



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:15 pm GMT

PDB ID : 6EML  
EMDB ID : EMD-3886  
Title : Cryo-EM structure of a late pre-40S ribosomal subunit from *Saccharomyces cerevisiae*  
Authors : Heuer, A.; Thomson, E.; Schmidt, C.; Berninghausen, O.; Becker, T.; Hurt, E.; Beckmann, R.  
Deposited on : 2017-10-02  
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
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

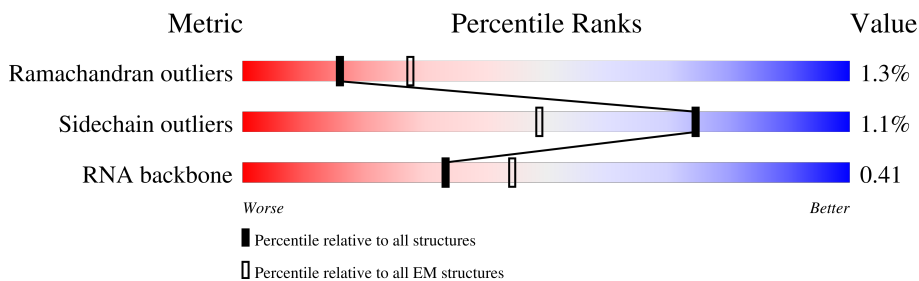
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	2	1800	
2	D	143	
3	B	225	
4	C	136	
5	E	142	
6	F	143	
7	H	146	
8	I	144	

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Mol	Chain	Length	Quality of chain
9	K	108	56% 55% 41%
10	L	67	82% 91% 7%
11	N	152	34% 30% 66%
12	P	252	7% 77% 18%
13	Q	255	26% 80% 16%
14	R	254	10% 82% 5% 13%
15	S	261	7% 94% 5%
16	T	236	11% 92%
17	U	190	38% 91% 6%
18	V	200	8% 88% 6% 6%
19	W	197	5% 88% 6% 6%
20	X	156	17% 94% 5%
21	Y	151	13% 93% 5%
22	Z	137	34% 90% 7%
23	a	87	6% 90% 9%
24	b	130	89% 9%
25	c	145	19% 89% 10%
26	d	135	7% 95%
27	f	82	10% 91% 7%
28	t	788	24% 77% 20%
29	g	63	51% 83% 11% 5%
30	p	274	27% 64% 32%
31	r	425	58% 61% 38%
32	e	483	44% 53% 46%

## 2 Entry composition i

There are 32 unique types of molecules in this entry. The entry contains 75886 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 pre-18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1675	35695	15958	6312	11750	1675	0	0

- Molecule 2 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	124	892	561	156	173	2	0	0

- Molecule 3 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	202	1592	998	296	295	3	0	0

- Molecule 4 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	114	871	541	169	159	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	117	928	590	172	159	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	141	1105	708	203	194	0	0

- Molecule 7 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	122	1009	636	193	178	2	0	0

- Molecule 8 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	143	1112	694	208	208	2	0	0

- Molecule 9 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	K	64	519	332	95	92	0	0

- Molecule 10 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	62	486	300	95	90	1	0	0

- Molecule 11 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	51	397	249	73	71	4	0	0

- Molecule 12 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	206	1577	1014	278	283	2	0	0

- Molecule 13 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Q	214	1709	1084	310	311	4	0	0

- Molecule 14 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	220	Total	C	N	O	S	0	0
			1662	1065	295	300	2		

- Molecule 15 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 16 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 17 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	U	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 18 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 19 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 20 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 21 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Y	150	1192	759	224	207	2	0	0

- Molecule 22 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Z	127	891	545	182	163	1	0	0

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	a	87	684	420	125	137	2	0	0

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	b	129	1021	650	188	180	3	0	0

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	c	144	1121	708	220	191	2	0	0

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	d	134	1073	676	208	189	0	0

- Molecule 27 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	f	81	610	382	110	113	5	0	0

- Molecule 28 is a protein called Ribosome biogenesis protein TSR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	t	633	Total	C	N	O	S	0	0
			5037	3220	875	929	13		

- Molecule 29 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 30 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	p	185	Total	C	N	O	S	0	0
			1473	942	267	260	4		

- Molecule 31 is a protein called Serine/threonine-protein kinase RIO2.

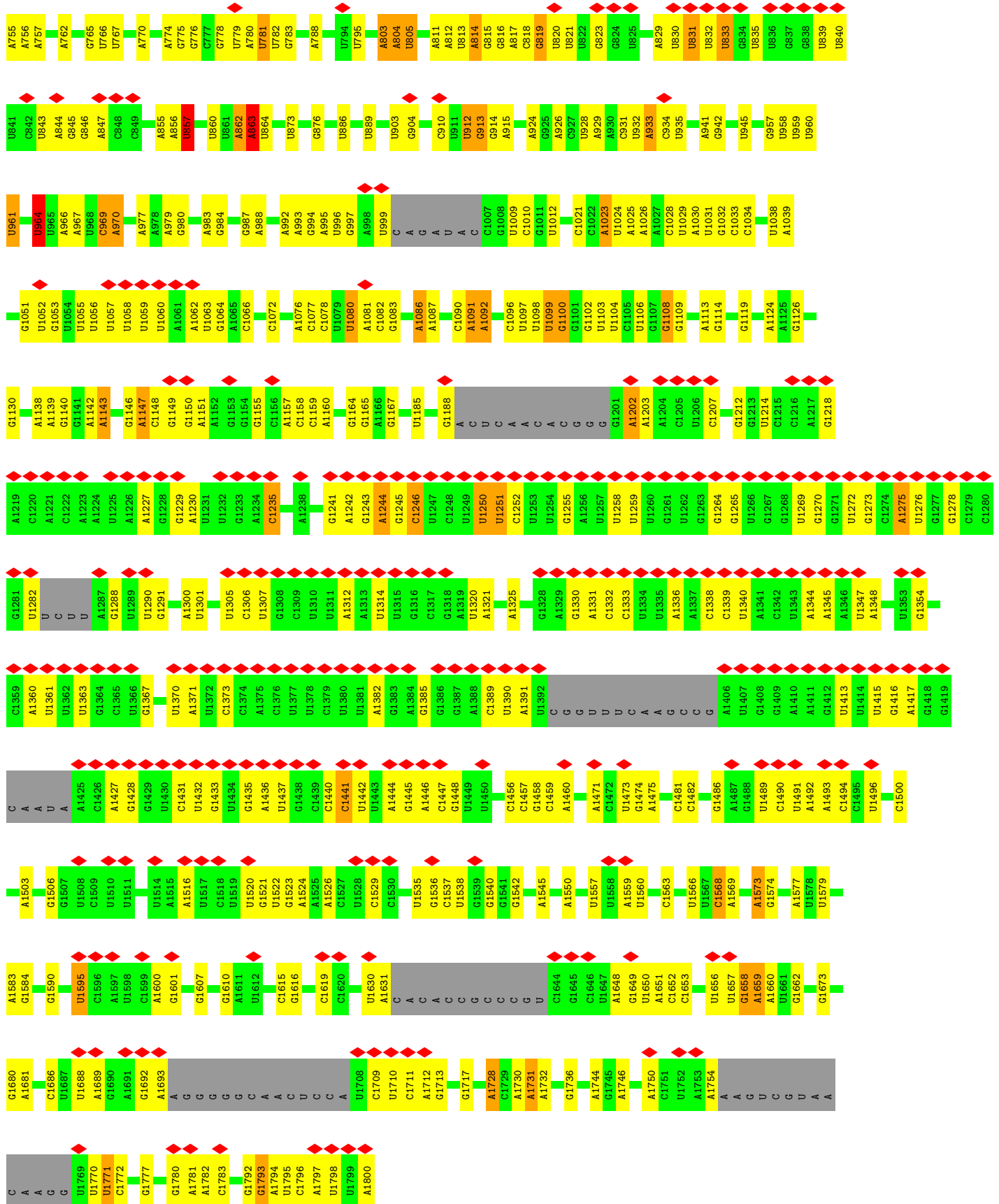
Mol	Chain	Residues	Atoms					AltConf	Trace
31	r	264	Total	C	N	O	S	0	0
			2166	1379	384	387	16		

- Molecule 32 is a protein called Essential nuclear protein 1.

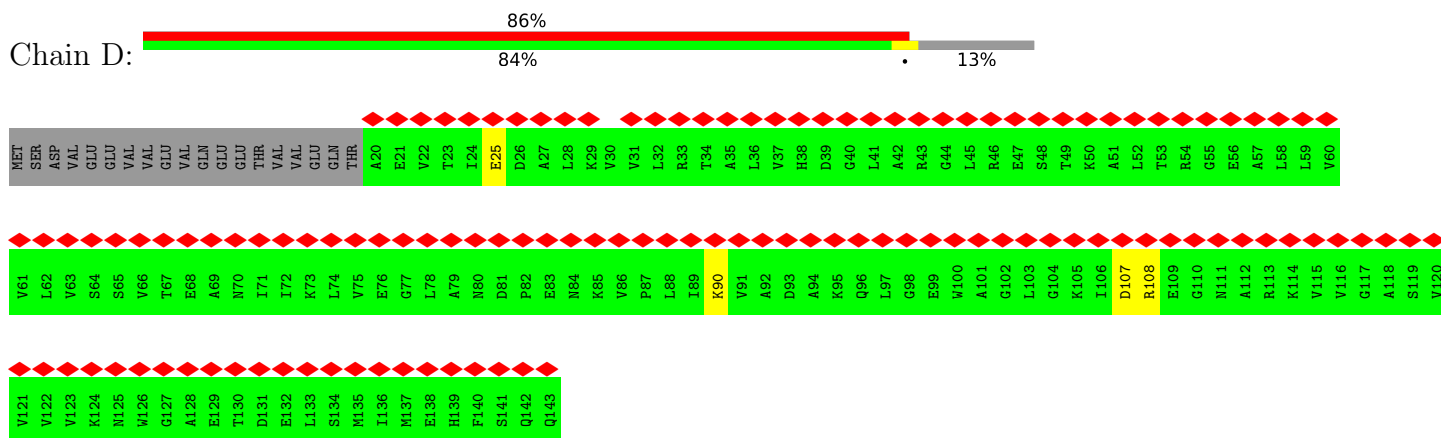
Mol	Chain	Residues	Atoms				AltConf	Trace
32	e	261	Total	C	N	O	0	0
			1045	523	261	261		



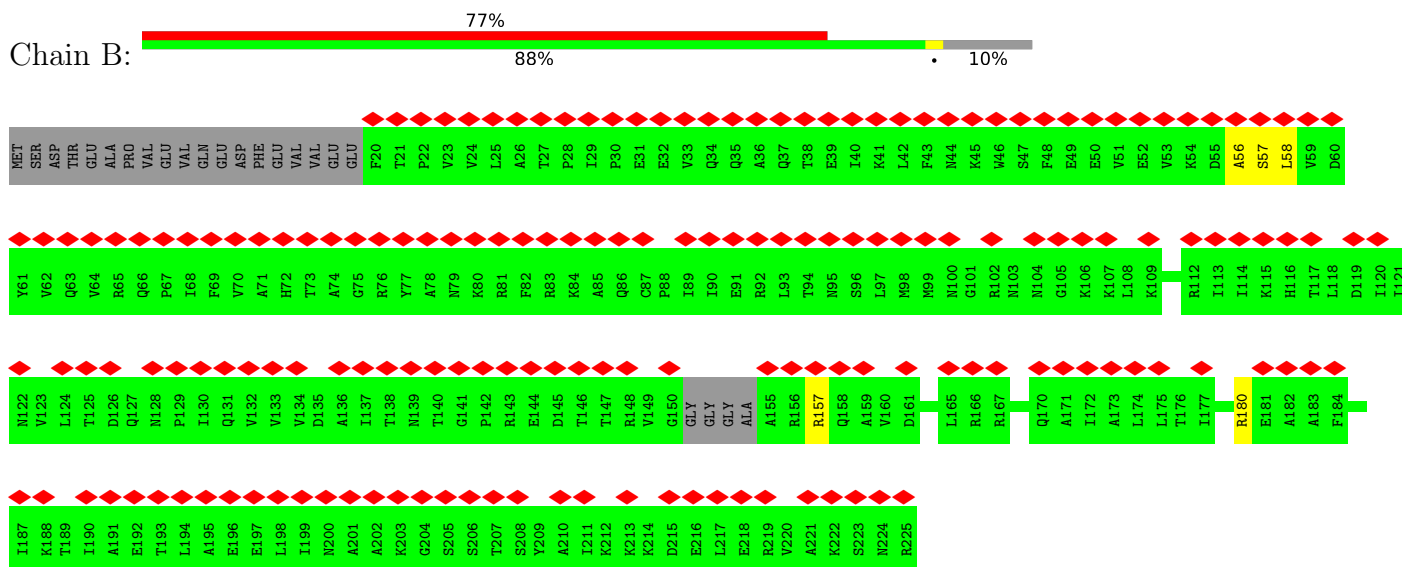




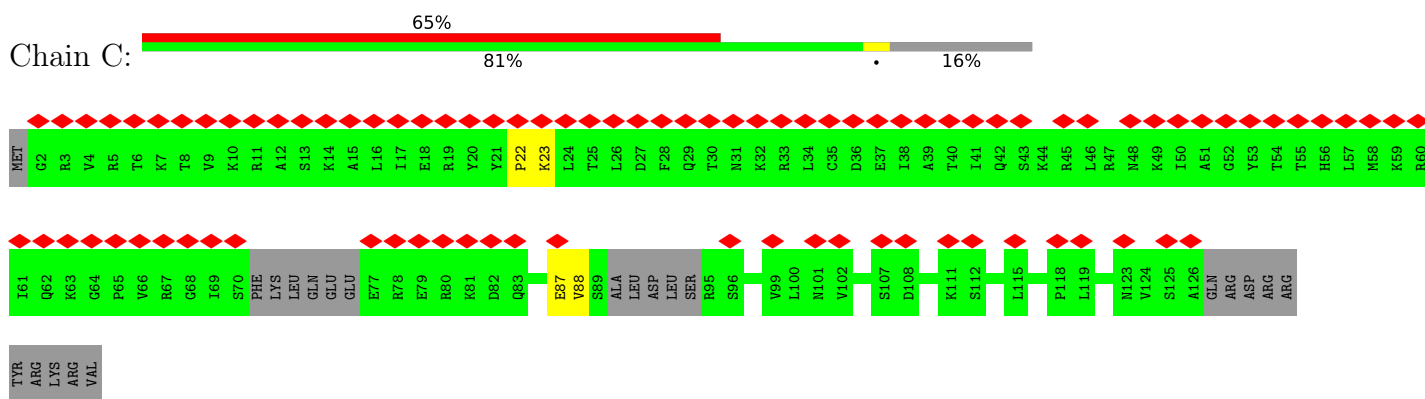
- Molecule 2: 40S ribosomal protein S12



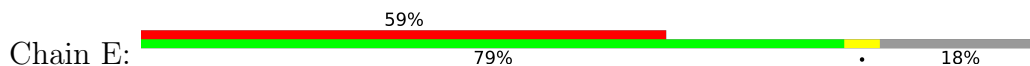
- Molecule 3: 40S ribosomal protein S5



- Molecule 4: 40S ribosomal protein S17-A

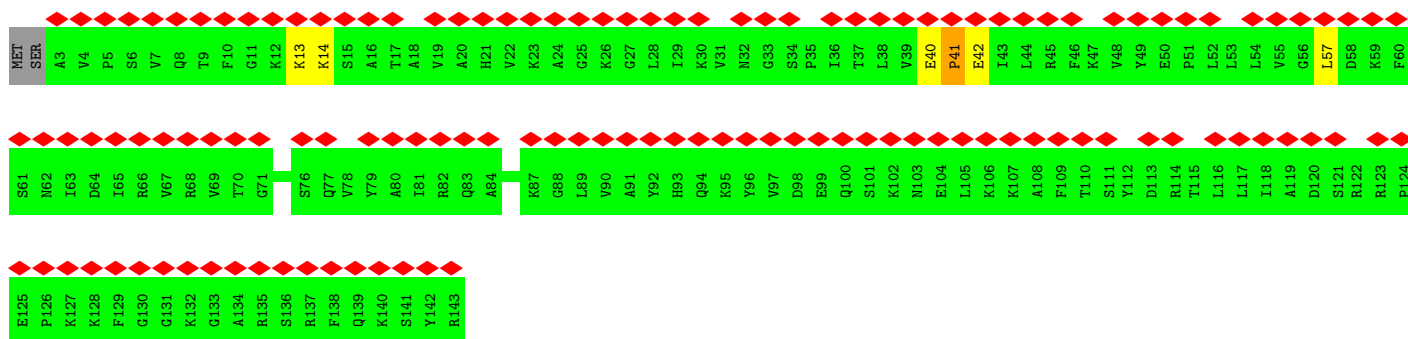
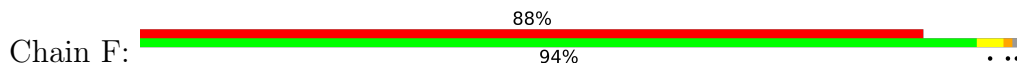


- Molecule 5: 40S ribosomal protein S15

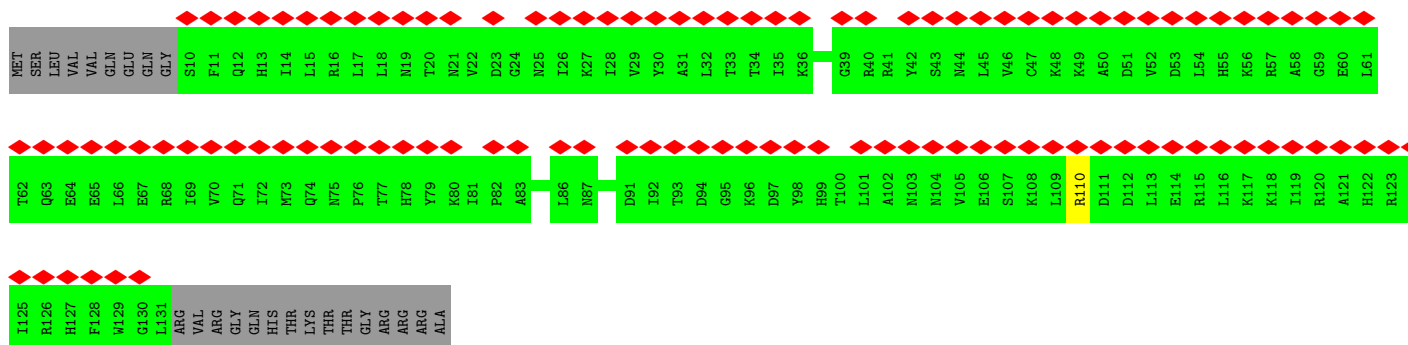
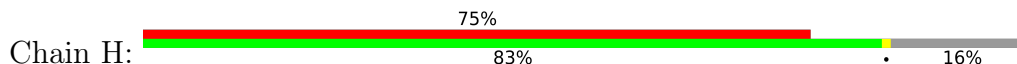




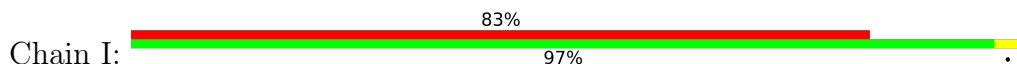
• Molecule 6: 40S ribosomal protein S16-A



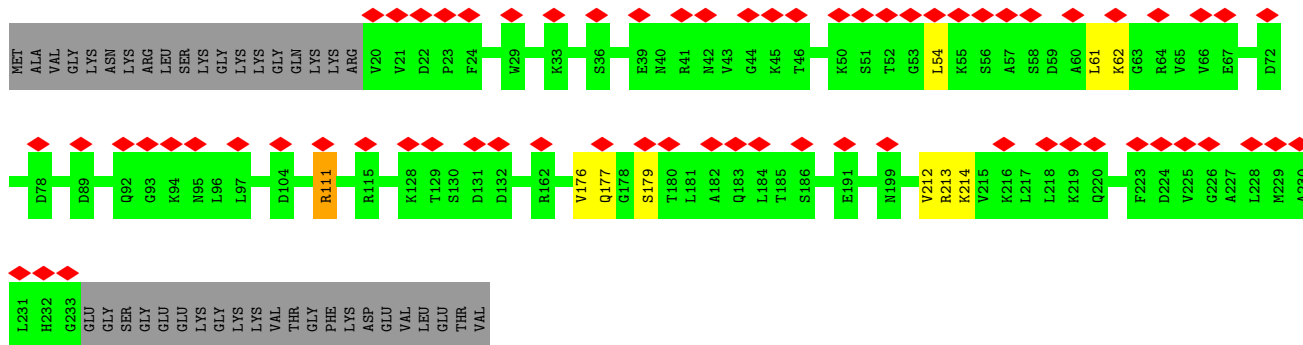
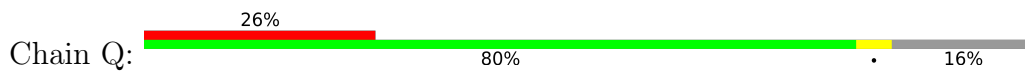
• Molecule 7: 40S ribosomal protein S18-A



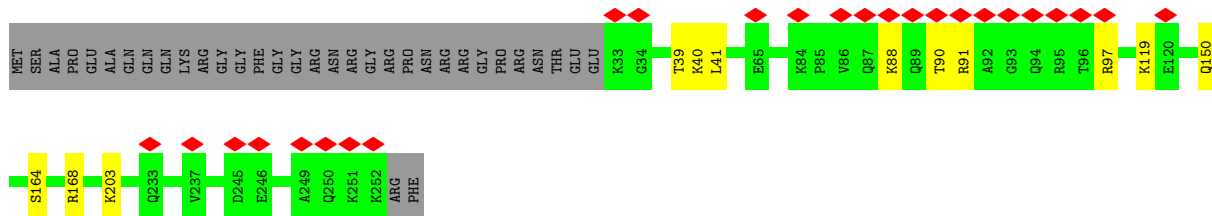
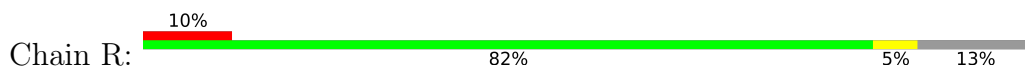
• Molecule 8: 40S ribosomal protein S19-A



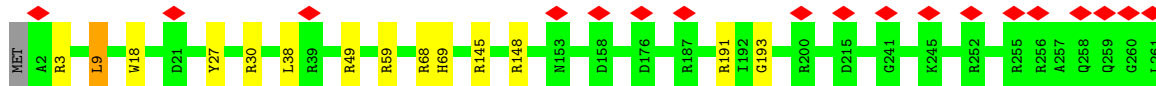
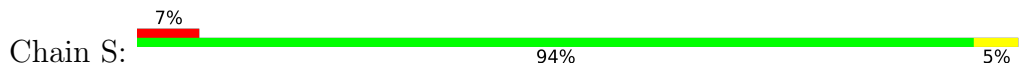




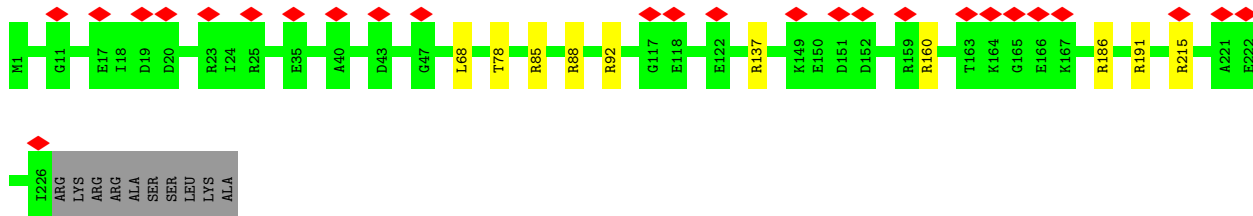
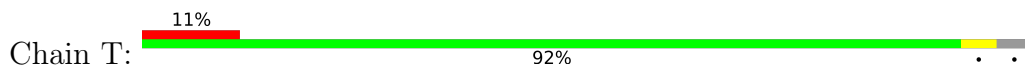
• Molecule 14: 40S ribosomal protein S2



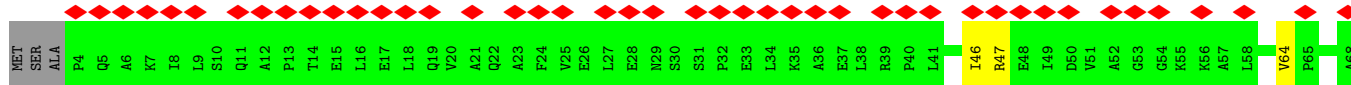
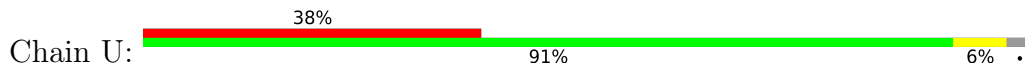
• Molecule 15: 40S ribosomal protein S4-A

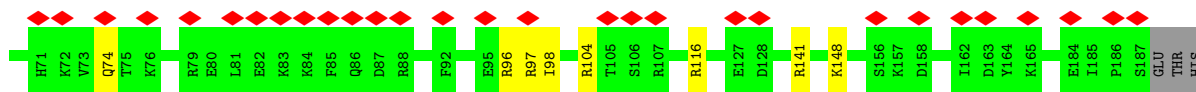


• Molecule 16: 40S ribosomal protein S6-A

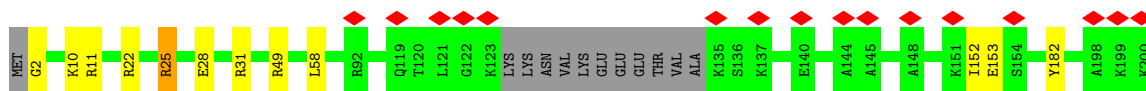
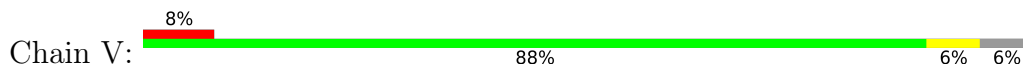


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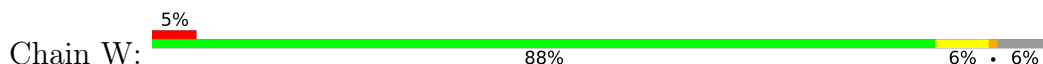




- Molecule 18: 40S ribosomal protein S8-A



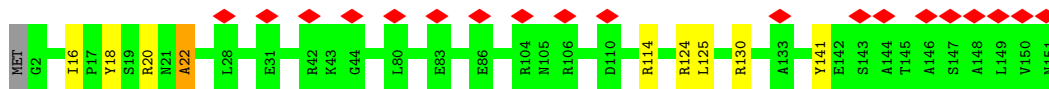
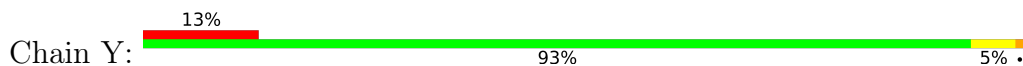
- Molecule 19: 40S ribosomal protein S9-A



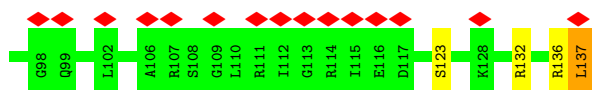
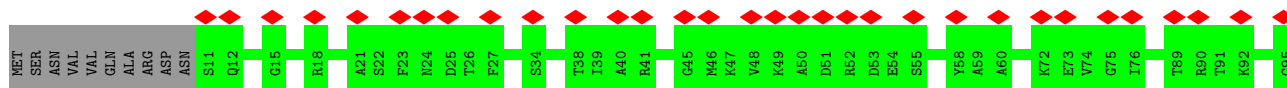
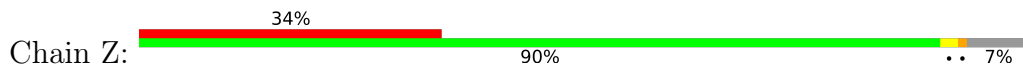
- Molecule 20: 40S ribosomal protein S11-A



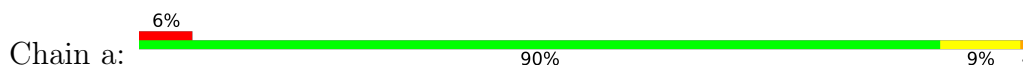
- Molecule 21: 40S ribosomal protein S13

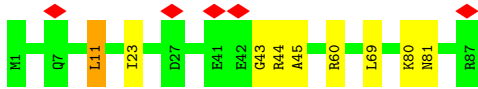


- Molecule 22: 40S ribosomal protein S14-A

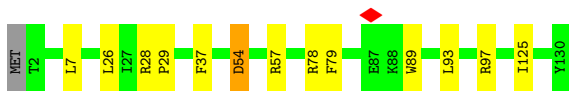
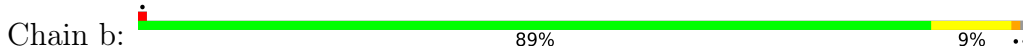


- Molecule 23: 40S ribosomal protein S21-A

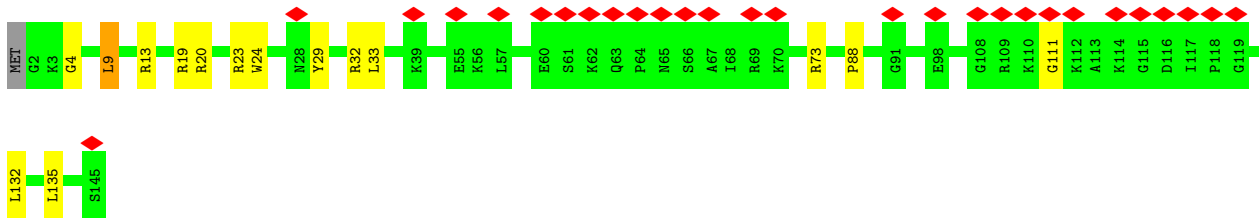
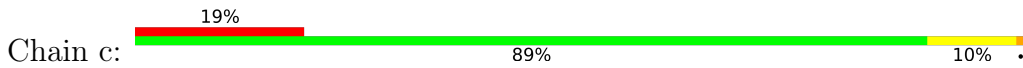




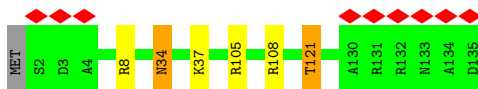
• Molecule 24: 40S ribosomal protein S22-A



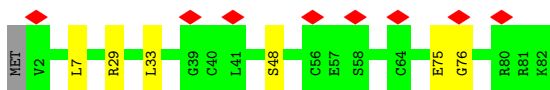
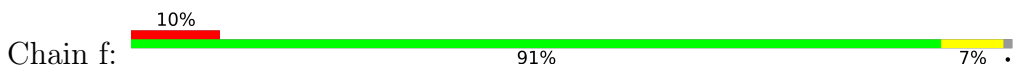
• Molecule 25: 40S ribosomal protein S23-A



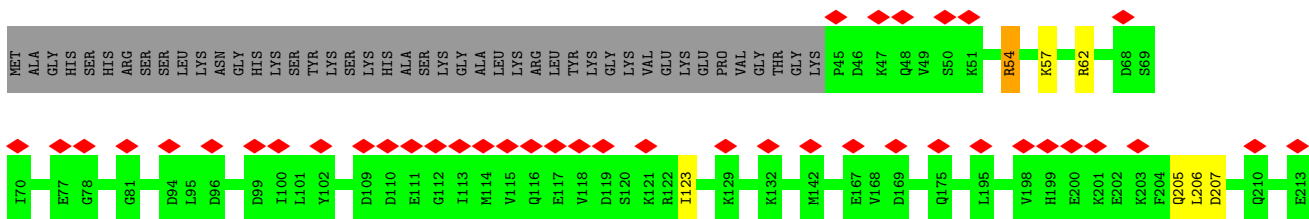
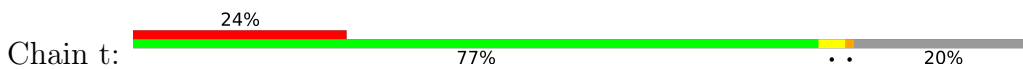
• Molecule 26: 40S ribosomal protein S24-A



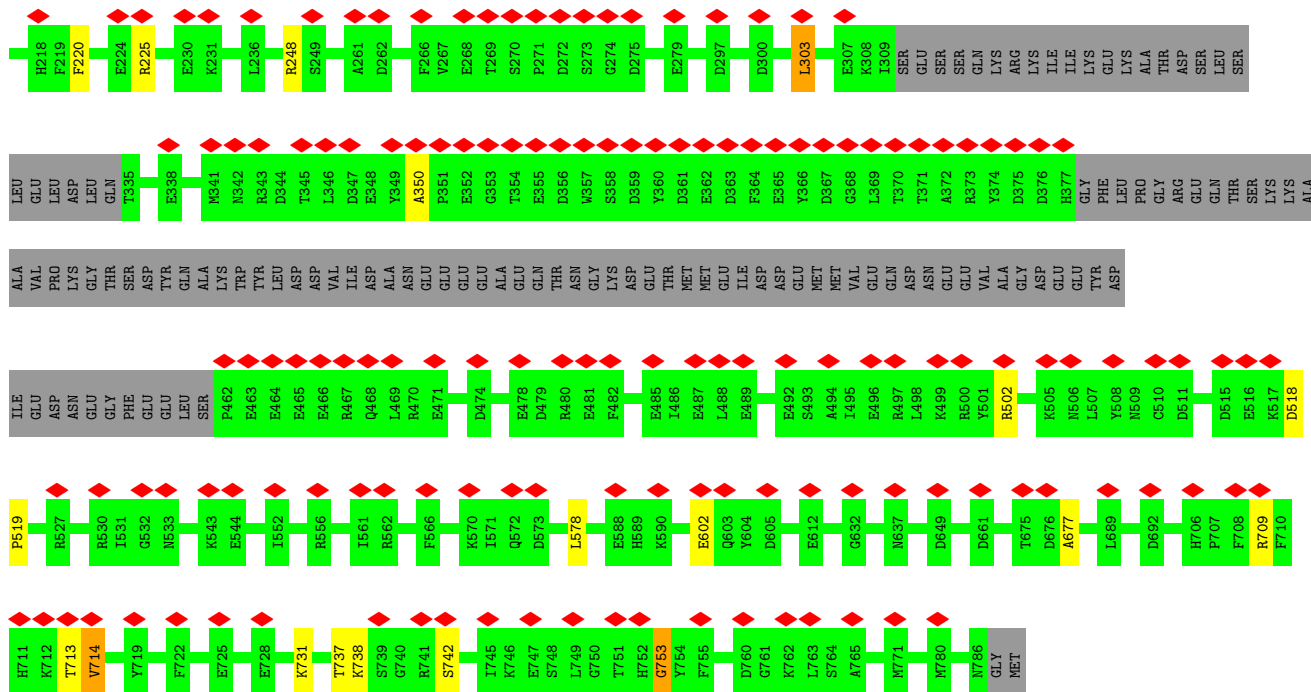
• Molecule 27: 40S ribosomal protein S27-A



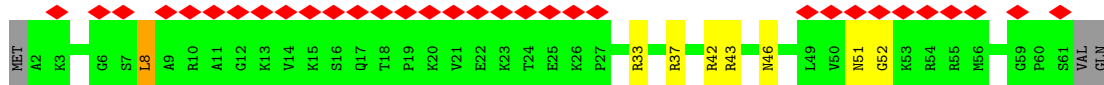
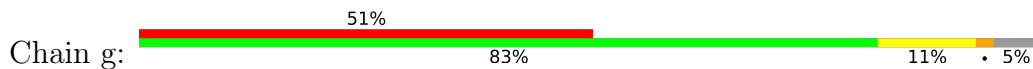
• Molecule 28: Ribosome biogenesis protein TSR1



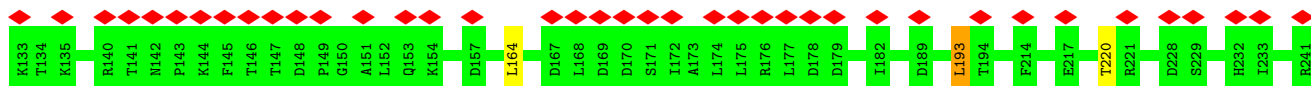
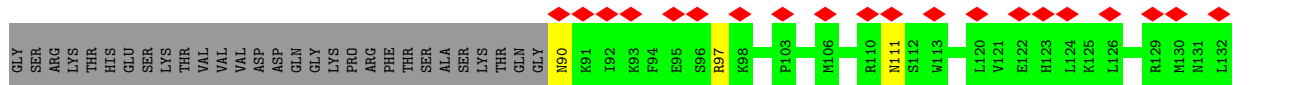
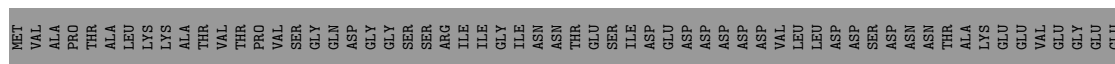




• Molecule 29: 40S ribosomal protein S30-A

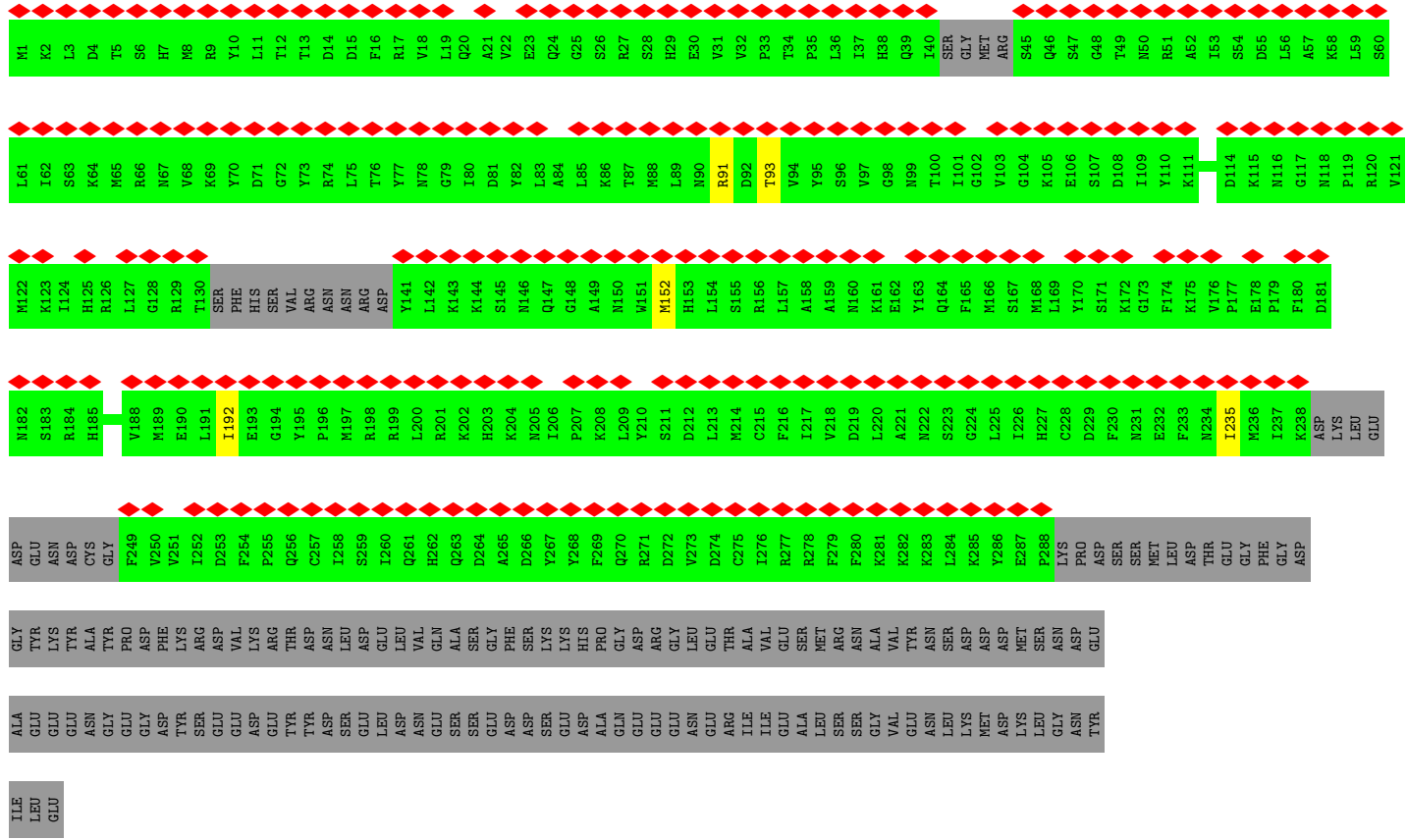


• Molecule 30: Pre-rRNA-processing protein PNO1

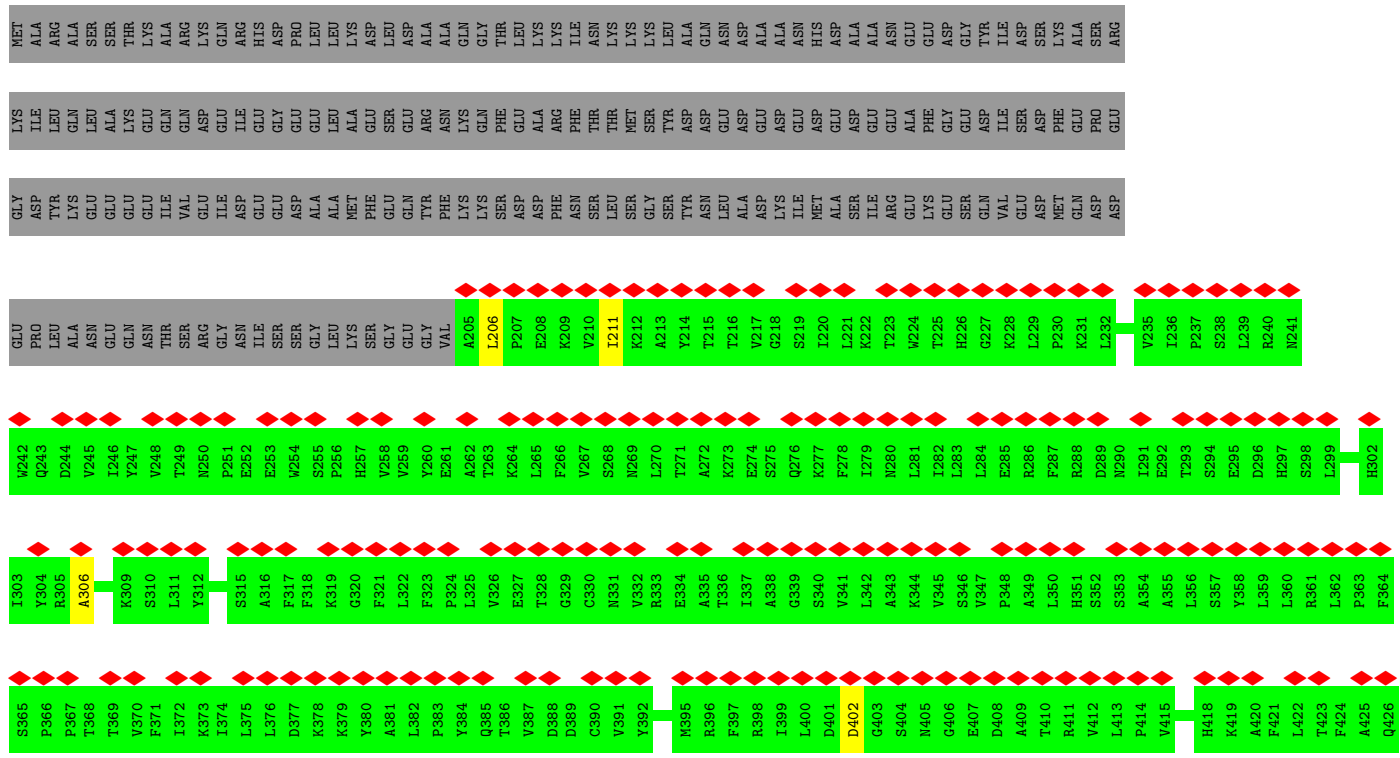
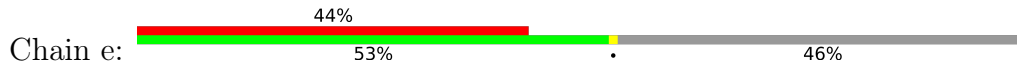


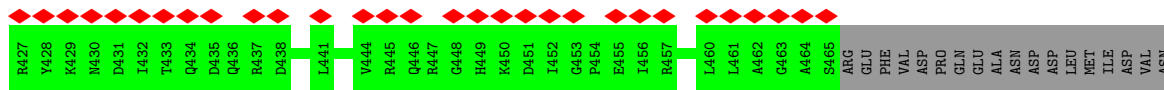
• Molecule 31: Serine/threonine-protein kinase RIO2





• Molecule 32: Essential nuclear protein 1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84100	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.523	Depositor
Minimum map value	-0.262	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0722	Depositor
Map size ( $\text{\AA}$ )	416.25598, 416.25598, 416.25598	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.084, 1.084, 1.084	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	1.27	181/39917 (0.5%)	1.13	242/62179 (0.4%)
2	D	0.44	0/900	0.76	0/1223
3	B	0.43	0/1611	0.75	3/2177 (0.1%)
4	C	0.45	0/878	0.76	0/1177
5	E	0.49	0/948	0.80	2/1273 (0.2%)
6	F	0.46	0/1125	0.73	0/1510
7	H	0.43	0/1027	0.72	1/1383 (0.1%)
8	I	0.45	0/1130	0.78	2/1517 (0.1%)
9	K	0.42	0/526	0.77	0/706
10	L	0.42	0/488	0.79	1/656 (0.2%)
11	N	0.46	0/404	0.76	0/542
12	P	0.90	2/1617 (0.1%)	0.93	4/2215 (0.2%)
13	Q	0.65	0/1735	0.85	2/2335 (0.1%)
14	R	0.94	1/1692 (0.1%)	0.94	2/2296 (0.1%)
15	S	1.05	2/2109 (0.1%)	1.07	12/2839 (0.4%)
16	T	0.78	0/1823	0.99	12/2439 (0.5%)
17	U	0.68	0/1506	0.94	5/2028 (0.2%)
18	V	1.00	4/1514 (0.3%)	1.07	6/2021 (0.3%)
19	W	1.02	1/1519 (0.1%)	1.10	7/2035 (0.3%)
20	X	1.21	4/1239 (0.3%)	1.17	7/1673 (0.4%)
21	Y	0.94	2/1215 (0.2%)	1.07	7/1638 (0.4%)
22	Z	0.60	0/901	0.87	2/1217 (0.2%)
23	a	0.96	0/693	1.08	2/935 (0.2%)
24	b	1.27	3/1038 (0.3%)	1.22	8/1395 (0.6%)
25	c	1.15	4/1139 (0.4%)	1.33	13/1518 (0.9%)
26	d	0.96	0/1087	1.01	6/1449 (0.4%)
27	f	0.83	1/620 (0.2%)	1.01	5/838 (0.6%)
28	t	0.70	1/5150 (0.0%)	0.81	7/6972 (0.1%)
29	g	0.85	0/483	1.15	5/643 (0.8%)
30	p	0.62	0/1500	0.84	2/2020 (0.1%)
31	r	0.29	0/2209	0.54	0/2965
32	e	0.27	0/1044	0.54	1/1304 (0.1%)
All	All	1.05	206/80787 (0.3%)	1.04	366/117118 (0.3%)

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
1	2	0	11
2	D	0	1
3	B	0	1
4	C	0	2
5	E	0	2
6	F	0	2
9	K	0	3
12	P	0	3
13	Q	0	5
14	R	0	1
15	S	0	1
17	U	0	3
18	V	0	1
19	W	0	2
20	X	0	1
21	Y	0	1
22	Z	0	1
23	a	0	3
24	b	0	1
25	c	0	1
28	t	0	8
29	g	0	1
31	r	0	2
All	All	0	57

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	220	A	C6-N1	-46.67	1.02	1.35
1	2	222	A	C6-N1	-43.87	1.04	1.35
1	2	831	U	C2-N3	34.00	1.61	1.37
1	2	833	U	C2-N3	32.63	1.60	1.37
1	2	863	A	C6-N1	-27.67	1.16	1.35
1	2	236	A	C6-N6	-23.83	1.14	1.33
1	2	831	U	C4-O4	-20.14	1.07	1.23
1	2	833	U	N3-C4	19.84	1.56	1.38
1	2	857	U	N3-C4	-17.50	1.22	1.38
1	2	831	U	N1-C2	16.56	1.53	1.38
1	2	440	U	N3-C4	-16.55	1.23	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	964	U	N3-C4	16.39	1.53	1.38
1	2	229	U	N3-C4	16.31	1.53	1.38
1	2	1057	U	C4-O4	-15.56	1.11	1.23
1	2	1595	U	N3-C4	-15.02	1.25	1.38
1	2	1235	C	N1-C2	14.20	1.54	1.40
1	2	401	A	O3'-P	14.11	1.78	1.61
1	2	831	U	N3-C4	13.68	1.50	1.38
1	2	1235	C	C1'-N1	13.24	1.68	1.48
1	2	863	A	C5-C6	-12.44	1.29	1.41
1	2	1086	A	N1-C2	12.30	1.45	1.34
1	2	1062	A	C6-N1	-12.13	1.27	1.35
1	2	229	U	C2-N3	11.85	1.46	1.37
1	2	440	U	C2-N3	-11.33	1.29	1.37
1	2	1595	U	C2-N3	-11.16	1.29	1.37
1	2	1038	U	N3-C4	-11.09	1.28	1.38
1	2	1057	U	N3-C4	-10.82	1.28	1.38
1	2	857	U	C2-N3	-10.76	1.30	1.37
1	2	1235	C	C2-O2	10.13	1.33	1.24
1	2	220	A	C6-N6	-10.09	1.25	1.33
1	2	1600	A	C6-N6	-10.08	1.25	1.33
1	2	236	A	C6-N1	-9.91	1.28	1.35
20	X	100	TYR	CG-CD1	-9.82	1.26	1.39
1	2	863	A	N1-C2	9.82	1.43	1.34
1	2	222	A	N1-C2	9.74	1.43	1.34
25	c	29	TYR	CE2-CZ	-9.55	1.26	1.38
1	2	481	A	C5-C6	9.46	1.49	1.41
1	2	964	U	C4-O4	-9.39	1.16	1.23
1	2	229	U	N1-C2	9.30	1.47	1.38
1	2	595	G	O3'-P	-9.21	1.50	1.61
1	2	505	A	C5-C6	-9.20	1.32	1.41
1	2	1143	A	N1-C2	-9.12	1.26	1.34
1	2	236	A	C2-N3	9.08	1.41	1.33
1	2	220	A	N1-C2	9.00	1.42	1.34
1	2	1235	C	C2-N3	8.88	1.42	1.35
1	2	1091	A	C6-N6	-8.87	1.26	1.33
1	2	833	U	N1-C2	8.85	1.46	1.38
1	2	1080	U	N3-C4	-8.64	1.30	1.38
1	2	967	A	O3'-P	-8.61	1.50	1.61
1	2	482	U	C4-C5	-8.50	1.35	1.43
1	2	814	A	C6-N6	-8.48	1.27	1.33
1	2	1235	C	C5-C6	8.43	1.41	1.34
1	2	805	U	O3'-P	-8.32	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	964	U	N1-C2	8.31	1.46	1.38
1	2	51	A	C6-N6	-8.01	1.27	1.33
20	X	100	TYR	CG-CD2	-7.96	1.28	1.39
1	2	831	U	N1-C6	-7.92	1.30	1.38
1	2	863	A	C6-N6	-7.76	1.27	1.33
1	2	1086	A	C2-N3	7.75	1.40	1.33
1	2	106	U	O3'-P	-7.73	1.51	1.61
1	2	481	A	N1-C2	7.72	1.41	1.34
1	2	833	U	N1-C6	-7.67	1.31	1.38
1	2	236	A	N1-C2	7.66	1.41	1.34
1	2	1235	C	C4-N4	7.65	1.40	1.33
1	2	1235	C	N1-C6	7.49	1.41	1.37
1	2	633	U	O3'-P	-7.38	1.52	1.61
1	2	472	U	O3'-P	-7.38	1.52	1.61
1	2	507	U	C4-C5	7.35	1.50	1.43
1	2	1143	A	C5-C6	7.33	1.47	1.41
19	W	146	PHE	CG-CD1	-7.24	1.27	1.38
1	2	423	G	O3'-P	7.21	1.69	1.61
1	2	596	C	O3'-P	-7.13	1.52	1.61
1	2	1731	A	O3'-P	-6.95	1.52	1.61
1	2	385	A	O3'-P	-6.93	1.52	1.61
1	2	964	U	C2-N3	6.91	1.42	1.37
1	2	1130	G	O3'-P	-6.90	1.52	1.61
1	2	1600	A	C6-N1	-6.89	1.30	1.35
1	2	377	G	O3'-P	-6.84	1.52	1.61
1	2	1087	A	C5-C6	-6.83	1.34	1.41
1	2	1062	A	C6-N6	-6.79	1.28	1.33
1	2	1142	A	O3'-P	-6.77	1.53	1.61
27	f	48	SER	CB-OG	-6.77	1.33	1.42
24	b	37	PHE	CG-CD1	-6.74	1.28	1.38
1	2	1092	A	C6-N6	-6.74	1.28	1.33
1	2	220	A	C5-C6	-6.61	1.35	1.41
1	2	1062	A	C5-C6	6.54	1.47	1.41
1	2	1083	G	C5-C6	-6.53	1.35	1.42
1	2	108	A	O3'-P	-6.52	1.53	1.61
1	2	347	G	O3'-P	-6.51	1.53	1.61
1	2	1142	A	C5-C6	-6.46	1.35	1.41
24	b	79	PHE	CG-CD2	-6.35	1.29	1.38
1	2	367	A	C5-C6	-6.34	1.35	1.41
1	2	612	U	O3'-P	-6.32	1.53	1.61
1	2	549	G	C2-N2	-6.32	1.28	1.34
1	2	152	U	C2-N3	6.28	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	457	G	C5-C6	-6.27	1.36	1.42
1	2	462	G	C5-C6	-6.26	1.36	1.42
1	2	961	U	O3'-P	-6.26	1.53	1.61
1	2	229	U	C5-C6	-6.24	1.28	1.34
1	2	325	G	O3'-P	-6.19	1.53	1.61
1	2	452	A	O3'-P	6.17	1.68	1.61
1	2	1600	A	N1-C2	-6.17	1.28	1.34
1	2	450	U	O3'-P	-6.16	1.53	1.61
1	2	447	U	O3'-P	-6.12	1.53	1.61
1	2	229	U	C4-O4	-6.12	1.18	1.23
1	2	958	U	O3'-P	-6.11	1.53	1.61
1	2	338	C	O3'-P	-6.10	1.53	1.61
1	2	374	U	O3'-P	-6.08	1.53	1.61
1	2	47	A	C5-C6	-6.04	1.35	1.41
1	2	625	C	O3'-P	-6.02	1.53	1.61
1	2	362	G	C5-C6	-6.00	1.36	1.42
1	2	977	A	C5-C6	-5.99	1.35	1.41
1	2	429	G	C5-C6	-5.98	1.36	1.42
1	2	1104	U	C4-O4	5.96	1.28	1.23
25	c	29	TYR	CG-CD1	-5.92	1.31	1.39
1	2	970	A	O3'-P	5.90	1.68	1.61
1	2	1057	U	C2-N3	-5.89	1.33	1.37
1	2	1545	A	C5-C6	5.87	1.46	1.41
1	2	592	A	C5-C6	-5.86	1.35	1.41
1	2	93	A	C5-C6	-5.86	1.35	1.41
25	c	24	TRP	CB-CG	-5.84	1.39	1.50
20	X	100	TYR	CE2-CZ	-5.80	1.31	1.38
1	2	863	A	C2-N3	5.78	1.38	1.33
1	2	379	U	P-OP2	5.76	1.58	1.49
1	2	363	G	C5-C6	-5.72	1.36	1.42
1	2	452	A	C3'-O3'	5.68	1.50	1.42
1	2	361	C	N1-C2	-5.67	1.34	1.40
1	2	863	A	N7-C5	-5.67	1.35	1.39
1	2	632	U	C2-O2	-5.65	1.17	1.22
1	2	102	U	O3'-P	-5.64	1.54	1.61
1	2	1235	C	N3-C4	5.64	1.38	1.33
1	2	1147	A	C5-C6	-5.64	1.35	1.41
18	V	182	TYR	CE1-CZ	-5.64	1.31	1.38
1	2	1108	G	C5-C6	-5.63	1.36	1.42
1	2	336	G	C5-C6	-5.63	1.36	1.42
1	2	401	A	C5-C6	-5.63	1.35	1.41
1	2	63	G	P-OP2	5.62	1.58	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	101	U	O3'-P	-5.60	1.54	1.61
1	2	600	U	C4-O4	5.60	1.28	1.23
25	c	19	ARG	CZ-NH2	5.59	1.40	1.33
1	2	804	A	C5-C6	-5.58	1.36	1.41
1	2	600	U	N3-C4	-5.58	1.33	1.38
1	2	770	A	O3'-P	-5.57	1.54	1.61
1	2	100	A	C5-C6	-5.57	1.36	1.41
1	2	1771	U	N3-C4	-5.56	1.33	1.38
1	2	964	U	C5-C6	-5.55	1.29	1.34
21	Y	141	TYR	CE1-CZ	-5.54	1.31	1.38
15	S	18	TRP	CZ3-CH2	-5.47	1.31	1.40
1	2	1566	U	C4-O4	5.47	1.28	1.23
1	2	1103	U	O3'-P	-5.46	1.54	1.61
1	2	401	A	P-OP1	5.45	1.58	1.49
12	P	174	TRP	CB-CG	-5.45	1.40	1.50
1	2	762	A	O3'-P	-5.45	1.54	1.61
21	Y	18	TYR	CG-CD2	-5.45	1.32	1.39
1	2	296	U	O3'-P	-5.44	1.54	1.61
1	2	7	G	C5-C6	-5.44	1.36	1.42
1	2	618	U	N3-C4	5.43	1.43	1.38
1	2	1062	A	N1-C2	-5.43	1.29	1.34
1	2	393	C	P-OP2	5.42	1.58	1.49
1	2	979	A	O3'-P	-5.42	1.54	1.61
1	2	964	U	C4-C5	5.41	1.48	1.43
14	R	164	SER	CB-OG	-5.40	1.35	1.42
1	2	404	G	O3'-P	5.38	1.67	1.61
1	2	399	A	C5-C6	-5.37	1.36	1.41
1	2	549	G	C5-C6	5.35	1.47	1.42
1	2	1099	U	O3'-P	5.35	1.67	1.61
1	2	561	G	C5-C6	-5.35	1.37	1.42
1	2	222	A	N3-C4	-5.34	1.31	1.34
1	2	1143	A	C6-N1	-5.33	1.31	1.35
1	2	1106	U	N3-C4	-5.32	1.33	1.38
1	2	612	U	N1-C2	-5.32	1.33	1.38
12	P	138	TYR	CG-CD1	-5.31	1.32	1.39
24	b	89	TRP	CB-CG	-5.31	1.40	1.50
28	t	602	GLU	CD-OE1	-5.29	1.19	1.25
1	2	863	A	C8-N7	-5.29	1.27	1.31
18	V	28	GLU	CD-OE1	5.29	1.31	1.25
1	2	402	C	C2-N3	-5.27	1.31	1.35
15	S	27	TYR	CE1-CZ	-5.25	1.31	1.38
1	2	1063	U	C4-O4	-5.24	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1600	A	C2-N3	-5.23	1.28	1.33
1	2	1038	U	C2-N3	-5.22	1.34	1.37
1	2	375	U	O3'-P	-5.21	1.54	1.61
1	2	383	G	C2-N2	-5.21	1.29	1.34
1	2	430	G	P-O5'	-5.20	1.54	1.59
1	2	590	C	C4-N4	-5.20	1.29	1.33
1	2	307	G	C5-C6	-5.17	1.37	1.42
1	2	281	G	C6-O6	-5.16	1.19	1.24
1	2	24	U	N3-C4	-5.14	1.33	1.38
1	2	298	C	O3'-P	-5.14	1.54	1.61
1	2	334	G	C5-C6	-5.14	1.37	1.42
1	2	357	G	O3'-P	-5.13	1.54	1.61
18	V	182	TYR	CG-CD2	-5.11	1.32	1.39
1	2	406	U	O3'-P	-5.08	1.55	1.61
1	2	1139	A	C5-C6	-5.08	1.36	1.41
20	X	99	ARG	NE-CZ	-5.08	1.26	1.33
1	2	969	C	N1-C2	-5.08	1.35	1.40
1	2	1038	U	C4-O4	-5.07	1.19	1.23
1	2	451	A	C6-N6	-5.06	1.29	1.33
1	2	553	G	O3'-P	-5.05	1.55	1.61
1	2	220	A	C5-C4	5.05	1.42	1.38
1	2	1057	U	N1-C2	5.04	1.43	1.38
1	2	300	A	C5-C6	5.02	1.45	1.41
18	V	2	GLY	N-CA	5.02	1.53	1.46
1	2	44	U	O3'-P	-5.02	1.55	1.61
1	2	375	U	N1-C6	-5.02	1.33	1.38
1	2	1728	A	C5-C6	-5.01	1.36	1.41

All (366) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	831	U	C2-N3-C4	-33.08	107.15	127.00
1	2	833	U	C2-N3-C4	-28.03	110.18	127.00
1	2	220	A	N1-C6-N6	-26.49	102.71	118.60
1	2	964	U	C2-N3-C4	-23.66	112.80	127.00
1	2	222	A	N1-C6-N6	-22.82	104.91	118.60
1	2	1062	A	N1-C6-N6	-21.97	105.42	118.60
1	2	220	A	C5-C6-N6	21.51	140.91	123.70
1	2	1595	U	N3-C4-O4	-19.45	105.78	119.40
1	2	222	A	C5-C6-N6	18.64	138.61	123.70
1	2	440	U	N3-C4-O4	-18.56	106.41	119.40
1	2	1595	U	C5-C4-O4	17.00	136.10	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	857	U	N3-C4-O4	-16.48	107.86	119.40
1	2	229	U	C2-N3-C4	-16.30	117.22	127.00
1	2	618	U	C2-N3-C4	-15.64	117.61	127.00
1	2	1062	A	C5-C6-N6	15.39	136.01	123.70
1	2	229	U	C5-C4-O4	-15.28	116.73	125.90
1	2	831	U	C5-C4-O4	-15.02	116.89	125.90
1	2	1086	A	C6-N1-C2	-14.99	109.60	118.60
1	2	1600	A	N1-C6-N6	-14.76	109.75	118.60
1	2	831	U	N1-C2-O2	-14.46	112.68	122.80
1	2	833	U	C5-C4-O4	-14.17	117.40	125.90
1	2	833	U	N1-C2-O2	-13.77	113.16	122.80
1	2	857	U	C5-C4-O4	13.64	134.08	125.90
1	2	1057	U	N3-C4-O4	-13.43	110.00	119.40
1	2	831	U	N3-C4-C5	13.41	122.65	114.60
25	c	23	ARG	NE-CZ-NH2	-13.13	113.73	120.30
1	2	440	U	C5-C4-O4	13.06	133.74	125.90
1	2	236	A	N1-C6-N6	-12.94	110.83	118.60
1	2	863	A	C6-C5-N7	-12.28	123.71	132.30
1	2	220	A	C2-N3-C4	-12.28	104.46	110.60
1	2	220	A	C6-N1-C2	12.25	125.95	118.60
25	c	19	ARG	NE-CZ-NH1	-12.10	114.25	120.30
1	2	1143	A	N1-C6-N6	-12.05	111.37	118.60
20	X	88	ARG	NE-CZ-NH1	11.84	126.22	120.30
17	U	141	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	2	323	A	O5'-P-OP1	-11.69	95.18	105.70
1	2	863	A	C4-C5-C6	11.47	122.74	117.00
1	2	1038	U	N3-C4-O4	-11.47	111.37	119.40
1	2	941	A	O5'-P-OP1	-11.46	95.39	105.70
21	Y	20	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	2	1080	U	N3-C4-O4	-10.92	111.76	119.40
1	2	1600	A	C5-C6-N6	10.83	132.36	123.70
1	2	380	U	O5'-P-OP2	-10.83	95.96	105.70
26	d	105	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	2	814	A	N1-C6-N6	-10.68	112.19	118.60
1	2	833	U	C4-C5-C6	10.68	126.11	119.70
1	2	302	U	O5'-P-OP1	-10.50	96.25	105.70
1	2	222	A	C2-N3-C4	-10.45	105.37	110.60
1	2	236	A	C5-C6-N1	10.26	122.83	117.70
24	b	97	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	2	831	U	C4-C5-C6	10.23	125.84	119.70
21	Y	20	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	2	831	U	N1-C2-N3	10.16	120.99	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	20	ARG	NE-CZ-NH1	9.97	125.28	120.30
1	2	833	U	N1-C2-N3	9.96	120.87	114.90
25	c	23	ARG	NE-CZ-NH1	9.88	125.24	120.30
18	V	22	ARG	NE-CZ-NH1	-9.88	115.36	120.30
1	2	857	U	N1-C2-O2	9.87	129.71	122.80
1	2	964	U	N3-C4-C5	9.83	120.50	114.60
16	T	88	ARG	NE-CZ-NH2	-9.74	115.43	120.30
18	V	25	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	2	236	A	C6-N1-C2	-9.68	112.79	118.60
1	2	1595	U	C2-N3-C4	9.63	132.78	127.00
1	2	1143	A	C5-C6-N6	9.60	131.38	123.70
1	2	857	U	N3-C2-O2	-9.53	115.53	122.20
20	X	67	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	2	473	A	O5'-P-OP1	-9.35	97.29	105.70
1	2	1595	U	N1-C2-O2	9.24	129.27	122.80
1	2	615	A	O5'-P-OP2	-9.07	97.54	105.70
1	2	1080	U	C5-C4-O4	9.01	131.31	125.90
1	2	229	U	C2-N1-C1'	9.00	128.50	117.70
1	2	1595	U	N3-C2-O2	-8.90	115.97	122.20
1	2	1057	U	C5-C4-O4	8.89	131.23	125.90
1	2	1057	U	N3-C2-O2	-8.88	115.98	122.20
29	g	8	LEU	CA-CB-CG	8.79	135.51	115.30
19	W	44	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	2	863	A	C2-N3-C4	-8.51	106.35	110.60
1	2	863	A	N9-C1'-C2'	-8.47	102.68	112.00
1	2	229	U	C6-N1-C1'	-8.45	109.37	121.20
25	c	32	ARG	NE-CZ-NH1	8.43	124.51	120.30
25	c	9	LEU	CB-CG-CD2	-8.41	96.70	111.00
1	2	440	U	N3-C2-O2	-8.36	116.35	122.20
25	c	73	ARG	NE-CZ-NH1	8.26	124.43	120.30
15	S	38	LEU	CB-CG-CD1	-8.23	97.00	111.00
1	2	440	U	N1-C2-O2	8.22	128.56	122.80
1	2	229	U	N3-C4-O4	8.22	125.15	119.40
1	2	1092	A	N1-C6-N6	-8.20	113.68	118.60
1	2	632	U	O5'-P-OP1	-8.18	98.34	105.70
1	2	831	U	C2-N1-C1'	8.16	127.49	117.70
12	P	101	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	2	381	C	O5'-P-OP2	-8.04	98.47	105.70
1	2	1235	C	O4'-C1'-N1	7.99	114.59	108.20
1	2	384	G	O5'-P-OP1	7.98	120.28	110.70
1	2	757	A	O5'-P-OP1	-7.97	98.53	105.70
1	2	152	U	C2-N3-C4	-7.96	122.22	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	301	A	O5'-P-OP1	-7.91	98.58	105.70
16	T	137	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	2	13	C	O5'-P-OP1	7.81	120.07	110.70
1	2	424	C	O5'-P-OP1	-7.77	98.71	105.70
1	2	16	G	O5'-P-OP1	7.77	120.02	110.70
1	2	51	A	N1-C6-N6	-7.75	113.95	118.60
16	T	88	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	2	833	U	N3-C4-O4	7.74	124.82	119.40
1	2	386	G	O5'-P-OP1	-7.74	98.74	105.70
13	Q	61	LEU	CA-CB-CG	7.64	132.88	115.30
1	2	814	A	C5-C6-N6	7.53	129.72	123.70
24	b	78	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	2	610	G	C4-N9-C1'	7.40	136.12	126.50
21	Y	114	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	2	857	U	C2-N3-C4	7.37	131.42	127.00
1	2	831	U	C6-N1-C1'	-7.36	110.90	121.20
17	U	96	ARG	NE-CZ-NH2	-7.36	116.62	120.30
20	X	71	LEU	CB-CG-CD1	-7.35	98.50	111.00
1	2	477	A	O5'-P-OP1	-7.33	99.10	105.70
15	S	49	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	2	1038	U	C5-C4-O4	7.28	130.27	125.90
27	f	29	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	2	129	U	O5'-P-OP2	-7.21	99.21	105.70
20	X	67	ARG	NE-CZ-NH2	-7.20	116.70	120.30
24	b	97	ARG	NE-CZ-NH2	-7.15	116.72	120.30
21	Y	124	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	2	1458	G	C4-N9-C1'	7.10	135.73	126.50
30	p	193	LEU	CA-CB-CG	7.05	131.52	115.30
8	I	35	ASP	CB-CG-OD1	7.02	124.61	118.30
1	2	863	A	N3-C4-N9	7.00	133.00	127.40
1	2	380	U	O5'-P-OP1	6.97	119.06	110.70
26	d	121	THR	CA-CB-CG2	-6.97	102.64	112.40
25	c	32	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	2	305	C	O5'-P-OP1	-6.94	99.45	105.70
1	2	1595	U	C4-C5-C6	-6.93	115.54	119.70
1	2	610	G	C8-N9-C1'	-6.93	117.99	127.00
19	W	90	LYS	CD-CE-NZ	6.93	127.63	111.70
15	S	145	ARG	NE-CZ-NH1	6.92	123.76	120.30
22	Z	132	ARG	NE-CZ-NH1	6.90	123.75	120.30
26	d	108	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	2	450	U	C2-N3-C4	-6.85	122.89	127.00
23	a	60	ARG	NE-CZ-NH1	-6.84	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	168	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	2	623	A	O5'-P-OP2	-6.78	99.59	105.70
20	X	129	ARG	NE-CZ-NH1	-6.73	116.94	120.30
1	2	1489	U	C2-N1-C1'	6.73	125.77	117.70
25	c	9	LEU	CB-CG-CD1	6.70	122.39	111.00
20	X	87	ARG	NE-CZ-NH2	-6.70	116.95	120.30
17	U	141	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	2	1389	C	C2-N1-C1'	6.66	126.13	118.80
1	2	449	C	O5'-P-OP1	-6.66	99.70	105.70
19	W	44	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	2	326	G	O5'-P-OP2	-6.65	99.72	105.70
1	2	20	G	O5'-P-OP1	-6.63	99.73	105.70
16	T	191	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	2	311	U	O5'-P-OP1	-6.63	99.74	105.70
1	2	215	A	O5'-P-OP1	-6.62	99.74	105.70
27	f	29	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	2	472	U	O5'-P-OP1	-6.59	99.77	105.70
1	2	1458	G	C8-N9-C1'	-6.59	118.43	127.00
1	2	13	C	O5'-P-OP2	-6.59	99.77	105.70
1	2	555	A	C4-N9-C1'	6.58	138.15	126.30
1	2	833	U	O4'-C1'-N1	6.58	113.47	108.20
1	2	1057	U	N1-C2-O2	6.57	127.40	122.80
1	2	958	U	P-O5'-C5'	-6.56	110.40	120.90
1	2	964	U	N1-C2-N3	6.56	118.84	114.90
1	2	1560	U	C2-N1-C1'	6.49	125.49	117.70
1	2	104	A	P-O3'-C3'	6.49	127.49	119.70
18	V	49	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	2	169	A	O5'-P-OP1	-6.47	99.87	105.70
19	W	23	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	2	555	A	C8-N9-C1'	-6.47	116.06	127.70
1	2	1389	C	N1-C1'-C2'	6.46	122.40	114.00
1	2	44	U	O5'-P-OP1	6.38	118.36	110.70
28	t	709	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	2	1091	A	N1-C6-N6	-6.37	114.78	118.60
1	2	863	A	N1-C6-N6	-6.36	114.78	118.60
1	2	162	A	C6-N1-C2	-6.34	114.79	118.60
16	T	160	ARG	NE-CZ-NH1	6.33	123.47	120.30
18	V	11	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	2	482	U	C2-N3-C4	6.31	130.78	127.00
1	2	222	A	C5-C6-N1	-6.30	114.55	117.70
1	2	959	U	C2-N1-C1'	6.28	125.23	117.70
28	t	62	ARG	NE-CZ-NH1	-6.25	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	S	59	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	2	462	G	O5'-P-OP1	-6.24	100.08	105.70
1	2	1086	A	C4-C5-C6	6.23	120.11	117.00
1	2	1251	U	N1-C1'-C2'	6.19	122.04	114.00
1	2	1143	A	C6-C5-N7	6.17	136.62	132.30
12	P	41	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	2	1100	G	P-O5'-C5'	-6.13	111.09	120.90
25	c	13	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	2	322	G	P-O3'-C3'	6.12	127.05	119.70
1	2	863	A	O5'-P-OP1	-6.12	100.19	105.70
3	B	180	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	2	16	G	O5'-P-OP2	-6.09	100.22	105.70
1	2	1246	C	O4'-C1'-N1	6.09	113.07	108.20
1	2	964	U	C5-C4-O4	-6.08	122.25	125.90
18	V	58	LEU	CB-CG-CD2	-6.07	100.68	111.00
22	Z	137	LEU	CA-CB-CG	6.05	129.21	115.30
1	2	1143	A	C4-C5-C6	-6.04	113.98	117.00
29	g	37	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	2	3	U	O5'-P-OP2	-6.03	100.27	105.70
25	c	33	LEU	CB-CG-CD1	-6.03	100.74	111.00
19	W	79	ARG	NE-CZ-NH2	-6.03	117.29	120.30
18	V	31	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	2	112	A	O5'-P-OP2	-6.01	100.29	105.70
1	2	1568	C	P-O3'-C3'	5.98	126.88	119.70
1	2	104	A	C2'-C3'-O3'	5.98	123.27	113.70
28	t	303	LEU	CA-CB-CG	5.97	129.04	115.30
1	2	1793	G	P-O3'-C3'	5.94	126.83	119.70
1	2	1090	C	O5'-P-OP1	-5.92	100.38	105.70
1	2	1057	U	N3-C4-C5	5.91	118.15	114.60
1	2	129	U	P-O3'-C3'	5.91	126.79	119.70
16	T	191	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	2	1560	U	O4'-C1'-N1	5.85	112.88	108.20
1	2	532	U	P-O5'-C5'	-5.83	111.58	120.90
1	2	776	G	C4-N9-C1'	5.83	134.07	126.50
1	2	1033	C	O5'-P-OP1	-5.83	100.45	105.70
1	2	1038	U	O5'-P-OP1	-5.83	100.46	105.70
1	2	121	U	P-O5'-C5'	-5.82	111.60	120.90
1	2	964	U	N1-C2-O2	-5.81	118.73	122.80
28	t	248	ARG	NE-CZ-NH1	-5.80	117.40	120.30
23	a	23	ILE	CG1-CB-CG2	-5.80	98.64	111.40
1	2	857	U	C4-C5-C6	-5.79	116.23	119.70
1	2	220	A	C4-C5-C6	5.76	119.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	803	A	P-O3'-C3'	5.76	126.61	119.70
1	2	1500	C	C2-N1-C1'	5.76	125.14	118.80
1	2	831	U	N3-C2-O2	5.75	126.23	122.20
1	2	1573	A	P-O3'-C3'	5.74	126.59	119.70
5	E	40	ARG	NE-CZ-NH1	5.74	123.17	120.30
29	g	42	ARG	NE-CZ-NH2	-5.73	117.44	120.30
24	b	54	ASP	CB-CG-OD2	5.72	123.45	118.30
16	T	160	ARG	NE-CZ-NH2	-5.71	117.44	120.30
16	T	186	ARG	NE-CZ-NH2	-5.70	117.45	120.30
30	p	97	ARG	NE-CZ-NH1	5.70	123.15	120.30
15	S	148	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	2	863	A	C4-C5-N7	5.69	113.54	110.70
1	2	1489	U	O4'-C1'-N1	5.68	112.75	108.20
15	S	145	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	2	440	U	C6-N1-C2	-5.68	117.59	121.00
1	2	957	G	OP1-P-OP2	-5.68	111.09	119.60
21	Y	130	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	2	222	A	C4-C5-C6	5.67	119.83	117.00
1	2	1658	G	C4-N9-C1'	5.66	133.85	126.50
1	2	1250	U	C2-N1-C1'	5.65	124.48	117.70
26	d	105	ARG	NE-CZ-NH2	-5.64	117.48	120.30
21	Y	125	LEU	CB-CG-CD1	-5.64	101.42	111.00
1	2	776	G	C8-N9-C1'	-5.62	119.69	127.00
1	2	1034	C	P-O5'-C5'	-5.62	111.91	120.90
1	2	384	G	P-O5'-C5'	-5.62	111.92	120.90
1	2	862	A	P-O3'-C3'	5.61	126.44	119.70
1	2	980	G	O5'-P-OP1	5.60	117.42	110.70
26	d	34	ASN	N-CA-CB	-5.60	100.52	110.60
1	2	138	A	C4-N9-C1'	5.59	136.36	126.30
1	2	594	A	O5'-P-OP2	-5.59	100.67	105.70
1	2	505	A	N1-C6-N6	5.58	121.95	118.60
1	2	229	U	N3-C4-C5	5.57	117.94	114.60
1	2	132	U	P-O3'-C3'	5.57	126.39	119.70
1	2	819	G	P-O3'-C3'	5.57	126.38	119.70
1	2	1389	C	C6-N1-C1'	-5.56	114.12	120.80
1	2	632	U	OP1-P-OP2	5.54	127.92	119.60
1	2	1244	A	C2'-C3'-O3'	5.54	122.57	113.70
15	S	30	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	2	699	U	C2'-C3'-O3'	5.53	122.54	113.70
25	c	20	ARG	NE-CZ-NH2	-5.53	117.54	120.30
19	W	77	ILE	CG1-CB-CG2	-5.52	99.25	111.40
1	2	66	U	O5'-P-OP1	5.51	117.31	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	S	9	LEU	CB-CG-CD1	5.51	120.37	111.00
1	2	587	C	C2-N1-C1'	5.51	124.86	118.80
1	2	964	U	C6-N1-C2	5.51	124.31	121.00
1	2	313	U	O5'-P-OP1	-5.51	100.74	105.70
12	P	109	ASN	O-C-N	5.49	131.49	122.70
17	U	116	ARG	NE-CZ-NH1	5.49	123.05	120.30
7	H	110	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	2	1235	C	N1-C2-O2	5.47	122.18	118.90
1	2	242	U	P-O3'-C3'	5.47	126.26	119.70
1	2	424	C	OP1-P-OP2	5.46	127.79	119.60
1	2	15	U	O5'-P-OP2	-5.43	100.81	105.70
1	2	913	G	P-O3'-C3'	5.42	126.20	119.70
1	2	1300	A	O5'-P-OP1	-5.42	100.82	105.70
1	2	139	C	P-O3'-C3'	5.41	126.19	119.70
12	P	101	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	2	236	A	N3-C4-C5	-5.40	123.02	126.80
1	2	795	U	O5'-P-OP1	-5.40	100.84	105.70
14	R	41	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	2	1456	C	C2-N1-C1'	5.40	124.74	118.80
15	S	3	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	2	379	U	O5'-P-OP1	-5.39	100.85	105.70
29	g	43	ARG	CG-CD-NE	-5.38	100.50	111.80
1	2	1658	G	C8-N9-C1'	-5.38	120.00	127.00
24	b	125	ILE	CG1-CB-CG2	-5.38	99.56	111.40
1	2	933	A	P-O3'-C3'	5.38	126.15	119.70
1	2	322	G	O4'-C1'-N9	-5.37	103.91	108.20
27	f	7	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	2	1038	U	N3-C2-O2	-5.34	118.46	122.20
28	t	578	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	2	1103	U	O5'-P-OP1	-5.32	100.92	105.70
1	2	229	U	C4-C5-C6	5.31	122.89	119.70
24	b	7	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	2	138	A	C8-N9-C1'	-5.30	118.17	127.70
1	2	833	U	N3-C2-O2	5.29	125.90	122.20
1	2	652	G	C2'-C3'-O3'	5.28	122.15	113.70
1	2	833	U	N3-C4-C5	5.28	117.77	114.60
3	B	157	ARG	NE-CZ-NH1	5.27	122.93	120.30
15	S	191	ARG	NE-CZ-NH1	5.27	122.93	120.30
16	T	215	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	2	1086	A	C4-N9-C1'	5.26	135.76	126.30
24	b	28	ARG	C-N-CD	-5.26	109.04	120.60
1	2	402	C	O5'-P-OP1	-5.25	100.98	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	t	57	LYS	CD-CE-NZ	5.25	123.77	111.70
1	2	242	U	C4'-C3'-O3'	5.24	123.49	113.00
1	2	924	A	N1-C6-N6	-5.24	115.45	118.60
1	2	863	A	N3-C4-C5	-5.23	123.14	126.80
16	T	85	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	2	555	A	P-O3'-C3'	5.22	125.97	119.70
24	b	57	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	2	857	U	C6-N1-C2	-5.22	117.87	121.00
1	2	1659	A	O4'-C1'-N9	5.21	112.37	108.20
1	2	93	A	N9-C1'-C2'	5.21	120.77	114.00
16	T	92	ARG	NE-CZ-NH1	-5.21	117.69	120.30
27	f	33	LEU	CB-CG-CD2	-5.21	102.15	111.00
3	B	180	ARG	NE-CZ-NH2	-5.20	117.70	120.30
15	S	193	GLY	N-CA-C	5.20	126.09	113.10
28	t	248	ARG	NE-CZ-NH2	5.17	122.89	120.30
8	I	105	LEU	CA-CB-CG	5.17	127.19	115.30
1	2	781	U	P-O3'-C3'	5.16	125.89	119.70
29	g	43	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	2	1658	G	P-O3'-C3'	5.16	125.89	119.70
1	2	1600	A	C4-C5-C6	-5.16	114.42	117.00
1	2	1560	U	C6-N1-C1'	-5.16	113.98	121.20
17	U	104	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	2	757	A	O5'-P-OP2	5.15	116.88	110.70
5	E	44	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	2	1202	A	C4-N9-C1'	5.15	135.57	126.30
1	2	440	U	C5-C6-N1	-5.14	120.13	122.70
27	f	7	LEU	CB-CG-CD1	5.13	119.73	111.00
1	2	152	U	N1-C2-O2	-5.13	119.21	122.80
10	L	29	ARG	NE-CZ-NH1	5.13	122.86	120.30
32	e	211	ILE	C-N-CA	5.13	134.52	121.70
16	T	186	ARG	NE-CZ-NH1	5.12	122.86	120.30
15	S	3	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	2	236	A	C4-N9-C1'	5.12	135.51	126.30
1	2	595	G	C5'-C4'-O4'	5.12	115.24	109.10
1	2	185	U	C2-N1-C1'	5.11	123.84	117.70
1	2	315	A	P-O3'-C3'	5.11	125.83	119.70
1	2	1023	A	C4'-C3'-O3'	5.10	123.21	113.00
1	2	121	U	C5'-C4'-C3'	-5.10	107.84	116.00
1	2	1092	A	C5-C6-N6	5.10	127.78	123.70
1	2	322	G	C2'-C3'-O3'	5.10	121.85	113.70
1	2	1251	U	C2-N1-C1'	-5.09	111.60	117.70
1	2	1441	C	P-O3'-C3'	5.08	125.79	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	135	LEU	CB-CG-CD1	-5.08	102.37	111.00
1	2	236	A	N3-C4-N9	5.07	131.45	127.40
1	2	440	U	C4-C5-C6	-5.07	116.66	119.70
13	Q	111	ARG	NE-CZ-NH1	5.06	122.83	120.30
21	Y	20	ARG	CG-CD-NE	5.05	122.40	111.80
1	2	1307	U	C2-N1-C1'	5.04	123.75	117.70
1	2	1731	A	O5'-P-OP2	-5.04	101.16	105.70
19	W	78	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	2	1091	A	C6-N1-C2	-5.03	115.58	118.60
20	X	136	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	2	1275	A	P-O3'-C3'	5.03	125.74	119.70
1	2	323	A	OP1-P-OP2	5.02	127.13	119.60
1	2	863	A	P-O3'-C3'	5.02	125.73	119.70
26	d	8	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	2	912	U	C2'-C3'-O3'	5.02	121.72	113.70
1	2	104	A	C4-N9-C1'	-5.01	117.28	126.30
1	2	139	C	OP2-P-O3'	5.01	116.22	105.20
1	2	104	A	C8-N9-C1'	5.01	136.71	127.70
1	2	1777	G	O5'-P-OP1	5.00	116.70	110.70

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	1086	A	Sidechain
1	2	1143	A	Sidechain
1	2	1595	U	Sidechain
1	2	222	A	Sidechain
1	2	236	A	Sidechain
1	2	440	U	Sidechain
1	2	507	U	Sidechain
1	2	618	U	Sidechain
1	2	857	U	Sidechain
1	2	863	A	Sidechain
1	2	964	U	Sidechain
3	B	57	SER	Peptide
4	C	22	PRO	Peptide
4	C	87	GLU	Peptide
2	D	107	ASP	Peptide
5	E	21	ASP	Peptide
5	E	45	PHE	Peptide
6	F	13	LYS	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
6	F	41	PRO	Peptide
9	K	103	ARG	Peptide
9	K	54	VAL	Peptide
9	K	96	SER	Peptide
12	P	110	TYR	Peptide
12	P	166	GLY	Peptide
12	P	190	ASP	Peptide
13	Q	176	VAL	Peptide
13	Q	177	GLN	Peptide
13	Q	179	SER	Peptide
13	Q	214	LYS	Peptide
13	Q	54	LEU	Peptide
14	R	39	THR	Peptide
15	S	68	ARG	Peptide
17	U	47	ARG	Peptide
17	U	64	VAL	Peptide
17	U	97	ARG	Peptide
18	V	25	ARG	Sidechain
19	W	119	ALA	Peptide
19	W	163	PRO	Peptide
20	X	5	LEU	Peptide
21	Y	22	ALA	Peptide
22	Z	123	SER	Peptide
23	a	43	GLY	Peptide
23	a	45	ALA	Peptide
23	a	80	LYS	Peptide
24	b	54	ASP	Peptide
25	c	111	GLY	Peptide
29	g	46	ASN	Peptide
31	r	152	MET	Peptide
31	r	91	ARG	Peptide
28	t	350	ALA	Peptide
28	t	518	ASP	Peptide
28	t	713	THR	Peptide
28	t	714	VAL	Peptide
28	t	731	LYS	Peptide
28	t	737	THR	Peptide
28	t	742	SER	Peptide
28	t	753	GLY	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	D	122/143 (85%)	89 (73%)	30 (25%)	3 (2%)	5	36
3	B	198/225 (88%)	168 (85%)	28 (14%)	2 (1%)	15	55
4	C	108/136 (79%)	92 (85%)	14 (13%)	2 (2%)	8	42
5	E	115/142 (81%)	93 (81%)	21 (18%)	1 (1%)	17	57
6	F	139/143 (97%)	121 (87%)	14 (10%)	4 (3%)	4	33
7	H	120/146 (82%)	107 (89%)	13 (11%)	0	100	100
8	I	141/144 (98%)	129 (92%)	11 (8%)	1 (1%)	22	61
9	K	62/108 (57%)	49 (79%)	10 (16%)	3 (5%)	2	22
10	L	60/67 (90%)	54 (90%)	6 (10%)	0	100	100
11	N	49/152 (32%)	32 (65%)	12 (24%)	5 (10%)	0	7
12	P	204/252 (81%)	168 (82%)	32 (16%)	4 (2%)	7	41
13	Q	212/255 (83%)	172 (81%)	38 (18%)	2 (1%)	17	57
14	R	218/254 (86%)	186 (85%)	29 (13%)	3 (1%)	11	48
15	S	258/261 (99%)	226 (88%)	31 (12%)	1 (0%)	34	71
16	T	224/236 (95%)	206 (92%)	17 (8%)	1 (0%)	34	71
17	U	182/190 (96%)	158 (87%)	22 (12%)	2 (1%)	14	53
18	V	184/200 (92%)	160 (87%)	21 (11%)	3 (2%)	9	46
19	W	183/197 (93%)	156 (85%)	24 (13%)	3 (2%)	9	46
20	X	153/156 (98%)	133 (87%)	19 (12%)	1 (1%)	22	61
21	Y	148/151 (98%)	130 (88%)	17 (12%)	1 (1%)	22	61
22	Z	125/137 (91%)	110 (88%)	15 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	a	85/87 (98%)	66 (78%)	16 (19%)	3 (4%)	3	30
24	b	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	19	59
25	c	142/145 (98%)	116 (82%)	23 (16%)	3 (2%)	7	40
26	d	132/135 (98%)	121 (92%)	9 (7%)	2 (2%)	10	47
27	f	79/82 (96%)	60 (76%)	17 (22%)	2 (2%)	5	36
28	t	627/788 (80%)	542 (86%)	78 (12%)	7 (1%)	14	53
29	g	58/63 (92%)	42 (72%)	14 (24%)	2 (3%)	3	31
30	p	183/274 (67%)	168 (92%)	15 (8%)	0	100	100
31	r	256/425 (60%)	227 (89%)	26 (10%)	3 (1%)	13	51
32	e	259/483 (54%)	242 (93%)	14 (5%)	3 (1%)	13	51
All	All	5153/6307 (82%)	4441 (86%)	644 (12%)	68 (1%)	16	50

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	K	97	LYS
11	N	148	TYR
12	P	110	TYR
12	P	111	ILE
15	S	69	HIS
17	U	98	ILE
19	W	120	LYS
23	a	11	LEU
28	t	677	ALA
29	g	52	GLY
31	r	235	ILE
32	e	306	ALA
2	D	90	LYS
3	B	56	ALA
4	C	88	VAL
11	N	142	GLY
11	N	147	VAL
14	R	40	LYS
14	R	97	ARG
18	V	10	LYS
23	a	81	ASN
26	d	34	ASN
28	t	54	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
28	t	205	GLN
28	t	519	PRO
31	r	93	THR
32	e	206	LEU
32	e	402	ASP
4	C	23	LYS
6	F	14	LYS
6	F	42	GLU
12	P	185	ARG
13	Q	213	ARG
25	c	4	GLY
25	c	132	LEU
26	d	37	LYS
27	f	75	GLU
27	f	76	GLY
2	D	25	GLU
2	D	108	ARG
3	B	58	LEU
5	E	54	ALA
9	K	55	PRO
9	K	96	SER
11	N	143	LYS
11	N	145	HIS
13	Q	62	LYS
16	T	68	LEU
18	V	152	ILE
18	V	153	GLU
25	c	88	PRO
28	t	207	ASP
28	t	738	LYS
6	F	40	GLU
12	P	196	SER
17	U	74	GLN
20	X	5	LEU
23	a	44	ARG
8	I	53	TRP
14	R	150	GLN
19	W	162	SER
21	Y	22	ALA
29	g	51	ASN
19	W	163	PRO
28	t	753	GLY

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Mol	Chain	Res	Type
31	r	192	ILE
6	F	41	PRO
24	b	29	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	
2	D	89/119 (75%)	89 (100%)	0	100	100
3	B	173/191 (91%)	173 (100%)	0	100	100
4	C	88/124 (71%)	88 (100%)	0	100	100
5	E	98/118 (83%)	98 (100%)	0	100	100
6	F	117/119 (98%)	116 (99%)	1 (1%)	78	90
7	H	109/129 (84%)	109 (100%)	0	100	100
8	I	115/116 (99%)	114 (99%)	1 (1%)	78	90
9	K	57/89 (64%)	57 (100%)	0	100	100
10	L	55/60 (92%)	55 (100%)	0	100	100
11	N	43/135 (32%)	40 (93%)	3 (7%)	15	48
12	P	164/210 (78%)	162 (99%)	2 (1%)	71	87
13	Q	191/224 (85%)	189 (99%)	2 (1%)	76	88
14	R	179/205 (87%)	174 (97%)	5 (3%)	43	72
15	S	221/222 (100%)	220 (100%)	1 (0%)	88	95
16	T	188/201 (94%)	187 (100%)	1 (0%)	88	95
17	U	165/170 (97%)	163 (99%)	2 (1%)	71	87
18	V	150/161 (93%)	150 (100%)	0	100	100
19	W	158/166 (95%)	157 (99%)	1 (1%)	86	94
20	X	129/137 (94%)	129 (100%)	0	100	100
21	Y	127/128 (99%)	126 (99%)	1 (1%)	81	91
22	Z	81/105 (77%)	79 (98%)	2 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	a	74/74 (100%)	72 (97%)	2 (3%)	44	73
24	b	110/111 (99%)	108 (98%)	2 (2%)	59	81
25	c	119/120 (99%)	118 (99%)	1 (1%)	81	91
26	d	112/113 (99%)	111 (99%)	1 (1%)	78	90
27	f	70/71 (99%)	70 (100%)	0	100	100
28	t	533/703 (76%)	525 (98%)	8 (2%)	65	84
29	g	51/54 (94%)	49 (96%)	2 (4%)	32	65
30	p	162/238 (68%)	154 (95%)	8 (5%)	25	59
31	r	242/384 (63%)	242 (100%)	0	100	100
All	All	4170/4997 (84%)	4124 (99%)	46 (1%)	74	88

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	57	LEU
8	I	114	VAL
11	N	143	LYS
11	N	145	HIS
11	N	146	SER
12	P	109	ASN
12	P	133	ILE
13	Q	111	ARG
13	Q	212	VAL
14	R	88	LYS
14	R	90	THR
14	R	91	ARG
14	R	119	LYS
14	R	203	LYS
15	S	9	LEU
16	T	78	THR
17	U	46	ILE
17	U	148	LYS
19	W	118	LEU
21	Y	16	ILE
22	Z	136	ARG
22	Z	137	LEU
23	a	11	LEU
23	a	69	LEU
24	b	26	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	b	93	LEU
25	c	9	LEU
26	d	121	THR
28	t	54	ARG
28	t	123	ILE
28	t	206	LEU
28	t	220	PHE
28	t	225	ARG
28	t	303	LEU
28	t	502	ARG
28	t	714	VAL
29	g	8	LEU
29	g	33	ARG
30	p	90	ASN
30	p	111	ASN
30	p	164	LEU
30	p	193	LEU
30	p	220	THR
30	p	244	ARG
30	p	258	LYS
30	p	262	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	B	100	ASN
3	B	103	ASN
3	B	116	HIS
4	C	105	GLN
5	E	98	ASN
5	E	103	ASN
5	E	104	GLN
6	F	32	ASN
6	F	139	GLN
7	H	19	ASN
7	H	89	GLN
8	I	12	GLN
8	I	129	GLN
11	N	145	HIS
12	P	15	GLN
12	P	30	GLN
13	Q	149	GLN

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Mol	Chain	Res	Type
14	R	209	ASN
15	S	69	HIS
15	S	98	ASN
16	T	139	ASN
17	U	5	GLN
18	V	32	GLN
18	V	103	GLN
18	V	138	ASN
19	W	38	ASN
20	X	14	GLN
20	X	104	HIS
21	Y	105	ASN
22	Z	80	HIS
24	b	15	ASN
24	b	80	ASN
25	c	75	GLN
26	d	133	ASN
28	t	53	GLN
28	t	116	GLN
28	t	194	ASN
28	t	199	HIS
28	t	294	HIS
28	t	509	ASN
28	t	766	GLN
30	p	90	ASN
30	p	111	ASN
31	r	146	ASN
31	r	182	ASN
31	r	222	ASN
31	r	234	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1664/1800 (92%)	589 (35%)	68 (4%)

All (589) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	4	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	5	U
1	2	8	U
1	2	9	U
1	2	14	C
1	2	16	G
1	2	17	C
1	2	25	C
1	2	26	A
1	2	32	U
1	2	34	G
1	2	42	G
1	2	43	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	59	C
1	2	60	U
1	2	63	G
1	2	66	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	71	A
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	78	A
1	2	79	C
1	2	80	A
1	2	93	A
1	2	99	C
1	2	100	A
1	2	101	U
1	2	104	A
1	2	105	A
1	2	111	U
1	2	114	C
1	2	116	U
1	2	120	U
1	2	121	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	126	A
1	2	127	G
1	2	128	U
1	2	129	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	138	A
1	2	139	C
1	2	140	A
1	2	142	G
1	2	145	A
1	2	155	U
1	2	159	U
1	2	160	C
1	2	161	U
1	2	166	C
1	2	168	A
1	2	170	U
1	2	171	A
1	2	176	C
1	2	178	U
1	2	179	A
1	2	185	U
1	2	188	A
1	2	189	C
1	2	191	C
1	2	193	U
1	2	194	U
1	2	195	G
1	2	197	A
1	2	199	G
1	2	211	U
1	2	215	A
1	2	216	U
1	2	222	A
1	2	223	U
1	2	225	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	227	U
1	2	228	G
1	2	231	U
1	2	233	C
1	2	234	G
1	2	238	U
1	2	240	U
1	2	241	U
1	2	243	G
1	2	249	U
1	2	250	C
1	2	255	U
1	2	257	A
1	2	259	U
1	2	260	U
1	2	261	U
1	2	265	A
1	2	274	G
1	2	275	C
1	2	278	U
1	2	280	U
1	2	281	G
1	2	287	G
1	2	299	A
1	2	313	U
1	2	314	C
1	2	315	A
1	2	316	A
1	2	320	U
1	2	321	C
1	2	322	G
1	2	323	A
1	2	337	G
1	2	338	C
1	2	340	U
1	2	349	U
1	2	350	U
1	2	351	C
1	2	352	A
1	2	353	A
1	2	359	A
1	2	361	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	387	A
1	2	390	G
1	2	396	G
1	2	397	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	417	A
1	2	418	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	430	G
1	2	434	G
1	2	435	C
1	2	436	A
1	2	437	A
1	2	439	U
1	2	444	C
1	2	445	A
1	2	448	C
1	2	452	A
1	2	453	U
1	2	454	U
1	2	455	C
1	2	459	G
1	2	460	A
1	2	461	G
1	2	468	A
1	2	471	A
1	2	477	A
1	2	483	A
1	2	484	C
1	2	488	G
1	2	491	C
1	2	492	A
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	510	G
1	2	520	A
1	2	527	A
1	2	532	U
1	2	534	A
1	2	537	G
1	2	538	A
1	2	539	G
1	2	541	A
1	2	542	A
1	2	544	A
1	2	548	G
1	2	551	G
1	2	554	C
1	2	555	A
1	2	556	A
1	2	558	U
1	2	559	C
1	2	561	G
1	2	562	G
1	2	564	G
1	2	565	C
1	2	566	C
1	2	568	G
1	2	576	G
1	2	577	G
1	2	579	A
1	2	580	A
1	2	581	U
1	2	582	U
1	2	594	A
1	2	595	G
1	2	596	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	599	A
1	2	608	U
1	2	610	G
1	2	611	U
1	2	613	G
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	625	C
1	2	638	U
1	2	639	U
1	2	641	G
1	2	644	C
1	2	645	C
1	2	648	G
1	2	650	U
1	2	652	G
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	678	A
1	2	681	U
1	2	684	A
1	2	687	G
1	2	688	G
1	2	690	G
1	2	694	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	736	C
1	2	739	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	741	C
1	2	742	U
1	2	744	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	779	U
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	788	A
1	2	803	A
1	2	804	A
1	2	805	U
1	2	811	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	816	G
1	2	817	A
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	832	U
1	2	833	U
1	2	835	U
1	2	839	U
1	2	840	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	843	U
1	2	844	A
1	2	845	G
1	2	846	G
1	2	847	A
1	2	855	A
1	2	856	A
1	2	857	U
1	2	860	U
1	2	862	A
1	2	863	A
1	2	864	U
1	2	873	U
1	2	876	G
1	2	886	U
1	2	889	U
1	2	903	U
1	2	904	G
1	2	910	C
1	2	913	G
1	2	914	G
1	2	915	A
1	2	926	A
1	2	928	U
1	2	929	A
1	2	931	C
1	2	932	U
1	2	933	A
1	2	934	C
1	2	935	U
1	2	942	G
1	2	945	U
1	2	960	U
1	2	961	U
1	2	964	U
1	2	966	A
1	2	969	C
1	2	970	A
1	2	983	A
1	2	984	G
1	2	987	G
1	2	988	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	992	A
1	2	993	A
1	2	994	G
1	2	995	A
1	2	996	U
1	2	997	G
1	2	999	U
1	2	1009	U
1	2	1010	C
1	2	1012	U
1	2	1021	C
1	2	1023	A
1	2	1024	U
1	2	1025	A
1	2	1026	A
1	2	1028	C
1	2	1029	U
1	2	1030	A
1	2	1031	U
1	2	1032	G
1	2	1039	A
1	2	1051	G
1	2	1052	U
1	2	1053	G
1	2	1055	U
1	2	1056	U
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1064	G
1	2	1066	C
1	2	1072	C
1	2	1076	A
1	2	1077	C
1	2	1078	C
1	2	1080	U
1	2	1081	A
1	2	1082	C
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1098	U
1	2	1099	U
1	2	1100	G
1	2	1102	G
1	2	1109	G
1	2	1113	A
1	2	1114	G
1	2	1119	G
1	2	1124	A
1	2	1126	G
1	2	1138	A
1	2	1140	G
1	2	1146	G
1	2	1147	A
1	2	1148	C
1	2	1149	G
1	2	1150	G
1	2	1151	A
1	2	1155	G
1	2	1158	C
1	2	1159	C
1	2	1160	A
1	2	1164	G
1	2	1165	G
1	2	1167	G
1	2	1185	U
1	2	1188	G
1	2	1202	A
1	2	1203	A
1	2	1207	C
1	2	1212	G
1	2	1214	U
1	2	1218	G
1	2	1227	A
1	2	1229	G
1	2	1230	A
1	2	1235	C
1	2	1241	G
1	2	1242	A
1	2	1243	G
1	2	1244	A
1	2	1245	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1246	C
1	2	1250	U
1	2	1251	U
1	2	1252	C
1	2	1255	G
1	2	1258	U
1	2	1259	U
1	2	1264	G
1	2	1265	G
1	2	1269	U
1	2	1270	G
1	2	1272	U
1	2	1273	G
1	2	1275	A
1	2	1276	U
1	2	1278	G
1	2	1282	U
1	2	1288	G
1	2	1290	U
1	2	1291	G
1	2	1301	U
1	2	1305	U
1	2	1306	C
1	2	1312	A
1	2	1314	U
1	2	1320	U
1	2	1321	A
1	2	1325	A
1	2	1330	G
1	2	1331	A
1	2	1333	C
1	2	1336	A
1	2	1338	C
1	2	1339	C
1	2	1340	U
1	2	1344	A
1	2	1345	A
1	2	1347	U
1	2	1348	A
1	2	1354	G
1	2	1360	A
1	2	1361	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1363	U
1	2	1367	G
1	2	1370	U
1	2	1371	A
1	2	1373	C
1	2	1382	A
1	2	1385	G
1	2	1390	U
1	2	1391	A
1	2	1413	U
1	2	1415	U
1	2	1416	G
1	2	1417	A
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1432	U
1	2	1433	G
1	2	1435	G
1	2	1436	A
1	2	1437	U
1	2	1440	C
1	2	1441	C
1	2	1442	U
1	2	1444	A
1	2	1445	G
1	2	1446	A
1	2	1447	C
1	2	1448	G
1	2	1457	C
1	2	1459	C
1	2	1460	A
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1482	C
1	2	1486	G
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1494	C
1	2	1496	U
1	2	1503	A
1	2	1506	G
1	2	1516	A
1	2	1520	U
1	2	1521	G
1	2	1522	U
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1529	C
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1540	G
1	2	1542	G
1	2	1550	A
1	2	1557	U
1	2	1559	A
1	2	1563	C
1	2	1569	A
1	2	1573	A
1	2	1574	G
1	2	1577	A
1	2	1579	U
1	2	1583	A
1	2	1584	G
1	2	1590	G
1	2	1601	G
1	2	1607	G
1	2	1610	G
1	2	1616	G
1	2	1619	C
1	2	1630	U
1	2	1631	A
1	2	1648	A
1	2	1650	U
1	2	1651	A
1	2	1652	C
1	2	1653	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1657	U
1	2	1658	G
1	2	1659	A
1	2	1660	A
1	2	1662	G
1	2	1673	G
1	2	1681	A
1	2	1686	C
1	2	1688	U
1	2	1689	A
1	2	1692	G
1	2	1693	A
1	2	1709	C
1	2	1710	U
1	2	1711	C
1	2	1712	A
1	2	1713	G
1	2	1717	G
1	2	1728	A
1	2	1730	A
1	2	1731	A
1	2	1732	A
1	2	1736	G
1	2	1744	A
1	2	1746	A
1	2	1750	A
1	2	1754	A
1	2	1770	U
1	2	1771	U
1	2	1772	C
1	2	1780	G
1	2	1781	A
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
1	2	1797	A
1	2	1798	U
1	2	1800	A

All (68) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	47	A
1	2	68	A
1	2	79	C
1	2	99	C
1	2	104	A
1	2	126	A
1	2	128	U
1	2	129	U
1	2	132	U
1	2	138	A
1	2	139	C
1	2	159	U
1	2	169	A
1	2	215	A
1	2	224	C
1	2	232	U
1	2	242	U
1	2	280	U
1	2	312	A
1	2	315	A
1	2	322	G
1	2	352	A
1	2	400	A
1	2	401	A
1	2	417	A
1	2	423	G
1	2	452	A
1	2	493	U
1	2	555	A
1	2	565	C
1	2	609	U
1	2	649	U
1	2	652	G
1	2	696	C
1	2	699	U
1	2	754	A
1	2	781	U
1	2	803	A
1	2	804	A
1	2	819	G
1	2	846	G
1	2	863	A

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Mol	Chain	Res	Type
1	2	912	U
1	2	913	G
1	2	1023	A
1	2	1058	U
1	2	1081	A
1	2	1097	U
1	2	1099	U
1	2	1108	G
1	2	1157	A
1	2	1244	A
1	2	1250	U
1	2	1332	C
1	2	1339	C
1	2	1344	A
1	2	1441	C
1	2	1446	A
1	2	1481	C
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1649	G
1	2	1656	U
1	2	1680	G
1	2	1793	G
1	2	1795	U

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

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

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	401:A	O3'	402:C	P	1.78

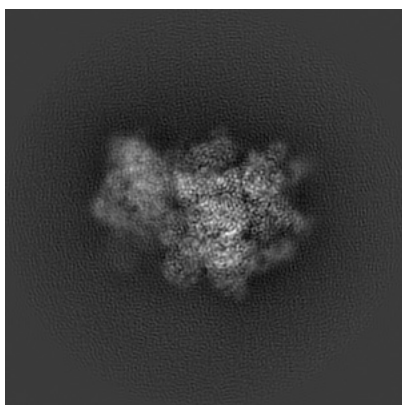
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3886. These allow visual inspection of the internal detail of the map and identification of artifacts.

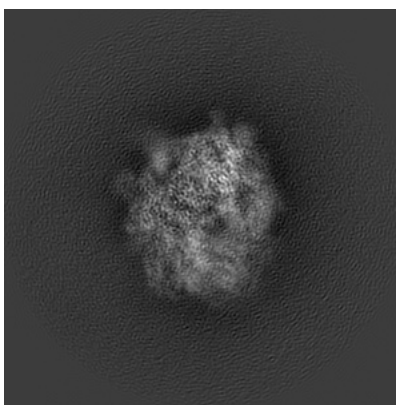
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

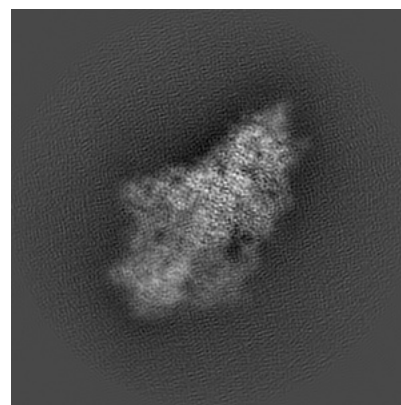
#### 6.1.1 Primary map



X



Y

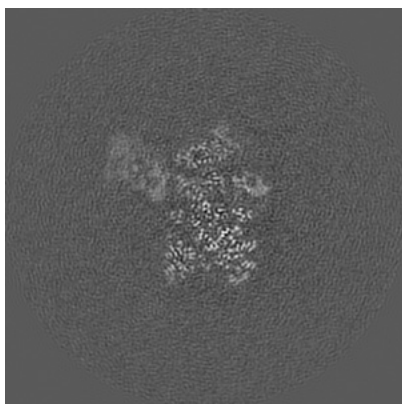


Z

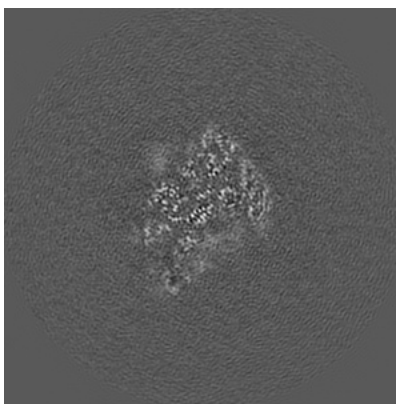
The images above show the map projected in three orthogonal directions.

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

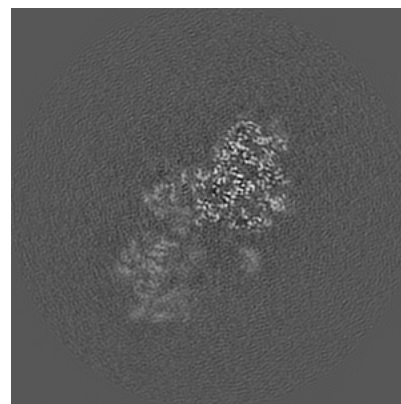
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

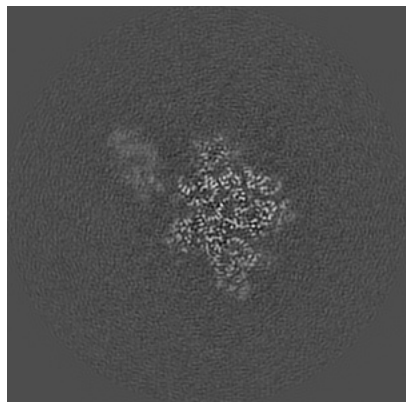


Z Index: 192

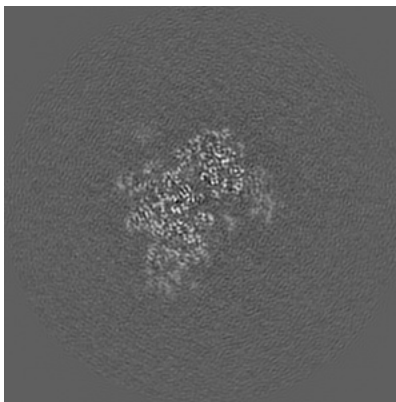
The images above show central slices of the map in three orthogonal directions.

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

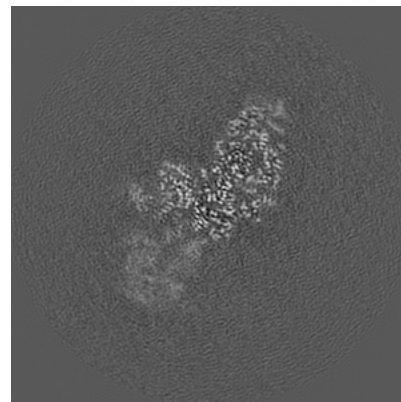
### 6.3.1 Primary map



X Index: 209



Y Index: 214

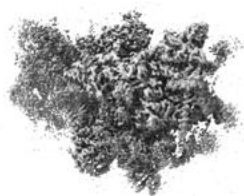


Z Index: 178

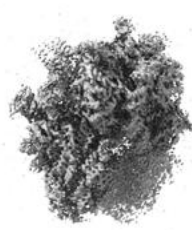
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 0.0722. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

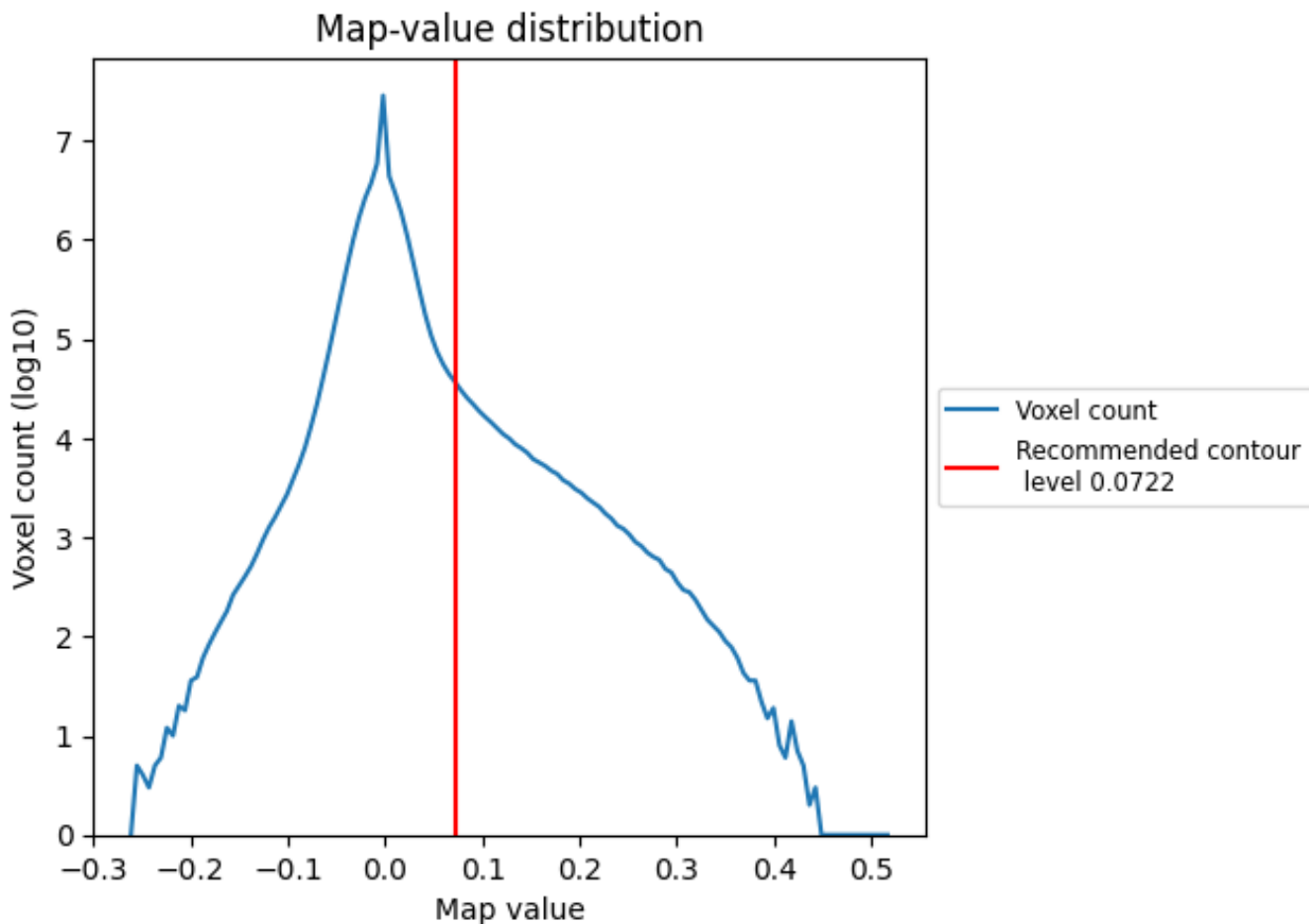
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

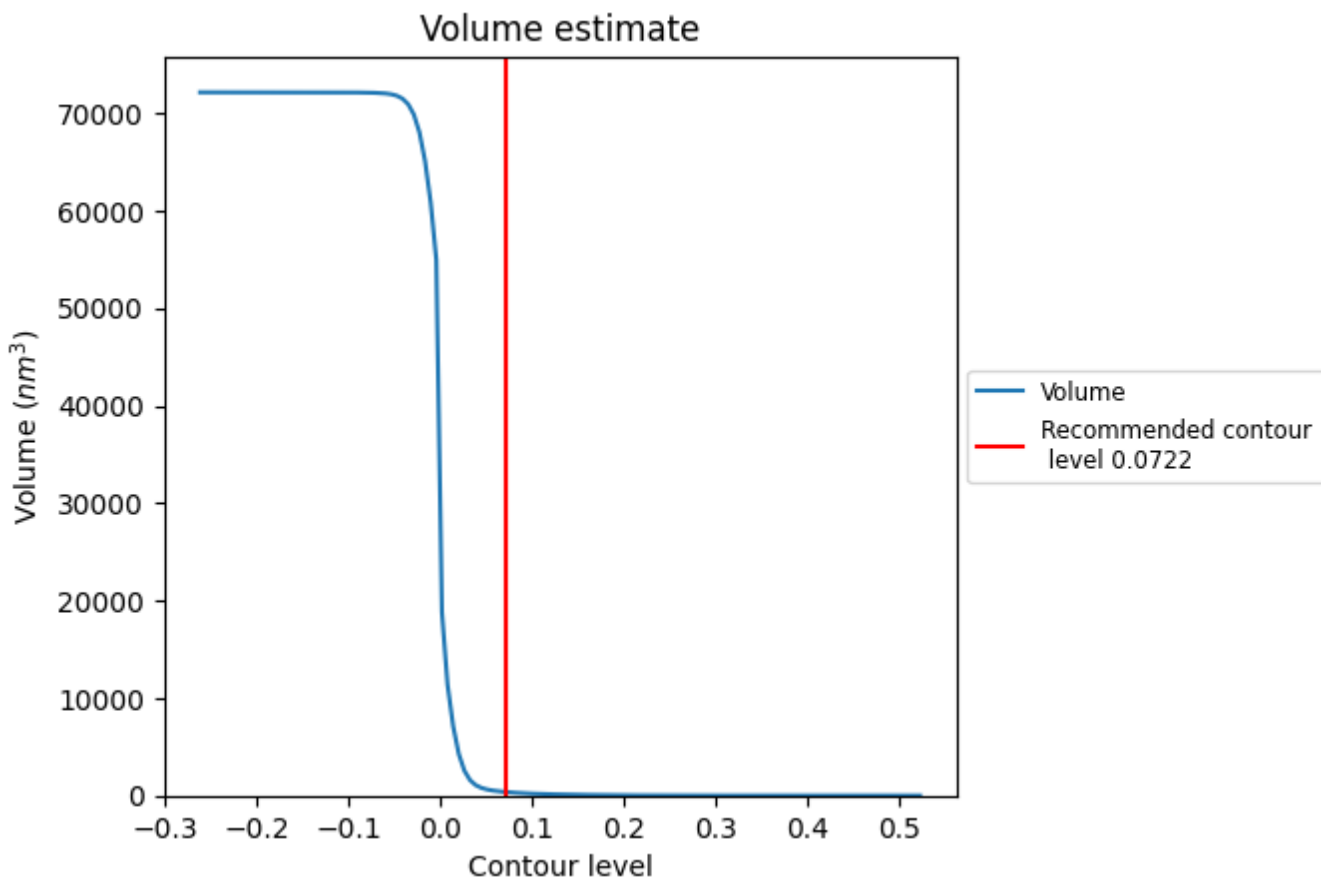
This section contains the results of statistical analysis of the map.

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



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

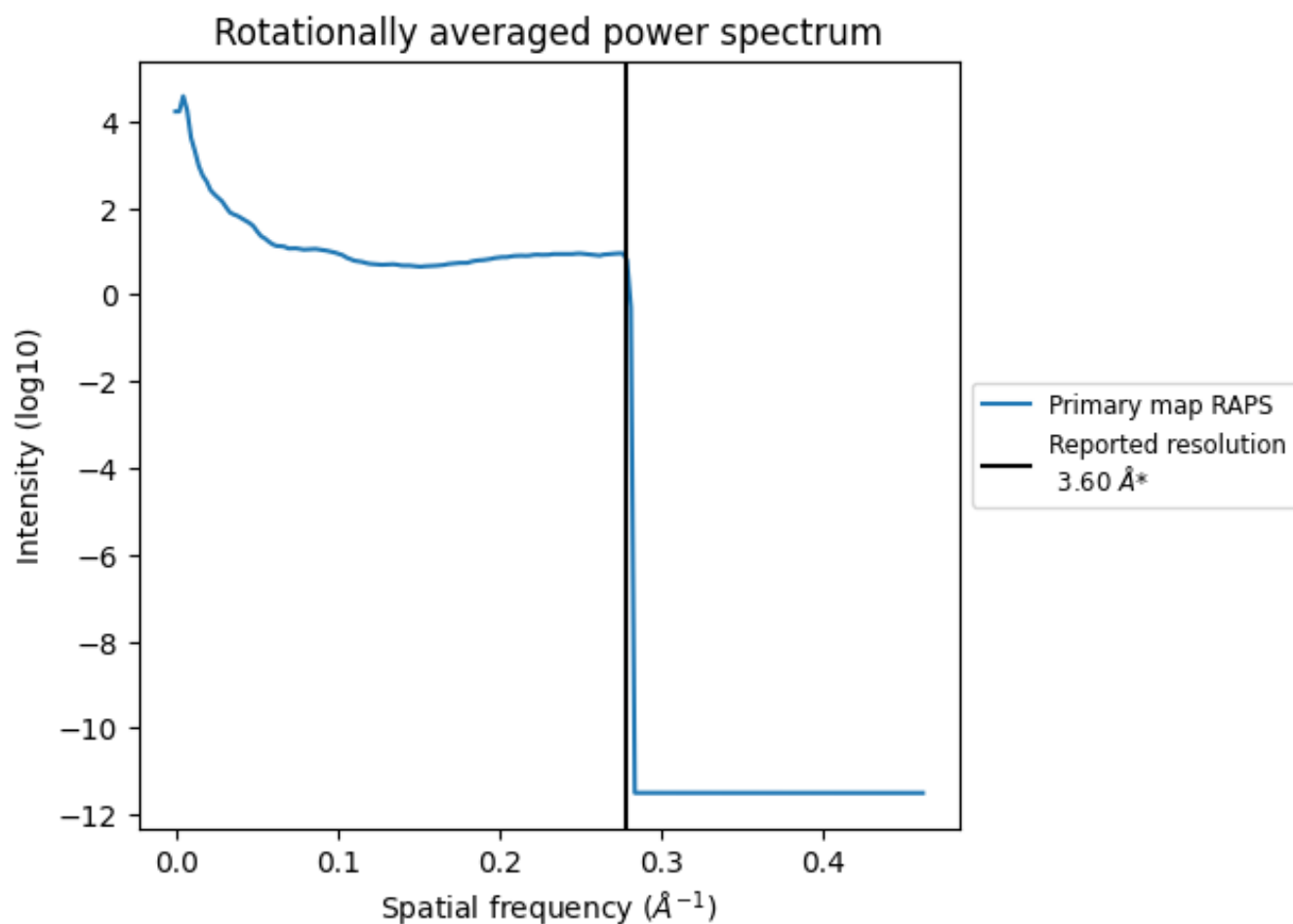
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 359  $\text{nm}^3$ ; this corresponds to an approximate mass of 324 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

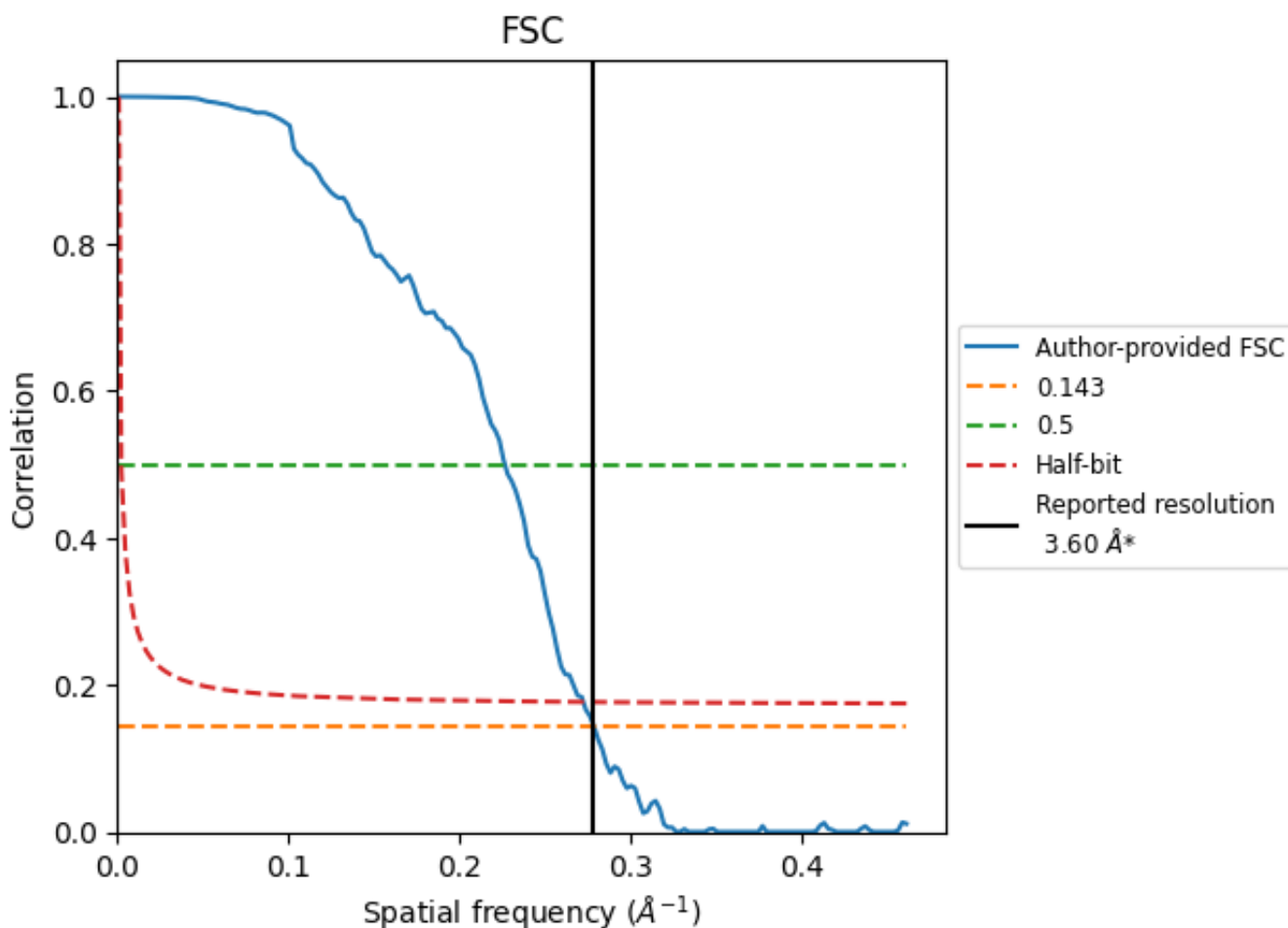


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

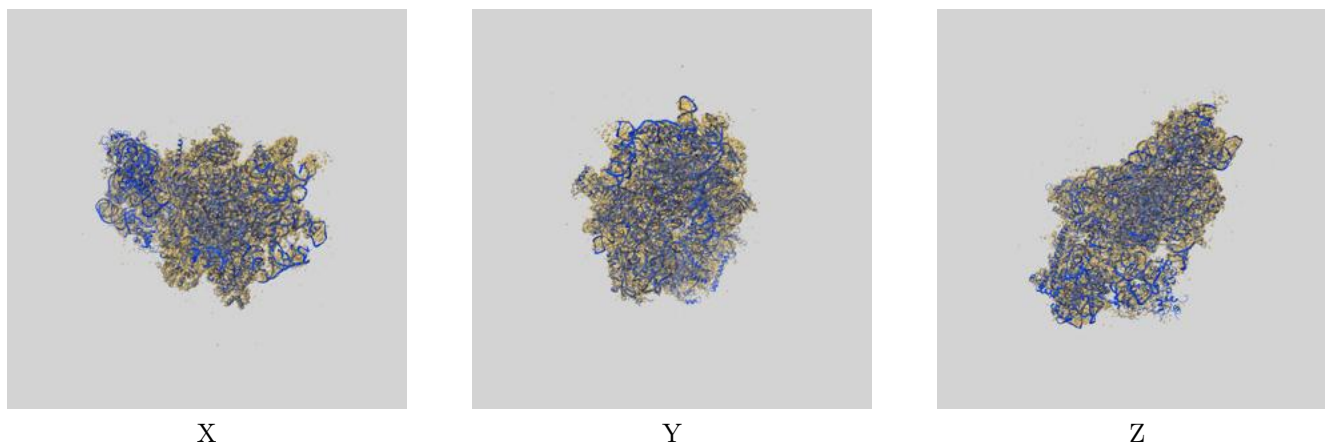
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.41	3.67
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

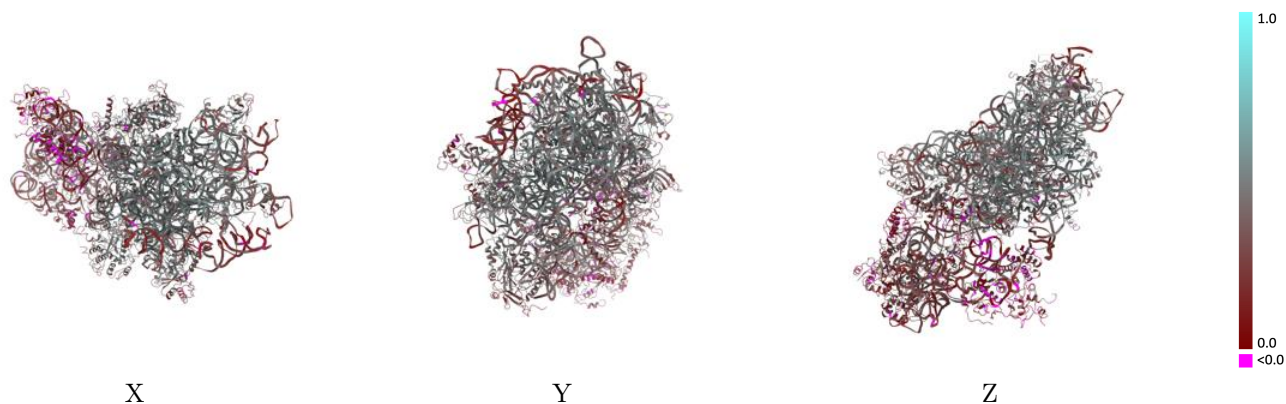
This section contains information regarding the fit between EMDB map EMD-3886 and PDB model 6EML. Per-residue inclusion information can be found in section 3 on page 9.

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



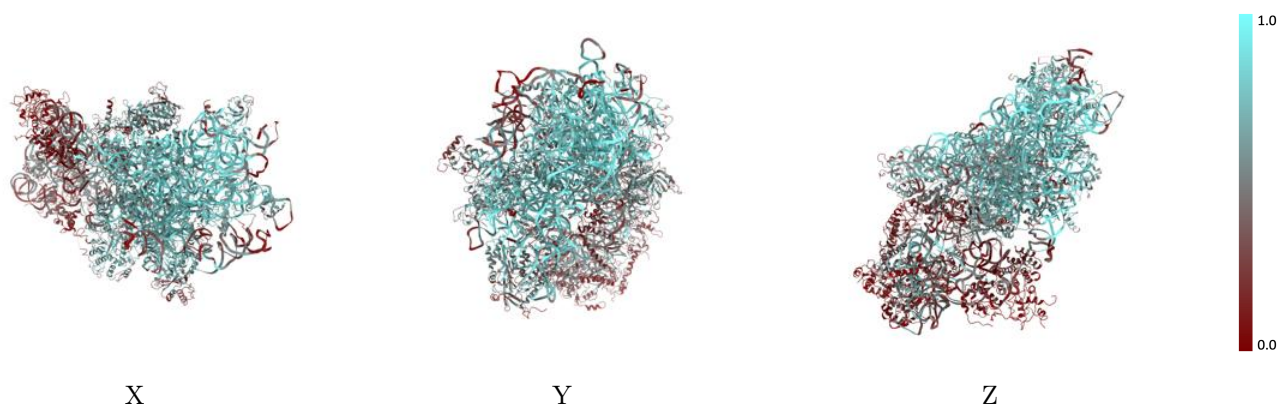
The images above show the 3D surface view of the map at the recommended contour level 0.0722 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



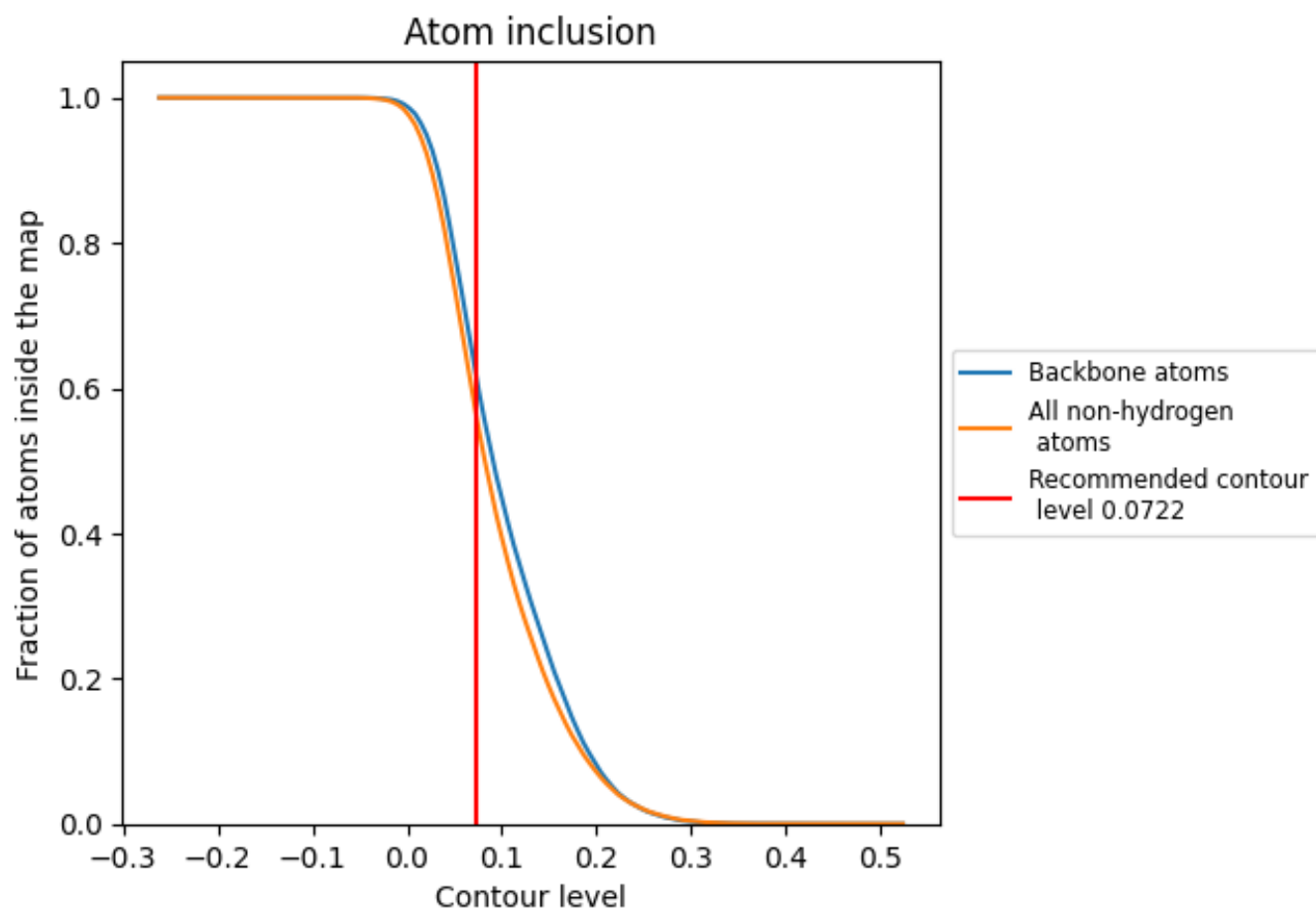
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0722).

## 9.4 Atom inclusion [i](#)





































































At the recommended contour level, 62% of all backbone atoms, 57% 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 (0.0722) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5678	 0.3710
2	 0.6673	 0.3790
B	 0.2304	 0.2400
C	 0.1811	 0.2180
D	 0.0454	 0.1680
E	 0.2594	 0.2530
F	 0.1603	 0.2270
H	 0.1814	 0.2510
I	 0.2109	 0.2440
K	 0.1054	 0.2120
L	 0.1752	 0.2370
N	 0.0310	 0.1090
P	 0.6649	 0.4400
Q	 0.5110	 0.3880
R	 0.6508	 0.4630
S	 0.7195	 0.4930
T	 0.6592	 0.4410
U	 0.4793	 0.3780
V	 0.7082	 0.4540
W	 0.7101	 0.4740
X	 0.6810	 0.4750
Y	 0.6996	 0.4510
Z	 0.4872	 0.3840
a	 0.6762	 0.4490
b	 0.7715	 0.5160
c	 0.6170	 0.4600
d	 0.6964	 0.4720
e	 0.1665	 0.1520
f	 0.6755	 0.4590
g	 0.3856	 0.3360
p	 0.4152	 0.3700
r	 0.1447	 0.1400
t	 0.5279	 0.4020

