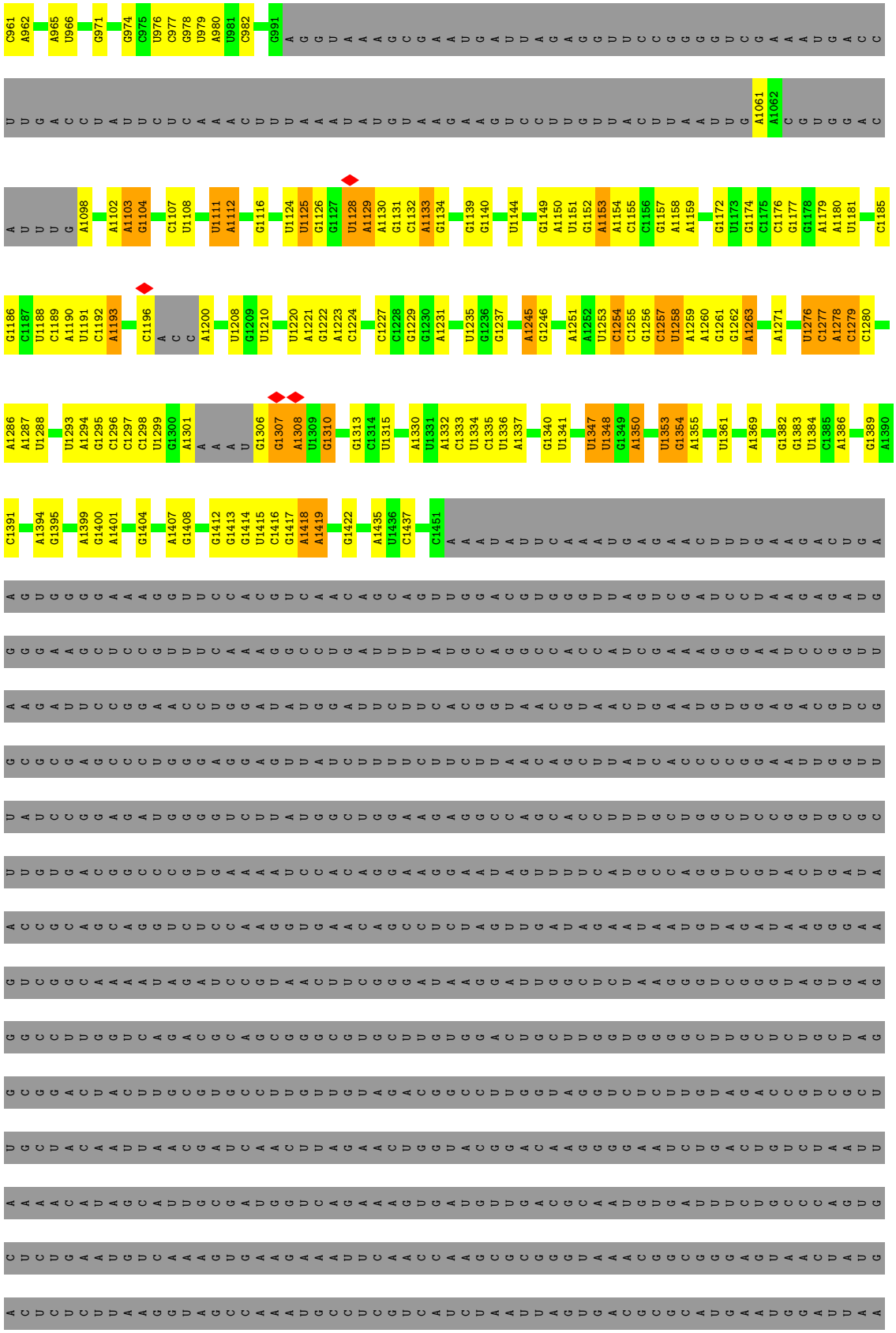
3 Residue-property plots (i)

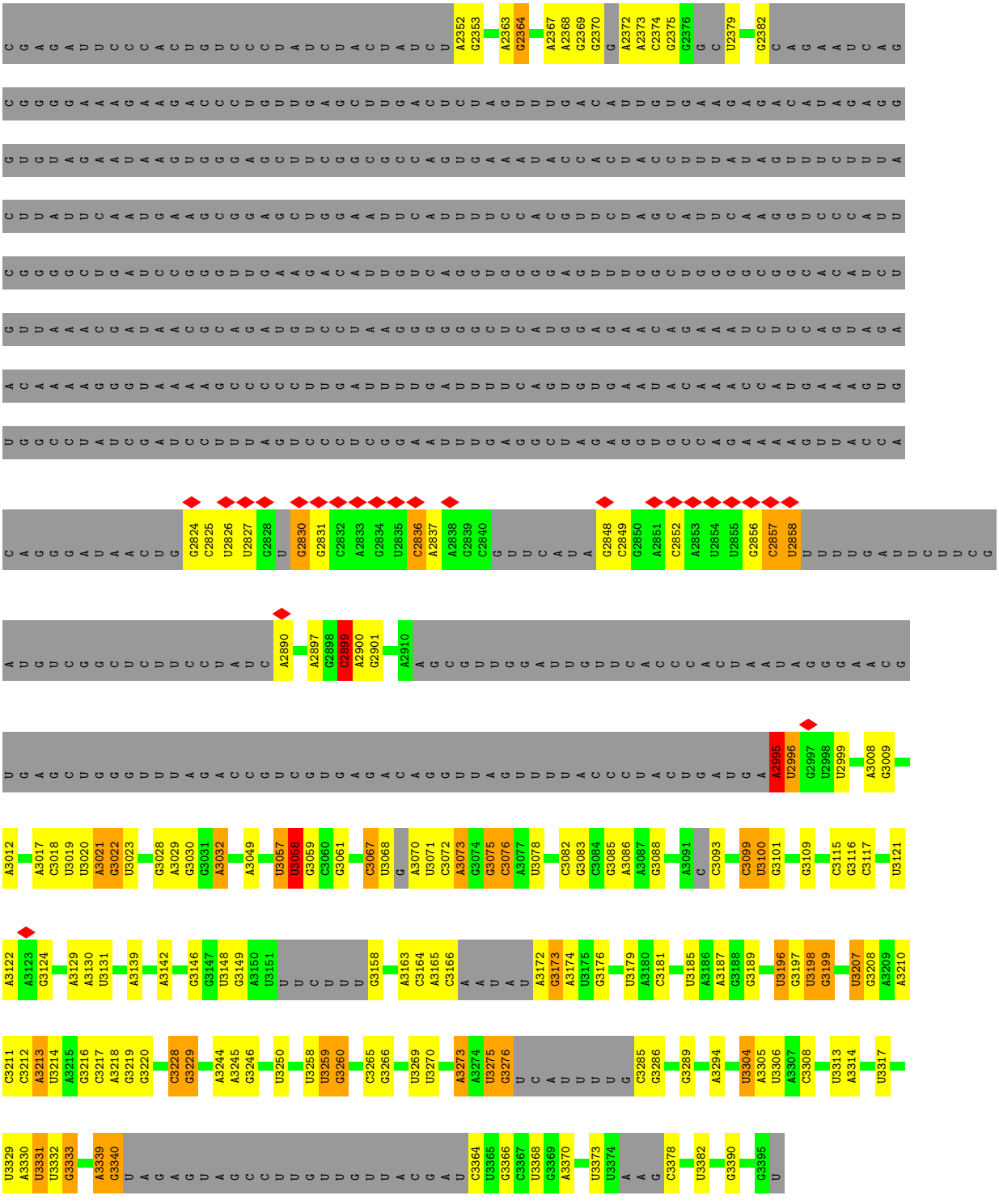
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 25S rRNA

Chain 1:

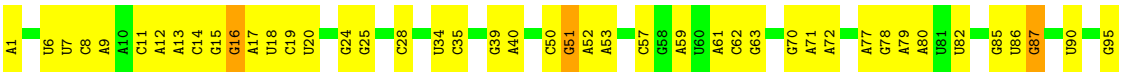


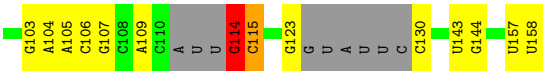




• Molecule 2: 5.8S rRNA

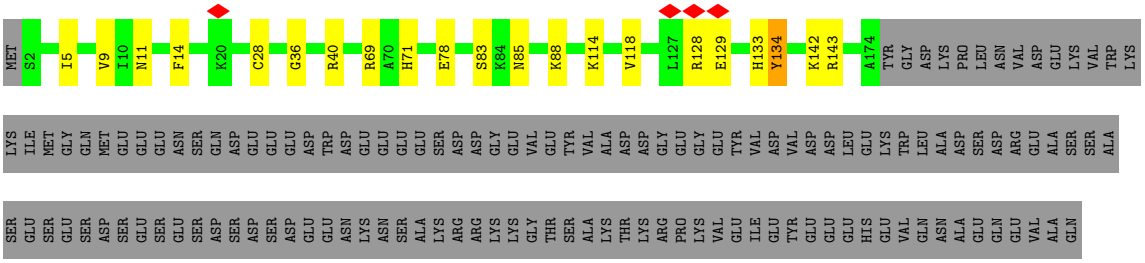
Chain 2:





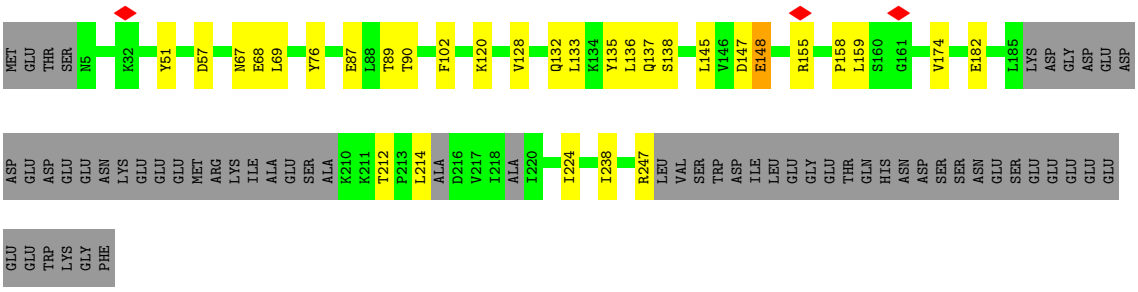
• Molecule 3: Protein MAK16

Chain 3:



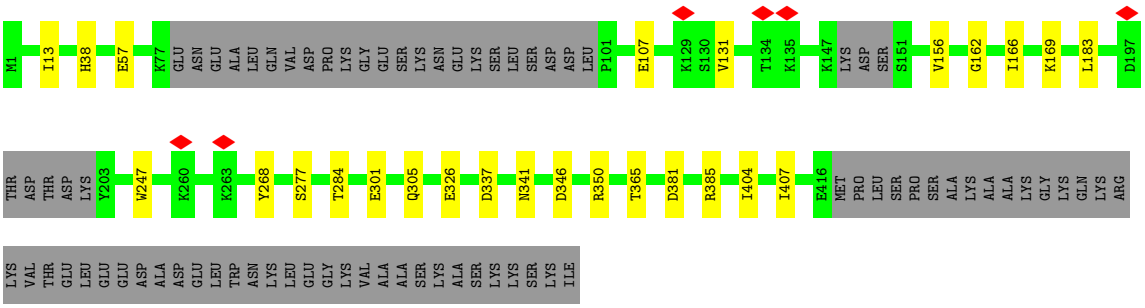
• Molecule 4: Ribosomal RNA-processing protein 1

Chain 4:



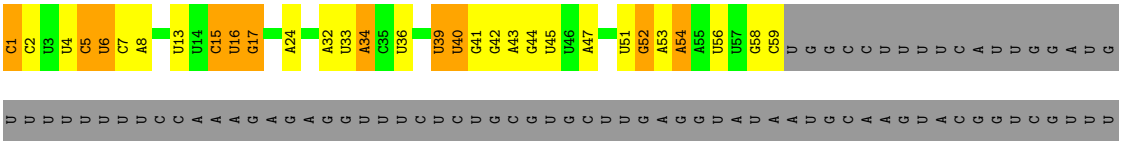
• Molecule 5: Ribosome biogenesis protein NSA1

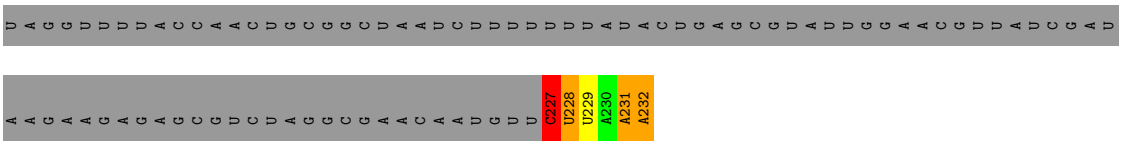
Chain 5:



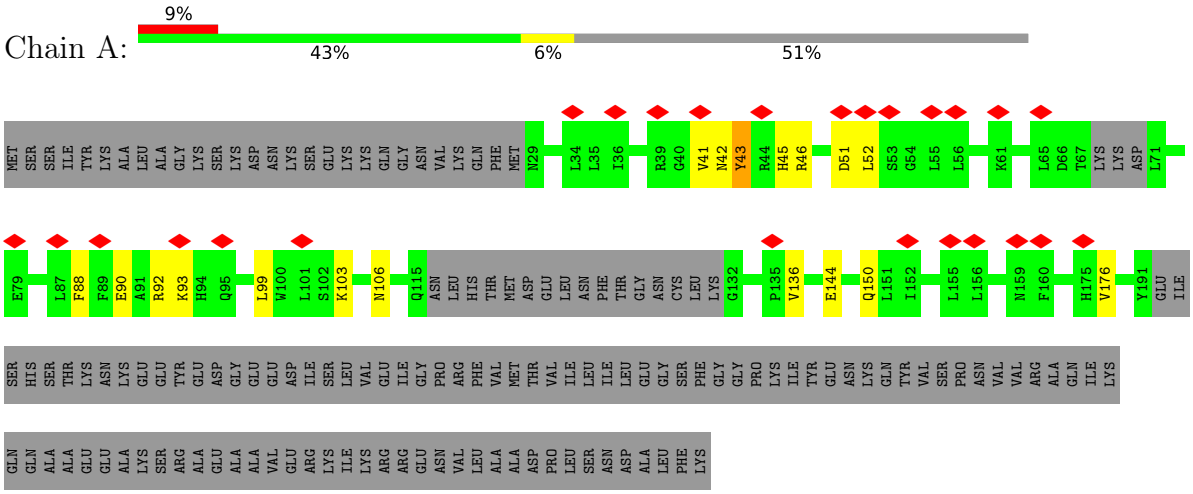
• Molecule 6: ITS2

Chain 6:

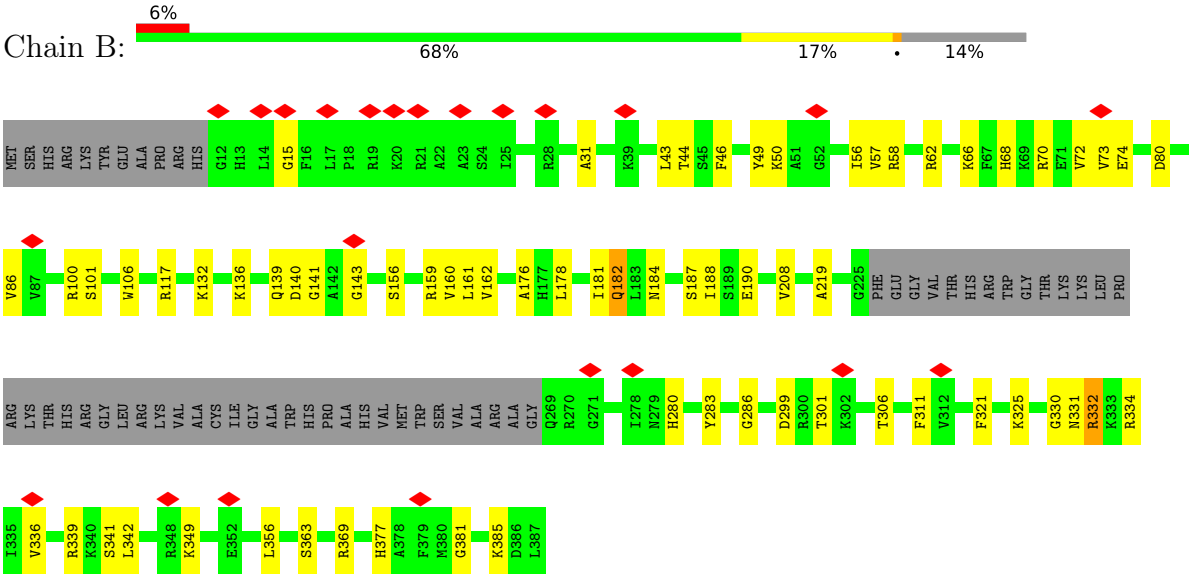




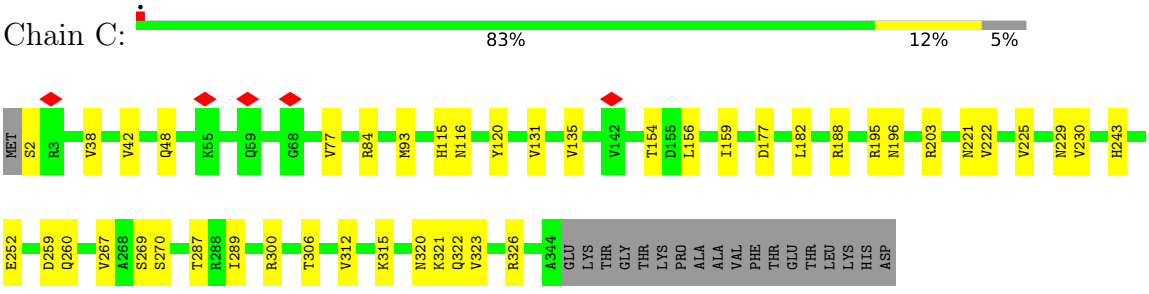
• Molecule 7: Ribosome biogenesis protein BRX1



• Molecule 8: 60S ribosomal protein L3

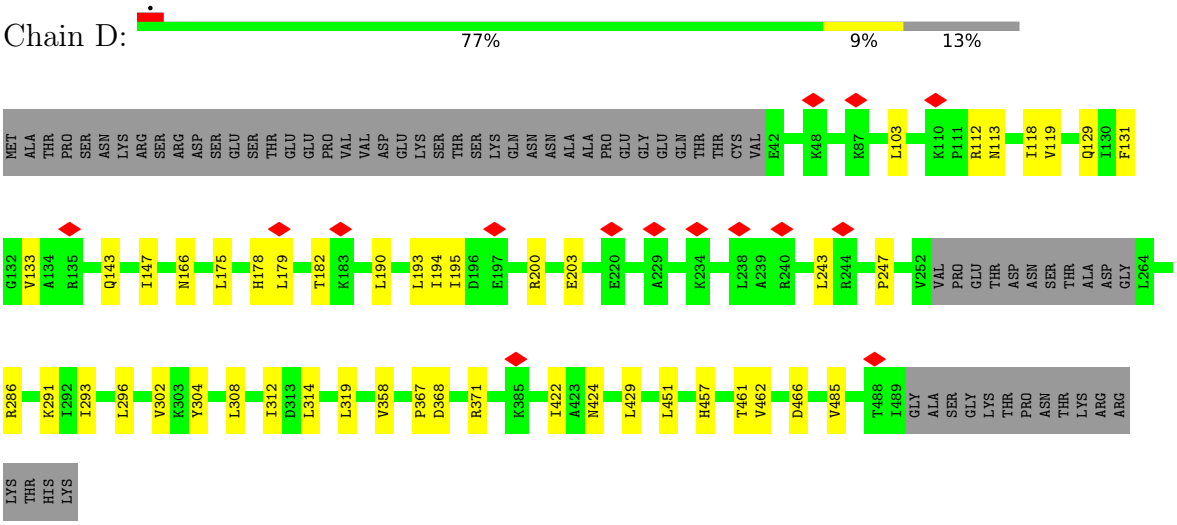


• Molecule 9: 60S ribosomal protein L4-A



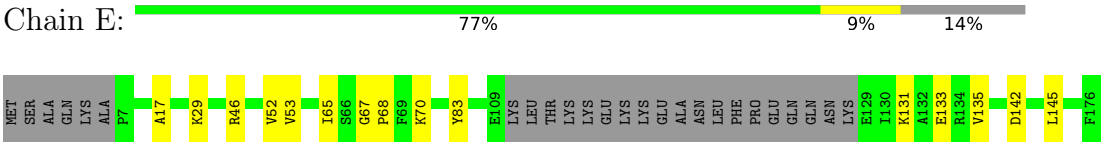
• Molecule 10: ATP-dependent RNA helicase HAS1

Chain D:



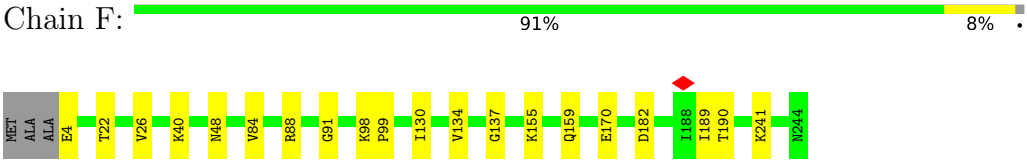
• Molecule 11: 60S ribosomal protein L6-A

Chain E:



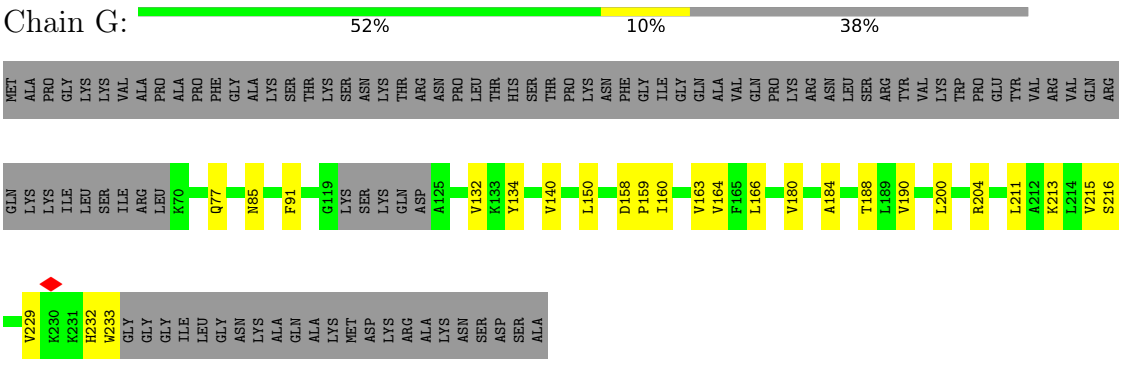
• Molecule 12: 60S ribosomal protein L7-A

Chain F:



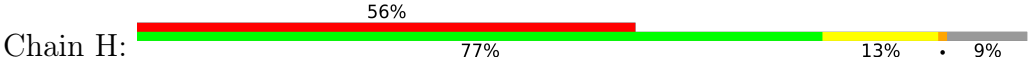
• Molecule 13: 60S ribosomal protein L8-A

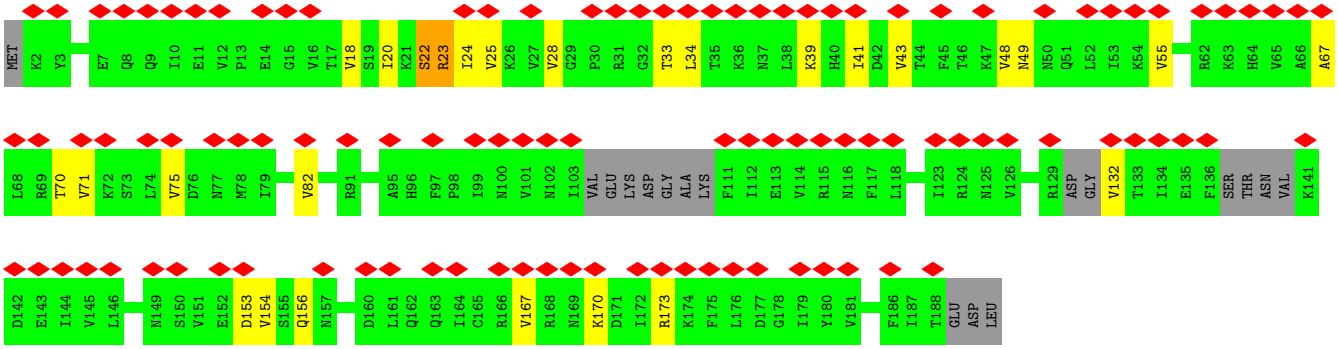
Chain G:



• Molecule 14: 60S ribosomal protein L9-A

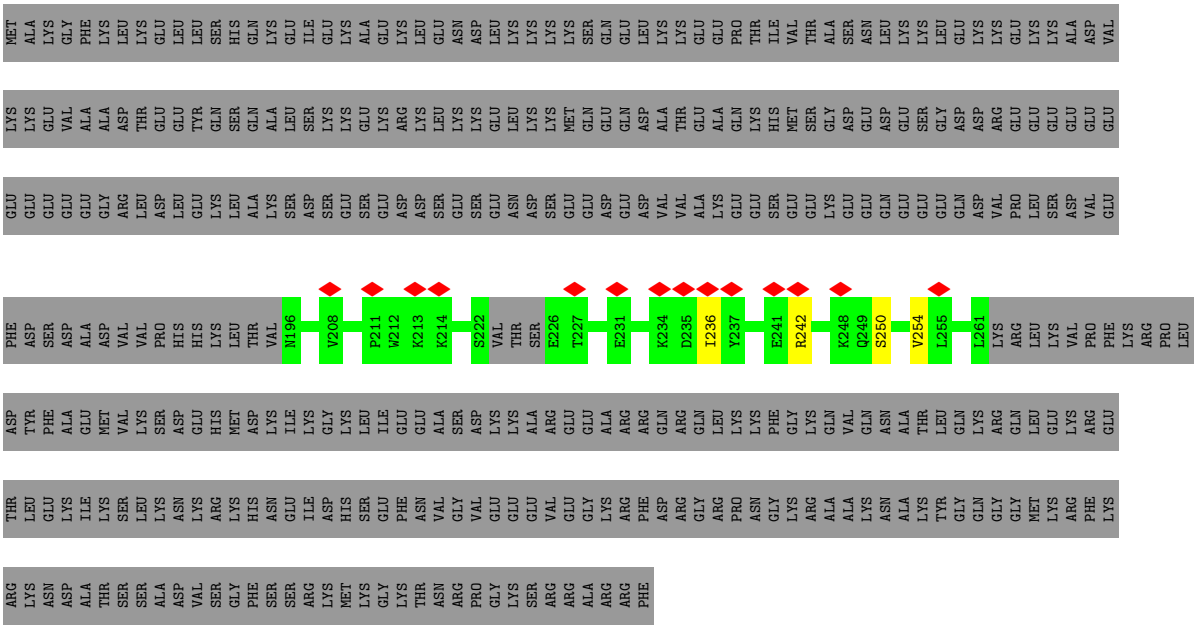
Chain H:





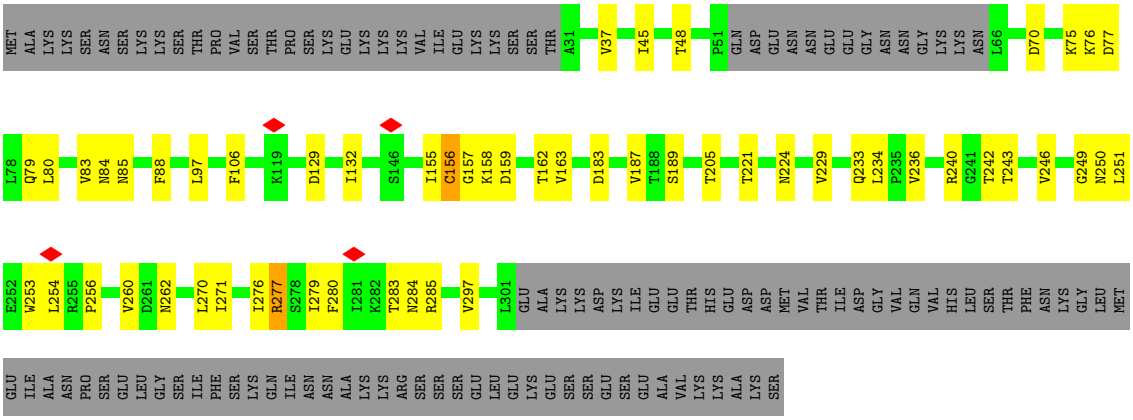
• Molecule 15: rRNA-processing protein EBP2

Chain J:



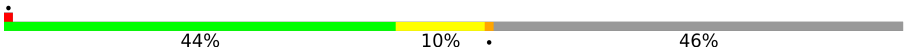
• Molecule 16: Proteasome-interacting protein CIC1

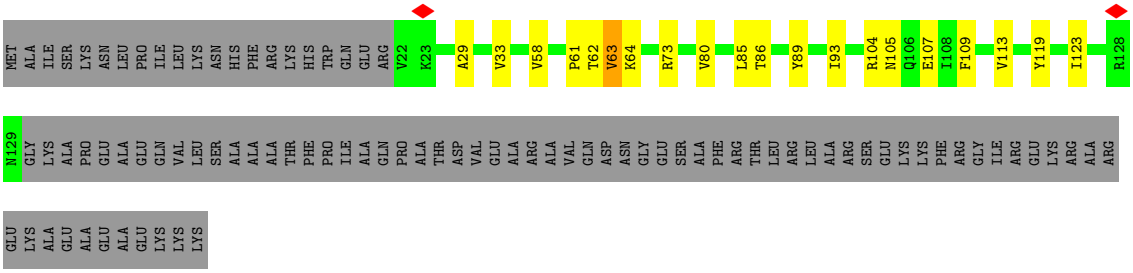
Chain K:



• Molecule 17: 60S ribosomal protein L13-A

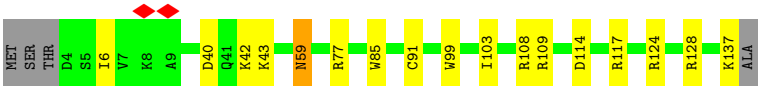
Chain L:





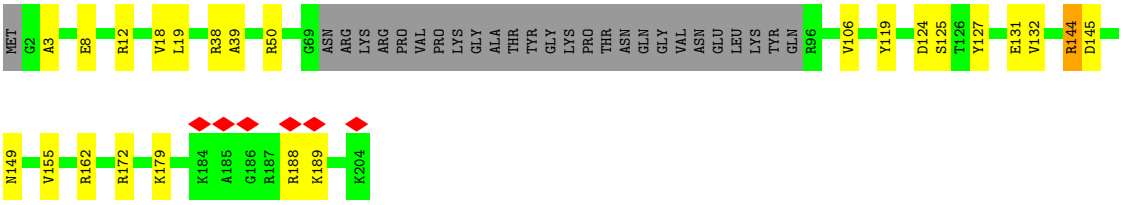
• Molecule 18: 60S ribosomal protein L14-A

Chain M:



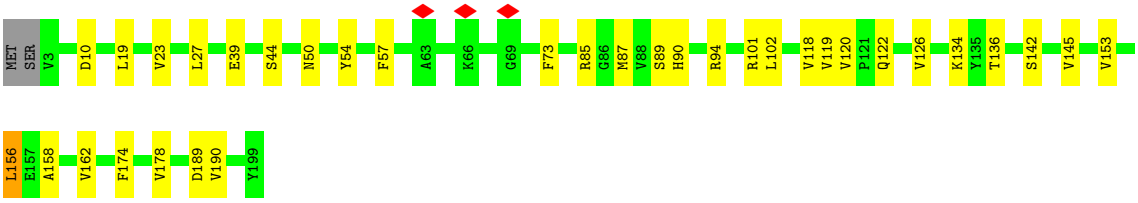
• Molecule 19: 60S ribosomal protein L15-A

Chain N:



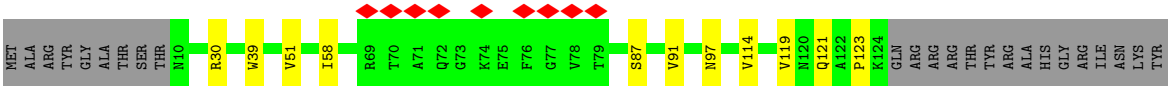
• Molecule 20: 60S ribosomal protein L16-A

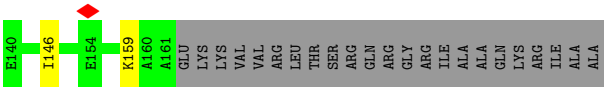
Chain O:



• Molecule 21: 60S ribosomal protein L17-A

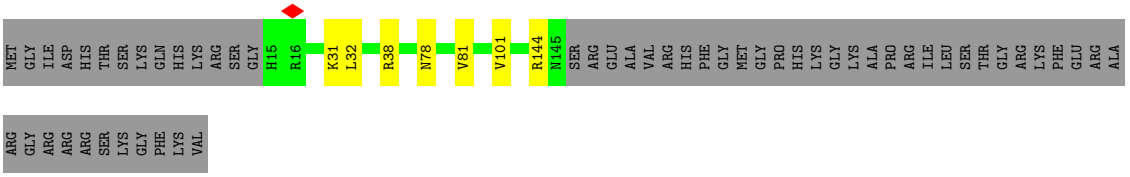
Chain P:





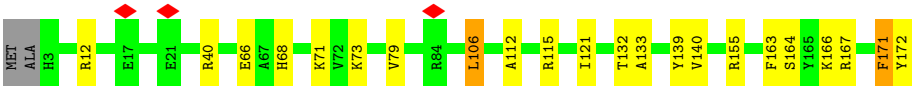
• Molecule 22: 60S ribosomal protein L18-A

Chain Q:



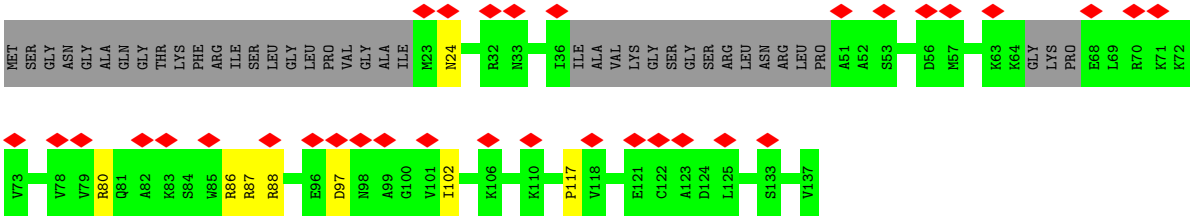
• Molecule 23: 60S ribosomal protein L20-A

Chain S:



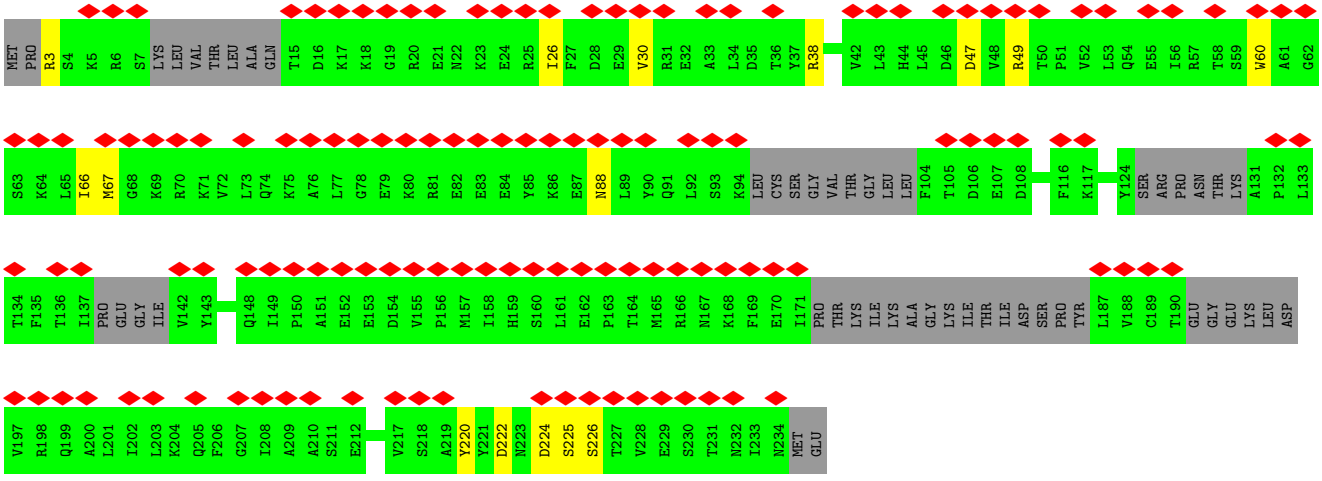
• Molecule 24: 60S ribosomal protein L23-A

Chain V:



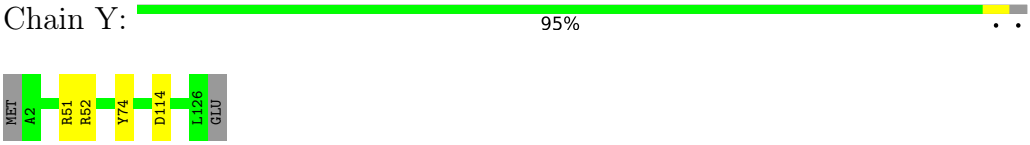
• Molecule 25: Ribosome assembly factor MRT4

Chain W:



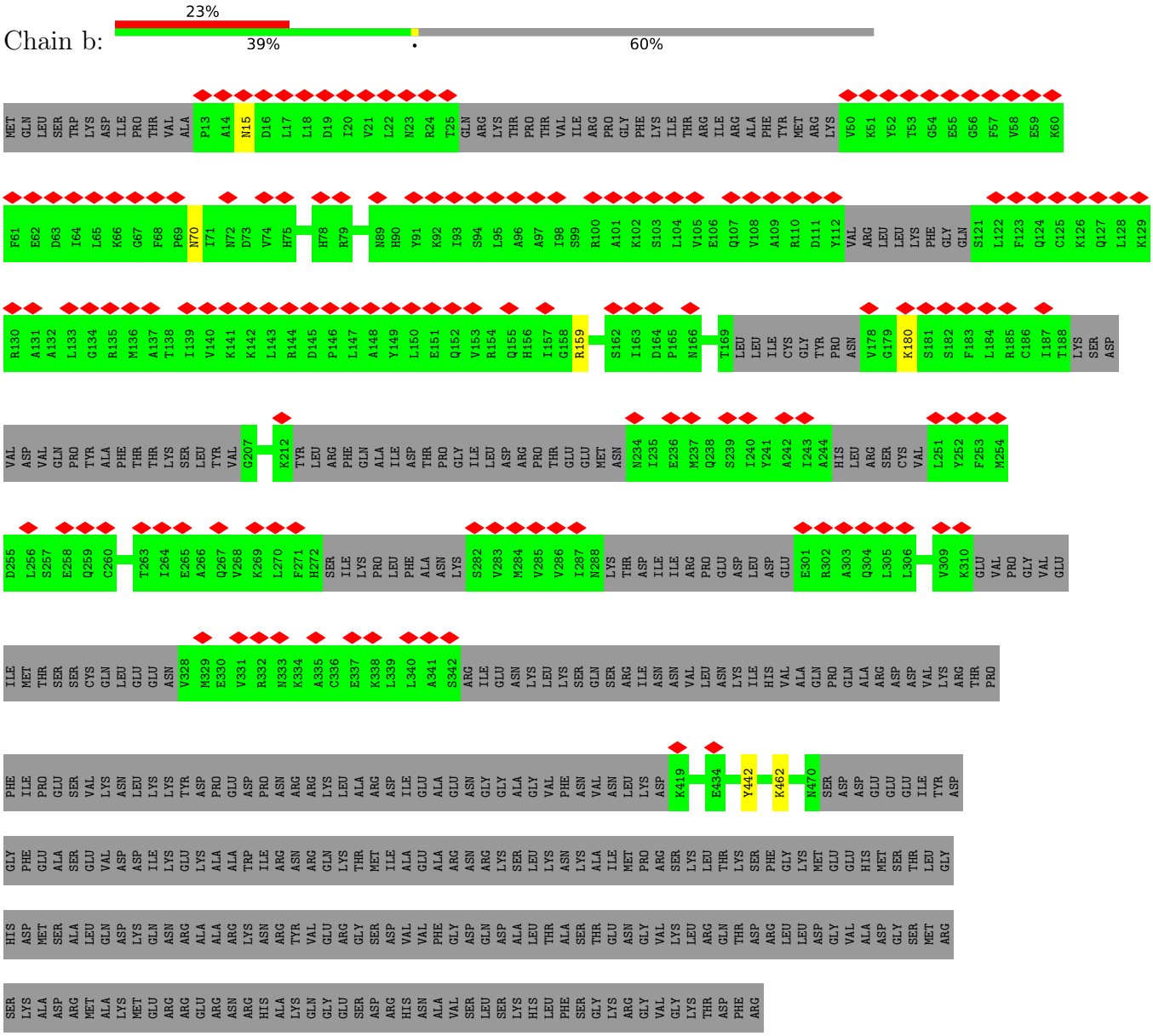
• Molecule 26: 60S ribosomal protein L26-A

Chain Y:



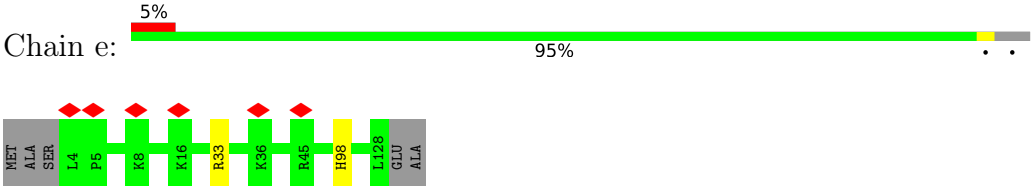
• Molecule 27: Nucleolar GTP-binding protein 1

Chain b:



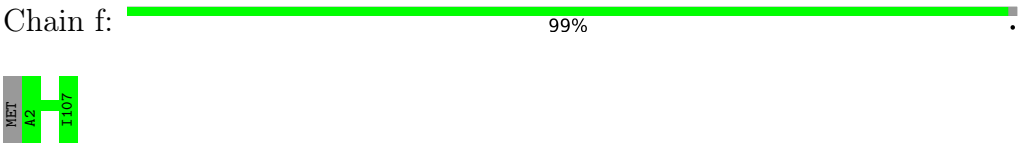
• Molecule 28: 60S ribosomal protein L32

Chain e:



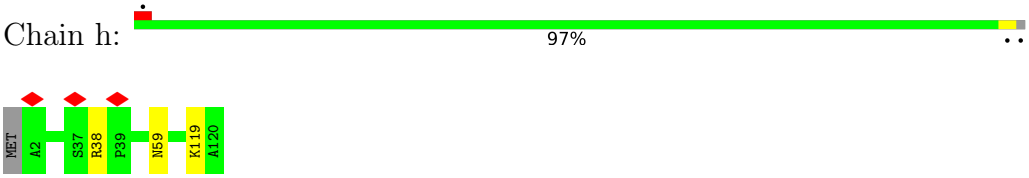
• Molecule 29: 60S ribosomal protein L33-A

Chain f:



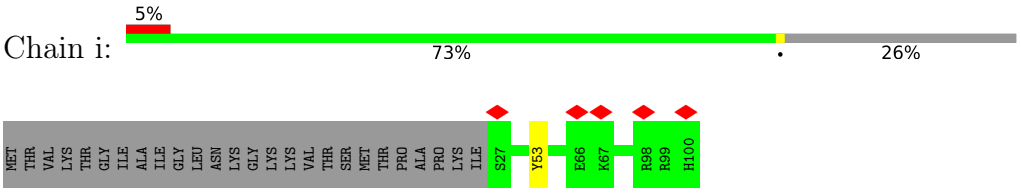
• Molecule 30: 60S ribosomal protein L35-A

Chain h:



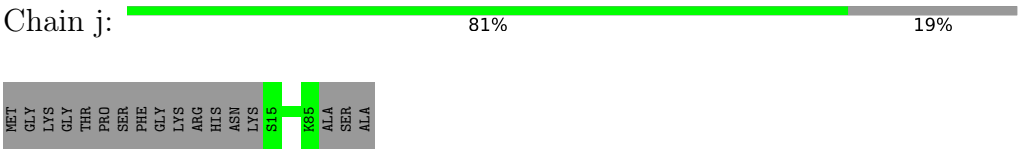
• Molecule 31: 60S ribosomal protein L36-A

Chain i:



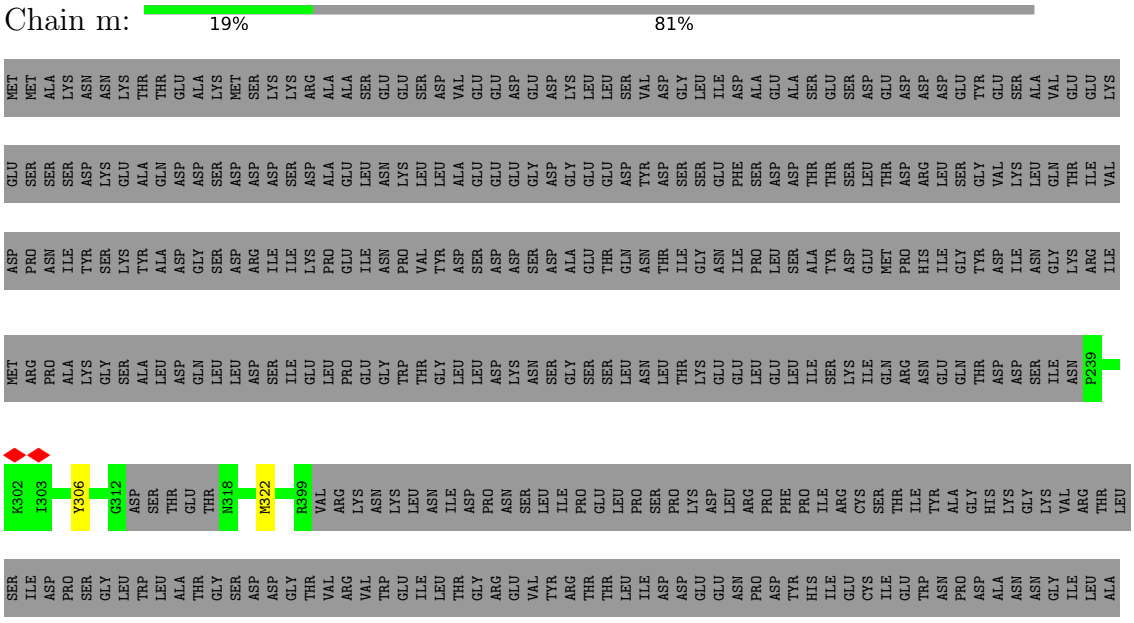
• Molecule 32: 60S ribosomal protein L37-A

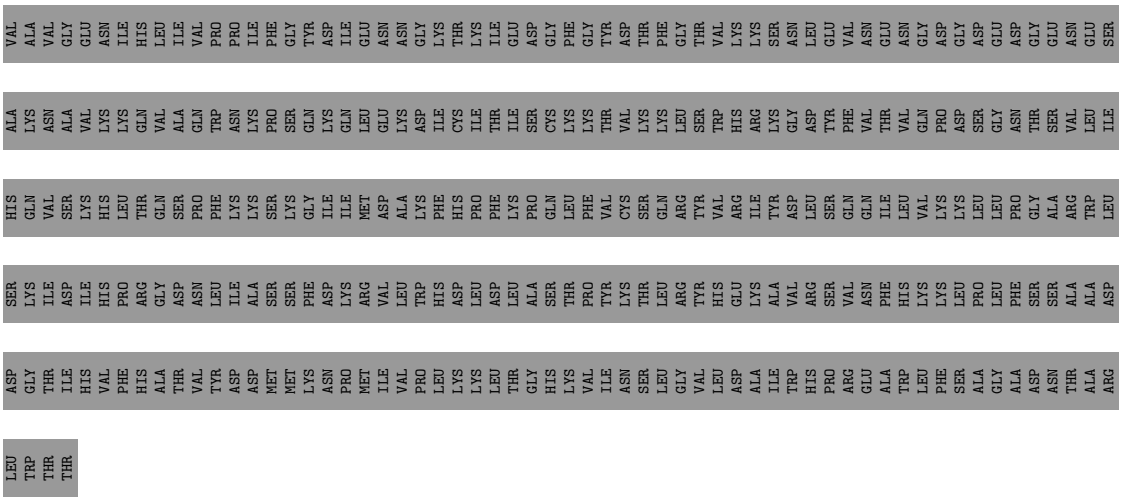
Chain j:



• Molecule 33: Ribosome biogenesis protein ERB1

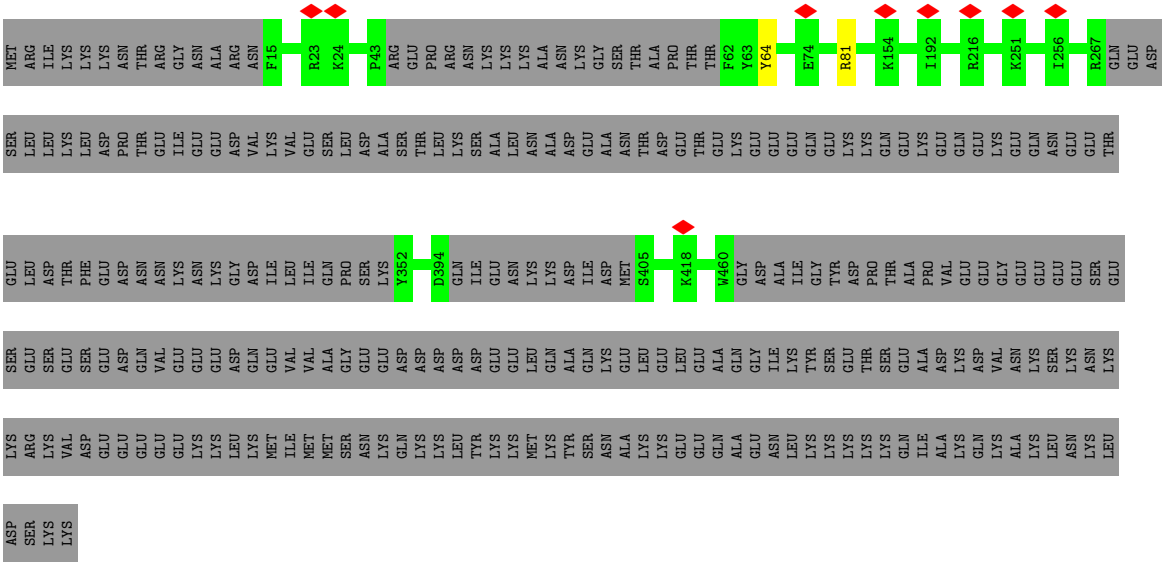
Chain m:





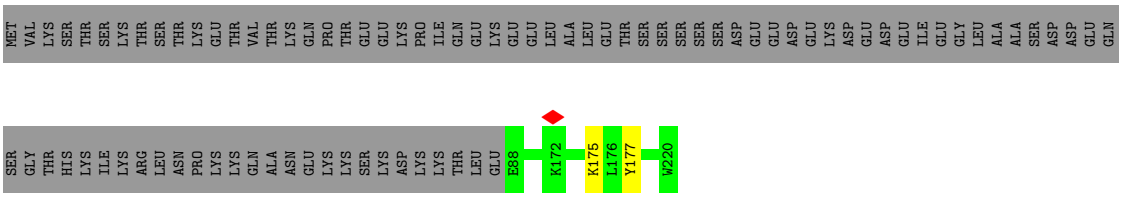
• Molecule 34: Pescadillo homolog

Chain n:



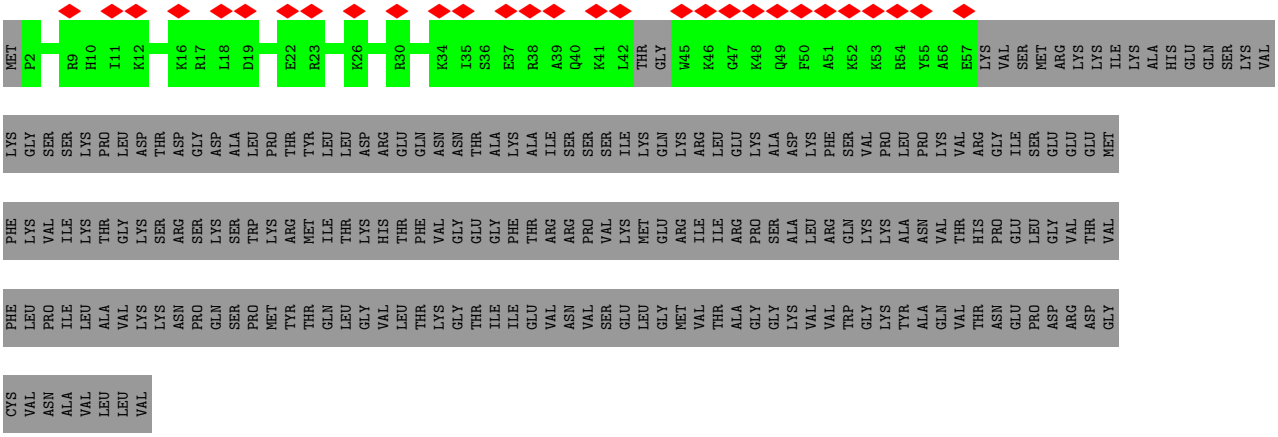
• Molecule 35: Ribosome biogenesis protein 15

Chain o:



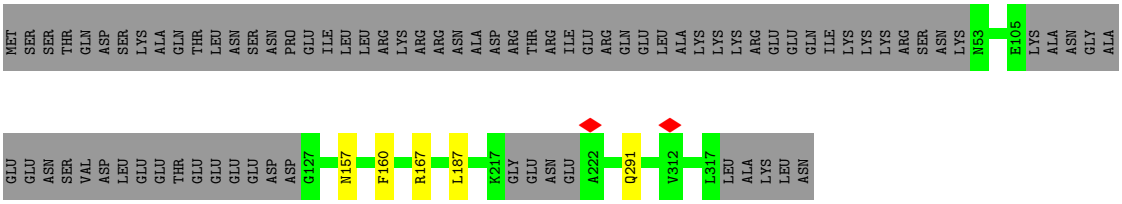
• Molecule 36: Ribosome biogenesis protein NSA2

Chain r:



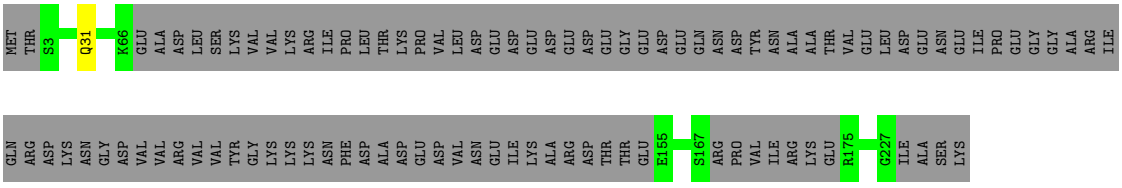
• Molecule 37: Ribosome biogenesis protein RLP7

Chain t:



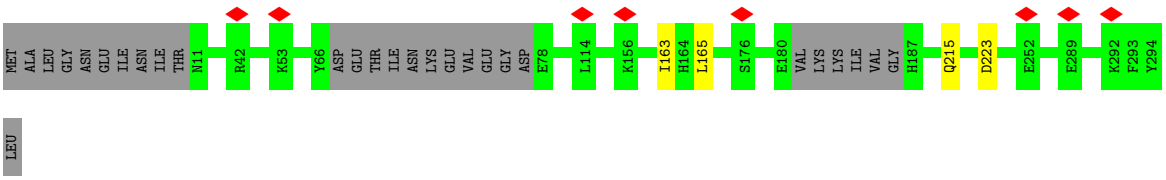
• Molecule 38: Nucleolar protein 16

Chain v:



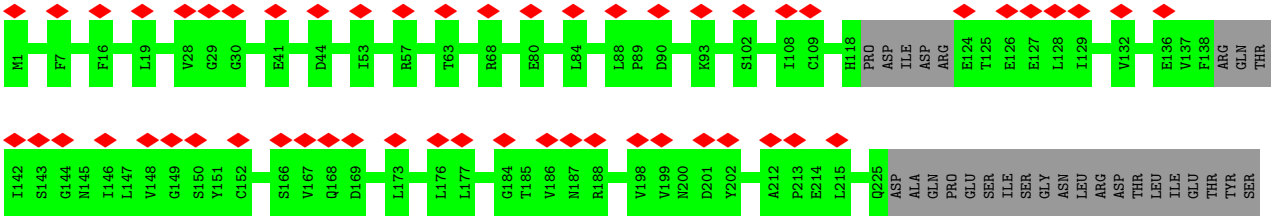
• Molecule 39: Ribosome production factor 1

Chain x:



• Molecule 40: Eukaryotic translation initiation factor 6

Chain y:


M1 F7 F16 L19 V28 G29 G30 E41 D44 I53 R57 T63 R68 E80 L84 L88 P89 D90 K93 S102 I108 C109 H118 PRO ASP ILE ASP ARG E124 T125 E126 E127 L128 I129 V132 E136 V137 F138 ARG GLN THR
I142 S143 G144 N145 I146 L147 V148 G149 S150 Y151 C152 S166 V167 Q168 D169 L173 L176 L177 G184 T185 V186 N187 R188 V198 V199 N200 D201 Y202 A212 P213 E214 L215 Q225 ASP ALA GLN PRO GLU SER ILE SER GLY ASN LEU ARG ASP THR LEU ILE GLU THR TYR SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37557	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 ($e^-/Å^2$)	86.09	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.042	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	425.40002, 425.40002, 425.40002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.16	0/39278	0.74	32/61189 (0.1%)
2	2	0.16	0/3536	0.75	3/5501 (0.1%)
3	3	0.24	0/1461	0.39	0/1958
4	4	0.24	0/1895	0.37	0/2549
5	5	0.23	0/3109	0.42	0/4187
6	6	0.16	0/1527	0.78	2/2371 (0.1%)
7	A	0.24	0/1235	0.41	0/1669
8	B	0.24	0/2699	0.42	0/3626
9	C	0.23	0/2660	0.40	0/3601
10	D	0.24	0/3552	0.39	0/4789
11	E	0.24	0/1226	0.39	0/1648
12	F	0.25	0/1974	0.38	0/2654
13	G	0.24	0/1252	0.41	0/1695
14	H	0.23	0/1412	0.42	0/1898
15	J	0.23	0/538	0.36	0/723
16	K	0.24	0/2107	0.39	0/2845
17	L	0.24	0/877	0.39	0/1179
18	M	0.24	0/1056	0.38	0/1421
19	N	0.23	0/1544	0.40	0/2065
20	O	0.24	0/1585	0.38	0/2128
21	P	0.24	0/1080	0.39	0/1455
22	Q	0.25	0/1024	0.44	1/1385 (0.1%)
23	S	0.24	0/1468	0.40	0/1973
24	V	0.24	0/747	0.41	0/1002
25	W	0.23	0/1543	0.40	0/2068
26	Y	0.23	0/995	0.40	0/1329
27	b	0.23	0/2133	0.36	0/2857
28	e	0.23	0/1030	0.40	0/1379
29	f	0.25	0/868	0.41	0/1168
30	h	0.24	0/978	0.37	0/1301
31	i	0.24	0/599	0.37	0/793
32	j	0.24	0/578	0.42	0/767

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	m	0.23	0/1363	0.37	0/1841
34	n	0.24	0/2802	0.36	0/3791
35	o	0.24	0/1129	0.39	0/1502
36	r	0.22	0/485	0.33	0/636
37	t	0.24	0/1930	0.40	0/2596
38	v	0.23	0/1100	0.37	0/1456
39	x	0.24	0/2313	0.40	0/3100
40	y	0.23	0/1650	0.43	0/2242
All	All	0.21	0/100338	0.59	38/144337 (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
14	H	0	1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	6	1	C	OP1-P-OP2	-6.95	109.17	119.60
1	1	310	U	OP1-P-OP2	-6.84	109.33	119.60
1	1	2890	A	OP1-P-OP2	-6.84	109.34	119.60
1	1	44	U	OP1-P-OP2	-6.80	109.40	119.60
1	1	3364	C	OP1-P-OP2	-6.79	109.41	119.60
1	1	714	G	OP1-P-OP2	-6.79	109.42	119.60
1	1	3070	A	OP1-P-OP2	-6.79	109.42	119.60
1	1	3285	C	OP1-P-OP2	-6.78	109.44	119.60
1	1	720	A	OP1-P-OP2	-6.77	109.44	119.60
1	1	2830	G	OP1-P-OP2	-6.77	109.44	119.60
1	1	2824	G	OP1-P-OP2	-6.77	109.44	119.60
2	2	114	G	OP1-P-OP2	-6.77	109.45	119.60
1	1	1306	G	OP1-P-OP2	-6.75	109.47	119.60
1	1	2379	U	OP1-P-OP2	-6.75	109.47	119.60
1	1	3093	C	OP1-P-OP2	-6.75	109.47	119.60
1	1	925	A	OP1-P-OP2	-6.75	109.48	119.60
1	1	3378	C	OP1-P-OP2	-6.75	109.48	119.60
1	1	1200	A	OP1-P-OP2	-6.75	109.48	119.60
1	1	2352	A	OP1-P-OP2	-6.75	109.48	119.60
6	6	227	C	OP1-P-OP2	-6.74	109.50	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	781	G	OP1-P-OP2	-6.73	109.50	119.60
1	1	2848	G	OP1-P-OP2	-6.73	109.50	119.60
2	2	1	A	OP1-P-OP2	-6.73	109.50	119.60
1	1	769	G	OP1-P-OP2	-6.73	109.51	119.60
1	1	3158	G	OP1-P-OP2	-6.73	109.51	119.60
1	1	2372	A	OP1-P-OP2	-6.72	109.51	119.60
1	1	1061	A	OP1-P-OP2	-6.72	109.52	119.60
1	1	3172	A	OP1-P-OP2	-6.72	109.52	119.60
1	1	2995	A	OP1-P-OP2	-6.72	109.53	119.60
1	1	93	C	OP1-P-OP2	-6.71	109.54	119.60
1	1	1098	A	OP1-P-OP2	-6.70	109.55	119.60
2	2	130	C	OP1-P-OP2	-6.70	109.55	119.60
1	1	1	G	OP1-P-OP2	-6.57	109.75	119.60
1	1	1254	C	N3-C2-O2	-6.29	117.50	121.90
1	1	2899	C	C2-N1-C1'	6.00	125.40	118.80
1	1	954	U	C2-N1-C1'	5.74	124.59	117.70
22	Q	31	LYS	CD-CE-NZ	5.72	124.85	111.70
1	1	3058	U	C2-N1-C1'	5.58	124.40	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	H	22	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	35107	17632	17660	363	0
2	2	3166	1601	1603	35	0
3	3	1434	1474	1473	11	0
4	4	1853	1891	1887	17	0
5	5	3055	3115	3113	14	0
6	6	1370	691	692	24	0
7	A	1203	1208	1205	9	0
8	B	2646	2728	2726	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	2611	2725	2724	29	0
10	D	3486	3620	3618	21	0
11	E	1205	1292	1291	10	0
12	F	1936	2033	2032	12	0
13	G	1231	1289	1287	18	0
14	H	1394	1468	1464	20	0
15	J	529	506	504	2	0
16	K	2073	2157	2155	36	0
17	L	864	918	917	14	0
18	M	1041	1138	1137	12	0
19	N	1513	1566	1564	17	0
20	O	1555	1660	1659	22	0
21	P	1062	1077	1075	10	0
22	Q	1009	1092	1091	4	0
23	S	1432	1472	1470	13	0
24	V	738	760	757	5	0
25	W	1522	1527	1520	10	0
26	Y	984	1076	1075	3	0
27	b	2105	2116	2106	0	0
28	e	1009	1081	1080	0	0
29	f	850	881	880	0	0
30	h	969	1079	1078	0	0
31	i	594	642	641	0	0
32	j	566	571	566	0	0
33	m	1325	1318	1317	0	0
34	n	2734	2782	2778	0	0
35	o	1107	1160	1159	0	0
36	r	477	485	484	0	0
37	t	1905	2018	2015	0	0
38	v	1087	1136	1133	0	0
39	x	2268	2305	2302	0	0
40	y	1632	1630	1628	0	0
41	j	1	0	0	0	0
All	All	94648	76920	76866	668	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (668) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3329:U:HO2'	8:B:363:SER:HG	1.03	0.99
1:1:3198:U:O2'	1:1:3199:G:OP1	1.81	0.99
1:1:625:G:O2'	1:1:1401:A:OP1	1.85	0.94
1:1:2899:C:O2'	1:1:2901:G:OP2	1.86	0.93
1:1:1347:U:O2'	1:1:1348:U:OP1	1.90	0.90
1:1:3228:C:O2'	1:1:3229:G:OP2	1.90	0.90
1:1:2857:C:O2'	1:1:2858:U:O5'	1.88	0.89
1:1:656:A:HO2'	2:2:17:A:HO2'	1.13	0.88
1:1:2995:A:O2'	1:1:2996:U:OP1	1.91	0.87
1:1:716:A:O2'	1:1:718:G:OP2	1.93	0.86
1:1:720:A:O2'	1:1:783:A:O2'	1.93	0.86
1:1:548:G:O2'	1:1:549:U:OP1	1.94	0.85
1:1:1278:A:O2'	1:1:1279:C:O5'	1.94	0.85
1:1:1395:G:O2'	2:2:18:U:O2	1.94	0.84
10:D:178:HIS:O	10:D:182:THR:OG1	1.94	0.84
1:1:2897:A:OP2	1:1:2899:C:N4	2.10	0.84
1:1:1152:G:N2	1:1:1152:G:OP2	2.10	0.83
1:1:518:G:OP2	1:1:518:G:N2	2.11	0.83
1:1:408:A:N3	1:1:655:C:O2'	2.10	0.83
1:1:1257:C:O2'	1:1:1258:U:O5'	1.95	0.82
1:1:2375:G:N2	1:1:2375:G:OP2	2.12	0.82
1:1:1254:C:O2'	1:1:1255:C:O4'	1.98	0.81
6:6:33:U:O4'	16:K:285:ARG:NE	2.13	0.81
1:1:476:G:O2'	1:1:477:A:O4'	1.99	0.81
1:1:3306:U:O2'	1:1:3308:C:OP2	1.99	0.80
1:1:1153:A:O2'	1:1:1154:A:O4'	2.00	0.80
1:1:164:A:O2'	1:1:166:C:O4'	1.99	0.80
1:1:200:C:N4	1:1:218:G:OP1	2.16	0.79
1:1:297:G:N2	1:1:297:G:OP2	2.16	0.79
1:1:399:A:O2'	1:1:403:C:O2'	1.98	0.79
8:B:66:LYS:O	8:B:70:ARG:NH2	2.15	0.78
1:1:691:A:N1	2:2:28:C:O2'	2.14	0.78
20:O:27:LEU:O	20:O:101:ARG:NH1	2.17	0.78
1:1:3099:C:O2'	1:1:3100:U:O5'	2.01	0.78
1:1:649:A:O2'	1:1:650:C:OP1	2.01	0.77
5:5:277:SER:OG	5:5:301:GLU:O	2.01	0.77
2:2:114:G:O2'	2:2:115:C:OP1	2.02	0.76
6:6:6:U:OP2	16:K:189:SER:OG	2.03	0.76
1:1:1394:A:N6	1:1:1416:C:O2	2.18	0.76
1:1:3115:C:O2	1:1:3117:C:N4	2.18	0.76
4:4:57:ASP:OD1	4:4:120:LYS:NZ	2.18	0.76
19:N:38:ARG:NH1	19:N:39:ALA:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:62:THR:O	17:L:64:LYS:N	2.18	0.75
6:6:44:G:N2	16:K:242:THR:OG1	2.20	0.75
1:1:755:A:O2'	1:1:756:U:O5'	2.03	0.75
1:1:399:A:HO2'	1:1:403:C:HO2'	1.29	0.75
1:1:600:G:N2	1:1:603:A:OP2	2.20	0.75
16:K:236:VAL:HG21	16:K:246:VAL:HG22	1.68	0.75
1:1:63:A:N3	1:1:78:U:O2'	2.20	0.74
1:1:1176:C:OP2	1:1:1177:G:O2'	2.01	0.74
1:1:348:A:N3	1:1:352:A:O2'	2.21	0.74
1:1:1231:A:OP2	25:W:49:ARG:NH2	2.18	0.74
2:2:50:C:OP2	2:2:51:G:N2	2.20	0.74
16:K:250:ASN:OD1	16:K:251:LEU:N	2.20	0.74
1:1:480:C:O2'	1:1:481:U:OP2	2.03	0.74
1:1:382:U:O2	21:P:97:ASN:ND2	2.20	0.74
1:1:1176:C:O2'	20:O:89:SER:OG	2.03	0.74
1:1:1259:A:OP1	25:W:67:MET:N	2.19	0.74
6:6:16:U:O2'	6:6:17:G:OP2	2.05	0.74
6:6:33:U:O2'	6:6:34:A:OP2	2.05	0.74
1:1:1315:U:OP2	20:O:44:SER:OG	2.01	0.73
8:B:57:VAL:HG12	8:B:73:VAL:HG23	1.68	0.73
6:6:54:A:OP1	13:G:213:LYS:NZ	2.20	0.73
1:1:720:A:HO2'	1:1:783:A:HO2'	1.27	0.73
1:1:68:C:OP2	1:1:301:G:N2	2.21	0.73
1:1:1384:U:O2	1:1:1422:G:O6	2.07	0.73
1:1:93:C:O2'	1:1:94:G:O5'	2.07	0.72
1:1:3116:G:N2	1:1:3116:G:OP1	2.21	0.72
1:1:755:A:O2'	1:1:756:U:O4'	2.05	0.72
12:F:88:ARG:NH1	12:F:91:GLY:O	2.23	0.72
6:6:5:C:N4	6:6:24:A:OP1	2.24	0.71
1:1:1307:G:O2'	1:1:1308:A:OP2	2.08	0.71
1:1:75:G:O2'	1:1:76:G:OP1	2.08	0.71
1:1:1235:U:N3	1:1:1237:G:O4'	2.24	0.71
6:6:58:G:N2	6:6:58:G:OP2	2.23	0.70
1:1:3228:C:HO2'	1:1:3229:G:P	2.14	0.70
1:1:117:U:O2'	1:1:119:U:OP2	2.06	0.69
6:6:51:U:O2'	6:6:54:A:N7	2.23	0.69
1:1:695:C:OP2	9:C:115:HIS:NE2	2.23	0.69
1:1:36:C:O2'	1:1:934:G:N3	2.26	0.69
2:2:13:A:O2'	21:P:121:GLN:O	2.10	0.69
2:2:103:G:OP2	2:2:105:A:O2'	2.10	0.69
1:1:177:U:O2	1:1:241:G:O6	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:310:U:O2'	1:1:311:C:O4'	2.12	0.68
1:1:656:A:O2'	2:2:17:A:O2'	2.04	0.68
6:6:45:U:O2'	16:K:243:THR:O	2.11	0.68
1:1:551:A:O2'	1:1:552:G:OP1	2.12	0.68
1:1:3165:A:O2'	1:1:3166:C:O4'	2.08	0.68
1:1:1:G:N2	1:1:1:G:OP1	2.26	0.68
1:1:195:U:O2'	1:1:1391:C:OP1	2.08	0.68
1:1:779:G:O3'	1:1:781:G:OP2	2.08	0.68
1:1:358:G:N2	1:1:361:A:OP2	2.26	0.68
25:W:38:ARG:NH2	25:W:222:ASP:OD1	2.26	0.68
1:1:3067:C:O2'	1:1:3068:U:O4'	2.12	0.68
4:4:67:ASN:OD1	4:4:68:GLU:N	2.26	0.68
1:1:1276:U:O2'	1:1:1277:C:OP1	2.11	0.67
8:B:219:ALA:HB2	8:B:336:VAL:HG12	1.75	0.67
23:S:79:VAL:HG21	23:S:106:LEU:HD21	1.76	0.67
8:B:187:SER:O	8:B:190:GLU:N	2.27	0.67
14:H:67:ALA:O	14:H:71:VAL:HG23	1.95	0.67
16:K:84:ASN:O	16:K:277:ARG:N	2.26	0.67
1:1:477:A:O2'	1:1:478:A:O5'	2.13	0.67
8:B:299:ASP:OD2	8:B:301:THR:OG1	2.12	0.66
1:1:3082:C:N4	1:1:3083:G:O6	2.29	0.66
1:1:3265:C:N4	1:1:3266:G:O6	2.28	0.66
10:D:203:GLU:OE1	10:D:371:ARG:NH1	2.27	0.66
23:S:40:ARG:NH2	23:S:121:ILE:O	2.29	0.66
1:1:549:U:O4	1:1:550:A:N6	2.29	0.66
1:1:1245:A:N7	1:1:1271:A:O2'	2.29	0.66
12:F:130:ILE:O	12:F:134:VAL:HG22	1.96	0.66
4:4:136:LEU:HB3	4:4:145:LEU:HD12	1.78	0.65
25:W:38:ARG:NH1	25:W:224:ASP:OD2	2.29	0.65
1:1:1158:A:OP1	12:F:91:GLY:N	2.30	0.65
1:1:759:U:O2'	1:1:760:G:O4'	2.15	0.65
1:1:2382:G:OP2	20:O:90:HIS:NE2	2.29	0.65
24:V:24:ASN:ND2	24:V:97:ASP:OD2	2.29	0.65
1:1:33:G:O6	1:1:49:A:O2'	2.13	0.65
24:V:102:ILE:O	24:V:102:ILE:HD12	1.97	0.65
8:B:74:GLU:OE1	8:B:325:LYS:NZ	2.27	0.65
1:1:213:A:N6	1:1:227:G:O2'	2.29	0.65
4:4:87:GLU:N	4:4:87:GLU:OE1	2.29	0.65
1:1:1:G:OP2	6:6:232:A:O3'	2.08	0.64
1:1:77:A:OP2	17:L:73:ARG:NH2	2.29	0.64
6:6:231:A:O2'	6:6:232:A:O5'	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3085:G:N2	1:1:3086:A:N7	2.46	0.64
1:1:1260:A:O2'	1:1:1279:C:O2	2.14	0.64
10:D:422:ILE:O	10:D:424:ASN:ND2	2.30	0.64
14:H:167:VAL:HG12	14:H:170:LYS:HB2	1.79	0.63
1:1:2857:C:HO2'	1:1:2858:U:P	2.22	0.63
7:A:51:ASP:OD1	7:A:52:LEU:N	2.31	0.63
13:G:132:VAL:HG12	13:G:200:LEU:HD21	1.81	0.63
1:1:3258:U:O2'	1:1:3260:G:OP1	2.17	0.63
13:G:184:ALA:O	13:G:188:THR:HG23	1.99	0.63
17:L:119:TYR:O	17:L:123:ILE:HG23	1.99	0.63
6:6:227:C:O2'	6:6:228:U:OP1	2.17	0.62
18:M:40:ASP:OD1	18:M:43:LYS:N	2.32	0.62
1:1:753:C:N3	1:1:781:G:N2	2.47	0.62
1:1:1102:A:OP1	12:F:155:LYS:NZ	2.32	0.62
18:M:42:LYS:O	18:M:59:ASN:ND2	2.32	0.62
1:1:1111:U:O2'	1:1:1112:A:O5'	2.12	0.62
1:1:1414:G:OP1	3:3:142:LYS:NZ	2.32	0.62
1:1:406:G:O2'	1:1:407:A:OP2	2.17	0.62
1:1:974:G:O2'	22:Q:144:ARG:NH1	2.32	0.62
5:5:162:GLY:O	5:5:183:LEU:N	2.33	0.62
16:K:83:VAL:HG21	16:K:270:LEU:HD13	1.81	0.62
20:O:10:ASP:OD2	23:S:167:ARG:NH2	2.33	0.62
1:1:1259:A:N3	1:1:1280:C:O2'	2.27	0.62
14:H:22:SER:O	14:H:24:ILE:N	2.33	0.62
1:1:674:G:O2'	9:C:116:ASN:ND2	2.33	0.61
10:D:119:VAL:HG13	10:D:194:ILE:HD11	1.80	0.61
1:1:3332:U:O2'	1:1:3333:G:O5'	2.19	0.61
21:P:39:TRP:O	21:P:114:VAL:HG12	2.00	0.61
1:1:717:C:O2'	1:1:718:G:O5'	2.15	0.61
1:1:3339:A:O2'	1:1:3340:G:OP1	2.17	0.61
10:D:131:PHE:CD2	10:D:147:ILE:HD11	2.34	0.61
1:1:80:G:O6	1:1:106:A:N6	2.34	0.61
1:1:102:C:O2'	17:L:62:THR:OG1	2.17	0.61
1:1:2899:C:O2	14:H:173:ARG:NH1	2.33	0.61
25:W:224:ASP:OD1	25:W:225:SER:N	2.33	0.61
7:A:41:VAL:HG13	7:A:45:HIS:HB2	1.83	0.61
1:1:1125:U:O2'	1:1:1126:G:O4'	2.13	0.60
3:3:69:ARG:NE	3:3:78:GLU:OE2	2.35	0.60
2:2:114:G:HO2'	2:2:115:C:P	2.23	0.60
6:6:231:A:O2'	6:6:232:A:N3	2.24	0.60
15:J:236:ILE:O	15:J:242:ARG:NH2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:312:ILE:HG22	10:D:312:ILE:O	2.02	0.60
25:W:88:ASN:ND2	25:W:226:SER:O	2.35	0.60
1:1:291:C:O2	1:1:292:U:N3	2.35	0.60
2:2:70:G:O2'	2:2:87:G:N2	2.35	0.60
11:E:52:VAL:HG21	11:E:65:ILE:CD1	2.31	0.59
19:N:8:GLU:OE2	19:N:50:ARG:NH2	2.34	0.59
1:1:2901:G:N2	1:1:3030:G:O2'	2.35	0.59
1:1:3198:U:HO2'	1:1:3199:G:P	2.22	0.59
9:C:315:LYS:HB2	9:C:323:VAL:HG21	1.85	0.59
1:1:3331:U:OP1	8:B:369:ARG:NH2	2.35	0.59
8:B:377:HIS:O	8:B:381:GLY:N	2.35	0.59
1:1:304:G:OP1	7:A:93:LYS:N	2.35	0.59
2:2:13:A:C2	2:2:14:C:C5	2.91	0.59
6:6:52:G:N2	13:G:216:SER:OG	2.34	0.59
12:F:189:ILE:HG23	12:F:190:THR:HG23	1.84	0.59
1:1:1103:A:O2'	1:1:1104:G:OP1	2.20	0.59
6:6:40:U:O2'	6:6:41:G:OP2	2.19	0.58
1:1:75:G:HO2'	1:1:76:G:P	2.24	0.58
1:1:126:U:OP1	19:N:144:ARG:NH2	2.36	0.58
1:1:146:U:N3	13:G:134:TYR:OH	2.36	0.58
12:F:48:ASN:ND2	12:F:182:ASP:OD1	2.36	0.58
13:G:163:VAL:HG23	13:G:166:LEU:HD12	1.85	0.58
1:1:442:G:O6	1:1:492:U:O2	2.22	0.58
1:1:3075:G:O2'	1:1:3076:C:O5'	2.17	0.58
4:4:51:TYR:OH	9:C:2:SER:O	2.19	0.58
10:D:293:ILE:HG13	10:D:358:VAL:HG21	1.85	0.58
18:M:99:TRP:CZ2	18:M:103:ILE:HD11	2.39	0.58
1:1:295:A:O2'	1:1:296:A:O5'	2.21	0.57
4:4:89:THR:O	4:4:90:THR:OG1	2.18	0.57
1:1:752:C:O2'	1:1:753:C:O5'	2.20	0.57
4:4:76:TYR:O	4:4:135:TYR:OH	2.17	0.57
8:B:86:VAL:HG22	8:B:162:VAL:HG12	1.85	0.57
1:1:250:U:O2'	1:1:251:G:OP2	2.14	0.57
10:D:118:ILE:HD12	10:D:190:LEU:HD13	1.86	0.57
21:P:30:ARG:HA	21:P:119:VAL:HG11	1.85	0.57
1:1:551:A:HO2'	1:1:552:G:P	2.28	0.57
8:B:56:ILE:HD12	8:B:356:LEU:HD22	1.86	0.56
1:1:1382:G:OP2	9:C:188:ARG:NH1	2.37	0.56
8:B:286:GLY:N	8:B:321:PHE:O	2.37	0.56
16:K:37:VAL:HG12	16:K:260:VAL:HG22	1.87	0.56
1:1:1237:G:O6	1:1:1251:A:N1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:182:GLU:OE1	4:4:247:ARG:NH1	2.39	0.56
14:H:71:VAL:O	14:H:75:VAL:HG23	2.04	0.56
1:1:3148:U:O2'	8:B:106:TRP:NE1	2.38	0.56
1:1:3273:A:H2	11:E:83:TYR:HH	1.54	0.56
4:4:155:ARG:O	4:4:159:LEU:HD12	2.06	0.56
9:C:260:GLN:O	9:C:270:SER:OG	2.10	0.56
1:1:534:U:OP1	23:S:132:THR:OG1	2.20	0.56
1:1:1177:G:OP1	1:1:1177:G:N2	2.30	0.55
12:F:40:LYS:NZ	12:F:170:GLU:OE2	2.28	0.55
13:G:140:VAL:HG21	19:N:3:ALA:HB2	1.88	0.55
11:E:52:VAL:HG21	11:E:65:ILE:HD13	1.89	0.55
13:G:134:TYR:CD1	13:G:190:VAL:HG21	2.42	0.55
1:1:637:C:O2'	1:1:638:C:OP2	2.20	0.55
1:1:752:C:H2'	1:1:753:C:C5	2.41	0.55
5:5:305:GLN:NE2	5:5:365:THR:O	2.39	0.55
4:4:174:VAL:HG21	4:4:238:ILE:HG22	1.88	0.55
9:C:38:VAL:O	9:C:42:VAL:HG23	2.07	0.55
1:1:209:A:O2'	1:1:211:A:OP2	2.17	0.55
14:H:41:ILE:CG2	14:H:43:VAL:HG22	2.37	0.55
1:1:3021:A:O2'	1:1:3022:G:OP2	2.21	0.55
20:O:19:LEU:O	20:O:23:VAL:HG23	2.07	0.55
8:B:49:TYR:O	8:B:80:ASP:N	2.37	0.54
14:H:28:VAL:HG22	14:H:33:THR:HG22	1.89	0.54
1:1:267:G:O4'	19:N:50:ARG:NH1	2.41	0.54
1:1:1229:G:O2'	25:W:47:ASP:OD2	2.23	0.54
6:6:44:G:O2'	16:K:240:ARG:O	2.24	0.54
1:1:3146:G:O2'	8:B:101:SER:O	2.24	0.54
9:C:154:THR:OG1	9:C:252:GLU:OE1	2.24	0.54
10:D:131:PHE:CG	10:D:147:ILE:HD11	2.42	0.54
10:D:143:GLN:OE1	10:D:166:ASN:ND2	2.38	0.54
2:2:72:A:OP1	26:Y:52:ARG:N	2.37	0.54
12:F:22:THR:O	12:F:26:VAL:HG23	2.08	0.54
1:1:3228:C:OP1	18:M:137:LYS:NZ	2.37	0.54
1:1:456:U:O2'	1:1:457:C:OP1	2.24	0.53
6:6:32:A:O2'	16:K:75:LYS:NZ	2.27	0.53
13:G:160:ILE:O	13:G:164:VAL:HG13	2.08	0.53
8:B:50:LYS:NZ	8:B:330:GLY:O	2.31	0.53
16:K:283:THR:HG22	16:K:284:ASN:H	1.71	0.53
5:5:381:ASP:OD2	5:5:385:ARG:NH1	2.41	0.53
13:G:134:TYR:CG	13:G:190:VAL:HG21	2.44	0.53
1:1:91:G:N2	1:1:95:A:OP2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:145:LEU:HD13	4:4:145:LEU:O	2.09	0.53
11:E:68:PRO:HG3	11:E:145:LEU:HD23	1.91	0.53
24:V:80:ARG:NH1	24:V:117:PRO:O	2.40	0.53
1:1:345:G:O2'	2:2:25:G:N3	2.42	0.53
1:1:726:G:N1	1:1:743:C:OP2	2.38	0.52
16:K:183:ASP:O	16:K:187:VAL:HG23	2.10	0.52
2:2:12:A:C2	2:2:13:A:C8	2.98	0.52
5:5:57:GLU:OE1	5:5:169:LYS:NZ	2.42	0.52
5:5:346:ASP:OD1	5:5:350:ARG:N	2.42	0.52
1:1:336:A:O2'	9:C:48:GLN:NE2	2.40	0.52
7:A:90:GLU:OE2	7:A:92:ARG:NH2	2.43	0.52
10:D:243:LEU:HD13	10:D:247:PRO:HB3	1.92	0.52
9:C:156:LEU:HD22	9:C:159:ILE:HD12	1.91	0.52
16:K:276:ILE:HD12	16:K:279:ILE:HD11	1.90	0.52
1:1:477:A:HO2'	1:1:478:A:P	2.32	0.52
1:1:337:G:OP2	9:C:196:ASN:ND2	2.41	0.52
4:4:147:ASP:OD1	4:4:148:GLU:N	2.43	0.52
9:C:229:ASN:OD1	9:C:230:VAL:N	2.43	0.52
18:M:85:TRP:HE1	18:M:91:CYS:HG	1.56	0.52
20:O:39:GLU:OE1	20:O:39:GLU:N	2.41	0.52
8:B:43:LEU:HB2	8:B:208:VAL:HG22	1.92	0.52
16:K:256:PRO:O	16:K:260:VAL:HG23	2.10	0.52
23:S:66:GLU:OE2	23:S:73:LYS:NZ	2.42	0.52
1:1:940:G:HO2'	1:1:1435:A:HO2'	1.53	0.51
1:1:401:U:O2'	1:1:402:A:OP2	2.15	0.51
1:1:456:U:O2'	1:1:457:C:P	2.68	0.51
1:1:34:A:H3'	1:1:48:A:H61	1.75	0.51
1:1:304:G:N2	1:1:312:C:O2	2.44	0.51
1:1:187:A:O2'	1:1:188:U:O4'	2.20	0.51
1:1:351:A:C4'	2:2:53:A:HO2'	2.22	0.51
1:1:1210:U:O4	25:W:3:ARG:NH2	2.43	0.51
1:1:1336:U:O2	1:1:1337:A:C8	2.63	0.51
1:1:3212:C:C2'	1:1:3213:A:O5'	2.59	0.51
23:S:155:ARG:NE	23:S:171:PHE:O	2.41	0.51
1:1:649:A:HO2'	1:1:650:C:P	2.34	0.51
9:C:131:VAL:O	9:C:135:VAL:HG23	2.10	0.51
1:1:3163:A:OP1	21:P:159:LYS:N	2.44	0.51
1:1:1108:U:O2	1:1:1108:U:O4'	2.29	0.51
16:K:70:ASP:N	16:K:70:ASP:OD1	2.40	0.50
14:H:55:VAL:HG21	14:H:71:VAL:HG11	1.94	0.50
1:1:609:G:O2'	9:C:312:VAL:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:289:A:C2	1:1:290:G:N7	2.80	0.50
1:1:720:A:O2'	1:1:721:G:P	2.69	0.50
1:1:1419:A:OP1	2:2:20:U:O2'	2.29	0.50
8:B:139:GLN:OE1	8:B:143:GLY:N	2.42	0.50
3:3:28:CYS:N	3:3:36:GLY:O	2.42	0.50
1:1:1192:C:H3'	1:1:1193:A:C5'	2.41	0.50
10:D:200:ARG:NH1	10:D:368:ASP:O	2.43	0.50
20:O:27:LEU:HD21	20:O:102:LEU:HB2	1.93	0.50
1:1:649:A:O2'	1:1:650:C:P	2.69	0.50
1:1:3109:G:N2	14:H:156:GLN:OE1	2.43	0.50
5:5:131:VAL:HG21	5:5:247:TRP:HZ3	1.76	0.50
1:1:631:U:O2	1:1:632:G:N7	2.45	0.49
20:O:54:TYR:OH	20:O:73:PHE:O	2.30	0.49
1:1:62:A:O2'	19:N:172:ARG:NH2	2.43	0.49
1:1:594:U:OP1	1:1:609:G:N1	2.42	0.49
1:1:1133:A:N6	1:1:1134:G:O6	2.45	0.49
1:1:437:G:O2'	1:1:621:A:N1	2.38	0.49
3:3:83:SER:OG	3:3:83:SER:O	2.29	0.49
19:N:155:VAL:O	19:N:162:ARG:NH2	2.43	0.49
20:O:120:VAL:HG12	20:O:122:GLN:HG2	1.94	0.49
1:1:611:A:O2'	1:1:612:U:OP2	2.25	0.49
1:1:2836:C:H5	1:1:2852:C:H41	1.60	0.49
16:K:254:LEU:HD22	16:K:254:LEU:H	1.77	0.49
19:N:124:ASP:OD2	19:N:125:SER:N	2.46	0.49
1:1:110:G:OP2	17:L:73:ARG:NH1	2.45	0.49
1:1:2:U:O2'	1:1:3:U:OP1	2.29	0.49
1:1:760:G:O2'	1:1:761:A:OP2	2.27	0.49
1:1:282:G:O6	1:1:286:U:N3	2.46	0.49
16:K:156:CYS:SG	16:K:157:GLY:N	2.85	0.49
1:1:3075:G:HO2'	1:1:3076:C:P	2.35	0.49
17:L:109:PHE:O	17:L:113:VAL:HG23	2.12	0.49
20:O:189:ASP:OD1	20:O:190:VAL:N	2.45	0.49
1:1:679:U:O2'	1:1:788:C:O2	2.29	0.48
2:2:11:C:C2	2:2:12:A:C8	3.01	0.48
14:H:41:ILE:HD13	14:H:71:VAL:HG22	1.94	0.48
17:L:105:ASN:ND2	17:L:107:GLU:OE1	2.44	0.48
1:1:3211:C:C2	1:1:3212:C:C5	3.01	0.48
1:1:80:G:OP1	19:N:189:LYS:NZ	2.31	0.48
1:1:593:C:O2'	1:1:594:U:O5'	2.24	0.48
1:1:1333:C:C2	1:1:1334:U:C5	3.02	0.48
1:1:1347:U:HO2'	1:1:1348:U:P	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:15:G:O3'	2:2:16:G:O4'	2.32	0.48
20:O:158:ALA:O	20:O:162:VAL:HG23	2.13	0.48
22:Q:81:VAL:HG13	22:Q:101:VAL:HG13	1.95	0.48
1:1:359:U:H4'	1:1:360:G:OP1	2.13	0.48
1:1:1278:A:O2'	1:1:1279:C:P	2.72	0.48
1:1:292:U:O2	1:1:292:U:O4'	2.32	0.48
2:2:14:C:H4'	21:P:123:PRO:HA	1.96	0.48
5:5:337:ASP:OD1	5:5:341:ASN:N	2.46	0.48
10:D:367:PRO:O	10:D:457:HIS:NE2	2.47	0.48
1:1:3212:C:OP2	18:M:124:ARG:NH2	2.46	0.48
11:E:52:VAL:HG21	11:E:65:ILE:HD12	1.95	0.48
11:E:70:LYS:N	11:E:142:ASP:OD2	2.45	0.48
20:O:174:PHE:O	20:O:178:VAL:HG23	2.14	0.48
1:1:2363:A:O2'	1:1:2364:G:O4'	2.21	0.48
9:C:156:LEU:CD2	9:C:159:ILE:HD12	2.44	0.48
1:1:1107:C:O2	1:1:1108:U:O2	2.32	0.47
1:1:3099:C:HO2'	1:1:3100:U:P	2.34	0.47
8:B:190:GLU:N	8:B:190:GLU:OE1	2.47	0.47
1:1:1416:C:OP1	3:3:143:ARG:NH1	2.43	0.47
8:B:159:ARG:NE	8:B:182:GLN:OE1	2.47	0.47
11:E:52:VAL:HG22	11:E:53:VAL:H	1.79	0.47
1:1:352:A:N7	1:1:367:A:N6	2.63	0.47
1:1:533:A:HO2'	1:1:535:G:H8	1.60	0.47
1:1:3121:U:H4'	1:1:3122:A:OP1	2.15	0.47
1:1:3210:A:OP1	18:M:109:ARG:NH1	2.44	0.47
5:5:404:ILE:HG21	5:5:407:ILE:HD11	1.95	0.47
9:C:222:VAL:HG13	9:C:225:VAL:HB	1.96	0.47
1:1:3208:G:O4'	1:1:3210:A:C8	2.68	0.47
16:K:159:ASP:O	16:K:163:VAL:HG12	2.15	0.47
1:1:3212:C:O2'	1:1:3213:A:O5'	2.29	0.47
14:H:23:ARG:O	14:H:25:VAL:HG23	2.14	0.47
1:1:720:A:O2'	1:1:721:G:OP2	2.32	0.47
1:1:1353:U:O2'	1:1:1354:G:N2	2.47	0.47
1:1:2826:U:N3	1:1:2827:U:O4	2.47	0.47
2:2:19:C:C2	2:2:20:U:C5	3.02	0.47
2:2:143:U:C2	2:2:144:G:C8	3.03	0.47
3:3:133:HIS:O	3:3:134:TYR:C	2.52	0.47
9:C:260:GLN:OE1	9:C:267:VAL:HG11	2.15	0.47
16:K:84:ASN:OD1	16:K:85:ASN:N	2.47	0.47
1:1:1296:C:N3	1:1:1297:C:C5	2.83	0.47
16:K:45:ILE:O	16:K:48:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:100:A:H3'	1:1:101:G:H21	1.80	0.47
10:D:461:THR:HG23	10:D:462:VAL:HG23	1.97	0.47
13:G:91:PHE:HE1	13:G:180:VAL:HG21	1.80	0.47
14:H:41:ILE:HG23	14:H:43:VAL:HG22	1.97	0.47
1:1:122:A:N6	1:1:146:U:O4'	2.47	0.47
1:1:1257:C:H4'	1:1:1258:U:OP1	2.15	0.47
1:1:3022:G:N2	1:1:3032:A:OP2	2.38	0.47
1:1:3207:U:H3	23:S:164:SER:HG	1.63	0.47
5:5:131:VAL:HG21	5:5:247:TRP:CZ3	2.49	0.47
7:A:88:PHE:O	7:A:99:LEU:HD12	2.15	0.47
1:1:296:A:O2'	1:1:297:G:O4'	2.24	0.46
1:1:665:A:N6	1:1:798:G:O6	2.48	0.46
1:1:1278:A:HO2'	1:1:1279:C:H6	1.59	0.46
1:1:3008:A:N6	1:1:3139:A:N6	2.63	0.46
10:D:291:LYS:HB2	10:D:358:VAL:HG23	1.97	0.46
20:O:153:VAL:O	20:O:156:LEU:HD23	2.15	0.46
1:1:752:C:HO2'	1:1:753:C:C5'	2.27	0.46
1:1:1172:G:O2'	1:1:1179:A:N1	2.38	0.46
1:1:3213:A:OP2	18:M:128:ARG:NH2	2.48	0.46
1:1:2382:G:OP1	20:O:85:ARG:NH1	2.47	0.46
1:1:2830:G:H2'	1:1:2831:G:C8	2.50	0.46
8:B:280:HIS:ND1	8:B:325:LYS:O	2.48	0.46
11:E:52:VAL:HG23	11:E:67:GLY:HA2	1.95	0.46
16:K:162:THR:HG23	16:K:163:VAL:N	2.31	0.46
1:1:196:G:N1	1:1:199:A:OP2	2.40	0.46
1:1:406:G:N2	2:2:16:G:C4	2.84	0.46
1:1:707:U:O4'	1:1:779:G:N2	2.48	0.46
1:1:1150:A:C8	1:1:1310:G:O4'	2.69	0.46
1:1:1276:U:O2'	1:1:1277:C:P	2.74	0.46
1:1:3019:U:O2	1:1:3019:U:O5'	2.34	0.46
4:4:132:GLN:O	4:4:133:LEU:HB2	2.14	0.46
8:B:132:LYS:O	8:B:136:LYS:N	2.43	0.46
9:C:289:ILE:HG21	22:Q:32:LEU:HD11	1.97	0.46
19:N:124:ASP:N	19:N:127:TYR:O	2.46	0.46
1:1:3020:U:H3'	1:1:3021:A:H5'	1.98	0.46
1:1:3313:U:O4	1:1:3314:A:N6	2.48	0.46
2:2:8:C:C2	2:2:9:A:C8	3.04	0.46
8:B:156:SER:O	8:B:188:ILE:HG21	2.16	0.46
21:P:87:SER:O	21:P:91:VAL:HG23	2.15	0.46
23:S:132:THR:O	23:S:133:ALA:HB3	2.16	0.46
1:1:717:C:HO2'	1:1:718:G:C5'	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:451:LEU:HD12	10:D:485:VAL:HG21	1.97	0.46
8:B:73:VAL:HG12	24:V:88:ARG:O	2.16	0.46
14:H:67:ALA:HA	14:H:70:THR:HG22	1.96	0.46
1:1:69:C:O2'	1:1:101:G:O2'	1.99	0.46
1:1:3220:G:C6	1:1:3266:G:N1	2.84	0.46
14:H:20:ILE:N	18:M:6:ILE:O	2.39	0.46
21:P:51:VAL:HG21	21:P:58:ILE:HD11	1.98	0.46
1:1:93:C:HO2'	1:1:94:G:C5'	2.26	0.46
1:1:563:U:OP1	23:S:68:HIS:NE2	2.49	0.46
8:B:31:ALA:O	8:B:339:ARG:NH1	2.46	0.46
1:1:400:G:O2'	1:1:401:U:OP2	2.27	0.46
1:1:752:C:H2'	1:1:753:C:C6	2.50	0.46
5:5:13:ILE:O	5:5:38:HIS:N	2.48	0.46
14:H:23:ARG:NH1	14:H:39:LYS:O	2.48	0.46
1:1:75:G:H5"	17:L:58:VAL:HG13	1.98	0.45
1:1:651:G:O2'	1:1:1435:A:OP1	2.35	0.45
1:1:3071:U:OP2	1:1:3073:A:N6	2.49	0.45
8:B:160:VAL:O	8:B:181:ILE:N	2.40	0.45
1:1:150:A:C2	1:1:151:A:C8	3.04	0.45
2:2:71:A:H4'	2:2:72:A:O5'	2.17	0.45
6:6:16:U:HO2'	6:6:17:G:P	2.30	0.45
8:B:57:VAL:HG12	8:B:73:VAL:CG2	2.43	0.45
8:B:140:ASP:OD1	8:B:141:GLY:N	2.50	0.45
1:1:548:G:HO2'	1:1:549:U:P	2.33	0.45
1:1:677:A:N6	1:1:786:A:O4'	2.49	0.45
16:K:158:LYS:O	16:K:162:THR:HG22	2.17	0.45
17:L:93:ILE:HG22	17:L:93:ILE:O	2.17	0.45
1:1:3059:G:O2'	1:1:3373:U:O2'	2.24	0.45
2:2:85:G:O6	26:Y:114:ASP:N	2.41	0.45
10:D:193:LEU:HD11	10:D:195:ILE:HD11	1.99	0.45
1:1:648:C:C2	1:1:649:A:C8	3.04	0.45
4:4:212:THR:O	4:4:214:LEU:N	2.50	0.45
1:1:151:A:C5	1:1:152:U:C5	3.05	0.45
7:A:136:VAL:HB	7:A:176:VAL:HG12	1.99	0.45
1:1:412:G:C6	2:2:12:A:C6	3.04	0.44
1:1:1257:C:H2'	1:1:1258:U:C6	2.52	0.44
1:1:3196:U:O2	1:1:3197:G:N1	2.50	0.44
1:1:3304:U:O3'	8:B:334:ARG:NH2	2.50	0.44
13:G:132:VAL:HG12	13:G:200:LEU:CD2	2.47	0.44
14:H:34:LEU:HD12	14:H:82:VAL:HG23	1.99	0.44
16:K:106:PHE:CE1	16:K:234:LEU:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:229:VAL:HG22	16:K:233:GLN:OE1	2.17	0.44
1:1:75:G:O2'	1:1:76:G:P	2.72	0.44
2:2:114:G:O2'	2:2:115:C:P	2.72	0.44
8:B:161:LEU:CD2	8:B:178:LEU:HD12	2.47	0.44
19:N:18:VAL:HG13	19:N:19:LEU:N	2.32	0.44
20:O:118:VAL:HG21	23:S:163:PHE:HB3	2.00	0.44
1:1:949:C:O2'	1:1:971:G:OP1	2.30	0.44
6:6:1:C:N4	13:G:85:ASN:OD1	2.50	0.44
12:F:84:VAL:HG12	12:F:137:GLY:O	2.17	0.44
14:H:48:VAL:HG13	14:H:49:ASN:N	2.33	0.44
15:J:250:SER:O	15:J:254:VAL:HG23	2.17	0.44
1:1:2367:A:N1	1:1:2368:A:N6	2.66	0.44
8:B:117:ARG:NE	8:B:176:ALA:O	2.39	0.44
1:1:164:A:HO2'	1:1:166:C:C1'	2.19	0.44
1:1:406:G:N2	2:2:16:G:O2'	2.50	0.44
1:1:1347:U:O2'	1:1:1348:U:P	2.74	0.44
1:1:3185:U:H2'	20:O:126:VAL:HG21	2.00	0.44
4:4:158:PRO:O	4:4:224:ILE:HD11	2.17	0.44
1:1:150:A:N3	1:1:150:A:H2'	2.32	0.44
1:1:208:C:H2'	1:1:209:A:O4'	2.17	0.44
17:L:86:THR:HG23	17:L:89:TYR:H	1.82	0.44
1:1:1412:G:C2	1:1:1413:G:C8	3.05	0.44
7:A:144:GLU:OE2	7:A:150:GLN:NE2	2.45	0.44
1:1:84:U:OP2	1:1:85:A:O2'	2.25	0.44
1:1:596:C:O2	9:C:326:ARG:NE	2.51	0.44
1:1:931:C:OP2	1:1:932:U:O2'	2.30	0.44
1:1:1174:G:N2	20:O:87:MET:SD	2.91	0.44
1:1:2369:G:O2'	1:1:2370:G:O5'	2.26	0.44
1:1:2900:A:C2	1:1:2901:G:C8	3.06	0.44
1:1:290:G:C5	1:1:291:C:C5	3.06	0.44
1:1:591:G:O2'	11:E:17:ALA:O	2.31	0.44
1:1:1413:G:C2	1:1:1414:G:N7	2.86	0.44
2:2:57:C:O2	2:2:61:A:O2'	2.32	0.44
6:6:33:U:OP2	16:K:285:ARG:NH1	2.51	0.44
8:B:331:ASN:ND2	8:B:332:ARG:O	2.50	0.44
11:E:131:LYS:O	11:E:135:VAL:HG23	2.18	0.44
13:G:77:GLN:HA	13:G:229:VAL:HG22	1.98	0.44
14:H:132:VAL:HG23	14:H:154:VAL:HG22	2.00	0.44
17:L:80:VAL:HG12	17:L:85:LEU:O	2.18	0.44
25:W:26:ILE:O	25:W:30:VAL:HG23	2.18	0.44
1:1:1157:G:H2'	1:1:1158:A:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1350:A:H62	9:C:287:THR:HG22	1.83	0.43
1:1:277:G:C6	1:1:289:A:C6	3.06	0.43
1:1:340:C:OP2	9:C:195:ARG:NH1	2.44	0.43
1:1:1340:G:H2'	1:1:1341:U:C6	2.53	0.43
1:1:1383:G:O2'	9:C:243:HIS:ND1	2.47	0.43
8:B:62:ARG:O	8:B:68:HIS:ND1	2.51	0.43
8:B:283:TYR:CD1	8:B:356:LEU:HD21	2.53	0.43
10:D:296:LEU:HD13	10:D:302:VAL:HG22	1.98	0.43
13:G:158:ASP:HB3	13:G:159:PRO:HD3	2.00	0.43
17:L:29:ALA:O	17:L:33:VAL:HG23	2.17	0.43
25:W:30:VAL:HG22	25:W:66:ILE:CG2	2.48	0.43
1:1:1188:U:OP1	1:1:1210:U:O2'	2.30	0.43
1:1:3018:C:C4	1:1:3019:U:C4	3.06	0.43
3:3:5:ILE:O	3:3:9:VAL:HG23	2.19	0.43
8:B:187:SER:OG	8:B:190:GLU:OE1	2.23	0.43
10:D:308:LEU:HD21	10:D:429:LEU:HD22	2.00	0.43
1:1:74:G:OP2	17:L:104:ARG:NH1	2.50	0.43
1:1:1150:A:C6	1:1:1151:U:C4	3.06	0.43
1:1:1307:G:HO2'	1:1:1308:A:P	2.37	0.43
1:1:1389:G:O2'	1:1:1418:A:N1	2.44	0.43
1:1:3017:A:C2	1:1:3018:C:C5	3.06	0.43
16:K:97:LEU:HD11	16:K:205:THR:HG23	2.00	0.43
16:K:155:ILE:HG22	16:K:156:CYS:N	2.33	0.43
19:N:106:VAL:HG11	19:N:132:VAL:HG11	2.00	0.43
1:1:645:A:H2'	1:1:646:A:O4'	2.19	0.43
1:1:655:C:H2'	1:1:656:A:H8	1.84	0.43
1:1:430:U:O4	1:1:630:A:N6	2.51	0.43
21:P:114:VAL:HG13	21:P:114:VAL:O	2.18	0.43
1:1:1294:A:C2	1:1:1295:G:C8	3.07	0.43
1:1:346:C:O2	1:1:348:A:N6	2.52	0.43
1:1:628:A:H2'	1:1:629:U:C6	2.54	0.43
1:1:791:A:C2	1:1:792:G:C5	3.07	0.43
1:1:1404:G:N2	1:1:1407:A:OP2	2.20	0.43
3:3:14:PHE:O	3:3:14:PHE:CG	2.70	0.43
5:5:326:GLU:OE1	5:5:326:GLU:N	2.52	0.43
16:K:83:VAL:HG21	16:K:270:LEU:CD1	2.46	0.43
1:1:369:A:O2'	1:1:370:U:H5"	2.19	0.43
1:1:628:A:H2'	1:1:629:U:O4'	2.19	0.43
1:1:1277:C:O2'	1:1:1278:A:OP2	2.32	0.43
1:1:1361:U:O2	12:F:159:GLN:NE2	2.52	0.43
1:1:3023:U:O2	1:1:3023:U:O4'	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:7:U:C2	2:2:8:C:C5	3.07	0.43
1:1:82:C:H2'	1:1:83:U:O4'	2.19	0.43
6:6:39:U:O2	6:6:39:U:O4'	2.37	0.43
9:C:320:ASN:O	9:C:322:GLN:N	2.52	0.43
16:K:77:ASP:O	16:K:251:LEU:N	2.52	0.43
20:O:118:VAL:HG22	20:O:119:VAL:H	1.83	0.43
1:1:3214:U:OP2	18:M:128:ARG:NH2	2.38	0.42
1:1:1415:U:H2'	1:1:1416:C:O4'	2.19	0.42
1:1:3020:U:H3'	1:1:3021:A:C5'	2.49	0.42
1:1:150:A:N1	1:1:151:A:C8	2.88	0.42
1:1:1128:U:O2'	1:1:1129:A:O3'	2.37	0.42
1:1:1188:U:O2'	1:1:1190:A:N7	2.47	0.42
1:1:1293:U:C2	1:1:1294:A:C8	3.08	0.42
1:1:1150:A:H2'	1:1:1150:A:N3	2.34	0.42
1:1:3305:A:OP1	8:B:334:ARG:NH2	2.52	0.42
1:1:30:G:OP1	19:N:172:ARG:NE	2.44	0.42
1:1:296:A:N3	1:1:299:G:O2'	2.53	0.42
1:1:753:C:H2'	1:1:754:G:O4'	2.19	0.42
1:1:3275:U:OP2	1:1:3276:G:N1	2.53	0.42
16:K:45:ILE:HD13	16:K:251:LEU:HD21	2.00	0.42
21:P:119:VAL:HG23	21:P:146:ILE:HG13	2.01	0.42
1:1:67:A:O2'	1:1:315:C:O2	2.29	0.42
1:1:311:C:H2'	1:1:312:C:O4'	2.20	0.42
1:1:400:G:H1'	1:1:401:U:OP2	2.20	0.42
1:1:976:U:O2	1:1:976:U:O5'	2.38	0.42
7:A:42:ASN:OD1	7:A:43:TYR:N	2.47	0.42
12:F:98:LYS:HB3	12:F:99:PRO:HD3	2.02	0.42
1:1:199:A:C2	1:1:219:A:C5	3.08	0.42
1:1:372:A:H2'	1:1:373:A:O4'	2.19	0.42
1:1:429:U:C2	1:1:430:U:C5	3.08	0.42
1:1:562:C:OP2	18:M:77:ARG:NH1	2.53	0.42
2:2:18:U:N3	2:2:19:C:C5	2.87	0.42
5:5:268:TYR:N	5:5:284:THR:OG1	2.53	0.42
1:1:341:G:N1	2:2:24:G:O6	2.53	0.42
1:1:82:C:N3	1:1:104:G:N1	2.67	0.42
1:1:90:C:HO2'	1:1:281:G:C2'	2.29	0.42
1:1:295:A:HO2'	1:1:296:A:C5'	2.33	0.42
1:1:1185:C:N4	1:1:1186:G:O6	2.52	0.42
1:1:3124:G:OP2	20:O:134:LYS:NZ	2.46	0.42
2:2:6:U:C2	2:2:7:U:C5	3.08	0.42
2:2:77:A:H2'	2:2:78:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:142:SER:HA	20:O:145:VAL:HG22	2.02	0.42
1:1:123:A:N1	1:1:150:A:C8	2.88	0.41
1:1:432:G:C6	1:1:628:A:N1	2.88	0.41
2:2:72:A:OP2	26:Y:52:ARG:NH2	2.52	0.41
1:1:126:U:C2	1:1:127:G:C8	3.08	0.41
1:1:648:C:H2'	1:1:648:C:O2	2.19	0.41
1:1:1224:C:O4'	1:1:1288:U:O2'	2.36	0.41
1:1:1298:C:H2'	1:1:1299:U:O2	2.19	0.41
1:1:1307:G:O2'	1:1:1308:A:P	2.78	0.41
1:1:3173:G:N3	1:1:3173:G:H2'	2.35	0.41
4:4:102:PHE:CE2	4:4:128:VAL:HG11	2.54	0.41
6:6:40:U:O2	6:6:40:U:O4'	2.38	0.41
8:B:58:ARG:O	8:B:72:VAL:N	2.46	0.41
1:1:72:C:H4'	17:L:63:VAL:HG22	2.03	0.41
1:1:303:G:OP1	19:N:179:LYS:NZ	2.53	0.41
1:1:385:A:C2'	1:1:386:A:O5'	2.68	0.41
1:1:626:U:H2'	1:1:627:U:C6	2.55	0.41
10:D:175:LEU:HD13	10:D:179:LEU:HD12	2.01	0.41
20:O:50:ASN:ND2	20:O:136:THR:OG1	2.54	0.41
1:1:303:G:H2'	1:1:304:G:C8	2.56	0.41
1:1:303:G:C6	1:1:313:A:N6	2.88	0.41
3:3:128:ARG:O	3:3:129:GLU:C	2.58	0.41
8:B:341:SER:O	8:B:342:LEU:HB2	2.21	0.41
16:K:79:GLN:N	16:K:249:GLY:O	2.46	0.41
1:1:454:C:H2'	1:1:455:C:C6	2.55	0.41
1:1:1278:A:O2'	1:1:1279:C:H6	2.03	0.41
1:1:1297:C:C2	1:1:1298:C:C5	3.09	0.41
3:3:114:LYS:O	3:3:118:VAL:HG23	2.20	0.41
16:K:276:ILE:O	16:K:297:VAL:HG21	2.20	0.41
18:M:114:ASP:OD1	18:M:117:ARG:NH1	2.51	0.41
1:1:546:C:OP1	1:1:548:G:N2	2.54	0.41
1:1:808:A:H2'	1:1:809:G:C8	2.55	0.41
13:G:232:HIS:O	13:G:233:TRP:C	2.59	0.41
1:1:199:A:C4	1:1:201:A:C8	3.08	0.41
1:1:1111:U:HO2'	1:1:1112:A:P	2.42	0.41
1:1:1192:C:H4'	1:1:1193:A:OP2	2.19	0.41
1:1:1256:G:H2'	1:1:1257:C:O4'	2.20	0.41
9:C:300:ARG:NH2	22:Q:38:ARG:O	2.53	0.41
14:H:18:VAL:HG23	14:H:18:VAL:O	2.21	0.41
23:S:71:LYS:HB3	23:S:73:LYS:HZ2	1.85	0.41
23:S:112:ALA:O	23:S:115:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:228:U:N3	1:1:229:G:N7	2.68	0.41
1:1:580:C:OP1	9:C:321:LYS:NZ	2.38	0.41
1:1:782:U:H2'	1:1:783:A:C1'	2.50	0.41
1:1:1257:C:HO2'	1:1:1258:U:P	2.39	0.41
1:1:1263:A:H2'	1:1:1263:A:N3	2.36	0.41
1:1:1334:U:C2	1:1:1335:C:C5	3.09	0.41
1:1:2995:A:HO2'	1:1:2996:U:P	2.33	0.41
1:1:209:A:N3	9:C:221:ASN:ND2	2.65	0.41
1:1:268:A:N7	19:N:12:ARG:NH1	2.69	0.41
1:1:271:C:C2	1:1:295:A:N6	2.89	0.41
1:1:432:G:H2'	1:1:433:A:O4'	2.21	0.41
1:1:965:A:H2'	1:1:966:U:O4'	2.20	0.41
1:1:1231:A:N6	1:1:1276:U:OP2	2.54	0.41
1:1:2367:A:C2	1:1:2368:A:N7	2.89	0.41
1:1:2901:G:O3'	14:H:170:LYS:NZ	2.52	0.41
1:1:3009:G:N2	8:B:15:GLY:O	2.49	0.41
3:3:85:ASN:OD1	3:3:88:LYS:HB3	2.21	0.41
4:4:137:GLN:O	4:4:138:SER:C	2.59	0.41
7:A:41:VAL:HG12	7:A:46:ARG:CG	2.51	0.41
1:1:2:U:HO2'	1:1:3:U:P	2.44	0.41
6:6:15:C:C4'	6:6:16:U:OP2	2.69	0.41
16:K:129:ASP:O	16:K:132:ILE:HG22	2.20	0.41
1:1:1208:U:O2	1:1:1208:U:O4'	2.39	0.40
1:1:1383:G:OP1	9:C:203:ARG:NE	2.52	0.40
1:1:2999:U:O2	1:1:3149:G:O6	2.39	0.40
19:N:119:TYR:OH	19:N:131:GLU:OE1	2.25	0.40
23:S:139:TYR:CE2	23:S:140:VAL:HG23	2.56	0.40
1:1:406:G:HO2'	1:1:407:A:P	2.44	0.40
8:B:44:THR:HG22	8:B:184:ASN:OD1	2.20	0.40
8:B:306:THR:HG23	8:B:311:PHE:CE2	2.57	0.40
16:K:221:THR:O	16:K:224:ASN:OD1	2.40	0.40
16:K:271:ILE:CG1	16:K:276:ILE:HD11	2.52	0.40
1:1:753:C:C4	1:1:754:G:C6	3.09	0.40
1:1:756:U:H3'	1:1:757:C:H5"	2.02	0.40
1:1:952:A:O3'	1:1:953:G:O4'	2.40	0.40
1:1:1149:G:C6	1:1:1152:G:OP2	2.75	0.40
1:1:3021:A:O4'	1:1:3023:U:C2	2.74	0.40
1:1:3216:G:O6	1:1:3259:U:O2'	2.32	0.40
13:G:150:LEU:HG	13:G:215:VAL:HG22	2.03	0.40
13:G:211:LEU:O	13:G:215:VAL:HG23	2.22	0.40
24:V:86:ARG:NH1	24:V:87:ARG:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:576:C:OP1	12:F:241:LYS:NZ	2.47	0.40
1:1:583:G:C2	1:1:584:G:C8	3.09	0.40
1:1:3057:U:H3'	1:1:3058:U:H4'	2.03	0.40
5:5:156:VAL:HG12	5:5:166:ILE:CD1	2.51	0.40
9:C:269:SER:O	9:C:270:SER:OG	2.39	0.40
10:D:129:GLN:O	10:D:133:VAL:HG23	2.21	0.40
19:N:145:ASP:O	19:N:149:ASN:N	2.54	0.40
1:1:498:A:C6	1:1:616:G:O6	2.75	0.40
1:1:706:A:N6	1:1:714:G:O6	2.53	0.40
1:1:951:A:N1	1:1:1369:A:C2	2.89	0.40
9:C:77:VAL:HG21	9:C:84:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	171/306 (56%)	161 (94%)	9 (5%)	1 (1%)	25	64
4	4	209/278 (75%)	191 (91%)	18 (9%)	0	100	100
5	5	377/463 (81%)	364 (97%)	13 (3%)	0	100	100
7	A	138/291 (47%)	124 (90%)	14 (10%)	0	100	100
8	B	329/387 (85%)	316 (96%)	13 (4%)	0	100	100
9	C	341/362 (94%)	323 (95%)	18 (5%)	0	100	100
10	D	433/505 (86%)	413 (95%)	20 (5%)	0	100	100
11	E	147/176 (84%)	142 (97%)	5 (3%)	0	100	100
12	F	239/244 (98%)	236 (99%)	3 (1%)	0	100	100
13	G	155/256 (60%)	151 (97%)	4 (3%)	0	100	100
14	H	166/191 (87%)	159 (96%)	6 (4%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	J	59/427 (14%)	59 (100%)	0	0	100	100
16	K	253/376 (67%)	240 (95%)	13 (5%)	0	100	100
17	L	106/199 (53%)	97 (92%)	7 (7%)	2 (2%)	8	40
18	M	132/138 (96%)	130 (98%)	2 (2%)	0	100	100
19	N	173/204 (85%)	171 (99%)	2 (1%)	0	100	100
20	O	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
21	P	133/184 (72%)	131 (98%)	2 (2%)	0	100	100
22	Q	129/186 (69%)	128 (99%)	1 (1%)	0	100	100
23	S	168/172 (98%)	156 (93%)	12 (7%)	0	100	100
24	V	92/137 (67%)	91 (99%)	1 (1%)	0	100	100
25	W	171/236 (72%)	167 (98%)	4 (2%)	0	100	100
26	Y	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
27	b	237/647 (37%)	230 (97%)	7 (3%)	0	100	100
28	e	123/130 (95%)	120 (98%)	3 (2%)	0	100	100
29	f	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
30	h	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
31	i	72/100 (72%)	70 (97%)	2 (3%)	0	100	100
32	j	69/88 (78%)	65 (94%)	4 (6%)	0	100	100
33	m	152/807 (19%)	145 (95%)	7 (5%)	0	100	100
34	n	326/605 (54%)	317 (97%)	9 (3%)	0	100	100
35	o	131/220 (60%)	127 (97%)	4 (3%)	0	100	100
36	r	50/261 (19%)	50 (100%)	0	0	100	100
37	t	234/322 (73%)	222 (95%)	12 (5%)	0	100	100
38	v	124/231 (54%)	118 (95%)	6 (5%)	0	100	100
39	x	261/295 (88%)	243 (93%)	18 (7%)	0	100	100
40	y	211/245 (86%)	206 (98%)	5 (2%)	0	100	100
All	All	6650/10222 (65%)	6385 (96%)	261 (4%)	4 (0%)	54	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	134	TYR
17	L	63	VAL

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Mol	Chain	Res	Type
14	H	23	ARG
17	L	61	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	3	155/274 (57%)	152 (98%)	3 (2%)	57 80
4	4	203/257 (79%)	201 (99%)	2 (1%)	76 88
5	5	343/410 (84%)	342 (100%)	1 (0%)	92 97
7	A	136/263 (52%)	133 (98%)	3 (2%)	52 78
8	B	280/323 (87%)	274 (98%)	6 (2%)	53 79
9	C	273/289 (94%)	267 (98%)	6 (2%)	52 78
10	D	381/440 (87%)	373 (98%)	8 (2%)	53 79
11	E	131/153 (86%)	128 (98%)	3 (2%)	50 77
12	F	204/205 (100%)	203 (100%)	1 (0%)	88 94
13	G	128/208 (62%)	127 (99%)	1 (1%)	81 91
14	H	157/171 (92%)	156 (99%)	1 (1%)	86 94
15	J	58/383 (15%)	58 (100%)	0	100 100
16	K	238/346 (69%)	230 (97%)	8 (3%)	37 68
17	L	87/159 (55%)	87 (100%)	0	100 100
18	M	106/109 (97%)	104 (98%)	2 (2%)	57 80
19	N	153/176 (87%)	151 (99%)	2 (1%)	69 86
20	O	160/162 (99%)	157 (98%)	3 (2%)	57 80
21	P	109/146 (75%)	109 (100%)	0	100 100
22	Q	107/151 (71%)	106 (99%)	1 (1%)	78 90
23	S	155/156 (99%)	150 (97%)	5 (3%)	39 69
24	V	77/105 (73%)	77 (100%)	0	100 100
25	W	169/213 (79%)	167 (99%)	2 (1%)	71 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	Y	108/110 (98%)	106 (98%)	2 (2%)	57 80
27	b	231/573 (40%)	225 (97%)	6 (3%)	46 74
28	e	108/111 (97%)	106 (98%)	2 (2%)	57 80
29	f	90/91 (99%)	90 (100%)	0	100 100
30	h	104/105 (99%)	101 (97%)	3 (3%)	42 71
31	i	61/82 (74%)	60 (98%)	1 (2%)	62 83
32	j	59/71 (83%)	59 (100%)	0	100 100
33	m	145/723 (20%)	143 (99%)	2 (1%)	67 85
34	n	302/548 (55%)	300 (99%)	2 (1%)	84 93
35	o	118/199 (59%)	116 (98%)	2 (2%)	60 82
36	r	48/229 (21%)	48 (100%)	0	100 100
37	t	213/287 (74%)	208 (98%)	5 (2%)	50 77
38	v	116/205 (57%)	115 (99%)	1 (1%)	78 90
39	x	252/276 (91%)	248 (98%)	4 (2%)	62 83
40	y	185/211 (88%)	185 (100%)	0	100 100
All	All	5950/8920 (67%)	5862 (98%)	88 (2%)	66 84

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	11	ASN
3	3	40	ARG
3	3	71	HIS
4	4	69	LEU
4	4	148	GLU
5	5	107	GLU
7	A	43	TYR
7	A	103	LYS
7	A	106	ASN
8	B	46	PHE
8	B	100	ARG
8	B	182	GLN
8	B	332	ARG
8	B	349	LYS
8	B	385	LYS
9	C	93	MET
9	C	120	TYR

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Mol	Chain	Res	Type
9	C	177	ASP
9	C	182	LEU
9	C	259	ASP
9	C	306	THR
10	D	103	LEU
10	D	112	ARG
10	D	113	ASN
10	D	286	ARG
10	D	304	TYR
10	D	314	LEU
10	D	319	LEU
10	D	466	ASP
11	E	29	LYS
11	E	46	ARG
11	E	133	GLU
12	F	4	GLU
13	G	204	ARG
14	H	153	ASP
16	K	76	LYS
16	K	80	LEU
16	K	88	PHE
16	K	156	CYS
16	K	253	TRP
16	K	262	ASN
16	K	277	ARG
16	K	280	PHE
18	M	59	ASN
18	M	108	ARG
19	N	144	ARG
19	N	188	ARG
20	O	57	PHE
20	O	94	ARG
20	O	156	LEU
22	Q	78	ASN
23	S	12	ARG
23	S	106	LEU
23	S	166	LYS
23	S	171	PHE
23	S	172	TYR
25	W	60	TRP
25	W	220	TYR
26	Y	51	ARG

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Mol	Chain	Res	Type
26	Y	74	TYR
27	b	15	ASN
27	b	70	ASN
27	b	159	ARG
27	b	180	LYS
27	b	442	TYR
27	b	462	LYS
28	e	33	ARG
28	e	98	HIS
30	h	38	ARG
30	h	59	ASN
30	h	119	LYS
31	i	53	TYR
33	m	306	TYR
33	m	322	MET
34	n	64	TYR
34	n	81	ARG
35	o	175	LYS
35	o	177	TYR
37	t	157	ASN
37	t	160	PHE
37	t	167	ARG
37	t	187	LEU
37	t	291	GLN
38	v	31	GLN
39	x	163	ILE
39	x	165	LEU
39	x	215	GLN
39	x	223	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	106	HIS
7	A	75	ASN
9	C	48	GLN
9	C	116	ASN
9	C	213	ASN
10	D	113	ASN
10	D	141	HIS
10	D	251	ASN
10	D	441	GLN

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Mol	Chain	Res	Type
12	F	157	ASN
13	G	145	ASN
14	H	59	ASN
16	K	262	ASN
18	M	41	GLN
18	M	59	ASN
20	O	50	ASN
22	Q	58	ASN
23	S	63	GLN
27	b	15	ASN
27	b	70	ASN
27	b	124	GLN
28	e	49	ASN
28	e	98	HIS
30	h	59	ASN
34	n	456	HIS
37	t	157	ASN
37	t	269	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1615/3396 (47%)	296 (18%)	27 (1%)
2	2	147/158 (93%)	25 (17%)	1 (0%)
6	6	64/232 (27%)	26 (40%)	2 (3%)
All	All	1826/3786 (48%)	347 (19%)	30 (1%)

All (347) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	3	U
1	1	20	A
1	1	26	A
1	1	34	A
1	1	38	U
1	1	49	A
1	1	60	A
1	1	65	A
1	1	66	A
1	1	76	G

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Mol	Chain	Res	Type
1	1	94	G
1	1	109	A
1	1	110	G
1	1	116	A
1	1	118	U
1	1	122	A
1	1	136	G
1	1	150	A
1	1	153	U
1	1	156	G
1	1	165	A
1	1	170	G
1	1	190	U
1	1	191	U
1	1	200	C
1	1	210	U
1	1	218	G
1	1	219	A
1	1	220	G
1	1	221	A
1	1	234	G
1	1	240	U
1	1	243	G
1	1	246	U
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	265	A
1	1	268	A
1	1	269	G
1	1	282	G
1	1	283	G
1	1	284	A
1	1	285	A
1	1	286	U
1	1	305	U
1	1	311	C
1	1	325	A
1	1	329	U
1	1	352	A
1	1	360	G

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Mol	Chain	Res	Type
1	1	368	G
1	1	370	U
1	1	375	A
1	1	376	G
1	1	383	G
1	1	384	A
1	1	385	A
1	1	386	A
1	1	388	G
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	404	G
1	1	421	G
1	1	422	A
1	1	429	U
1	1	438	A
1	1	439	C
1	1	442	G
1	1	454	C
1	1	457	C
1	1	459	G
1	1	462	C
1	1	463	C
1	1	464	U
1	1	465	U
1	1	468	G
1	1	478	A
1	1	479	U
1	1	480	C
1	1	481	U
1	1	482	C
1	1	521	A
1	1	533	A
1	1	544	C
1	1	545	U
1	1	547	G
1	1	548	G
1	1	549	U
1	1	551	A

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Mol	Chain	Res	Type
1	1	552	G
1	1	555	U
1	1	556	U
1	1	557	A
1	1	559	A
1	1	569	A
1	1	578	A
1	1	579	G
1	1	589	A
1	1	592	A
1	1	604	G
1	1	611	A
1	1	619	A
1	1	621	A
1	1	636	C
1	1	638	C
1	1	645	A
1	1	647	A
1	1	650	C
1	1	660	A
1	1	661	G
1	1	677	A
1	1	681	U
1	1	705	A
1	1	716	A
1	1	717	C
1	1	718	G
1	1	721	G
1	1	722	G
1	1	725	G
1	1	735	A
1	1	737	G
1	1	750	G
1	1	753	C
1	1	756	U
1	1	757	C
1	1	761	A
1	1	775	A
1	1	777	U
1	1	779	G
1	1	783	A
1	1	784	A

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Mol	Chain	Res	Type
1	1	785	G
1	1	806	A
1	1	817	A
1	1	926	A
1	1	930	U
1	1	933	A
1	1	937	G
1	1	938	C
1	1	944	C
1	1	951	A
1	1	953	G
1	1	956	U
1	1	957	C
1	1	959	C
1	1	961	C
1	1	962	A
1	1	977	C
1	1	978	G
1	1	979	U
1	1	980	A
1	1	982	C
1	1	1103	A
1	1	1104	G
1	1	1111	U
1	1	1112	A
1	1	1116	G
1	1	1124	U
1	1	1125	U
1	1	1129	A
1	1	1130	A
1	1	1131	G
1	1	1132	C
1	1	1133	A
1	1	1139	G
1	1	1140	G
1	1	1144	U
1	1	1153	A
1	1	1155	C
1	1	1159	A
1	1	1180	A
1	1	1181	U
1	1	1189	C

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Mol	Chain	Res	Type
1	1	1191	U
1	1	1193	A
1	1	1196	C
1	1	1220	U
1	1	1221	A
1	1	1222	G
1	1	1223	A
1	1	1227	C
1	1	1245	A
1	1	1246	G
1	1	1253	U
1	1	1258	U
1	1	1261	G
1	1	1262	G
1	1	1263	A
1	1	1277	C
1	1	1278	A
1	1	1279	C
1	1	1286	A
1	1	1287	A
1	1	1301	A
1	1	1307	G
1	1	1308	A
1	1	1310	G
1	1	1313	G
1	1	1330	A
1	1	1332	A
1	1	1348	U
1	1	1350	A
1	1	1353	U
1	1	1354	G
1	1	1355	A
1	1	1386	A
1	1	1399	A
1	1	1400	G
1	1	1408	G
1	1	1417	G
1	1	1418	A
1	1	1419	A
1	1	1437	C
1	1	2353	G
1	1	2364	G

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Mol	Chain	Res	Type
1	1	2373	A
1	1	2374	C
1	1	2825	C
1	1	2836	C
1	1	2837	A
1	1	2849	C
1	1	2856	G
1	1	2858	U
1	1	2899	C
1	1	2996	U
1	1	3012	A
1	1	3021	A
1	1	3022	G
1	1	3028	G
1	1	3029	A
1	1	3032	A
1	1	3049	A
1	1	3057	U
1	1	3058	U
1	1	3061	G
1	1	3067	C
1	1	3072	C
1	1	3073	A
1	1	3075	G
1	1	3076	C
1	1	3078	U
1	1	3088	G
1	1	3099	C
1	1	3100	U
1	1	3101	G
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3164	C
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3181	C
1	1	3187	A
1	1	3189	G

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Mol	Chain	Res	Type
1	1	3196	U
1	1	3198	U
1	1	3199	G
1	1	3207	U
1	1	3213	A
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3229	G
1	1	3244	A
1	1	3245	A
1	1	3246	G
1	1	3250	U
1	1	3259	U
1	1	3260	G
1	1	3270	U
1	1	3273	A
1	1	3275	U
1	1	3276	G
1	1	3286	G
1	1	3289	G
1	1	3294	A
1	1	3304	U
1	1	3317	U
1	1	3330	A
1	1	3331	U
1	1	3333	G
1	1	3340	G
1	1	3366	G
1	1	3368	U
1	1	3370	A
1	1	3382	U
1	1	3390	G
2	2	16	G
2	2	34	U
2	2	35	C
2	2	39	G
2	2	40	A
2	2	51	G
2	2	52	A
2	2	59	A
2	2	62	C

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Mol	Chain	Res	Type
2	2	63	G
2	2	79	A
2	2	80	A
2	2	82	U
2	2	86	U
2	2	87	G
2	2	90	U
2	2	95	G
2	2	104	A
2	2	106	C
2	2	107	G
2	2	109	A
2	2	115	C
2	2	123	G
2	2	157	U
2	2	158	U
6	6	2	C
6	6	4	U
6	6	5	C
6	6	6	U
6	6	7	C
6	6	8	A
6	6	13	U
6	6	15	C
6	6	16	U
6	6	17	G
6	6	34	A
6	6	36	U
6	6	39	U
6	6	40	U
6	6	42	G
6	6	43	A
6	6	47	A
6	6	52	G
6	6	53	A
6	6	54	A
6	6	56	U
6	6	59	C
6	6	228	U
6	6	229	U
6	6	231	A
6	6	232	A

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	75	G
1	1	93	C
1	1	155	G
1	1	250	U
1	1	310	U
1	1	359	U
1	1	400	G
1	1	401	U
1	1	456	U
1	1	477	A
1	1	480	C
1	1	548	G
1	1	551	A
1	1	649	A
1	1	659	G
1	1	720	A
1	1	755	A
1	1	1128	U
1	1	1257	C
1	1	1276	U
1	1	1347	U
1	1	2857	C
1	1	2995	A
1	1	3218	A
1	1	3228	C
1	1	3269	U
1	1	3339	A
2	2	114	G
6	6	15	C
6	6	227	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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

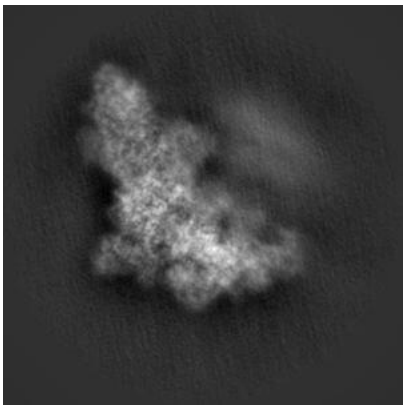
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12911. These allow visual inspection of the internal detail of the map and identification of artifacts.

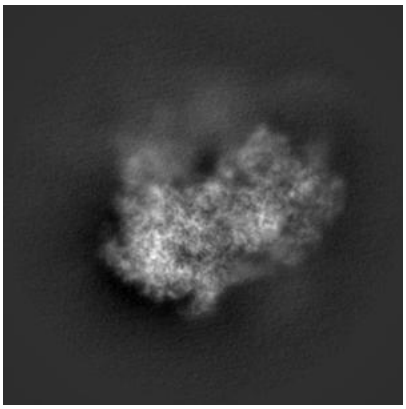
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

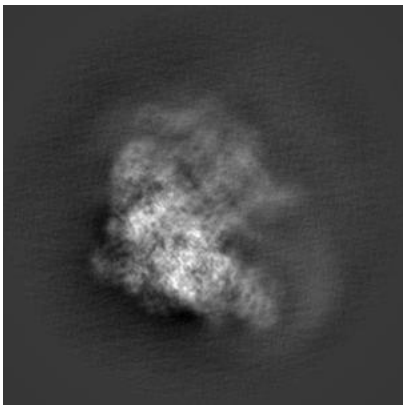
6.1.1 Primary map



X

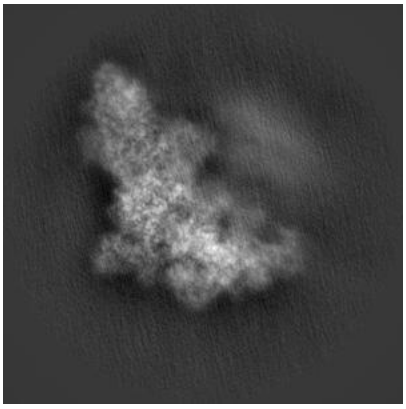


Y

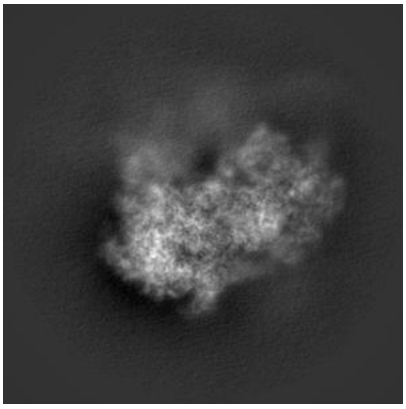


Z

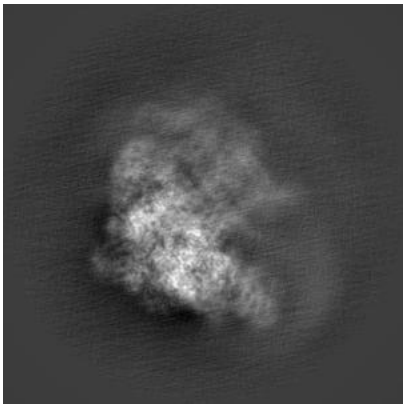
6.1.2 Raw map



X



Y

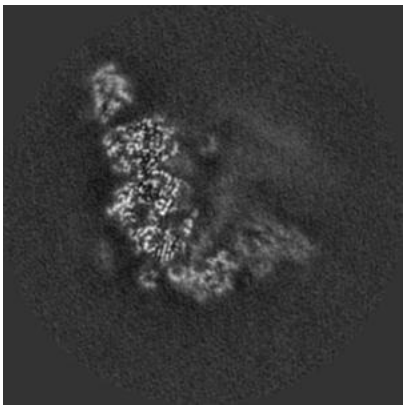


Z

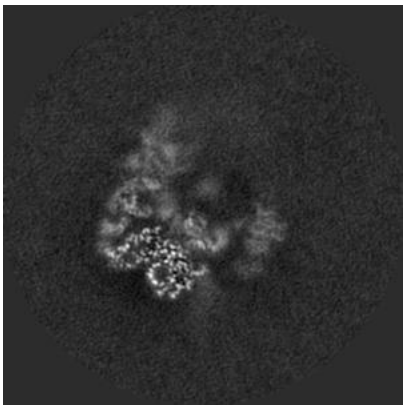
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

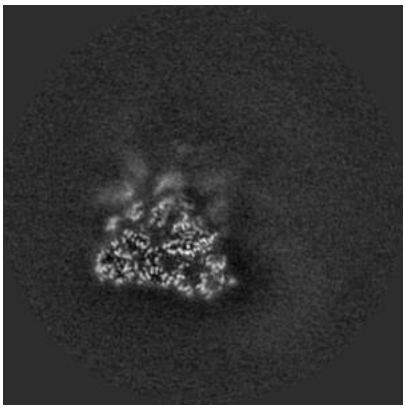
6.2.1 Primary map



X Index: 200

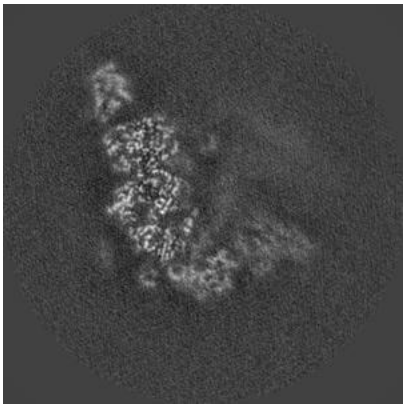


Y Index: 200

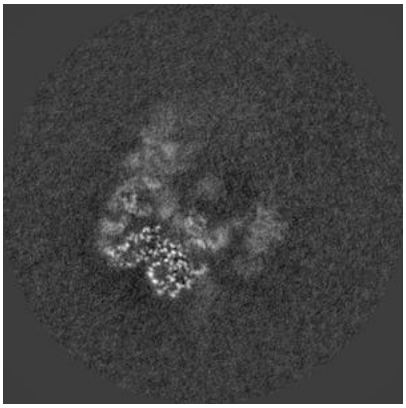


Z Index: 200

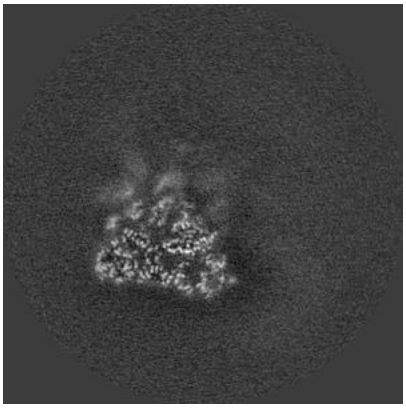
6.2.2 Raw map



X Index: 200



Y Index: 200

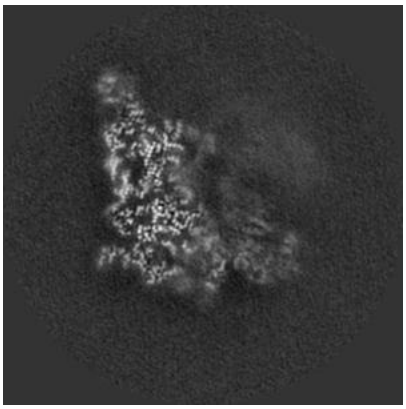


Z Index: 200

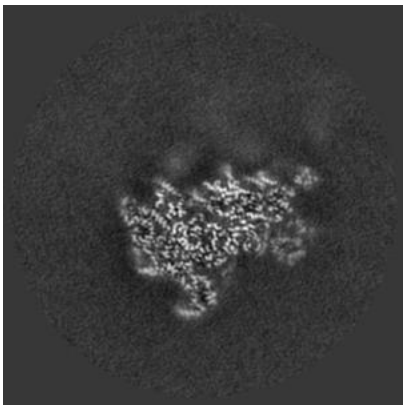
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

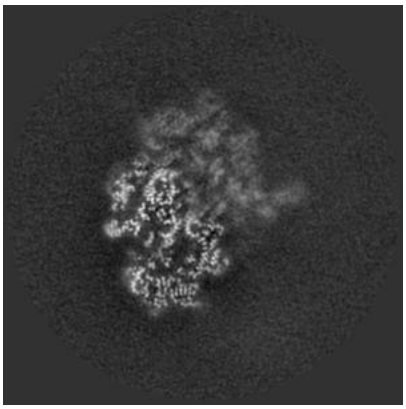
6.3.1 Primary map



X Index: 188

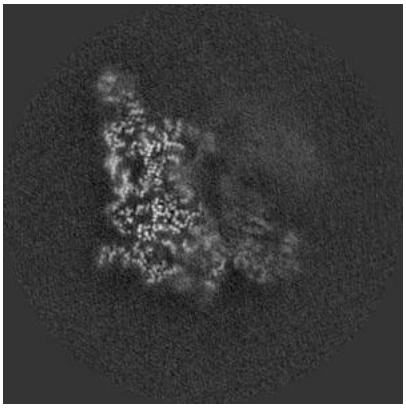


Y Index: 146

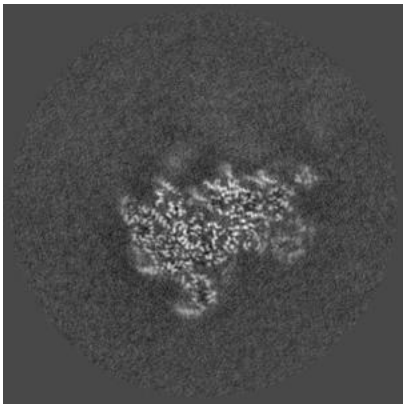


Z Index: 155

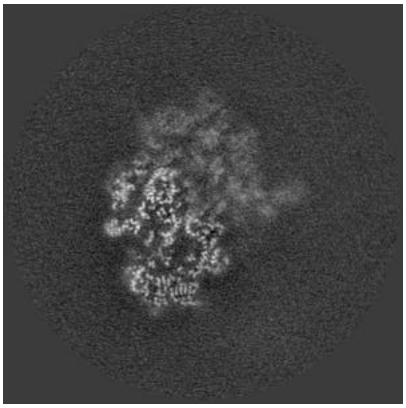
6.3.2 Raw map



X Index: 188



Y Index: 146



Z Index: 155

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 0.021. 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.

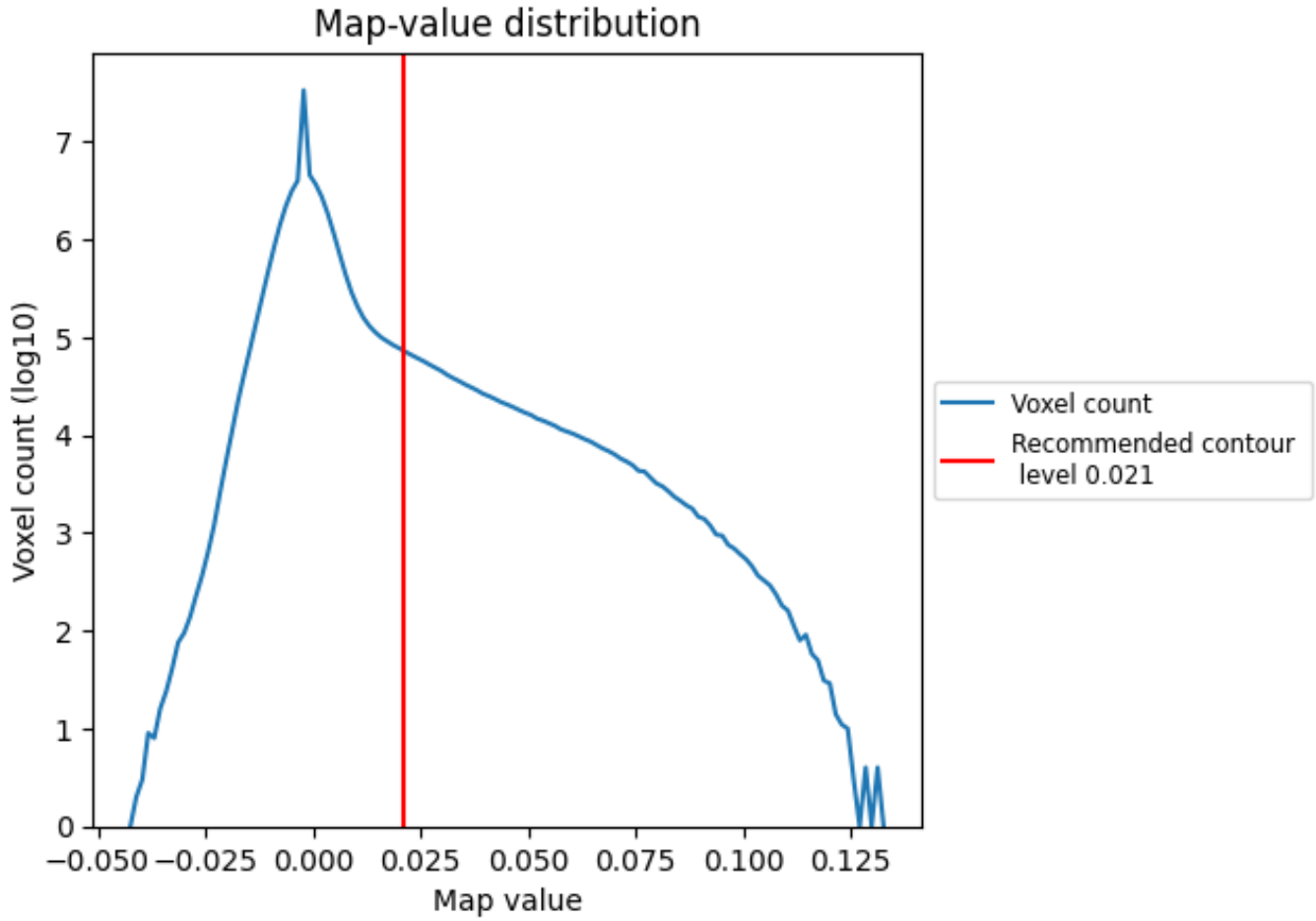
6.5 Mask visualisation (i)

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

7 Map analysis

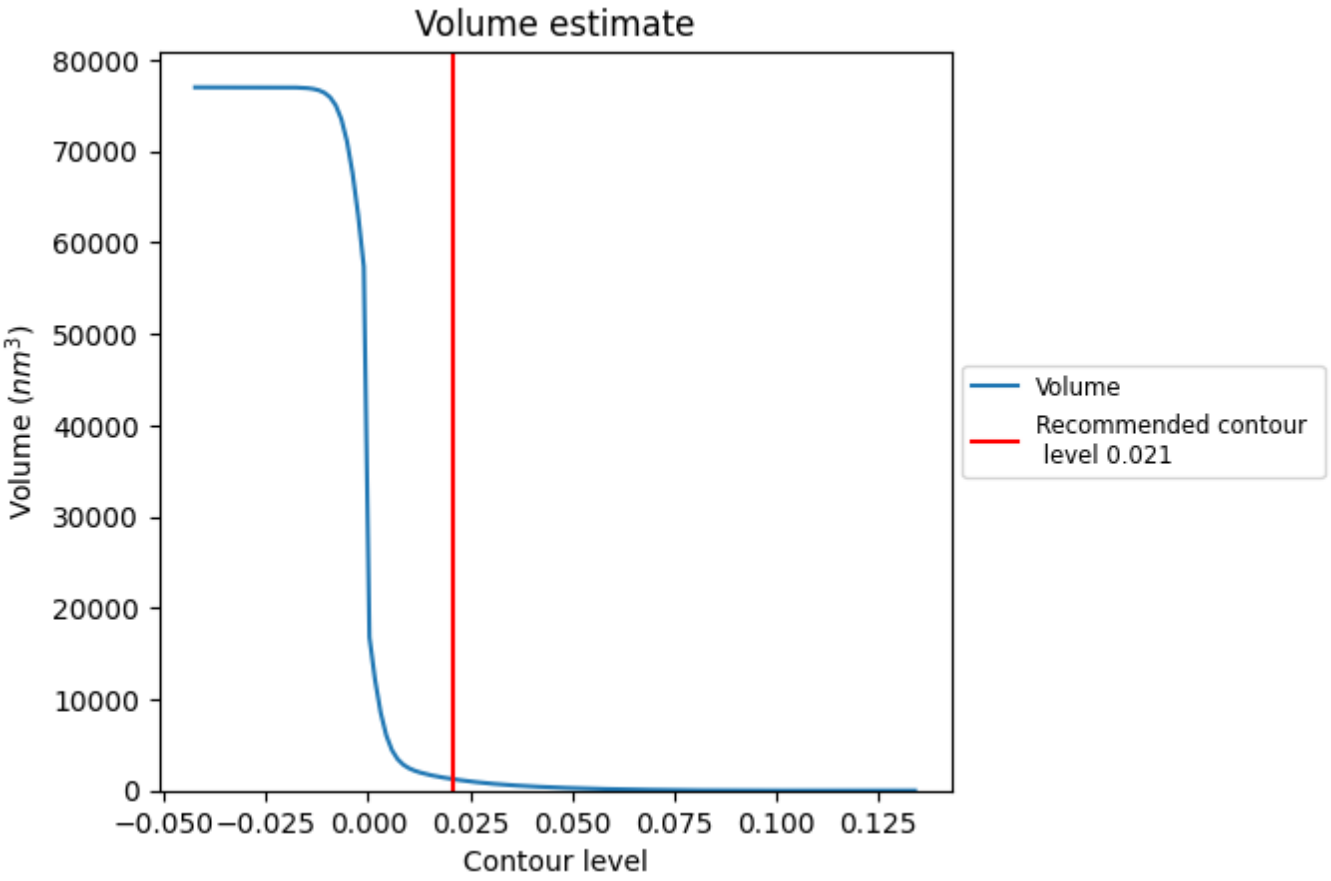
This section contains the results of statistical analysis of the map.

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.

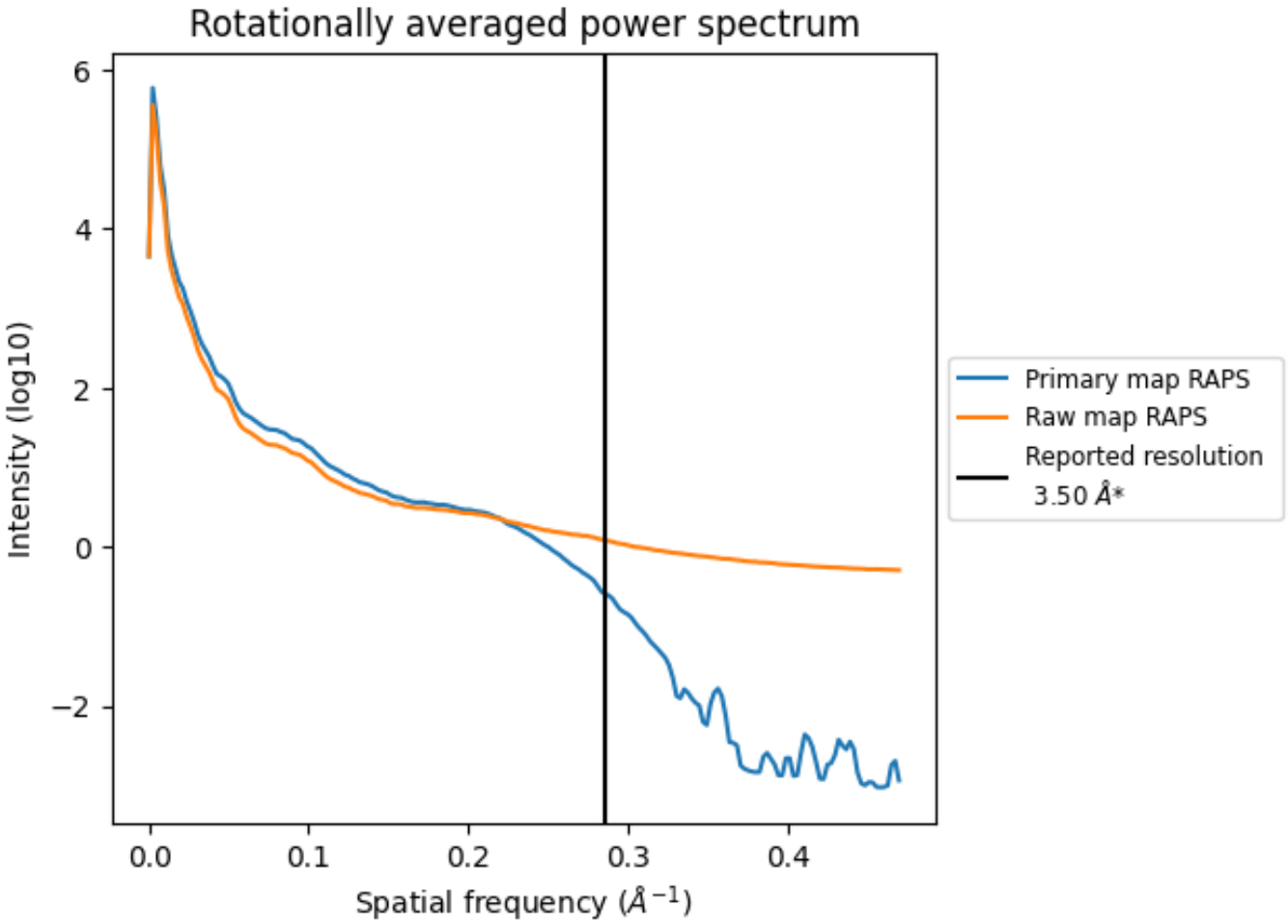
7.2 Volume estimate



The volume at the recommended contour level is 1238 nm^3; this corresponds to an approximate mass of 1119 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)

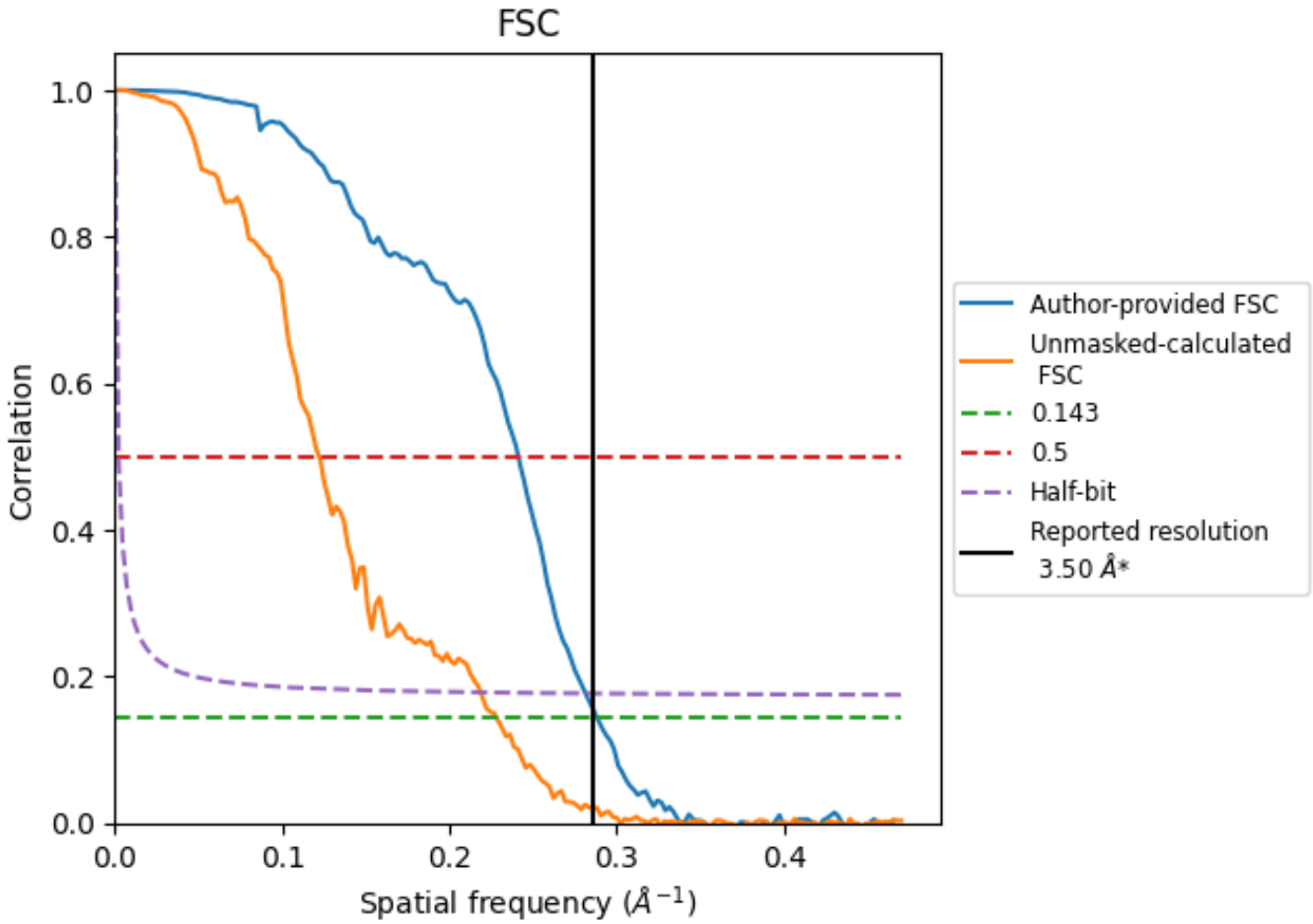


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

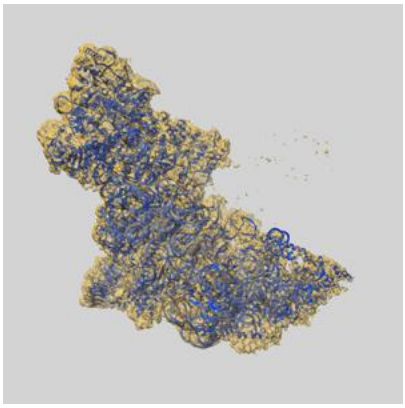
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	4.15	3.55
Unmasked-calculated*	4.38	8.19	4.57

*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 4.38 differs from the reported value 3.5 by more than 10 %

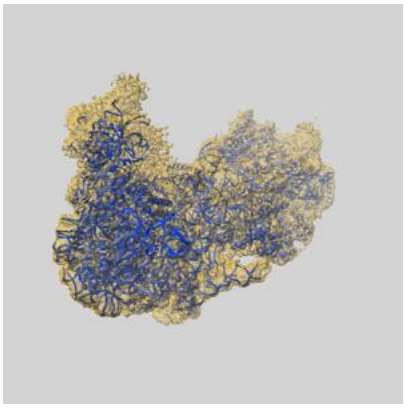
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12911 and PDB model 7OHW. Per-residue inclusion information can be found in section 3 on page 11.

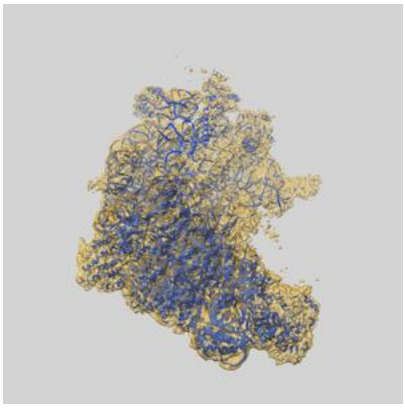
9.1 Map-model overlay



X



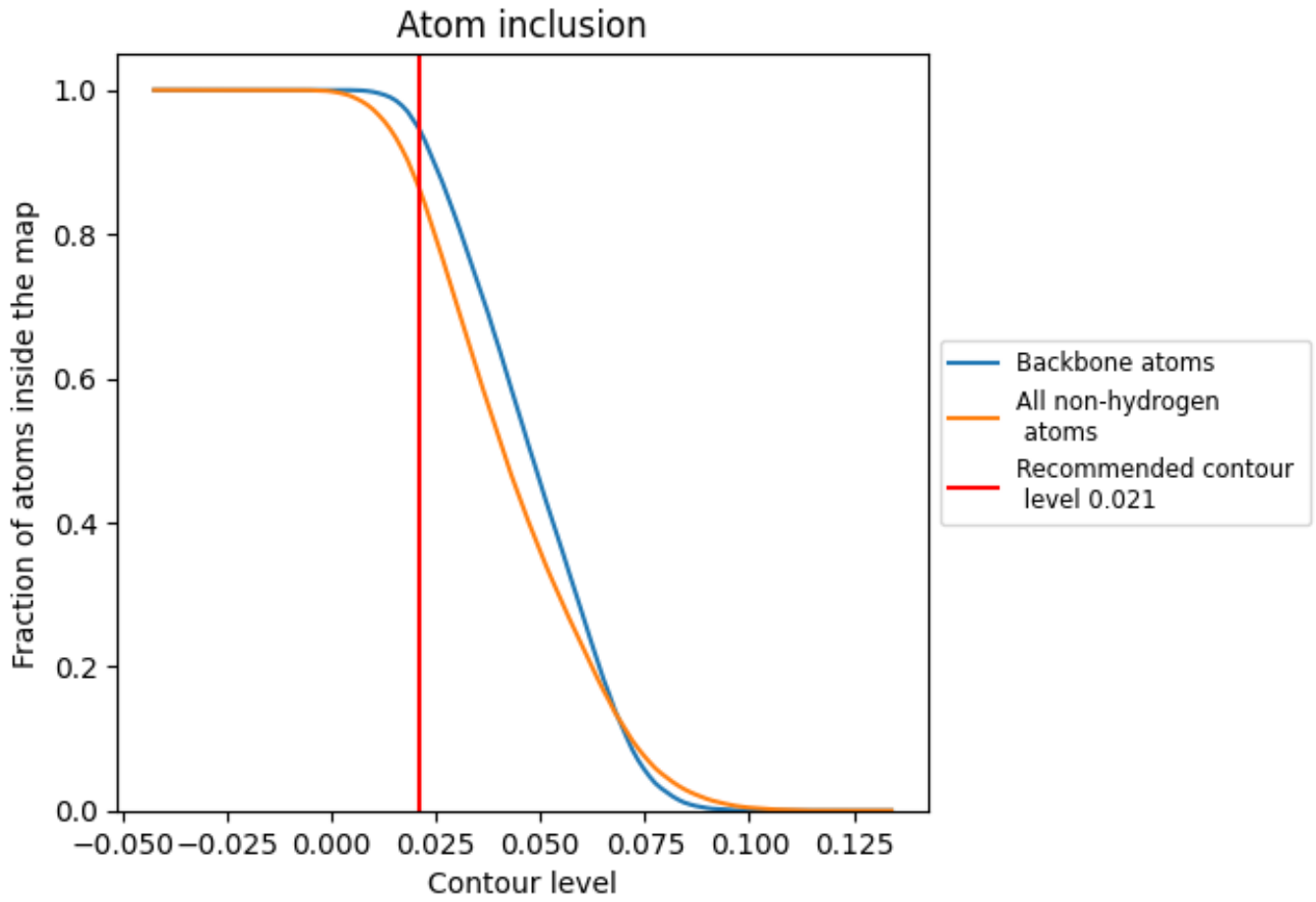
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.021 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 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.