



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:16 PM UTC

PDB ID : 6YLX / pdb_00006ylx
EMDB ID : EMD-10841
Title : pre-60S State NE1 (TAP-Flag-Nop53)
Authors : Kater, L.; Beckmann, R.
Deposited on : 2020-04-07
Resolution : 3.90 Å (reported)
Based on initial models : 3JCT, 6ELZ, 6N8J

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

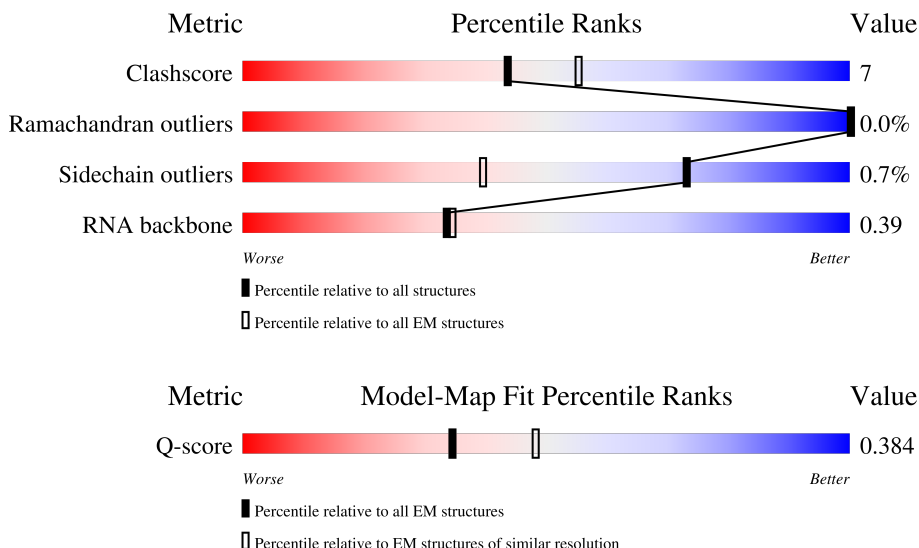
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

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



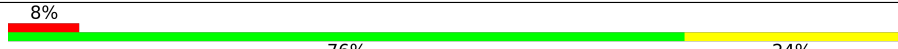
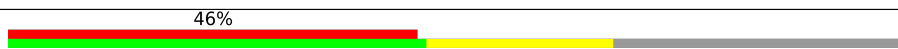
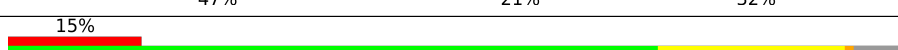
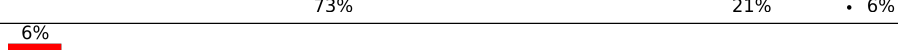
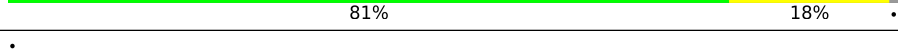
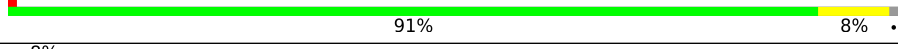
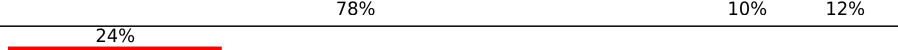
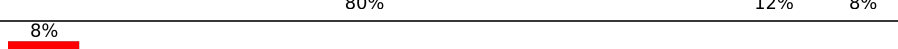
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	B	387	13% 75% 25%
2	C	362	• 83% 15% •
3	E	176	5% 70% 18% • 11%

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Mol	Chain	Length	Quality of chain
4	F	244	
5	G	256	
6	H	191	
7	K	376	
8	L	199	
9	M	138	
10	N	204	
11	O	199	
12	P	184	
13	Q	186	
14	R	189	
15	S	172	
16	T	160	
17	U	121	
18	V	137	
19	W	236	
20	X	142	
21	Y	127	
22	Z	136	
23	a	149	
24	b	647	
25	c	105	
26	d	113	
27	e	130	
28	f	107	

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Mol	Chain	Length	Quality of chain
29	g	121	
30	h	120	
31	i	100	
32	j	88	
33	k	78	
34	l	51	
35	n	605	
36	o	220	
37	q	455	
38	r	261	
39	s	520	
40	t	322	
41	u	199	
42	y	245	
43	z	106	
44	1	3396	
45	2	158	
46	6	232	
47	w	841	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 118882 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 protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 2 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 3 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 4 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 5 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	192	Total	C	N	O	S	0	0
			1515	974	267	272	2		

- Molecule 6 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 7 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	256	Total	C	N	O	S	0	0
			2064	1332	342	387	3		

- Molecule 8 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	187	Total	C	N	O	S	0	0
			1499	934	307	258			

- Molecule 9 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 10 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	180	Total	C	N	O	S	0	0
			1543	968	325	249	1		

- Molecule 11 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 12 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	176	Total	C	N	O	S	0	0
			1397	868	279	250			

- Molecule 13 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	134	Total	C	N	O	S	0	0
			1035	659	196	179	1		

- Molecule 14 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	R	156	Total	C	N	O	0	0
			1258	781	265	212		

- Molecule 15 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 16 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	56	Total	C	N	O	S	0	0
			434	268	86	79	1		

- Molecule 17 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	U	106	Total	C	N	O	0	0
			844	545	138	161		

- Molecule 18 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 19 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	234	Total	C	N	O	S	0	0
			1885	1194	323	362	6		

- Molecule 20 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	141	Total	C	N	O	S	0	0
			1100	705	196	197	2		

- Molecule 21 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 22 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	Z	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 23 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	93	Total	C	N	O	S	0	0
			735	479	130	125	1		

- Molecule 24 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	470	Total	C	N	O	S	0	0
			3814	2424	663	709	18		

- Molecule 25 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 26 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 27 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 28 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 29 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 33 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 34 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 35 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	371	Total	C	N	O	S	0	0
			3030	1963	523	534	10		

- Molecule 36 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 37 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	q	87	Total	C	N	O	S	0	0
			723	450	129	143	1		

- Molecule 38 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	r	217	Total	C	N	O	S	0	0
			1760	1110	334	309	7		

- Molecule 39 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	s	36	Total	C	N	O	S	0	0
			301	184	69	46	2		

- Molecule 40 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	t	287	Total	C	N	O	S	0	0
			2306	1459	427	417	3		

- Molecule 41 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	u	123	Total	C	N	O	S	0	0
			1040	652	211	168	9		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

- Molecule 43 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 44 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	2534	Total	C	N	O	P	0	0
			54232	24220	9799	17679	2534		

- Molecule 45 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 46 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	6	65	Total	C	N	O	P	0	0
			1370	614	228	463	65		

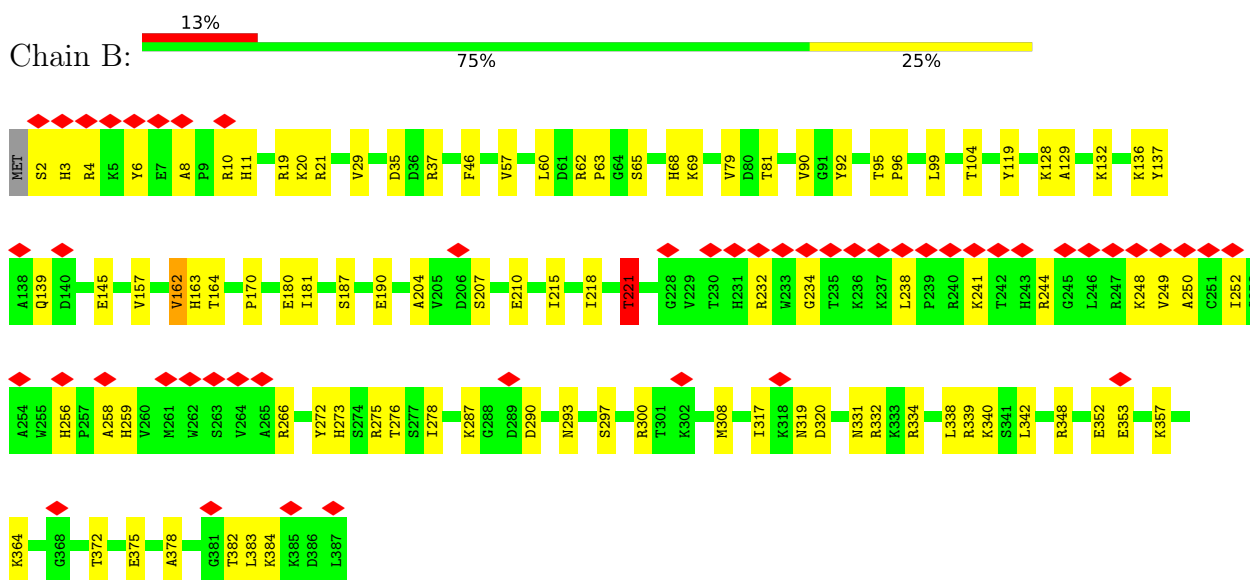
- Molecule 47 is a protein called 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	360	Total	C	N	O	S	0	0
			2898	1860	507	516	15		

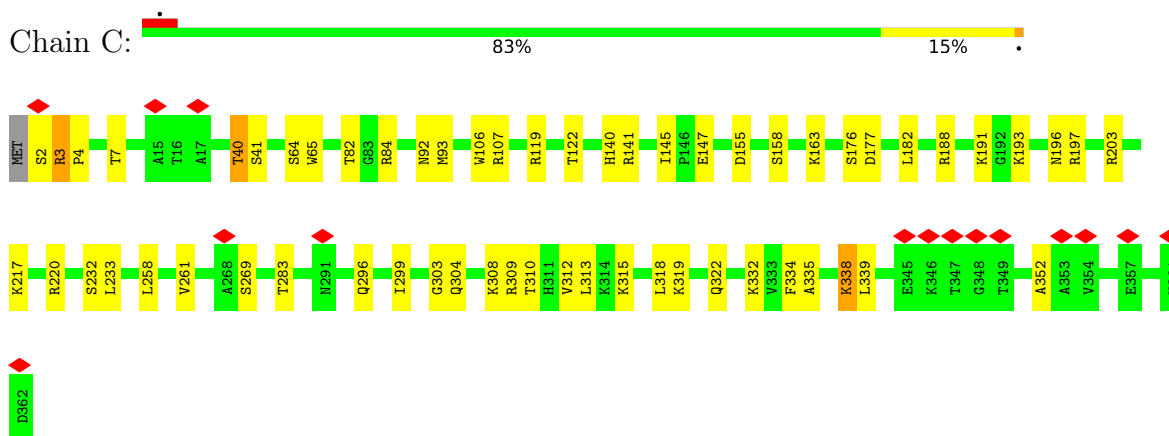
3 Residue-property plots

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

- Molecule 1: 60S ribosomal protein L3

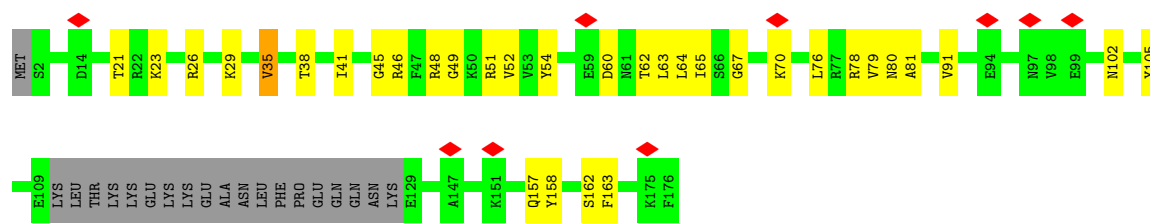


- Molecule 2: 60S ribosomal protein L4-A

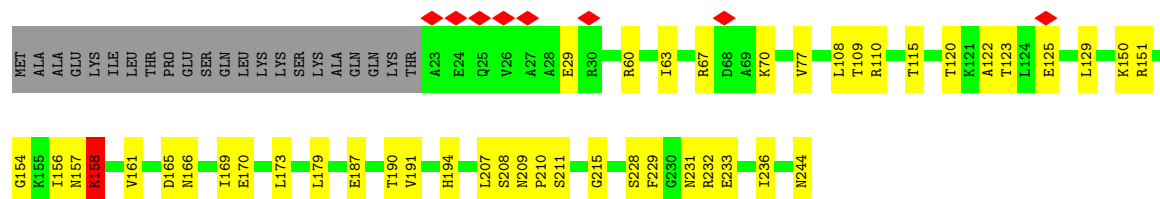


- Molecule 3: 60S ribosomal protein L6-A

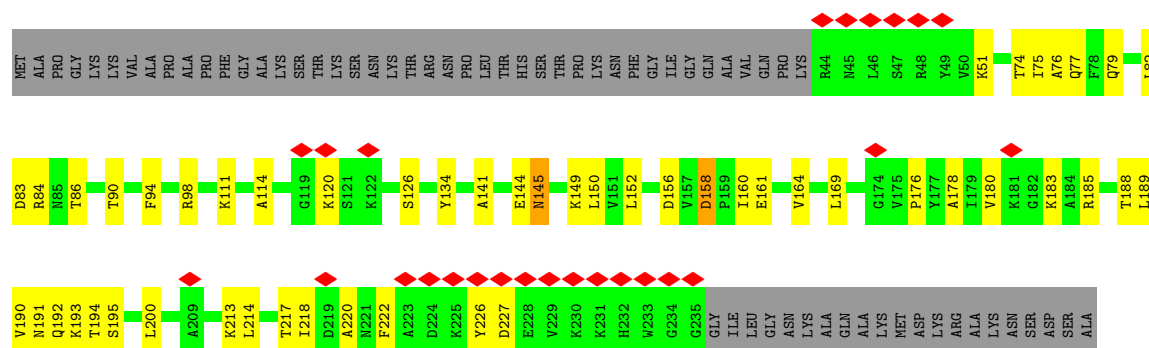




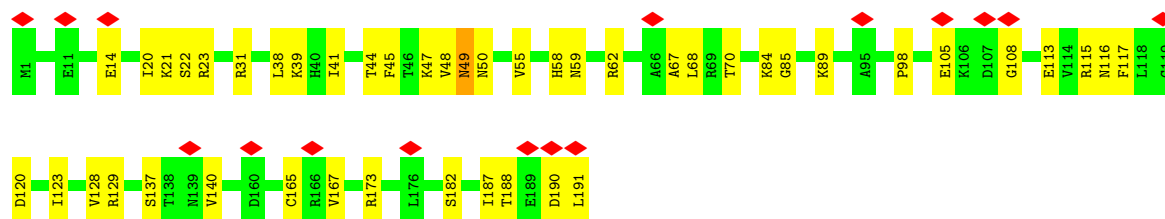
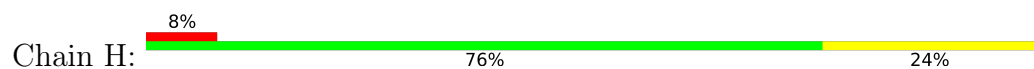
• Molecule 4: 60S ribosomal protein L7-A



• Molecule 5: 60S ribosomal protein L8-A

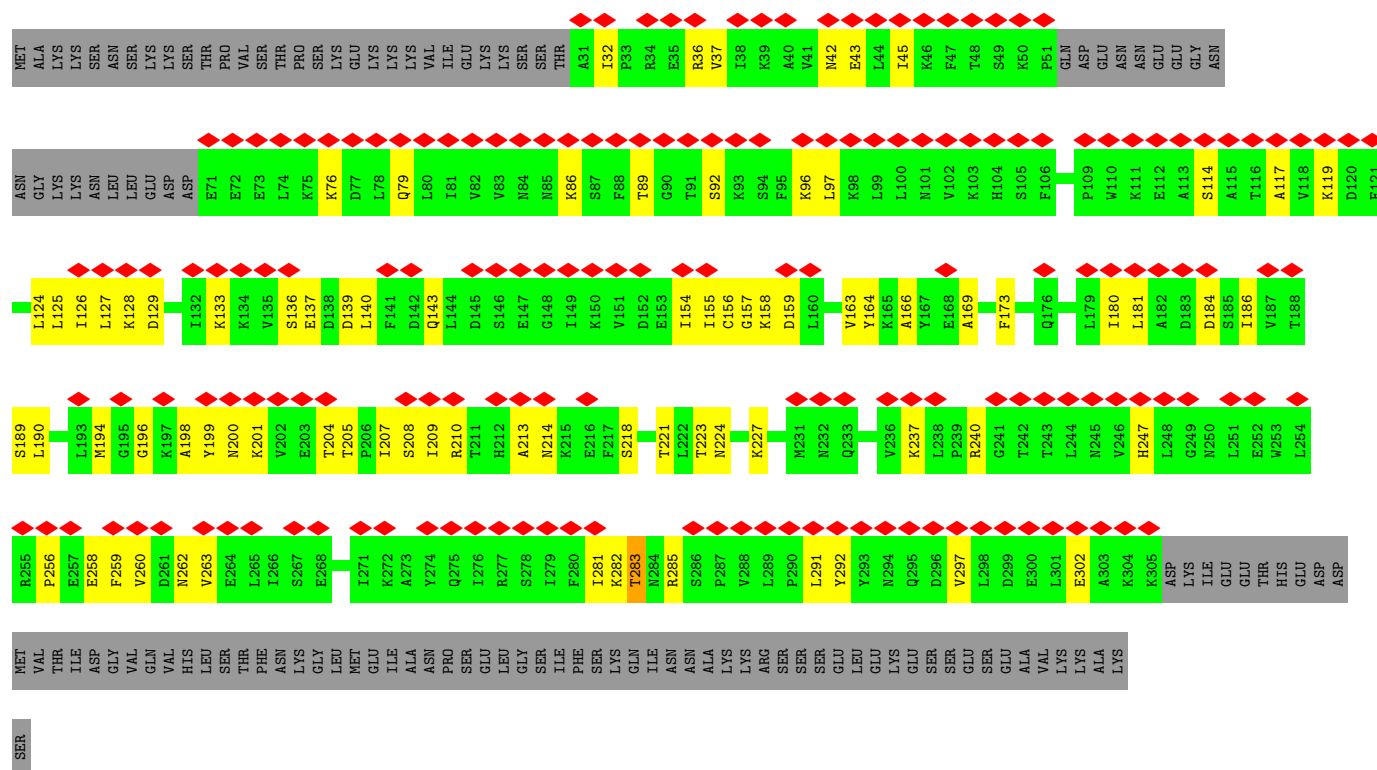


• Molecule 6: 60S ribosomal protein L9-A

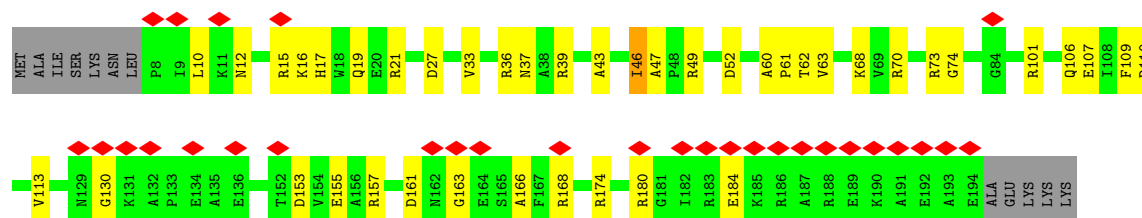


• Molecule 7: Proteasome-interacting protein CIC1

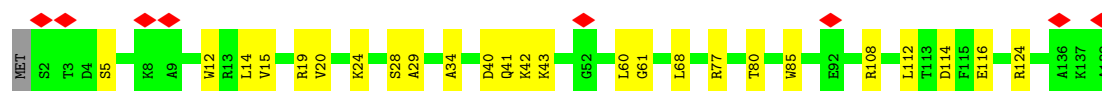
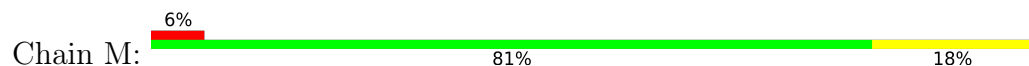




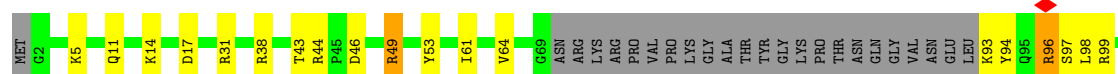
• Molecule 8: 60S ribosomal protein L13-A



• Molecule 9: 60S ribosomal protein L14-A



• Molecule 10: 60S ribosomal protein L15-A





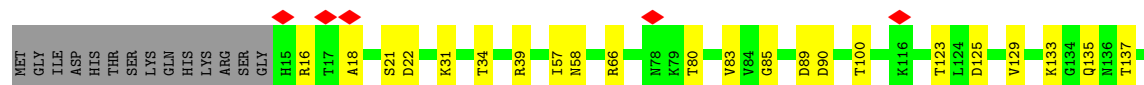
- Molecule 11: 60S ribosomal protein L16-A



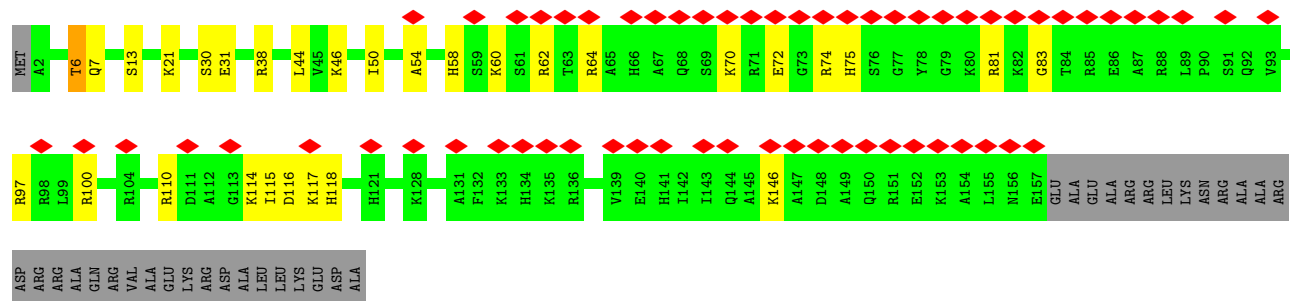
- Molecule 12: 60S ribosomal protein L17-A



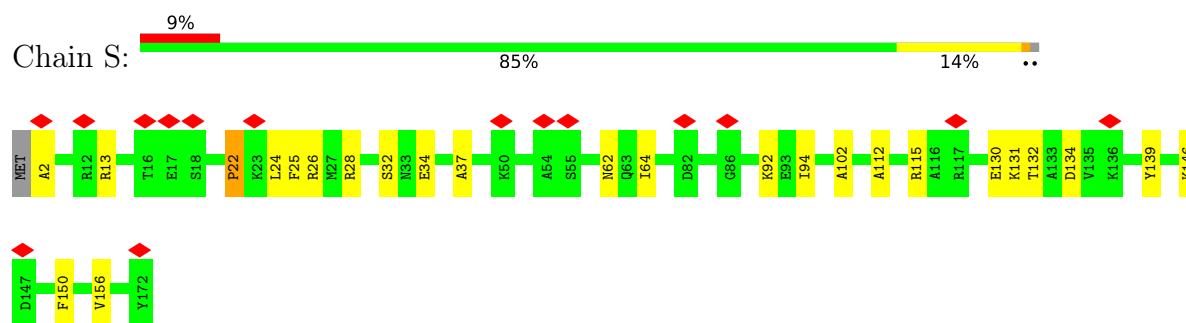
- Molecule 13: 60S ribosomal protein L18-A



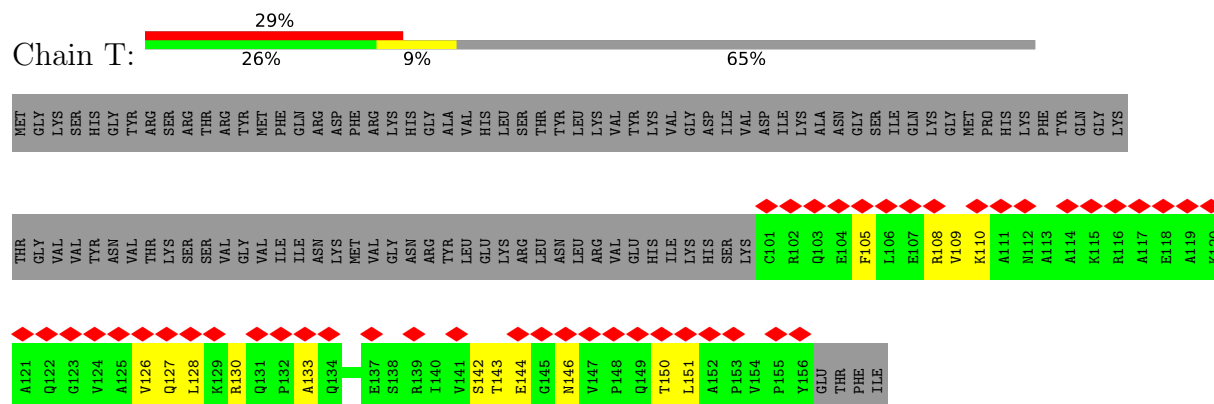
- Molecule 14: 60S ribosomal protein L19-A



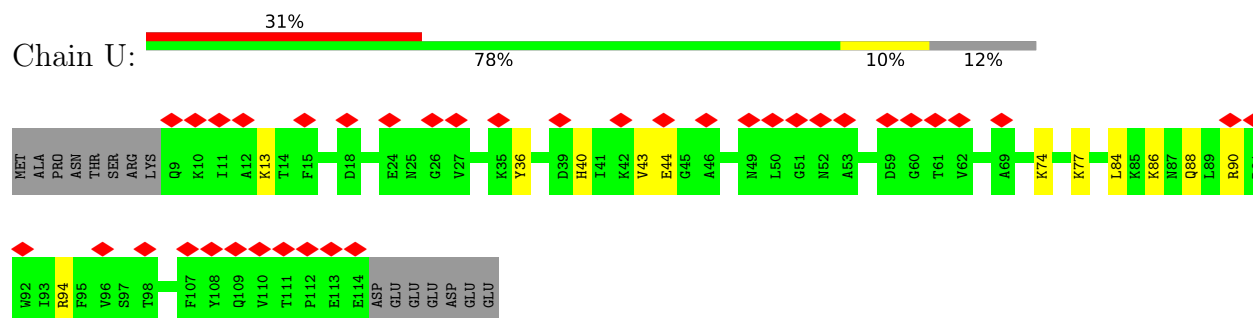
- Molecule 15: 60S ribosomal protein L20-A



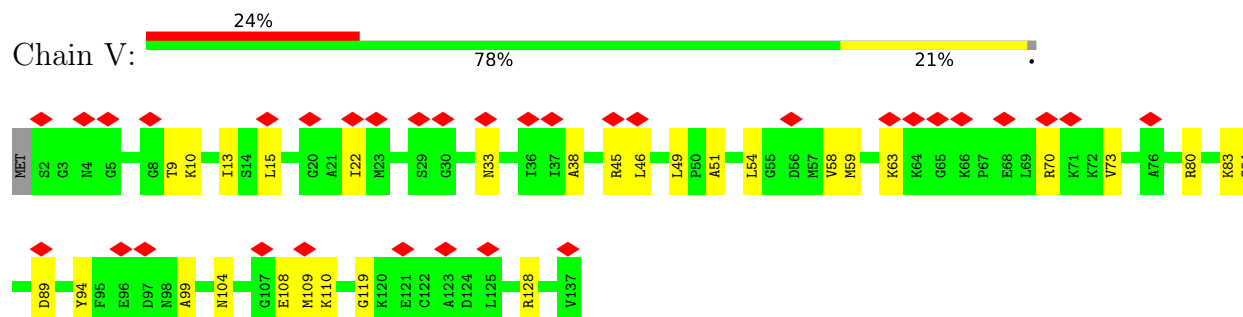
- Molecule 16: 60S ribosomal protein L21-A



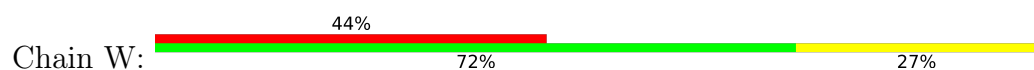
- Molecule 17: 60S ribosomal protein L22-A

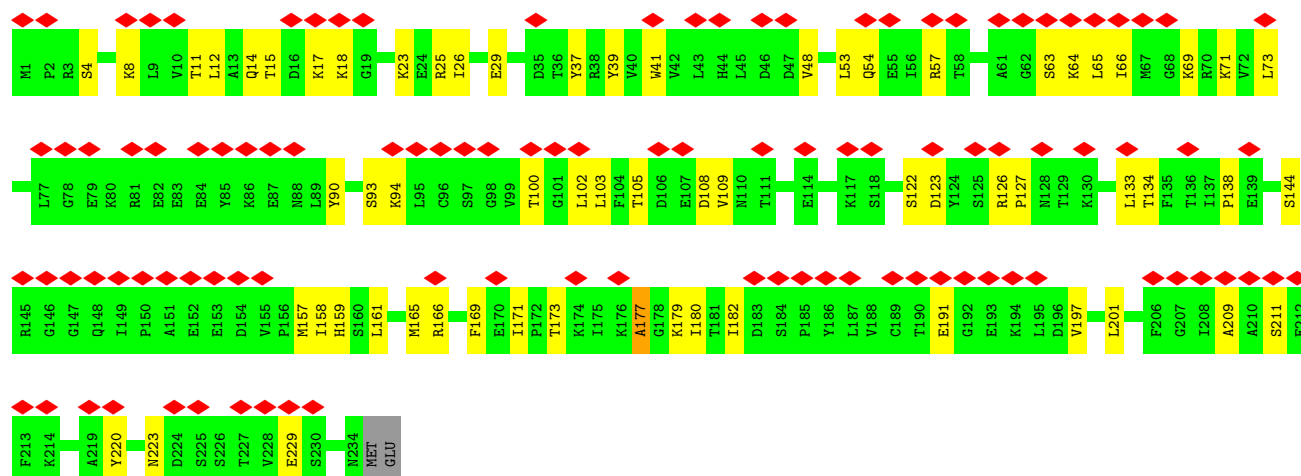


- Molecule 18: 60S ribosomal protein L23-A

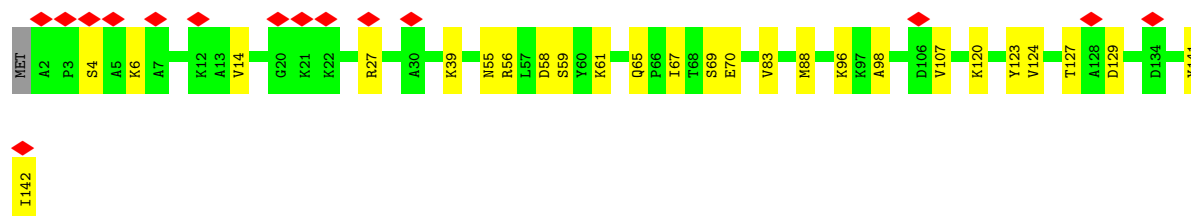
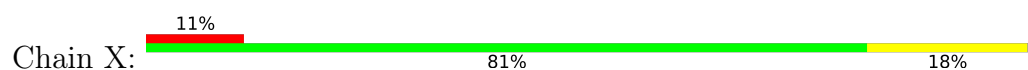


- Molecule 19: Ribosome assembly factor MRT4

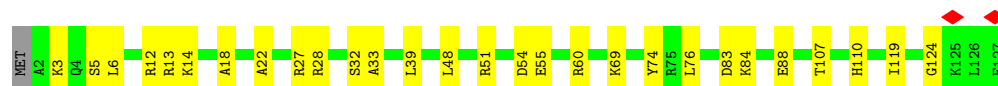
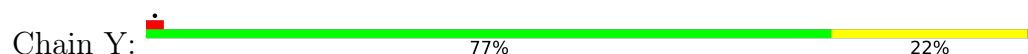




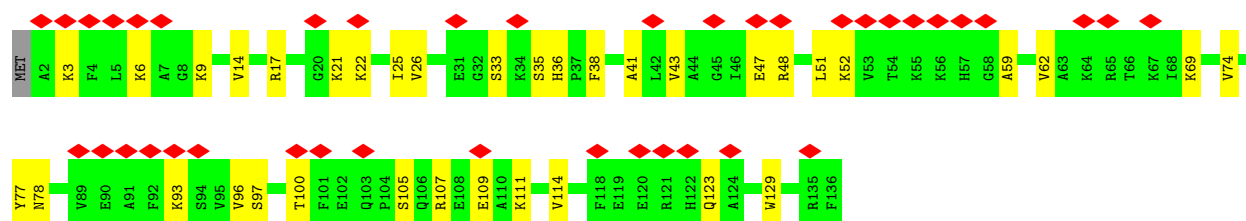
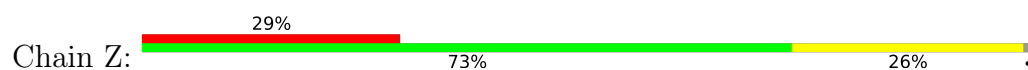
- Molecule 20: 60S ribosomal protein L25



- Molecule 21: 60S ribosomal protein L26-A

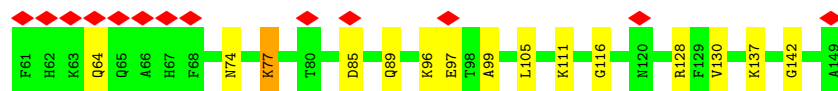
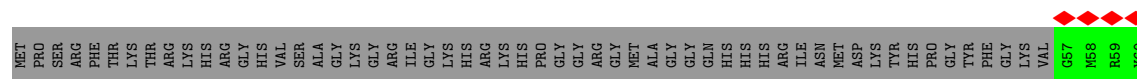


- Molecule 22: 60S ribosomal protein L27-A

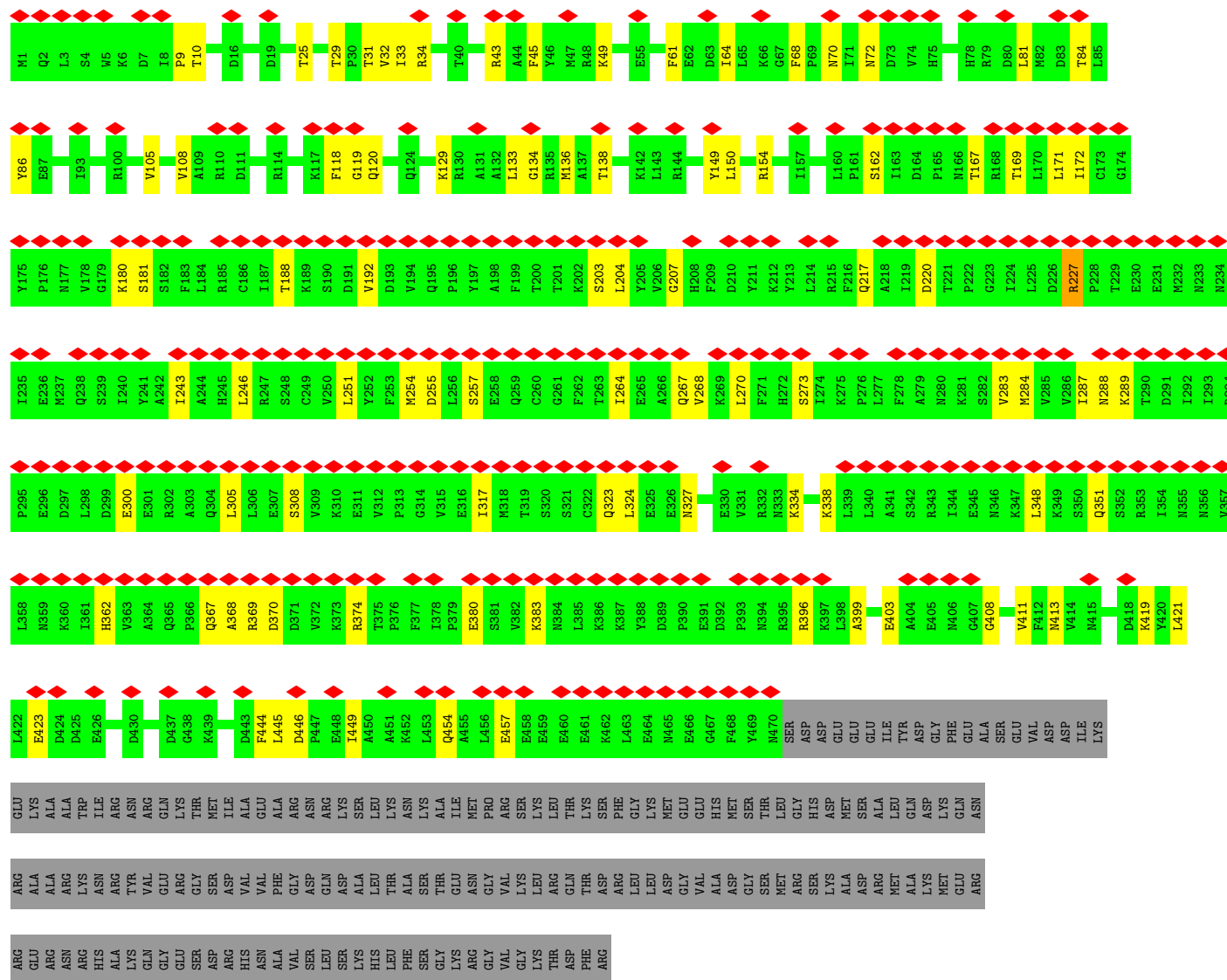
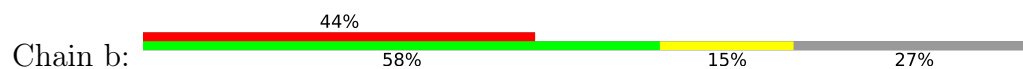


- Molecule 23: 60S ribosomal protein L28

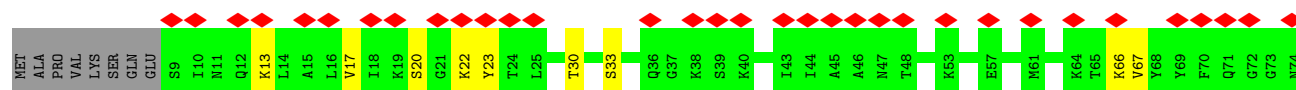
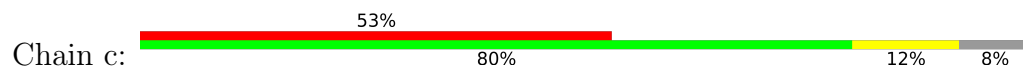


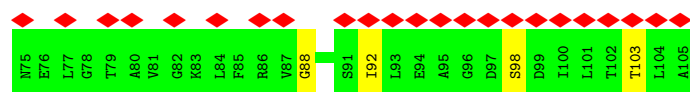


• Molecule 24: Nucleolar GTP-binding protein 1

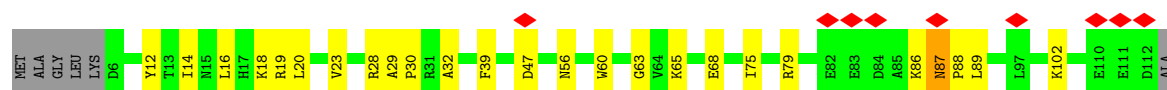
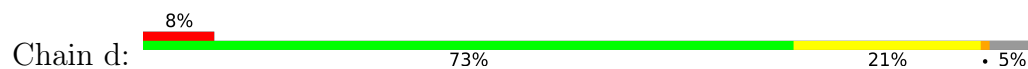


• Molecule 25: 60S ribosomal protein L30

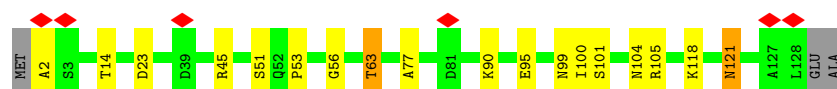
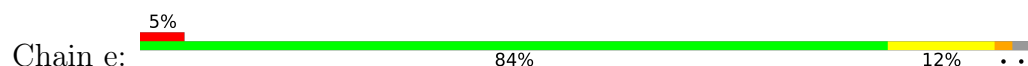




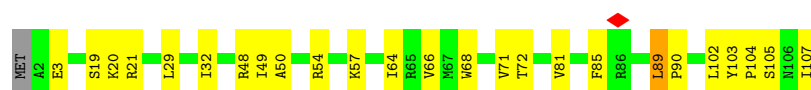
- Molecule 26: 60S ribosomal protein L31-A



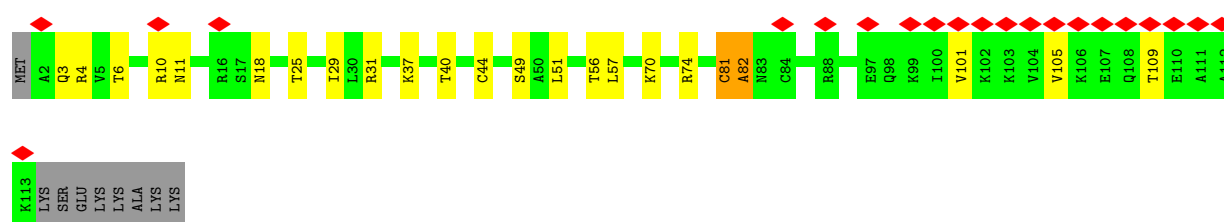
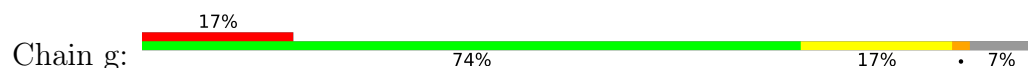
- Molecule 27: 60S ribosomal protein L32



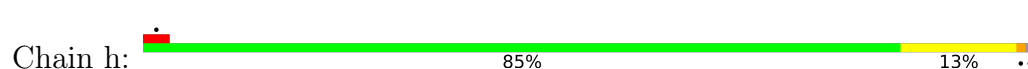
- Molecule 28: 60S ribosomal protein L33-A



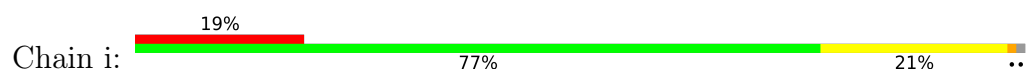
- Molecule 29: 60S ribosomal protein L34-A

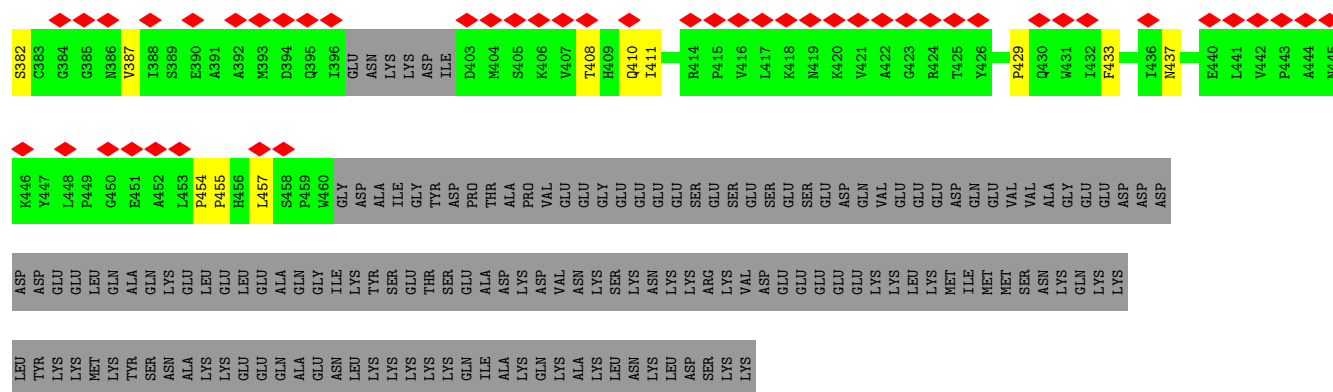


- Molecule 30: 60S ribosomal protein L35-A

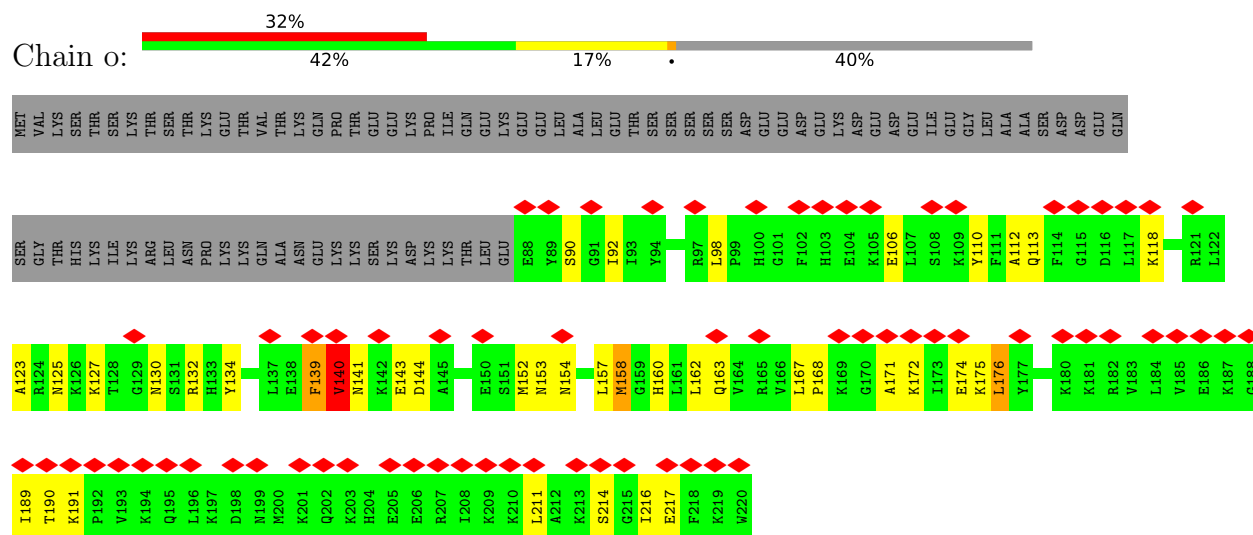


- Molecule 31: 60S ribosomal protein L36-A

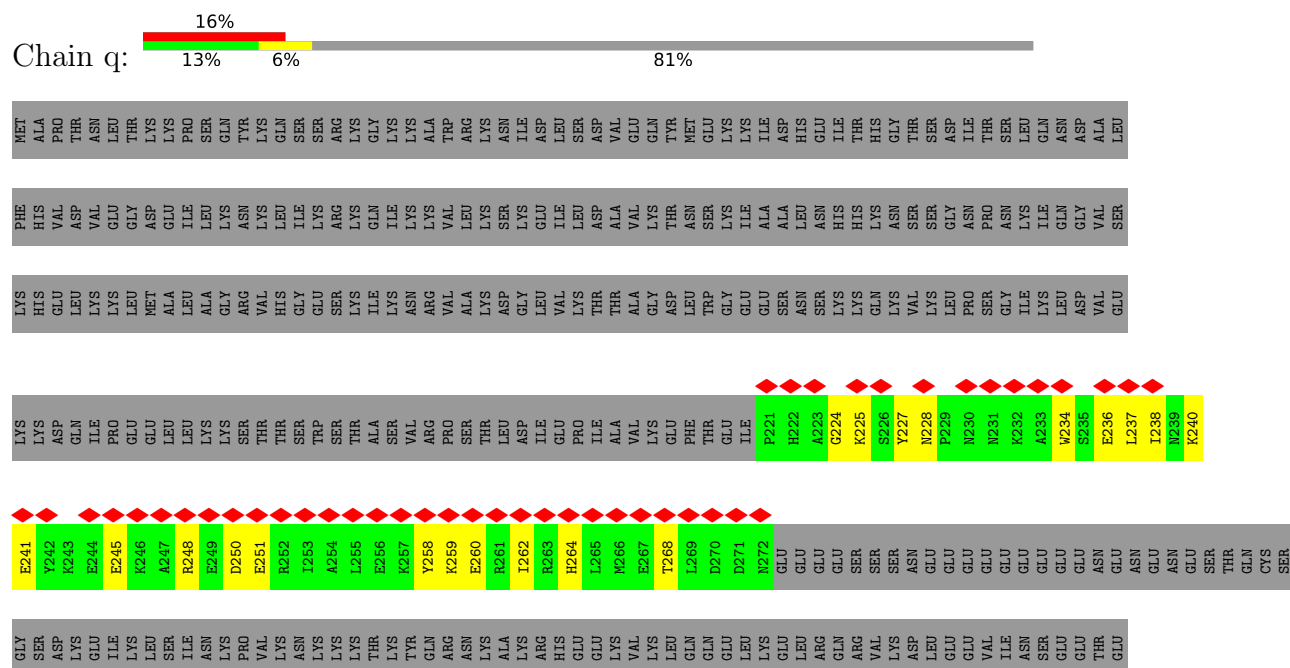




• Molecule 36: Ribosome biogenesis protein 15



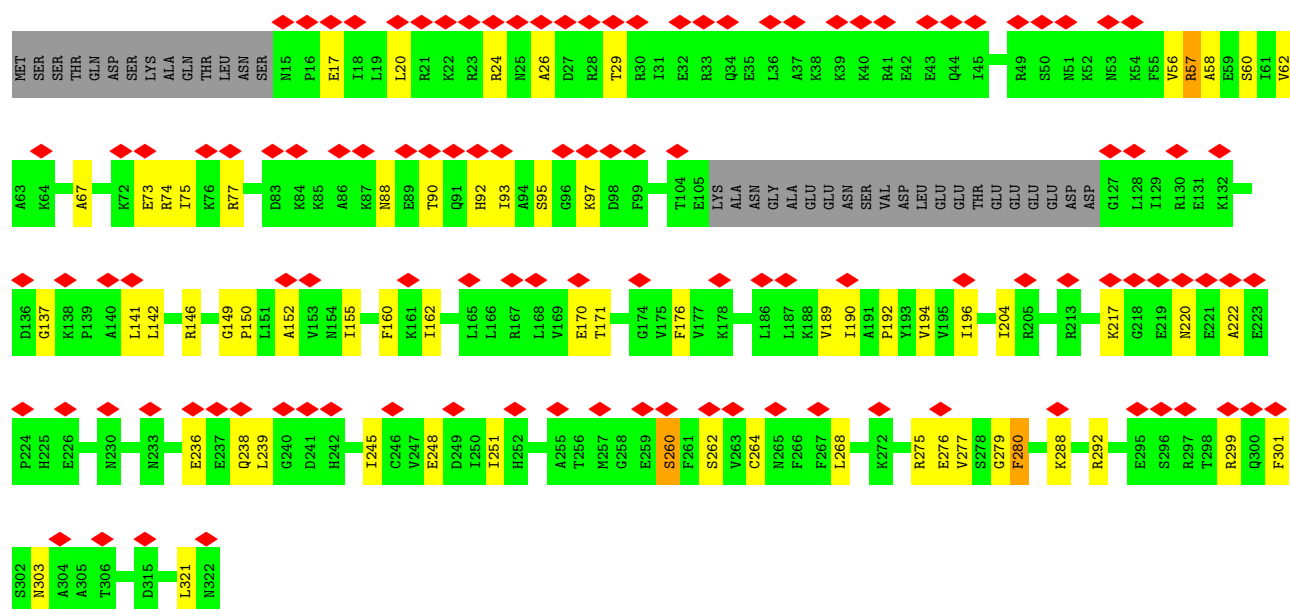
• Molecule 37: Ribosome biogenesis protein NOP53



ILE VAL SER GLU THR TRP ASP LYS PHE ASP ASP LEU GLY LEU PHE SER SER LEU ASP LYS ASP ALA ILE ASP ALA SER LYS ASP ASP THR MET MET GLU

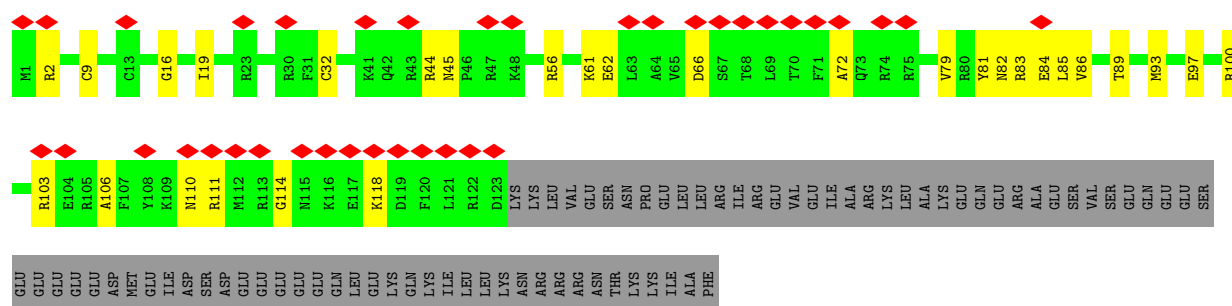
• Molecule 40: Ribosome biogenesis protein RLP7

Chain t: 



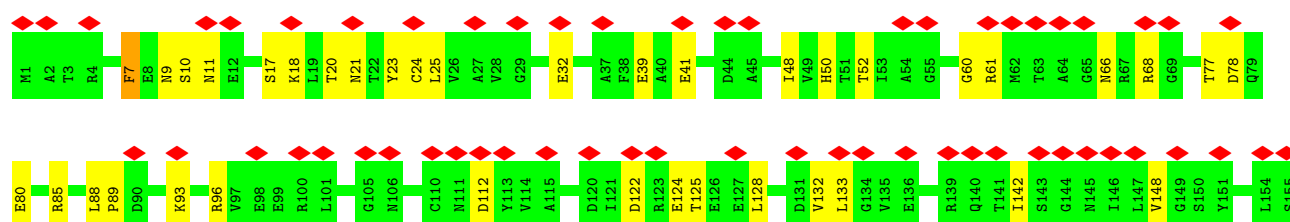
• Molecule 41: Ribosome biogenesis protein RLP24

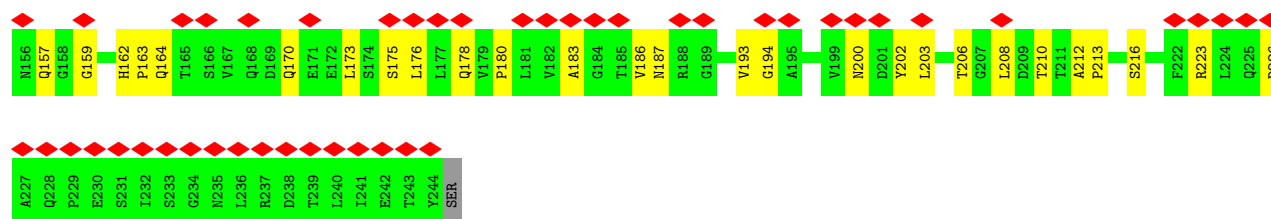
Chain u: 



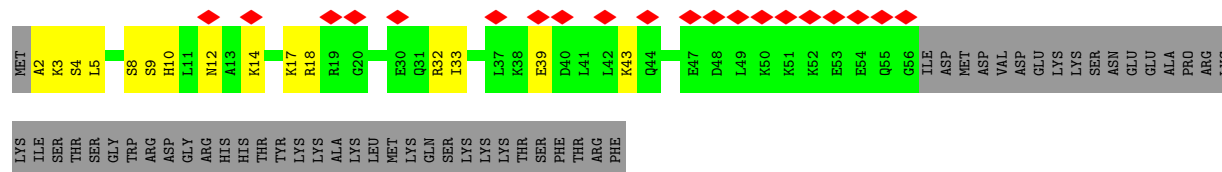
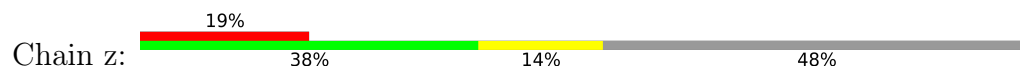
• Molecule 42: Eukaryotic translation initiation factor 6

Chain y: 

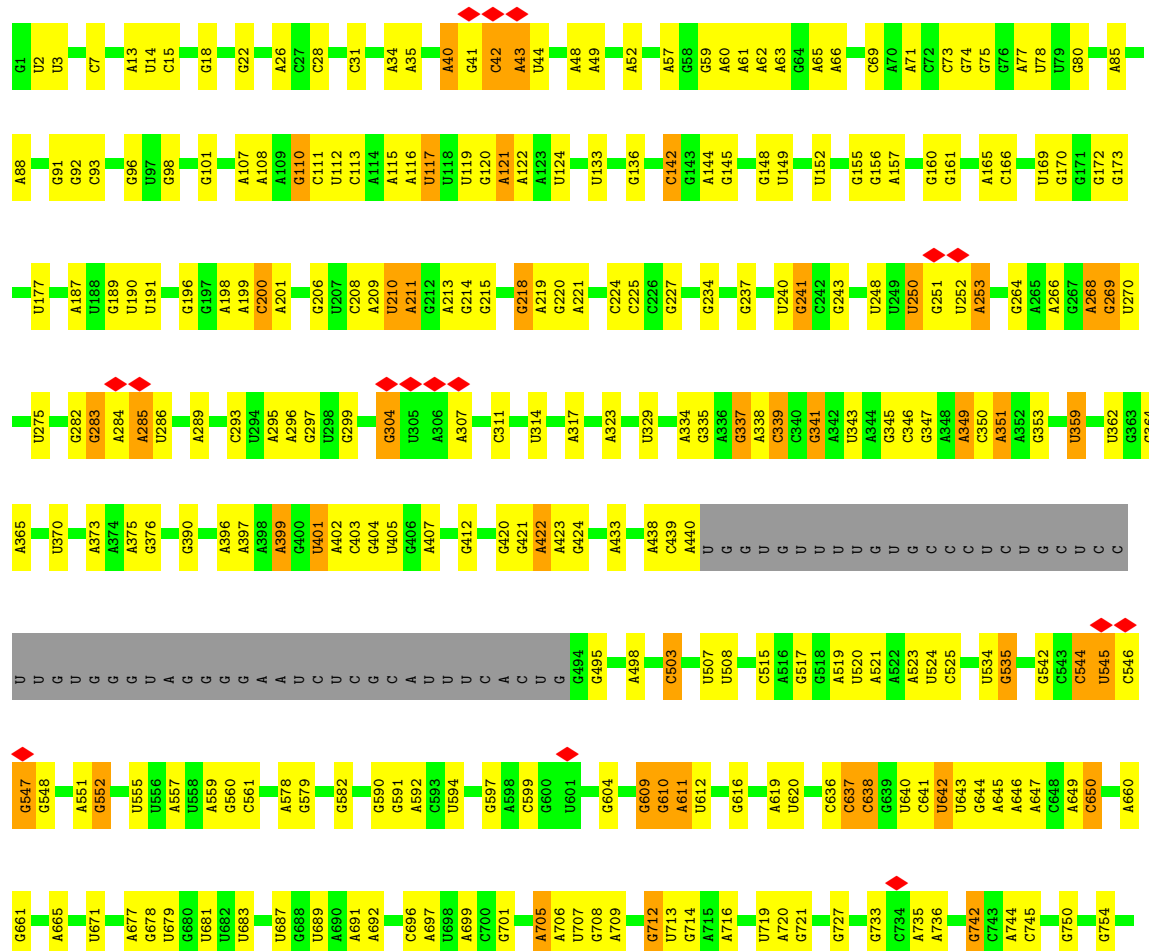
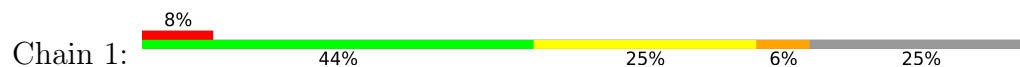




• Molecule 43: UPF0642 protein YBL028C

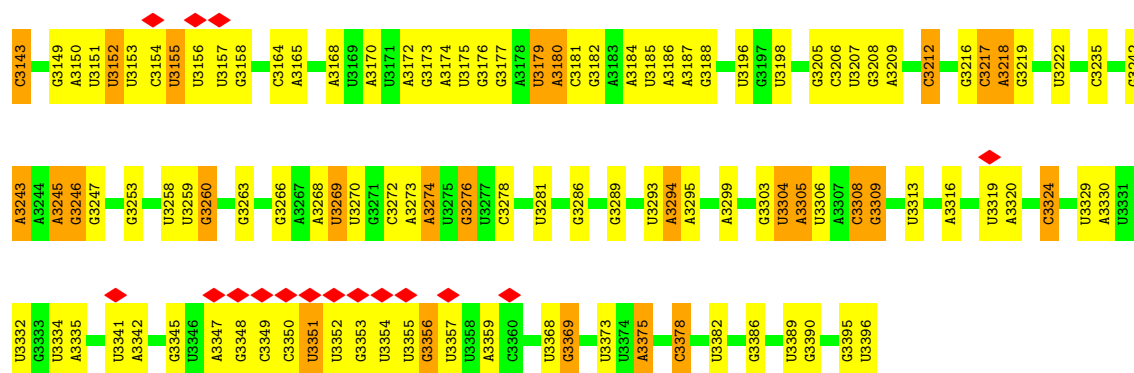


• Molecule 44: 25S rRNA

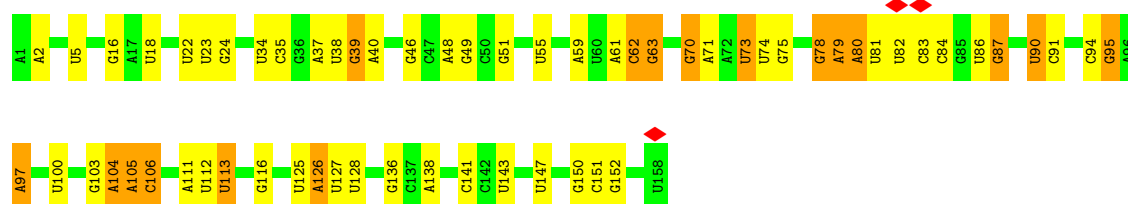




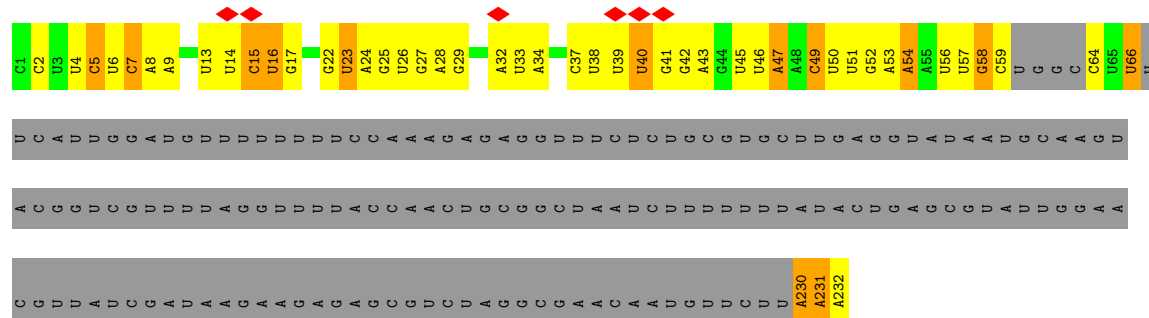




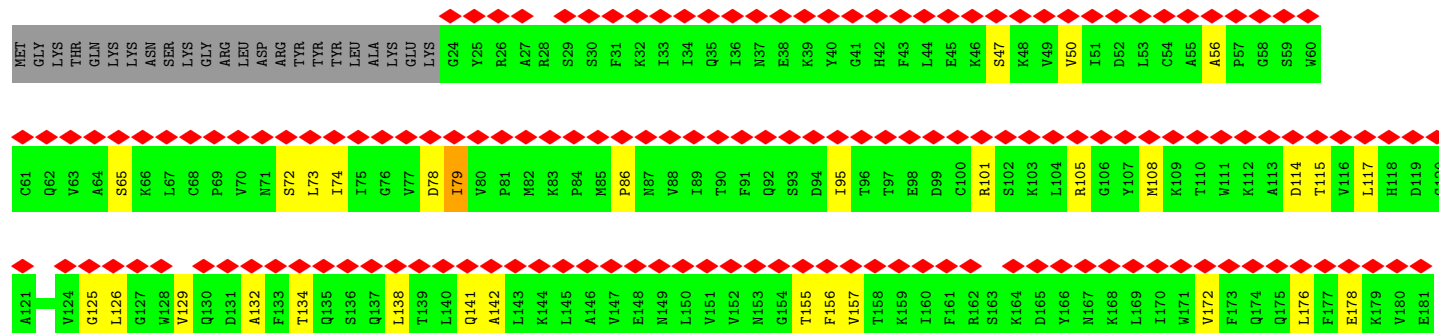
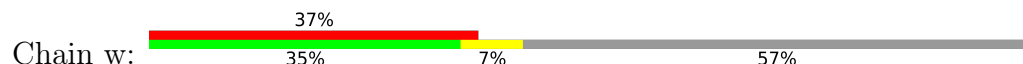
• Molecule 45: 5.8S rRNA

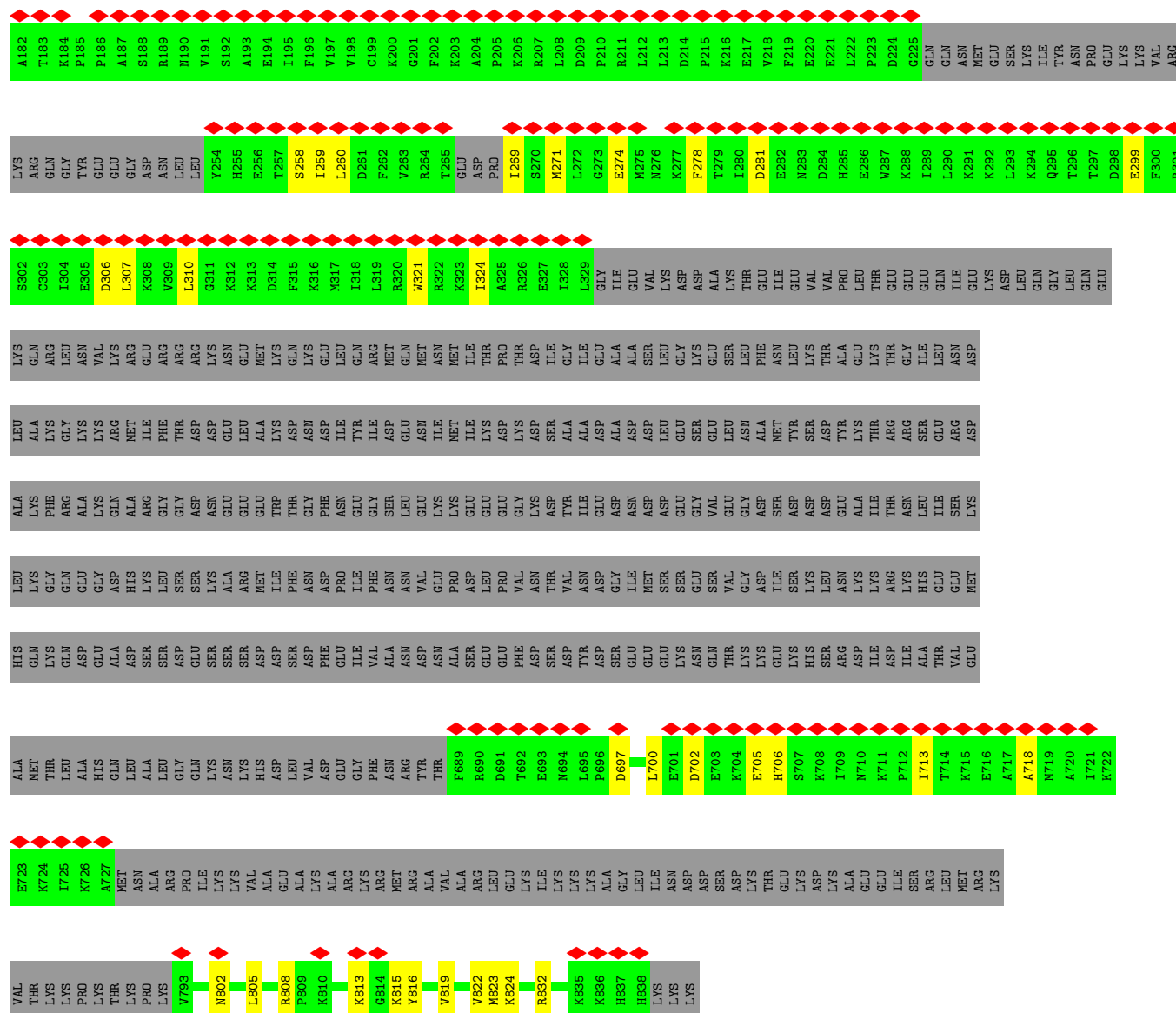


• Molecule 46: ITS2



• Molecule 47: 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29163	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 ($e^-/\text{\AA}^2$)	24	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	0.483	Depositor
Minimum map value	-0.257	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.055	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 ⓘ

5.1 Standard geometry ⓘ

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	B	1.10	1/3152 (0.0%)	0.96	1/4239 (0.0%)
2	C	1.36	1/2801 (0.0%)	1.03	4/3792 (0.1%)
3	E	0.98	0/1260	0.85	1/1694 (0.1%)
4	F	1.22	2/1821 (0.1%)	1.03	6/2451 (0.2%)
5	G	0.91	0/1542	0.89	3/2083 (0.1%)
6	H	0.88	0/1539	0.93	2/2073 (0.1%)
7	K	0.44	0/2098	0.77	4/2830 (0.1%)
8	L	1.12	0/1524	0.97	2/2046 (0.1%)
9	M	1.07	0/1074	0.89	0/1446
10	N	1.47	3/1575 (0.2%)	1.06	1/2106 (0.0%)
11	O	1.53	1/1585 (0.1%)	0.95	0/2128
12	P	1.34	3/1419 (0.2%)	0.94	0/1904
13	Q	1.13	0/1050	0.91	0/1419
14	R	0.74	1/1275 (0.1%)	0.78	0/1702
15	S	0.97	0/1473	0.92	0/1980
16	T	0.44	0/440	0.85	0/594
17	U	0.52	0/861	0.71	0/1167
18	V	0.69	0/1018	0.80	0/1369
19	W	0.48	0/1918	0.76	2/2586 (0.1%)
20	X	1.13	0/1116	0.84	0/1503
21	Y	1.19	0/1004	0.97	0/1341
22	Z	0.51	0/1118	0.74	0/1497
23	a	0.87	0/751	0.90	2/1013 (0.2%)
24	b	0.54	0/3885	0.82	0/5242
25	c	0.41	0/751	0.66	0/1008
26	d	1.02	0/887	0.90	4/1191 (0.3%)
27	e	1.43	2/1041 (0.2%)	1.00	1/1394 (0.1%)
28	f	1.71	4/868 (0.5%)	1.07	3/1168 (0.3%)
29	g	0.84	0/891	0.90	2/1191 (0.2%)
30	h	1.20	0/978	0.96	2/1301 (0.2%)
31	i	0.78	0/778	0.79	0/1034
32	j	1.44	2/696 (0.3%)	1.06	1/923 (0.1%)
33	k	0.64	0/618	0.78	0/826
34	l	0.70	0/443	0.92	0/588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	n	0.74	0/3101	0.91	4/4187 (0.1%)
36	o	0.53	0/1129	0.89	4/1502 (0.3%)
37	q	0.42	0/733	0.80	0/977
38	r	0.64	0/1789	0.87	2/2389 (0.1%)
39	s	0.75	0/301	0.97	0/386
40	t	0.57	0/2333	0.89	3/3128 (0.1%)
41	u	0.73	1/1061 (0.1%)	0.97	2/1410 (0.1%)
42	y	0.54	0/1872	0.75	0/2548
43	z	0.67	0/445	0.89	0/585
44	1	0.91	1/60703 (0.0%)	0.75	3/94630 (0.0%)
45	2	1.16	0/3746	0.87	0/5832
46	6	0.46	0/1527	0.59	0/2371
47	w	0.43	0/2952	0.68	1/3965 (0.0%)
All	All	0.93	22/126942 (0.0%)	0.81	60/184739 (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
1	B	0	7
2	C	0	6
4	F	0	2
5	G	0	5
6	H	0	3
7	K	0	1
8	L	0	5
9	M	0	1
10	N	0	1
12	P	0	1
14	R	0	1
15	S	0	2
18	V	0	1
19	W	0	2
20	X	0	1
23	a	0	2
24	b	0	3
26	d	0	1
27	e	0	1
28	f	0	2
29	g	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
30	h	0	3
31	i	0	2
33	k	0	2
35	n	0	11
36	o	0	5
37	q	0	1
38	r	0	1
39	s	0	1
40	t	0	5
41	u	0	2
42	y	0	1
47	w	0	2
All	All	0	86

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	146	ALA	CA-C	-8.06	1.38	1.52
28	f	102	LEU	C-N	-7.29	1.16	1.33
1	B	96	PRO	C-N	-6.53	1.24	1.33
10	N	153	ASP	C-N	-6.45	1.26	1.34
28	f	104	PRO	CB-CG	-6.41	1.26	1.51
32	j	26	SER	CA-CB	-6.39	1.43	1.53
10	N	184	LYS	CA-CB	-6.35	1.42	1.53
28	f	32	ILE	CG1-CD1	-5.96	1.28	1.51
12	P	143	PRO	CB-CG	-5.73	1.21	1.49
41	u	2	ARG	C-N	-5.72	1.26	1.33
11	O	15	LEU	CG-CD2	-5.72	1.33	1.52
14	R	58	HIS	CA-CB	-5.71	1.44	1.53
27	e	53	PRO	CB-CG	-5.59	1.21	1.49
4	F	207	LEU	CA-CB	-5.56	1.44	1.53
32	j	45	ARG	CZ-NH2	-5.47	1.26	1.33
2	C	193	LYS	CB-CG	-5.38	1.36	1.52
12	P	122	ALA	CA-CB	-5.23	1.47	1.54
4	F	236	ILE	CG1-CD1	-5.23	1.31	1.51
28	f	29	LEU	CG-CD2	-5.20	1.35	1.52
27	e	51	SER	C-N	-5.19	1.25	1.33
12	P	29	THR	CB-CG2	-5.18	1.35	1.52
44	1	945	C	C4-C5	-5.02	1.32	1.43

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	156	ILE	CA-C-N	9.47	139.63	121.54
4	F	156	ILE	C-N-CA	9.47	139.63	121.54
35	n	5	LYS	N-CA-C	7.26	119.41	110.91
3	E	35	VAL	N-CA-C	-6.92	103.52	109.19
4	F	157	ASN	CA-C-N	6.73	134.40	121.54
4	F	157	ASN	C-N-CA	6.73	134.40	121.54
38	r	16	LYS	CB-CA-C	-6.67	97.15	110.42
28	f	103	TYR	CA-CB-CG	6.46	125.53	113.90
26	d	87	ASN	CA-C-N	6.30	142.11	127.00
26	d	87	ASN	C-N-CA	6.30	142.11	127.00
40	t	137	GLY	CA-C-N	6.01	132.52	121.70
40	t	137	GLY	C-N-CA	6.01	132.52	121.70
38	r	16	LYS	CA-CB-CG	5.91	125.91	114.10
36	o	214	SER	CA-C-N	5.88	132.29	121.70
36	o	214	SER	C-N-CA	5.88	132.29	121.70
8	L	62	THR	CA-C-N	5.84	132.49	121.97
8	L	62	THR	C-N-CA	5.84	132.49	121.97
6	H	188	THR	CA-C-N	5.74	132.02	121.70
6	H	188	THR	C-N-CA	5.74	132.02	121.70
32	j	49	TRP	CA-CB-CG	5.72	124.47	113.60
47	w	79	ILE	N-CA-C	-5.65	106.70	111.56
26	d	88	PRO	N-CA-C	5.64	126.77	112.10
2	C	40	THR	CB-CA-C	-5.63	101.80	110.81
36	o	140	VAL	N-CA-C	-5.63	107.17	111.62
4	F	158	LYS	N-CA-C	-5.62	98.84	110.80
23	a	77	LYS	CA-C-N	5.61	132.25	121.54
23	a	77	LYS	C-N-CA	5.61	132.25	121.54
44	l	3269	U	C4'-C3'-O3'	5.60	117.81	109.40
41	u	32	CYS	CA-CB-SG	5.59	127.26	114.40
26	d	87	ASN	C-N-CD	-5.55	108.38	120.60
30	h	91	ALA	CA-C-N	5.53	132.09	121.54
30	h	91	ALA	C-N-CA	5.53	132.09	121.54
35	n	374	ASP	CA-C-N	-5.47	117.77	122.96
35	n	374	ASP	C-N-CA	-5.47	117.77	122.96
41	u	81	TYR	N-CA-C	5.45	117.29	110.91
28	f	90	PRO	CA-N-CD	-5.43	104.40	112.00
28	f	48	ARG	NE-CZ-NH1	-5.41	116.09	121.50
29	g	81	CYS	CA-C-N	5.38	131.82	121.54
29	g	81	CYS	C-N-CA	5.38	131.82	121.54
44	l	314	U	N1-C1'-C2'	5.38	120.08	112.00
5	G	75	ILE	N-CA-C	-5.38	104.13	110.21
35	n	39	LYS	N-CA-C	5.38	116.83	111.07
2	C	140	HIS	N-CA-C	5.37	117.19	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	t	57	ARG	N-CA-C	5.36	117.19	110.91
10	N	150	TRP	CA-CB-CG	5.34	123.75	113.60
27	e	53	PRO	CA-N-CD	-5.32	104.55	112.00
4	F	229	PHE	CA-CB-CG	5.28	119.08	113.80
1	B	221	THR	N-CA-C	5.20	116.87	108.34
19	W	100	THR	CA-C-N	5.06	130.80	121.70
19	W	100	THR	C-N-CA	5.06	130.80	121.70
44	1	1159	A	O4'-C1'-N9	5.05	115.78	108.20
36	o	172	LYS	N-CA-C	5.04	118.20	111.24
5	G	145	ASN	CA-C-N	5.04	130.77	121.70
5	G	145	ASN	C-N-CA	5.04	130.77	121.70
7	K	283	THR	CA-C-N	5.04	131.16	121.54
7	K	283	THR	C-N-CA	5.04	131.16	121.54
2	C	106	TRP	CA-CB-CG	5.03	123.15	113.60
7	K	214	ASN	CA-C-N	5.02	130.74	121.70
7	K	214	ASN	C-N-CA	5.02	130.74	121.70
2	C	319	LYS	N-CA-C	-5.01	101.80	108.86

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	170	PRO	Peptide
1	B	221	THR	Peptide
1	B	241	LYS	Peptide
1	B	340	LYS	Peptide
1	B	35	ASP	Peptide
1	B	353	GLU	Peptide
1	B	37	ARG	Peptide
2	C	182	LEU	Peptide
2	C	269	SER	Peptide
2	C	3	ARG	Peptide
2	C	318	LEU	Peptide
2	C	338	LYS	Peptide
2	C	4	PRO	Peptide
4	F	158	LYS	Peptide
4	F	215	GLY	Peptide
5	G	120	LYS	Peptide
5	G	226	TYR	Peptide
5	G	76	ALA	Peptide
5	G	79	GLN	Peptide
5	G	83	ASP	Peptide

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Mol	Chain	Res	Type	Group
6	H	20	ILE	Peptide
6	H	21	LYS	Peptide
6	H	49	ASN	Peptide
7	K	164	TYR	Peptide
8	L	12	ASN	Peptide
8	L	130	GLY	Peptide
8	L	166	ALA	Mainchain
8	L	27	ASP	Peptide
8	L	46	ILE	Peptide
9	M	12	TRP	Peptide
10	N	93	LYS	Peptide
12	P	144	SER	Peptide
14	R	54	ALA	Peptide
15	S	13	ARG	Peptide
15	S	22	PRO	Peptide
18	V	89	ASP	Peptide
19	W	127	PRO	Peptide
19	W	177	ALA	Peptide
20	X	65	GLN	Peptide
23	a	77	LYS	Peptide
23	a	97	GLU	Peptide
24	b	227	ARG	Peptide
24	b	368	ALA	Peptide
24	b	399	ALA	Peptide
26	d	87	ASN	Peptide
27	e	121	ASN	Peptide
28	f	66	VAL	Peptide
28	f	89	LEU	Peptide
29	g	6	THR	Peptide
29	g	82	ALA	Mainchain
30	h	119	LYS	Peptide
30	h	83	LYS	Peptide
30	h	91	ALA	Peptide
31	i	49	GLY	Peptide
31	i	78	GLY	Peptide
33	k	32	ASN	Peptide
33	k	33	LYS	Peptide
35	n	1	MET	Peptide
35	n	123	PRO	Peptide
35	n	240	SER	Peptide
35	n	3	ILE	Peptide
35	n	374	ASP	Peptide

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Mol	Chain	Res	Type	Group
35	n	375	ILE	Peptide
35	n	455	PRO	Peptide
35	n	53	ASN	Peptide
35	n	54	LYS	Peptide
35	n	55	GLY	Peptide
35	n	73	HIS	Peptide
36	o	139	PHE	Peptide
36	o	140	VAL	Peptide
36	o	158	MET	Peptide
36	o	171	ALA	Peptide
36	o	176	LEU	Peptide
37	q	225	LYS	Peptide
38	r	45	TRP	Mainchain
39	s	2	ARG	Peptide
40	t	150	PRO	Peptide
40	t	170	GLU	Peptide
40	t	220	ASN	Peptide
40	t	260	SER	Peptide
40	t	280	PHE	Peptide
41	u	61	LYS	Peptide
41	u	79	VAL	Peptide
47	w	126	LEU	Peptide
47	w	56	ALA	Peptide
42	y	7	PHE	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	B	3081	0	3165	70	0
2	C	2749	0	2863	40	0
3	E	1239	0	1326	20	0
4	F	1784	0	1862	29	0
5	G	1515	0	1596	31	0
6	H	1518	0	1587	31	0
7	K	2064	0	2156	57	0
8	L	1499	0	1558	27	0
9	M	1059	0	1154	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	N	1543	0	1594	29	0
11	O	1555	0	1659	17	0
12	P	1397	0	1436	23	0
13	Q	1035	0	1115	16	0
14	R	1258	0	1342	25	0
15	S	1437	0	1475	17	0
16	T	434	0	450	14	0
17	U	844	0	855	11	0
18	V	1003	0	1048	19	0
19	W	1885	0	1921	49	0
20	X	1100	0	1187	18	0
21	Y	993	0	1081	22	0
22	Z	1092	0	1155	24	0
23	a	735	0	776	9	0
24	b	3814	0	3875	71	0
25	c	743	0	797	11	0
26	d	873	0	914	17	0
27	e	1020	0	1090	15	0
28	f	850	0	880	12	0
29	g	881	0	945	17	0
30	h	969	0	1078	9	0
31	i	771	0	849	16	0
32	j	681	0	687	15	0
33	k	612	0	682	5	0
34	l	436	0	475	15	0
35	n	3030	0	3107	37	0
36	o	1107	0	1159	35	0
37	q	723	0	722	18	0
38	r	1760	0	1850	25	0
39	s	301	0	359	9	0
40	t	2306	0	2454	40	0
41	u	1040	0	1067	20	0
42	y	1849	0	1836	46	0
43	z	444	0	478	13	0
44	1	54232	0	26854	497	0
45	2	3353	0	1655	31	0
46	6	1370	0	692	42	0
47	w	2898	0	3002	39	0
All	All	118882	0	91868	1303	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 7.

All (1303) 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)
45:2:39:G:N2	45:2:106:C:N3	1.99	1.09
44:1:1392:G:N3	44:1:1418:A:N6	2.16	0.92
44:1:1538:G:H21	44:1:1583:A:H62	1.18	0.90
44:1:1449:A:H62	44:1:2355:G:H21	1.14	0.89
44:1:1392:G:H21	44:1:1418:A:H62	1.26	0.81
44:1:616:G:H21	44:1:3274:A:H61	1.29	0.79
21:Y:32:SER:HG	44:1:225:C:HO2'	1.21	0.79
44:1:88:A:H62	44:1:98:G:H21	1.30	0.78
44:1:1481:A:H62	44:1:1872:C:N4	1.81	0.78
44:1:1392:G:N2	44:1:1418:A:H62	1.82	0.77
1:B:29:VAL:HG22	1:B:218:ILE:HD11	1.66	0.77
44:1:1303:A:O2'	44:1:1304:A:O4'	2.03	0.76
24:b:172:ILE:HG23	24:b:251:LEU:HD22	1.68	0.75
1:B:90:VAL:HG12	1:B:104:THR:HG22	1.69	0.75
7:K:213:ALA:HB2	7:K:221:THR:HG21	1.68	0.75
44:1:1481:A:N6	44:1:1872:C:H42	1.83	0.75
44:1:1449:A:H62	44:1:2355:G:N2	1.83	0.75
29:g:37:LYS:NZ	44:1:1656:A:OP2	2.19	0.75
8:L:70:ARG:NH2	44:1:75:G:O2'	2.21	0.74
44:1:339:C:OP1	44:1:1380:G:O2'	2.04	0.74
12:P:62:ARG:NH1	44:1:412:G:OP1	2.20	0.74
35:n:51:LYS:NZ	44:1:1619:A:OP2	2.20	0.74
9:M:24:LYS:NZ	9:M:61:GLY:O	2.21	0.74
4:F:228:SER:O	4:F:232:ARG:NH2	2.21	0.73
27:e:99:ASN:O	44:1:1388:U:O2'	2.05	0.73
34:l:10:LYS:NZ	44:1:1834:U:OP2	2.21	0.73
44:1:1433:A:O2'	44:1:1434:G:O4'	2.05	0.73
2:C:188:ARG:NH1	44:1:1382:G:OP2	2.21	0.73
8:L:73:ARG:NH1	44:1:110:G:OP2	2.22	0.73
11:O:74:ARG:NH1	44:1:3008:A:OP2	2.22	0.73
44:1:1524:A:O2'	44:1:1526:U:OP2	2.06	0.73
4:F:120:THR:OG1	16:T:133:ALA:O	2.07	0.73
19:W:8:LYS:NZ	44:1:1289:G:O3'	2.22	0.73
9:M:77:ARG:O	9:M:80:THR:OG1	2.06	0.72
4:F:110:ARG:NH1	44:1:1364:C:OP1	2.23	0.72
44:1:1188:U:OP1	44:1:1210:U:O2'	2.07	0.72
44:1:1193:A:O2'	44:1:1298:C:OP1	2.07	0.72
1:B:331:ASN:OD1	1:B:334:ARG:NE	2.22	0.72
35:n:242:LEU:HD11	35:n:264:LEU:HD23	1.72	0.72
44:1:1189:C:N4	44:1:1316:C:OP2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:156:CYS:SG	7:K:158:LYS:NZ	2.62	0.72
36:o:153:ASN:O	36:o:163:GLN:NE2	2.23	0.72
44:1:1308:A:O2'	44:1:1311:G:OP1	2.07	0.72
44:1:2394:G:OP2	44:1:2946:A:N6	2.23	0.72
35:n:42:TYR:OH	35:n:121:ARG:NH2	2.22	0.72
26:d:47:ASP:OD1	26:d:86:LYS:NZ	2.23	0.71
40:t:288:LYS:NZ	46:6:230:A:OP2	2.23	0.71
1:B:266:ARG:NH1	44:1:2392:C:O2'	2.23	0.71
42:y:85:ARG:NH1	42:y:89:PRO:O	2.23	0.71
34:l:36:ARG:NH2	44:1:401:U:O2'	2.24	0.71
42:y:157:GLN:O	42:y:223:ARG:NH1	2.24	0.71
44:1:1064:A:O2'	44:1:1093:A:N6	2.24	0.71
21:Y:60:ARG:NH1	44:1:200:C:OP1	2.24	0.71
24:b:129:LYS:NZ	44:1:2828:G:OP2	2.23	0.71
5:G:86:THR:O	5:G:90:THR:OG1	2.08	0.71
5:G:213:LYS:NZ	46:6:54:A:OP1	2.23	0.71
10:N:172:ARG:NH2	44:1:62:A:O2'	2.23	0.71
4:F:169:ILE:HD11	4:F:173:LEU:HD12	1.73	0.71
12:P:27:LYS:NZ	44:1:1447:G:OP2	2.24	0.71
25:c:66:LYS:NZ	25:c:67:VAL:O	2.23	0.71
8:L:36:ARG:NH2	44:1:687:U:OP2	2.24	0.71
4:F:158:LYS:NZ	44:1:1103:A:OP1	2.23	0.70
19:W:23:LYS:NZ	44:1:1221:A:N3	2.39	0.70
44:1:1252:A:N7	44:1:1263:A:O2'	2.23	0.70
22:Z:22:LYS:NZ	22:Z:129:TRP:O	2.22	0.70
32:j:3:LYS:NZ	44:1:919:U:OP1	2.21	0.70
8:L:46:ILE:HG22	8:L:49:ARG:HB2	1.73	0.70
30:h:106:LYS:NZ	44:1:152:U:OP1	2.25	0.70
42:y:9:ASN:ND2	44:1:3019:U:OP2	2.24	0.70
1:B:69:LYS:NZ	24:b:413:ASN:OD1	2.24	0.70
24:b:118:PHE:O	24:b:120:GLN:NE2	2.24	0.70
35:n:57:THR:O	44:1:1810:A:O2'	2.07	0.70
36:o:125:ASN:ND2	36:o:127:LYS:O	2.24	0.70
20:X:6:LYS:NZ	36:o:112:ALA:O	2.25	0.70
1:B:4:ARG:NH2	44:1:2881:C:OP2	2.25	0.70
5:G:214:LEU:O	5:G:217:THR:OG1	2.10	0.70
44:1:1480:G:O4'	44:1:1483:G:N2	2.25	0.70
44:1:1481:A:N6	44:1:1872:C:N4	2.39	0.70
12:P:135:ARG:NE	44:1:879:U:O2'	2.24	0.70
29:g:11:ASN:O	29:g:18:ASN:ND2	2.24	0.70
41:u:16:GLY:O	44:1:3050:U:O2'	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:O	44:1:3004:C:O2'	2.10	0.70
7:K:285:ARG:NH2	46:6:32:A:O2'	2.25	0.70
28:f:21:ARG:NH2	44:1:1151:U:OP1	2.25	0.70
8:L:74:GLY:O	8:L:101:ARG:NH1	2.24	0.70
39:s:2:ARG:NH2	44:1:2886:U:OP2	2.25	0.70
44:1:978:G:O2'	44:1:1103:A:O2'	2.08	0.70
7:K:224:ASN:ND2	46:6:17:G:OP1	2.24	0.69
21:Y:12:ARG:NH1	44:1:215:G:OP1	2.25	0.69
40:t:301:PHE:O	40:t:303:ASN:ND2	2.25	0.69
1:B:128:LYS:NZ	44:1:3294:A:OP1	2.26	0.69
37:q:241:GLU:OE2	37:q:395:GLU:N	2.25	0.69
40:t:217:LYS:NZ	40:t:222:ALA:O	2.26	0.69
31:i:35:ASN:ND2	44:1:264:G:OP1	2.26	0.69
44:1:835:G:O2'	44:1:857:G:N2	2.25	0.69
1:B:180:GLU:OE1	44:1:3002:C:O2'	2.10	0.69
19:W:64:LYS:NZ	19:W:65:LEU:O	2.26	0.69
19:W:71:LYS:NZ	44:1:1222:G:N7	2.40	0.69
24:b:162:SER:OG	44:1:3027:A:N6	2.26	0.69
40:t:95:SER:OG	46:6:8:A:O2'	2.10	0.69
1:B:297:SER:O	1:B:300:ARG:NH1	2.25	0.69
14:R:62:ARG:NH2	44:1:3070:A:OP1	2.25	0.69
16:T:143:THR:OG1	16:T:146:ASN:O	2.09	0.69
39:s:8:SER:OG	39:s:9:ARG:N	2.21	0.69
46:6:51:U:O2'	46:6:54:A:N7	2.23	0.69
44:1:551:A:O2'	44:1:552:G:O4'	2.10	0.69
7:K:79:GLN:OE1	7:K:283:THR:OG1	2.11	0.69
29:g:3:GLN:NE2	29:g:4:ARG:O	2.26	0.69
17:U:86:LYS:O	17:U:88:GLN:NE2	2.26	0.68
30:h:49:LYS:NZ	45:2:63:G:O3'	2.26	0.68
4:F:210:PRO:O	44:1:1167:U:O2'	2.11	0.68
40:t:97:LYS:NZ	46:6:8:A:O2'	2.26	0.68
45:2:70:G:O2'	45:2:87:G:N2	2.26	0.68
7:K:136:SER:OG	7:K:137:GLU:OE1	2.10	0.68
9:M:108:ARG:NH2	11:O:196:ALA:O	2.26	0.68
10:N:49:ARG:NH1	44:1:115:A:OP1	2.27	0.68
16:T:108:ARG:NH1	44:1:1062:A:O2'	2.26	0.68
17:U:86:LYS:NZ	44:1:1684:U:OP1	2.27	0.68
19:W:37:TYR:O	19:W:223:ASN:ND2	2.26	0.68
8:L:33:VAL:O	8:L:37:ASN:ND2	2.25	0.68
8:L:39:ARG:NH1	44:1:107:A:OP1	2.26	0.68
8:L:43:ALA:O	8:L:47:ALA:HA	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:145:ASN:ND2	44:1:745:C:OP1	2.26	0.68
22:Z:97:SER:N	22:Z:100:THR:OG1	2.27	0.68
38:r:183:ASN:ND2	44:1:2857:C:O2	2.27	0.68
44:1:2360:C:O2'	44:1:2362:C:OP2	2.12	0.68
36:o:130:ASN:ND2	46:6:27:G:OP1	2.26	0.68
43:z:17:LYS:NZ	44:1:3037:U:OP2	2.26	0.68
13:Q:66:ARG:NH1	44:1:744:A:OP1	2.27	0.68
3:E:46:ARG:NH2	44:1:3268:A:OP1	2.26	0.68
6:H:117:PHE:N	6:H:120:ASP:OD1	2.26	0.68
44:1:40:A:O2'	44:1:41:G:N7	2.25	0.68
34:l:13:MET:SD	44:1:1493:G:O2'	2.49	0.68
23:a:74:ASN:OD1	44:1:705:A:N6	2.23	0.68
41:u:66:ASP:OD2	41:u:103:ARG:NH1	2.27	0.68
44:1:275:U:OP2	44:1:285:A:N6	2.27	0.68
2:C:315:LYS:NZ	44:1:609:G:OP2	2.27	0.67
6:H:59:ASN:OD1	9:M:41:GLN:NE2	2.27	0.67
7:K:198:ALA:O	7:K:204:THR:OG1	2.09	0.67
21:Y:28:ARG:NH2	45:2:71:A:OP1	2.27	0.67
36:o:158:MET:HE2	46:6:2:C:H41	1.59	0.67
7:K:218:SER:O	7:K:221:THR:OG1	2.09	0.67
22:Z:105:SER:OG	22:Z:109:GLU:OE1	2.12	0.67
24:b:169:THR:OG1	24:b:217:GLN:NE2	2.27	0.67
25:c:88:GLY:N	44:1:1729:A:OP1	2.28	0.67
27:e:118:LYS:NZ	44:1:438:A:OP1	2.27	0.67
47:w:105:ARG:NH2	47:w:108:MET:O	2.27	0.67
1:B:256:HIS:O	44:1:2943:G:O2'	2.11	0.67
13:Q:123:THR:OG1	13:Q:125:ASP:OD1	2.08	0.67
38:r:30:ARG:NH1	44:1:3109:G:OP2	2.28	0.67
42:y:212:ALA:O	42:y:216:SER:OG	2.10	0.67
10:N:44:ARG:NH1	44:1:269:G:OP2	2.27	0.67
11:O:161:LYS:NZ	44:1:3182:G:O3'	2.27	0.67
44:1:362:U:O2'	44:1:928:C:O2'	2.12	0.67
44:1:1646:G:O2'	44:1:1808:G:N2	2.26	0.67
44:1:2994:A:OP2	44:1:3142:A:N6	2.27	0.67
24:b:227:ARG:NH2	44:1:1242:G:OP2	2.27	0.67
44:1:616:G:N2	44:1:3274:A:H61	1.93	0.67
4:F:151:ARG:NH1	4:F:244:ASN:OD1	2.28	0.67
5:G:126:SER:OG	44:1:121:A:N6	2.27	0.67
41:u:97:GLU:OE2	41:u:100:ARG:NH1	2.27	0.67
44:1:831:G:O2'	44:1:1864:A:N3	2.26	0.67
1:B:19:ARG:N	44:1:2990:G:OP1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:131:LYS:NZ	15:S:132:THR:OG1	2.28	0.67
42:y:32:GLU:OE1	42:y:50:HIS:NE2	2.28	0.67
42:y:132:VAL:HG13	42:y:133:LEU:HD12	1.76	0.67
42:y:175:SER:O	42:y:178:GLN:NE2	2.28	0.67
44:1:177:U:O2	44:1:241:G:N2	2.28	0.67
4:F:211:SER:OG	44:1:508:U:OP1	2.10	0.67
7:K:128:LYS:NZ	46:6:6:U:O2'	2.28	0.67
44:1:642:U:O4'	47:w:832:ARG:NH1	2.28	0.67
44:1:1605:A:O2'	44:1:1607:U:OP2	2.11	0.67
44:1:3055:U:O2'	44:1:3057:U:OP2	2.13	0.67
20:X:127:THR:OG1	20:X:129:ASP:OD2	2.12	0.66
24:b:454:GLN:NE2	24:b:457:GLU:OE1	2.29	0.66
44:1:696:C:O2'	44:1:697:A:O4'	2.14	0.66
5:G:161:GLU:OE2	10:N:11:GLN:NE2	2.28	0.66
40:t:275:ARG:NH2	46:6:66:U:OP1	2.28	0.66
44:1:1259:A:N3	44:1:1280:C:O2'	2.23	0.66
7:K:237:LYS:NZ	46:6:46:U:OP1	2.26	0.66
19:W:15:THR:OG1	44:1:1278:A:N3	2.27	0.66
44:1:1390:A:N6	44:1:1418:A:O2'	2.28	0.66
44:1:2860:U:O2'	44:1:2864:A:N6	2.29	0.66
3:E:60:ASP:OD2	3:E:78:ARG:NH2	2.28	0.66
42:y:78:ASP:OD1	42:y:96:ARG:NH1	2.29	0.66
44:1:283:G:N2	44:1:285:A:OP1	2.29	0.66
7:K:36:ARG:NH1	7:K:291:LEU:O	2.29	0.66
12:P:120:ASN:OD1	12:P:120:ASN:N	2.24	0.66
17:U:94:ARG:NH2	44:1:1679:A:OP1	2.29	0.66
6:H:47:LYS:NZ	9:M:5:SER:O	2.27	0.66
41:u:44:ARG:NH1	44:1:2112:U:O4'	2.29	0.66
44:1:2919:A:O2'	47:w:125:GLY:O	2.12	0.66
2:C:119:ARG:O	2:C:122:THR:OG1	2.12	0.66
7:K:86:LYS:NZ	7:K:297:VAL:O	2.28	0.66
10:N:193:ARG:NH1	44:1:80:G:OP1	2.29	0.66
14:R:100:ARG:NH1	44:1:1722:U:OP1	2.29	0.66
15:S:62:ASN:ND2	44:1:519:A:OP1	2.28	0.66
22:Z:69:LYS:NZ	44:1:1632:A:OP1	2.27	0.66
32:j:26:SER:O	32:j:26:SER:OG	2.08	0.66
36:o:92:ILE:HG23	36:o:167:LEU:HB2	1.75	0.66
44:1:1696:A:OP2	44:1:1749:A:N6	2.28	0.66
44:1:3157:U:O2'	44:1:3158:G:N7	2.28	0.66
1:B:232:ARG:NH1	1:B:266:ARG:O	2.28	0.66
11:O:85:ARG:NH1	44:1:2382:G:OP1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:80:THR:OG1	13:Q:100:THR:O	2.13	0.66
38:r:39:ALA:O	44:1:1206:G:N2	2.29	0.66
42:y:93:LYS:NZ	42:y:132:VAL:O	2.24	0.66
44:1:1189:C:O2	44:1:1190:A:N6	2.28	0.66
44:1:1529:A:OP2	44:1:1592:G:N2	2.27	0.66
6:H:31:ARG:NH2	6:H:84:LYS:O	2.27	0.65
8:L:19:GLN:NE2	44:1:800:G:OP1	2.29	0.65
21:Y:3:LYS:NZ	21:Y:5:SER:O	2.29	0.65
42:y:122:ASP:O	42:y:125:THR:OG1	2.13	0.65
8:L:68:LYS:NZ	44:1:699:A:OP1	2.30	0.65
27:e:105:ARG:NH2	44:1:1412:G:OP1	2.29	0.65
29:g:31:ARG:NH2	44:1:1598:G:OP2	2.29	0.65
30:h:5:LYS:NZ	45:2:87:G:OP2	2.26	0.65
44:1:544:C:O2'	44:1:547:G:N2	2.29	0.65
44:1:924:G:OP1	47:w:815:LYS:NZ	2.29	0.65
44:1:1713:G:O2'	44:1:1730:G:N2	2.29	0.65
44:1:2837:A:O2'	44:1:2850:G:N2	2.29	0.65
26:d:28:ARG:NH2	44:1:3058:U:OP1	2.29	0.65
44:1:2143:A:N6	44:1:2145:A:O4'	2.30	0.65
14:R:64:ARG:NH1	44:1:1689:U:OP1	2.28	0.65
17:U:74:LYS:NZ	44:1:1678:G:N7	2.44	0.65
18:V:63:LYS:O	18:V:70:ARG:NH2	2.29	0.65
24:b:181:SER:OG	24:b:192:VAL:O	2.12	0.65
32:j:48:ASN:OD1	32:j:54:LYS:NZ	2.28	0.65
26:d:18:LYS:NZ	44:1:3324:C:OP2	2.21	0.65
44:1:3258:U:O2'	44:1:3260:G:OP1	2.10	0.65
2:C:332:LYS:NZ	44:1:599:C:OP1	2.24	0.65
10:N:112:ASN:ND2	45:2:141:C:O2	2.30	0.65
14:R:46:LYS:NZ	44:1:1766:G:N7	2.41	0.65
9:M:77:ARG:NH2	44:1:524:U:OP1	2.30	0.65
13:Q:21:SER:OG	13:Q:22:ASP:N	2.30	0.65
36:o:190:THR:N	46:6:38:U:OP1	2.30	0.65
37:q:260:GLU:OE1	37:q:264:HIS:NE2	2.28	0.65
42:y:187:ASN:OD1	42:y:210:THR:OG1	2.14	0.65
44:1:727:G:OP2	44:1:742:G:N2	2.29	0.65
5:G:141:ALA:O	5:G:145:ASN:ND2	2.30	0.65
24:b:171:LEU:HD13	24:b:243:ILE:HD13	1.79	0.65
27:e:63:THR:O	27:e:63:THR:OG1	2.12	0.65
29:g:74:ARG:NH2	44:1:1639:C:OP2	2.30	0.65
35:n:217:ILE:O	35:n:220:THR:OG1	2.15	0.65
42:y:17:SER:OG	42:y:25:LEU:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:2:ALA:N	15:S:32:SER:HG	1.95	0.65
19:W:18:LYS:NZ	44:1:1279:C:O2'	2.29	0.65
39:s:24:SER:OG	39:s:27:ARG:NH2	2.30	0.65
44:1:117:U:O2'	44:1:119:U:OP2	2.11	0.65
19:W:93:SER:OG	19:W:94:LYS:NZ	2.29	0.65
38:r:52:LYS:NZ	44:1:2852:C:O3'	2.27	0.65
28:f:3:GLU:N	28:f:3:GLU:OE1	2.30	0.64
34:l:6:SER:OG	45:2:113:U:OP2	2.11	0.64
44:1:214:G:O6	44:1:227:G:N2	2.30	0.64
6:H:22:SER:OG	6:H:39:LYS:NZ	2.30	0.64
29:g:40:THR:HG21	44:1:1655:G:OP1	1.96	0.64
44:1:1449:A:O2'	44:1:2983:C:N4	2.29	0.64
5:G:74:THR:O	5:G:77:GLN:NE2	2.30	0.64
20:X:96:LYS:NZ	20:X:107:VAL:O	2.31	0.64
42:y:68:ARG:NH1	42:y:112:ASP:O	2.30	0.64
44:1:1222:G:N2	44:1:1285:G:O2'	2.29	0.64
44:1:3155:U:O2'	44:1:3158:G:O4'	2.08	0.64
11:O:117:ARG:NH2	44:1:3182:G:OP1	2.30	0.64
34:l:20:ASN:ND2	34:l:42:ARG:O	2.31	0.64
43:z:18:ARG:NH2	44:1:3100:U:OP1	2.30	0.64
37:q:423:LEU:O	37:q:426:SER:OG	2.09	0.64
1:B:210:GLU:OE2	43:z:32:ARG:NH1	2.30	0.64
4:F:208:SER:OG	4:F:209:ASN:N	2.29	0.64
19:W:122:SER:OG	19:W:209:ALA:O	2.14	0.64
44:1:994:G:O2'	44:1:995:U:O4'	2.12	0.64
44:1:2117:A:HO2'	44:1:3080:G:HO2'	1.43	0.64
2:C:155:ASP:OD1	2:C:158:SER:OG	2.16	0.64
3:E:70:LYS:NZ	44:1:3266:G:OP2	2.27	0.64
10:N:188:ARG:NH2	44:1:31:C:OP2	2.31	0.64
15:S:131:LYS:NZ	44:1:534:U:OP2	2.31	0.64
36:o:191:LYS:NZ	46:6:38:U:OP2	2.25	0.64
44:1:1277:C:O2'	44:1:1278:A:O5'	2.14	0.64
6:H:85:GLY:HA3	6:H:187:ILE:HD12	1.80	0.64
19:W:90:TYR:O	19:W:94:LYS:NZ	2.29	0.64
20:X:39:LYS:O	35:n:26:GLN:NE2	2.30	0.64
30:h:43:LYS:O	30:h:46:THR:OG1	2.14	0.64
24:b:9:PRO:O	24:b:154:ARG:NH2	2.31	0.63
44:1:616:G:H21	44:1:3274:A:N6	1.96	0.63
1:B:290:ASP:O	1:B:293:ASN:ND2	2.31	0.63
36:o:174:GLU:N	36:o:174:GLU:OE1	2.31	0.63
23:a:85:ASP:O	23:a:89:GLN:NE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:3375:A:O2'	44:1:3378:C:OP2	2.17	0.63
1:B:129:ALA:O	44:1:3149:G:O2'	2.10	0.63
44:1:1489:A:C5	44:1:1838:G:N2	2.66	0.63
44:1:1657:C:O2'	44:1:1797:A:OP2	2.13	0.63
6:H:113:GLU:OE2	6:H:115:ARG:NE	2.32	0.63
2:C:64:SER:OG	2:C:65:TRP:N	2.28	0.63
7:K:196:GLY:O	7:K:200:ASN:ND2	2.31	0.63
24:b:68:PHE:CZ	24:b:150:LEU:HD12	2.34	0.63
44:1:2385:G:N7	44:1:3143:C:O2'	2.27	0.63
1:B:95:THR:HG22	44:1:3243:A:H4'	1.81	0.63
4:F:187:GLU:OE1	4:F:194:HIS:N	2.31	0.63
27:e:121:ASN:ND2	44:1:1411:C:O2'	2.32	0.63
28:f:19:SER:OG	28:f:20:LYS:N	2.27	0.63
44:1:1094:U:O2'	44:1:1096:U:OP1	2.12	0.63
7:K:166:ALA:O	7:K:169:ALA:N	2.32	0.62
42:y:21:ASN:O	42:y:202:TYR:OH	2.11	0.62
19:W:14:GLN:O	38:r:72:LYS:NZ	2.22	0.62
44:1:2926:A:O2'	44:1:2927:C:O4'	2.10	0.62
44:1:3308:C:OP2	44:1:3309:G:N2	2.32	0.62
7:K:129:ASP:O	7:K:133:LYS:NZ	2.33	0.62
19:W:166:ARG:NH1	38:r:18:LEU:O	2.32	0.62
34:l:48:LYS:NZ	44:1:1492:G:O2'	2.33	0.62
44:1:1278:A:O2'	44:1:1279:C:O5'	2.16	0.62
5:G:222:PHE:O	5:G:227:ASP:N	2.33	0.62
16:T:142:SER:OG	16:T:144:GLU:OE2	2.17	0.62
35:n:167:LEU:HB2	35:n:259:LEU:HD11	1.81	0.62
44:1:1223:A:OP2	44:1:1285:G:N2	2.32	0.62
44:1:1449:A:N6	44:1:2355:G:H21	1.92	0.62
44:1:1483:G:O6	44:1:1873:U:O4	2.18	0.62
45:2:150:G:O2'	45:2:152:G:OP1	2.10	0.62
44:1:3351:U:H3	44:1:3356:G:HO2'	1.46	0.62
4:F:120:THR:O	4:F:123:THR:OG1	2.14	0.62
22:Z:25:ILE:HA	22:Z:43:VAL:HG12	1.82	0.62
44:1:3152:U:OP2	44:1:3395:G:N1	2.33	0.62
24:b:25:THR:O	24:b:29:THR:OG1	2.12	0.61
24:b:305:LEU:O	24:b:308:SER:OG	2.12	0.61
34:l:45:ARG:NH2	44:1:1841:A:N3	2.48	0.61
42:y:52:THR:OG1	42:y:80:GLU:OE1	2.17	0.61
8:L:16:LYS:NZ	44:1:98:G:OP1	2.32	0.61
44:1:2187:G:O2'	44:1:2188:A:OP1	2.16	0.61
3:E:49:GLY:O	3:E:163:PHE:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:u:85:LEU:O	41:u:89:THR:HG23	2.00	0.61
44:1:914:A:OP2	44:1:2136:C:O2'	2.17	0.61
47:w:65:SER:OG	47:w:86:PRO:O	2.13	0.61
21:Y:22:ALA:O	21:Y:27:ARG:NE	2.31	0.61
22:Z:33:SER:OG	22:Z:35:SER:O	2.13	0.61
7:K:208:SER:OG	7:K:209:ILE:N	2.31	0.61
10:N:112:ASN:N	10:N:112:ASN:OD1	2.34	0.61
46:6:13:U:O2	46:6:16:U:N3	2.34	0.61
14:R:118:HIS:HE2	44:1:1716:U:HO2'	1.47	0.61
21:Y:18:ALA:O	21:Y:22:ALA:HB2	2.00	0.61
7:K:89:THR:OG1	7:K:92:SER:OG	2.19	0.61
8:L:161:ASP:OD1	8:L:163:GLY:N	2.33	0.61
23:a:64:GLN:NE2	44:1:71:A:OP2	2.34	0.60
32:j:72:ARG:NH1	45:2:95:G:OP2	2.33	0.60
39:s:8:SER:O	39:s:9:ARG:NH1	2.34	0.60
44:1:826:G:OP1	44:1:1590:G:O2'	2.18	0.60
45:2:112:U:O2'	45:2:113:U:O5'	2.17	0.60
1:B:238:LEU:HD22	1:B:250:ALA:HB2	1.83	0.60
5:G:158:ASP:OD1	5:G:158:ASP:N	2.33	0.60
28:f:49:ILE:HD11	28:f:71:VAL:HG23	1.83	0.60
44:1:1635:G:N2	44:1:1638:A:OP2	2.30	0.60
8:L:107:GLU:OE1	8:L:107:GLU:N	2.35	0.60
22:Z:3:LYS:O	22:Z:6:LYS:NZ	2.23	0.60
22:Z:26:VAL:HG21	22:Z:96:VAL:HG21	1.82	0.60
30:h:12:LYS:NZ	30:h:20:GLN:OE1	2.34	0.60
35:n:380:ILE:HD13	35:n:387:VAL:HG23	1.83	0.60
44:1:1813:A:O2'	44:1:1816:A:N3	2.24	0.60
6:H:62:ARG:NH2	19:W:4:SER:OG	2.35	0.60
19:W:54:GLN:NE2	44:1:1257:C:O2	2.34	0.60
45:2:126:A:O2'	45:2:128:U:OP2	2.12	0.60
24:b:154:ARG:NH1	44:1:2899:C:OP1	2.35	0.60
44:1:198:A:N3	44:1:218:G:O2'	2.33	0.60
5:G:150:LEU:HD12	5:G:176:PRO:O	2.01	0.60
5:G:191:ASN:O	5:G:192:GLN:NE2	2.34	0.60
20:X:83:VAL:HG12	20:X:123:TYR:HD1	1.67	0.60
21:Y:5:SER:OG	21:Y:6:LEU:N	2.32	0.60
24:b:257:SER:OG	24:b:288:ASN:O	2.19	0.60
42:y:23:TYR:OH	42:y:66:ASN:O	2.16	0.60
8:L:153:ASP:OD1	8:L:157:ARG:NH2	2.34	0.60
38:r:21:GLU:N	38:r:21:GLU:OE1	2.34	0.60
44:1:283:G:N2	44:1:304:G:O2'	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:1901:A:O2'	44:1:2918:G:OP1	2.19	0.59
1:B:21:ARG:NH2	44:1:2991:A:O3'	2.34	0.59
1:B:258:ALA:O	1:B:259:HIS:ND1	2.33	0.59
8:L:155:GLU:OE1	8:L:155:GLU:N	2.36	0.59
21:Y:76:LEU:HD23	34:l:31:THR:HG21	1.83	0.59
38:r:203:ASN:ND2	38:r:214:VAL:O	2.35	0.59
44:1:1240:A:N6	44:1:1241:U:O4	2.36	0.59
2:C:197:ARG:NH2	44:1:339:C:OP2	2.36	0.59
14:R:60:LYS:NZ	44:1:1671:C:OP1	2.33	0.59
36:o:132:ARG:NE	46:6:28:A:OP1	2.33	0.59
43:z:14:LYS:NZ	44:1:3100:U:OP2	2.34	0.59
44:1:733:G:N2	44:1:736:A:OP2	2.31	0.59
44:1:2117:A:O2'	44:1:3080:G:O2'	2.13	0.59
32:j:30:GLN:NE2	44:1:817:A:OP1	2.35	0.59
44:1:1929:G:O2'	44:1:2322:C:OP1	2.09	0.59
22:Z:41:ALA:HB2	22:Z:77:TYR:HE1	1.67	0.59
35:n:17:THR:OG1	35:n:18:ARG:N	2.35	0.59
44:1:1595:U:O2'	44:1:1606:U:O2	2.20	0.59
44:1:1863:G:H21	44:1:1867:A:H62	1.50	0.59
10:N:5:LYS:NZ	44:1:266:A:OP1	2.25	0.59
25:c:22:LYS:NZ	25:c:23:TYR:O	2.35	0.59
35:n:379:LEU:O	35:n:382:SER:OG	2.12	0.59
44:1:359:U:O4	44:1:815:G:O2'	2.20	0.59
7:K:210:ARG:NH1	46:6:7:C:N3	2.51	0.59
36:o:90:SER:OG	36:o:168:PRO:O	2.12	0.59
2:C:308:LYS:NZ	44:1:594:U:O2'	2.35	0.58
24:b:254:MET:HG3	24:b:287:ILE:HG22	1.83	0.58
44:1:364:G:O2'	44:1:365:A:O4'	2.19	0.58
44:1:407:A:OP2	45:2:16:G:N2	2.35	0.58
44:1:913:A:N7	44:1:2135:U:O2'	2.33	0.58
44:1:1481:A:OP2	44:1:1859:A:N6	2.36	0.58
23:a:105:LEU:HD11	23:a:128:ARG:NH2	2.18	0.58
36:o:140:VAL:HG23	36:o:141:ASN:HB2	1.85	0.58
40:t:279:GLY:O	44:1:1570:U:O2'	2.20	0.58
2:C:82:THR:HG23	2:C:84:ARG:H	1.68	0.58
18:V:104:ASN:OD1	18:V:108:GLU:N	2.35	0.58
4:F:67:ARG:NH2	44:1:517:G:OP1	2.37	0.58
13:Q:31:LYS:O	13:Q:34:THR:OG1	2.18	0.58
1:B:145:GLU:OE1	1:B:145:GLU:N	2.37	0.58
7:K:156:CYS:SG	7:K:157:GLY:N	2.76	0.58
24:b:134:GLY:O	24:b:138:THR:OG1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:f:54:ARG:NH1	28:f:64:ILE:HD11	2.19	0.58
1:B:352:GLU:OE1	1:B:352:GLU:N	2.37	0.58
4:F:110:ARG:NH2	44:1:1159:A:N7	2.52	0.58
44:1:1464:G:N2	44:1:1467:A:OP2	2.37	0.58
21:Y:54:ASP:OD2	21:Y:110:HIS:N	2.36	0.58
5:G:193:LYS:NZ	44:1:144:A:OP1	2.29	0.58
23:a:111:LYS:NZ	44:1:714:G:N7	2.50	0.58
44:1:679:U:O2'	44:1:788:C:O2	2.21	0.58
19:W:63:SER:HB2	19:W:103:LEU:HD11	1.84	0.57
31:i:76:ARG:O	44:1:293:C:O2'	2.19	0.57
41:u:106:ALA:O	41:u:110:ASN:ND2	2.37	0.57
44:1:650:C:OP2	44:1:2397:A:N6	2.37	0.57
24:b:369:ARG:NE	42:y:175:SER:O	2.30	0.57
44:1:1378:U:N3	44:1:1430:U:O2	2.36	0.57
21:Y:51:ARG:NH1	45:2:71:A:OP2	2.37	0.57
24:b:172:ILE:HG22	24:b:180:LYS:NZ	2.18	0.57
44:1:2860:U:O2	44:1:2864:A:N6	2.37	0.57
2:C:335:ALA:O	2:C:338:LYS:NZ	2.30	0.57
19:W:57:ARG:NH1	44:1:1259:A:OP1	2.36	0.57
27:e:104:ASN:ND2	44:1:1389:G:OP1	2.37	0.57
44:1:1347:U:O2	44:1:1357:G:O6	2.22	0.57
23:a:105:LEU:HD11	23:a:128:ARG:HH21	1.68	0.57
24:b:403:GLU:O	24:b:408:GLY:N	2.38	0.57
35:n:366:TYR:O	35:n:410:GLN:NE2	2.37	0.57
2:C:217:LYS:NZ	44:1:210:U:O2	2.37	0.57
17:U:84:LEU:HD23	17:U:90:ARG:HD2	1.85	0.57
44:1:35:A:OP2	44:1:48:A:N6	2.37	0.57
1:B:187:SER:OG	1:B:190:GLU:OE2	2.16	0.57
7:K:119:LYS:NZ	46:6:49:C:OP2	2.37	0.57
12:P:22:LEU:HD12	12:P:146:ILE:HD12	1.87	0.57
12:P:64:ASN:HA	12:P:67:ILE:HD12	1.87	0.57
19:W:158:ILE:CG1	19:W:161:LEU:HD23	2.35	0.57
1:B:132:LYS:NZ	44:1:3151:U:OP2	2.37	0.57
12:P:62:ARG:NE	45:2:5:U:OP1	2.38	0.57
24:b:283:VAL:O	24:b:338:LYS:NZ	2.37	0.57
36:o:125:ASN:OD1	36:o:132:ARG:NH2	2.38	0.57
44:1:2845:A:O2'	44:1:2848:G:O6	2.18	0.57
2:C:163:LYS:NZ	44:1:208:C:OP2	2.34	0.57
15:S:25:PHE:HD2	16:T:151:LEU:HD21	1.69	0.57
38:r:224:ASN:OD1	38:r:226:SER:OG	2.15	0.57
1:B:57:VAL:HG13	1:B:357:LYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:23:LYS:NZ	44:1:611:A:O5'	2.39	0.56
5:G:213:LYS:O	5:G:217:THR:HG23	2.05	0.56
14:R:6:THR:OG1	44:1:1498:A:OP1	2.23	0.56
37:q:259:LYS:HA	37:q:262:ILE:HD12	1.87	0.56
1:B:92:TYR:OH	44:1:3003:G:O2'	2.15	0.56
24:b:268:VAL:HG11	24:b:305:LEU:HD12	1.87	0.56
5:G:188:THR:OG1	5:G:189:LEU:N	2.39	0.56
17:U:90:ARG:NH1	44:1:1682:U:O4	2.37	0.56
24:b:86:TYR:O	24:b:149:TYR:OH	2.23	0.56
36:o:175:LYS:NZ	46:6:58:G:O3'	2.38	0.56
44:1:1347:U:C2	44:1:1357:G:O6	2.58	0.56
13:Q:135:GLN:O	13:Q:137:THR:HG23	2.05	0.56
37:q:258:TYR:CZ	37:q:262:ILE:HD11	2.41	0.56
44:1:2875:U:O2'	44:1:2952:G:N2	2.38	0.56
47:w:705:GLU:OE2	47:w:706:HIS:NE2	2.39	0.56
8:L:174:ARG:NH2	44:1:713:U:OP2	2.38	0.56
35:n:47:ARG:NH2	45:2:128:U:O4	2.38	0.56
47:w:307:LEU:HA	47:w:310:LEU:HD13	1.88	0.56
2:C:2:SER:OG	2:C:3:ARG:N	2.36	0.56
14:R:146:LYS:NZ	44:1:2093:A:OP1	2.38	0.56
36:o:118:LYS:NZ	36:o:140:VAL:O	2.25	0.56
7:K:76:LYS:O	7:K:283:THR:HG22	2.05	0.56
26:d:60:TRP:O	26:d:63:GLY:N	2.39	0.56
35:n:209:ILE:HG22	35:n:211:SER:H	1.71	0.56
40:t:75:ILE:HD12	40:t:189:VAL:HG23	1.88	0.56
44:1:923:C:O2'	44:1:924:G:OP2	2.22	0.56
44:1:1203:A:O2'	44:1:1204:A:OP2	2.17	0.56
44:1:3092:C:O2'	44:1:3094:A:OP2	2.16	0.56
33:k:42:LYS:NZ	44:1:1748:G:OP2	2.38	0.56
35:n:144:ASN:ND2	35:n:203:PHE:O	2.38	0.56
5:G:156:ASP:O	5:G:183:LYS:NZ	2.28	0.56
12:P:171:ARG:NH2	44:1:3274:A:N7	2.54	0.56
22:Z:9:LYS:O	22:Z:25:ILE:HG22	2.06	0.56
43:z:4:SER:OG	44:1:3013:U:OP1	2.17	0.56
7:K:186:ILE:O	7:K:189:SER:OG	2.24	0.55
19:W:64:LYS:O	19:W:103:LEU:HD12	2.06	0.55
39:s:22:LYS:NZ	44:1:2824:G:OP2	2.37	0.55
6:H:137:SER:OG	6:H:140:VAL:O	2.23	0.55
7:K:43:GLU:OE2	36:o:217:GLU:N	2.39	0.55
25:c:13:LYS:O	25:c:17:VAL:HG23	2.07	0.55
10:N:38:ARG:NH1	45:2:143:U:OP2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:f:105:SER:OG	28:f:107:ILE:O	2.24	0.55
44:1:820:A:N3	44:1:911:C:O2'	2.37	0.55
14:R:83:GLY:N	44:1:1864:A:OP1	2.39	0.55
35:n:364:VAL:O	35:n:408:THR:OG1	2.24	0.55
44:1:3177:G:O2'	44:1:3179:U:OP1	2.14	0.55
12:P:47:TYR:OH	12:P:57:ALA:O	2.12	0.55
9:M:112:LEU:HD11	9:M:116:GLU:HB3	1.89	0.55
19:W:133:LEU:N	19:W:191:GLU:OE1	2.40	0.55
44:1:250:U:O2'	44:1:253:A:N6	2.39	0.55
9:M:28:SER:OG	9:M:29:ALA:N	2.39	0.55
21:Y:55:GLU:OE2	21:Y:69:LYS:NZ	2.40	0.55
39:s:17:GLU:OE2	39:s:20:LYS:NZ	2.37	0.55
34:l:9:ILE:HG22	34:l:13:MET:HE3	1.89	0.55
42:y:7:PHE:O	42:y:10:SER:N	2.37	0.55
42:y:9:ASN:ND2	44:1:3018:C:OP1	2.40	0.55
42:y:132:VAL:HG13	42:y:133:LEU:CD1	2.36	0.55
5:G:51:LYS:NZ	44:1:1557:A:OP1	2.24	0.55
12:P:171:ARG:NH1	44:1:3276:G:O6	2.40	0.55
21:Y:14:LYS:NZ	44:1:335:G:OP2	2.40	0.55
44:1:545:U:O4	44:1:548:G:N2	2.35	0.55
7:K:42:ASN:HA	7:K:45:ILE:HD12	1.89	0.55
29:g:4:ARG:NH1	44:1:1481:A:N3	2.55	0.55
42:y:200:ASN:OD1	42:y:203:LEU:N	2.39	0.55
44:1:1565:G:O2'	44:1:1567:U:OP2	2.18	0.55
6:H:58:HIS:O	44:1:3186:A:N6	2.40	0.54
17:U:77:LYS:NZ	44:1:1678:G:OP2	2.38	0.54
1:B:275:ARG:NH2	44:1:3046:A:OP1	2.40	0.54
4:F:187:GLU:O	4:F:191:VAL:HA	2.07	0.54
10:N:94:TYR:O	44:1:289:A:O2'	2.26	0.54
44:1:1481:A:C5	44:1:1872:C:N4	2.75	0.54
4:F:29:GLU:OE1	4:F:29:GLU:N	2.40	0.54
16:T:128:LEU:HD13	44:1:1097:G:C8	2.42	0.54
20:X:56:ARG:O	20:X:61:LYS:NZ	2.26	0.54
42:y:21:ASN:ND2	42:y:112:ASP:OD2	2.41	0.54
3:E:45:GLY:O	3:E:48:ARG:NH2	2.41	0.54
7:K:37:VAL:HG11	7:K:260:VAL:HG22	1.90	0.54
38:r:200:VAL:HG11	38:r:213:GLY:HA2	1.88	0.54
44:1:88:A:H62	44:1:98:G:N2	2.01	0.54
1:B:204:ALA:O	1:B:207:SER:OG	2.24	0.54
2:C:107:ARG:NH2	44:1:1429:G:OP2	2.39	0.54
5:G:160:ILE:O	5:G:164:VAL:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:128:ARG:HD2	12:P:136:ILE:HD11	1.89	0.54
32:j:14:LYS:NZ	44:1:1492:G:OP1	2.28	0.54
46:6:14:U:O2'	46:6:16:U:O4'	2.12	0.54
46:6:58:G:OP1	46:6:58:G:N2	2.40	0.54
2:C:141:ARG:NH1	44:1:1385:C:OP1	2.38	0.54
12:P:40:GLU:OE1	12:P:42:THR:N	2.40	0.54
22:Z:109:GLU:OE1	22:Z:109:GLU:N	2.40	0.54
22:Z:123:GLN:OE1	37:q:258:TYR:OH	2.15	0.54
44:1:1792:C:O2	44:1:1794:G:O2'	2.13	0.54
5:G:84:ARG:NE	20:X:14:VAL:O	2.41	0.54
19:W:93:SER:HG	19:W:94:LYS:HZ3	1.56	0.54
2:C:191:LYS:NZ	44:1:341:G:OP2	2.28	0.54
29:g:49:SER:OG	29:g:81:CYS:SG	2.66	0.54
40:t:73:GLU:OE2	40:t:77:ARG:NH2	2.40	0.54
11:O:25:LYS:NZ	44:1:1176:C:OP1	2.25	0.53
12:P:24:VAL:HG23	12:P:86:LYS:HD3	1.91	0.53
26:d:19:ARG:NH1	44:1:3324:C:OP1	2.41	0.53
43:z:4:SER:OG	43:z:5:LEU:N	2.42	0.53
44:1:1002:A:N6	44:1:1049:C:O5'	2.41	0.53
31:i:37:THR:OG1	31:i:41:ARG:NH1	2.42	0.53
39:s:29:LYS:NZ	44:1:1128:U:O4	2.42	0.53
43:z:3:LYS:NZ	44:1:2892:A:O3'	2.38	0.53
14:R:81:ARG:O	44:1:1914:G:N2	2.42	0.53
24:b:348:LEU:O	24:b:351:GLN:NE2	2.41	0.53
42:y:18:LYS:HB2	42:y:25:LEU:HD13	1.90	0.53
44:1:1778:G:O2'	44:1:1780:G:OP2	2.26	0.53
5:G:149:LYS:N	5:G:200:LEU:O	2.40	0.53
24:b:383:LYS:NZ	42:y:226:ASP:OD1	2.41	0.53
42:y:18:LYS:NZ	42:y:60:GLY:O	2.26	0.53
44:1:1481:A:N6	44:1:1872:C:C4	2.73	0.53
44:1:2113:A:O2'	44:1:2114:C:O5'	2.14	0.53
5:G:194:THR:OG1	5:G:195:SER:N	2.42	0.53
10:N:38:ARG:NH2	45:2:143:U:OP1	2.42	0.53
10:N:96:ARG:NH2	44:1:1546:A:O2'	2.42	0.53
13:Q:89:ASP:OD1	13:Q:90:ASP:N	2.41	0.53
9:M:116:GLU:N	9:M:116:GLU:OE1	2.41	0.53
12:P:64:ASN:O	12:P:80:LYS:NZ	2.40	0.53
20:X:70:GLU:N	20:X:70:GLU:OE1	2.41	0.53
32:j:66:TYR:OH	32:j:73:ARG:NH2	2.42	0.53
44:1:1483:G:C6	44:1:1873:U:O4	2.61	0.53
1:B:372:THR:HG23	1:B:375:GLU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:43:ARG:NH2	24:b:119:GLY:O	2.42	0.53
25:c:17:VAL:O	25:c:20:SER:C	2.52	0.53
35:n:88:ARG:NE	45:2:147:U:OP2	2.39	0.53
44:1:28:C:O2'	44:1:61:A:N3	2.42	0.53
44:1:551:A:O2'	44:1:552:G:O5'	2.26	0.53
46:6:39:U:O2'	46:6:40:U:O2	2.26	0.53
47:w:47:SER:OG	47:w:115:THR:HG21	2.07	0.53
47:w:117:LEU:HD13	47:w:157:VAL:HG23	1.90	0.53
2:C:155:ASP:O	2:C:158:SER:OG	2.24	0.53
4:F:70:LYS:NZ	44:1:519:A:O5'	2.36	0.53
11:O:126:VAL:HG21	44:1:3185:U:H6	1.73	0.53
12:P:135:ARG:HE	44:1:879:U:HO2'	1.53	0.53
42:y:128:LEU:O	42:y:132:VAL:HG12	2.08	0.53
42:y:186:VAL:HG22	42:y:193:VAL:HG12	1.91	0.53
44:1:296:A:N3	44:1:299:G:O2'	2.40	0.53
44:1:3245:A:N7	44:1:3246:G:N2	2.56	0.53
47:w:819:VAL:HG13	47:w:823:MET:HE2	1.90	0.53
2:C:196:ASN:ND2	44:1:337:G:OP2	2.40	0.53
44:1:3303:G:O2'	44:1:3305:A:N6	2.42	0.53
11:O:159:LYS:NZ	44:1:3242:G:OP1	2.38	0.53
19:W:159:HIS:HA	19:W:180:ILE:HD11	1.89	0.53
24:b:287:ILE:HG23	24:b:317:ILE:HD11	1.90	0.53
9:M:40:ASP:OD1	9:M:43:LYS:N	2.41	0.52
19:W:158:ILE:HG12	19:W:161:LEU:HD23	1.92	0.52
31:i:19:SER:OG	31:i:20:MET:N	2.41	0.52
34:l:27:ILE:O	34:l:33:ASN:ND2	2.40	0.52
42:y:159:GLY:N	42:y:180:PRO:O	2.42	0.52
44:1:1392:G:C2	44:1:1418:A:N6	2.72	0.52
6:H:38:LEU:O	6:H:41:ILE:HG22	2.10	0.52
9:M:124:ARG:NH2	44:1:3212:C:OP2	2.41	0.52
19:W:66:ILE:HD12	44:1:1259:A:OP1	2.08	0.52
35:n:367:VAL:HG22	35:n:411:ILE:HD12	1.91	0.52
44:1:1538:G:N2	44:1:1583:A:H62	1.98	0.52
20:X:4:SER:OG	36:o:144:ASP:OD1	2.22	0.52
37:q:227:TYR:CD1	37:q:409:LEU:HD11	2.44	0.52
44:1:422:A:O2'	44:1:423:A:O4'	2.26	0.52
44:1:801:A:O2'	44:1:802:C:OP2	2.23	0.52
7:K:181:LEU:HD12	7:K:207:ILE:O	2.09	0.52
10:N:97:SER:OG	10:N:98:LEU:N	2.42	0.52
26:d:56:ASN:ND2	44:1:1459:C:O4'	2.43	0.52
27:e:45:ARG:NH2	44:1:1160:C:N3	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:y:206:THR:OG1	42:y:210:THR:OG1	2.21	0.52
24:b:81:LEU:O	24:b:84:THR:OG1	2.26	0.52
25:c:13:LYS:NZ	25:c:103:THR:OG1	2.42	0.52
28:f:50:ALA:HB2	28:f:68:TRP:CZ3	2.44	0.52
43:z:2:ALA:N	44:1:2891:U:O3'	2.43	0.52
44:1:1131:G:O2'	44:1:2822:U:O4	2.28	0.52
1:B:81:THR:HG23	1:B:320:ASP:HB2	1.90	0.52
24:b:188:THR:HG21	24:b:207:GLY:HA3	1.90	0.52
45:2:55:U:O4	45:2:62:C:N3	2.43	0.52
1:B:60:LEU:HD21	1:B:62:ARG:CZ	2.39	0.52
1:B:339:ARG:NH2	1:B:342:LEU:HD11	2.24	0.52
2:C:92:ASN:OD1	2:C:93:MET:N	2.43	0.52
24:b:33:ILE:HD11	24:b:45:PHE:CG	2.44	0.52
24:b:70:ASN:ND2	24:b:72:ASN:OD1	2.42	0.52
1:B:65:SER:OG	1:B:68:HIS:N	2.42	0.52
21:Y:119:ILE:HG22	21:Y:124:GLY:HA3	1.91	0.52
26:d:68:GLU:N	26:d:68:GLU:OE2	2.42	0.52
35:n:454:PRO:HB2	35:n:457:LEU:HD23	1.92	0.52
44:1:952:A:N3	44:1:1114:U:O2'	2.42	0.52
44:1:1418:A:O2'	44:1:1419:A:OP2	2.21	0.52
44:1:1489:A:N6	44:1:1838:G:H21	2.07	0.52
4:F:231:ASN:ND2	4:F:233:GLU:OE2	2.43	0.52
2:C:40:THR:OG1	2:C:41:SER:N	2.39	0.52
2:C:176:SER:OG	2:C:177:ASP:N	2.43	0.52
2:C:312:VAL:HG21	44:1:610:G:C8	2.45	0.52
15:S:146:LYS:NZ	44:1:535:G:O5'	2.43	0.52
44:1:2316:G:N2	44:1:2316:G:OP2	2.43	0.52
3:E:158:TYR:OH	9:M:114:ASP:OD2	2.13	0.51
21:Y:119:ILE:O	21:Y:124:GLY:N	2.43	0.51
22:Z:21:LYS:NZ	22:Z:47:GLU:O	2.38	0.51
37:q:245:GLU:OE1	37:q:248:ARG:NH1	2.42	0.51
44:1:869:G:O6	44:1:870:G:N2	2.40	0.51
47:w:50:VAL:HB	47:w:74:ILE:HG23	1.92	0.51
12:P:24:VAL:HG22	12:P:25:SER:H	1.75	0.51
20:X:27:ARG:NH2	45:2:150:G:OP1	2.44	0.51
34:l:2:ALA:N	44:1:1490:A:OP2	2.43	0.51
35:n:186:VAL:O	35:n:200:LEU:HD23	2.09	0.51
20:X:55:ASN:OD1	20:X:58:ASP:N	2.43	0.51
25:c:17:VAL:O	25:c:20:SER:O	2.28	0.51
4:F:122:ALA:O	44:1:986:U:O2'	2.28	0.51
7:K:199:TYR:HA	7:K:205:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:HIS:ND1	1:B:164:THR:O	2.44	0.51
7:K:181:LEU:HD11	7:K:209:ILE:HB	1.93	0.51
19:W:138:PRO:O	19:W:182:ILE:HD11	2.11	0.51
38:r:150:MET:HE1	38:r:172:ILE:HG21	1.91	0.51
44:1:2837:A:OP2	44:1:2845:A:N6	2.43	0.51
1:B:348:ARG:NH2	24:b:411:VAL:O	2.43	0.51
19:W:41:TRP:CZ2	19:W:109:VAL:HG12	2.46	0.51
44:1:1761:C:O2'	44:1:1762:C:O5'	2.15	0.51
18:V:108:GLU:OE1	18:V:128:ARG:NH1	2.43	0.51
40:t:77:ARG:NE	46:6:5:C:N3	2.59	0.51
42:y:163:PRO:HA	42:y:183:ALA:HB1	1.93	0.51
44:1:921:A:OP1	44:1:922:U:N3	2.44	0.51
44:1:1220:U:OP1	44:1:1221:A:O2'	2.28	0.51
44:1:1482:A:OP2	44:1:1858:A:O2'	2.28	0.51
47:w:306:ASP:OD1	47:w:306:ASP:N	2.43	0.51
1:B:248:LYS:NZ	44:1:2393:G:OP2	2.42	0.51
34:l:37:TYR:O	44:1:351:A:N6	2.44	0.51
44:1:2364:G:HO2'	44:1:2365:C:P	2.33	0.51
1:B:210:GLU:HG2	43:z:33:ILE:HD11	1.93	0.51
7:K:190:LEU:HD22	7:K:194:MET:HE3	1.92	0.51
8:L:17:HIS:NE2	44:1:932:U:OP2	2.44	0.51
9:M:80:THR:HG21	44:1:561:C:P	2.50	0.51
27:e:2:ALA:O	27:e:90:LYS:NZ	2.44	0.51
44:1:1436:U:C5	47:w:822:VAL:HG11	2.46	0.51
5:G:98:ARG:NH1	5:G:188:THR:O	2.44	0.50
7:K:201:LYS:NZ	46:6:49:C:OP2	2.44	0.50
2:C:197:ARG:NH1	44:1:1381:A:OP1	2.44	0.50
22:Z:48:ARG:NH2	44:1:1631:C:OP2	2.45	0.50
44:1:2920:U:O2'	44:1:2921:U:OP1	2.22	0.50
2:C:322:GLN:OE1	2:C:322:GLN:N	2.45	0.50
14:R:7:GLN:OE1	14:R:7:GLN:N	2.42	0.50
15:S:134:ASP:OD2	15:S:134:ASP:N	2.43	0.50
23:a:116:GLY:O	23:a:137:LYS:NZ	2.31	0.50
3:E:29:LYS:NZ	44:1:582:G:OP1	2.27	0.50
10:N:203:ARG:NH1	44:1:665:A:OP1	2.43	0.50
21:Y:88:GLU:OE1	21:Y:88:GLU:N	2.44	0.50
30:h:27:GLU:O	30:h:31:LEU:HD13	2.11	0.50
36:o:106:GLU:OE1	36:o:106:GLU:N	2.45	0.50
22:Z:78:ASN:ND2	44:1:1711:C:OP1	2.45	0.50
27:e:45:ARG:NH2	44:1:1366:A:O2'	2.44	0.50
44:1:1392:G:O2'	44:1:1417:G:N1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:ARG:NH2	44:1:1383:G:OP1	2.43	0.50
12:P:78:VAL:HG12	12:P:80:LYS:H	1.77	0.50
16:T:130:ARG:NE	44:1:1098:A:OP1	2.38	0.50
28:f:54:ARG:HH12	28:f:64:ILE:HD11	1.75	0.50
40:t:149:GLY:HA2	46:6:64:C:H42	1.77	0.50
44:1:1704:A:N7	44:1:1740:U:N3	2.60	0.50
1:B:136:LYS:O	1:B:139:GLN:NE2	2.44	0.50
2:C:310:THR:O	2:C:310:THR:OG1	2.28	0.50
35:n:34:ARG:HG2	35:n:220:THR:HG21	1.92	0.50
38:r:7:ILE:HD12	44:1:2898:G:C4	2.47	0.50
40:t:26:ALA:O	40:t:29:THR:OG1	2.30	0.50
44:1:1128:U:O2'	44:1:1130:A:N7	2.37	0.50
2:C:352:ALA:N	4:F:70:LYS:O	2.43	0.50
26:d:12:TYR:CD2	26:d:75:ILE:HD12	2.47	0.50
28:f:105:SER:OG	28:f:107:ILE:N	2.44	0.50
47:w:808:ARG:NH1	47:w:813:LYS:O	2.45	0.50
1:B:2:SER:OG	1:B:3:HIS:N	2.45	0.49
6:H:45:PHE:CE2	6:H:55:VAL:HG12	2.46	0.49
10:N:160:GLU:OE2	10:N:160:GLU:N	2.41	0.49
18:V:15:LEU:HD12	18:V:51:ALA:CB	2.42	0.49
24:b:31:THR:OG1	44:1:2827:U:O2	2.27	0.49
25:c:17:VAL:HG22	25:c:98:SER:CB	2.41	0.49
4:F:170:GLU:OE2	4:F:179:LEU:HD12	2.12	0.49
33:k:4:GLU:OE1	33:k:4:GLU:N	2.41	0.49
44:1:1492:G:OP2	44:1:1493:G:N2	2.45	0.49
44:1:1657:C:N4	44:1:1798:A:OP2	2.29	0.49
28:f:57:LYS:NZ	44:1:433:A:OP2	2.36	0.49
36:o:157:LEU:HD23	36:o:158:MET:HB2	1.94	0.49
44:1:112:U:HO2'	44:1:113:C:P	2.35	0.49
1:B:384:LYS:NZ	44:1:3368:U:OP1	2.27	0.49
3:E:80:ASN:OD1	3:E:81:ALA:N	2.45	0.49
9:M:42:LYS:HA	9:M:60:LEU:HD12	1.93	0.49
15:S:112:ALA:O	15:S:115:ARG:NH1	2.45	0.49
19:W:169:PHE:O	19:W:171:ILE:HG23	2.13	0.49
44:1:52:A:N3	44:1:811:U:O2'	2.45	0.49
44:1:341:G:O2'	45:2:22:U:O4	2.30	0.49
44:1:1463:U:O4	44:1:1467:A:N7	2.46	0.49
15:S:130:GLU:N	15:S:130:GLU:OE2	2.45	0.49
18:V:80:ARG:HB2	18:V:99:ALA:HB3	1.93	0.49
24:b:254:MET:CG	24:b:287:ILE:HG22	2.42	0.49
47:w:129:VAL:O	47:w:132:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:281:ASP:OD1	47:w:281:ASP:N	2.43	0.49
3:E:51:ARG:NH1	3:E:162:SER:O	2.45	0.49
44:1:1913:A:O2'	44:1:2120:A:N3	2.37	0.49
2:C:334:PHE:O	2:C:338:LYS:HA	2.13	0.49
14:R:30:SER:OG	14:R:31:GLU:OE1	2.30	0.49
15:S:28:ARG:NH2	15:S:64:ILE:HD13	2.27	0.49
44:1:2984:C:OP2	44:1:2985:C:N4	2.45	0.49
44:1:2991:A:O2'	44:1:3309:G:N7	2.45	0.49
5:G:178:ALA:HB2	5:G:218:ILE:HG12	1.95	0.49
6:H:44:THR:OG1	44:1:3186:A:N3	2.37	0.49
13:Q:80:THR:HG22	13:Q:137:THR:HG22	1.95	0.49
13:Q:125:ASP:O	13:Q:129:VAL:HG23	2.12	0.49
26:d:102:LYS:NZ	44:1:3373:U:OP2	2.27	0.49
12:P:119:VAL:O	44:1:412:G:O2'	2.23	0.49
19:W:102:LEU:HD12	19:W:103:LEU:H	1.78	0.49
32:j:19:CYS:SG	32:j:20:ASN:N	2.86	0.49
44:1:63:A:N3	44:1:78:U:O2'	2.38	0.49
8:L:109:PHE:CE1	31:i:20:MET:HE1	2.47	0.49
37:q:258:TYR:CE2	37:q:262:ILE:HD11	2.48	0.49
6:H:105:GLU:OE2	6:H:108:GLY:N	2.44	0.48
7:K:127:LEU:HD23	7:K:154:ILE:HG13	1.95	0.48
11:O:49:ARG:NH2	44:1:1193:A:OP1	2.46	0.48
27:e:100:ILE:O	27:e:105:ARG:NH1	2.46	0.48
32:j:17:THR:HG22	32:j:18:LEU:H	1.77	0.48
44:1:1533:U:H3	44:1:1587:A:H62	1.59	0.48
44:1:3351:U:N3	44:1:3356:G:O2'	2.43	0.48
45:2:73:U:N3	45:2:90:U:OP1	2.46	0.48
47:w:134:THR:O	47:w:138:LEU:HD23	2.13	0.48
47:w:321:TRP:HA	47:w:324:ILE:HD12	1.94	0.48
1:B:278:ILE:O	44:1:3097:C:O2'	2.31	0.48
6:H:49:ASN:N	6:H:49:ASN:OD1	2.46	0.48
7:K:223:THR:O	7:K:227:LYS:NZ	2.25	0.48
24:b:61:PHE:HA	24:b:64:ILE:HD12	1.94	0.48
24:b:445:LEU:CD1	41:u:89:THR:HG21	2.43	0.48
1:B:221:THR:O	1:B:272:TYR:N	2.37	0.48
2:C:92:ASN:ND2	44:1:803:C:O2'	2.47	0.48
19:W:103:LEU:HG	19:W:105:THR:HG23	1.95	0.48
21:Y:13:ARG:NH1	45:2:24:G:OP2	2.45	0.48
38:r:59:VAL:HG12	38:r:62:ARG:HH12	1.78	0.48
4:F:187:GLU:O	4:F:190:THR:O	2.32	0.48
6:H:98:PRO:O	6:H:116:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:57:ILE:HD12	44:1:671:U:OP2	2.14	0.48
24:b:171:LEU:HD12	24:b:246:LEU:HD21	1.94	0.48
31:i:40:VAL:HA	31:i:43:LEU:HD12	1.94	0.48
44:1:1178:G:N2	44:1:1329:U:O4'	2.47	0.48
1:B:10:ARG:NH1	1:B:11:HIS:O	2.46	0.48
1:B:382:THR:C	1:B:383:LEU:HD12	2.38	0.48
3:E:26:ARG:NH1	44:1:503:C:O5'	2.47	0.48
7:K:180:ILE:HD11	7:K:194:MET:HE1	1.96	0.48
7:K:281:ILE:HG12	7:K:291:LEU:HD22	1.95	0.48
8:L:180:ARG:O	8:L:184:GLU:N	2.43	0.48
19:W:93:SER:HG	19:W:94:LYS:NZ	2.10	0.48
19:W:220:TYR:O	19:W:229:GLU:N	2.44	0.48
20:X:88:MET:HE2	34:l:7:PHE:CZ	2.49	0.48
32:j:19:CYS:SG	32:j:21:ARG:N	2.84	0.48
32:j:24:ARG:NH2	44:1:362:U:O4	2.45	0.48
36:o:123:ALA:HA	36:o:176:LEU:HD23	1.94	0.48
41:u:111:ARG:NH2	44:1:3369:G:OP1	2.46	0.48
4:F:165:ASP:OD1	4:F:166:ASN:N	2.47	0.48
7:K:159:ASP:O	7:K:163:VAL:HG22	2.13	0.48
16:T:105:PHE:O	16:T:109:VAL:HG23	2.13	0.48
21:Y:83:ASP:OD1	21:Y:84:LYS:N	2.46	0.48
29:g:70:LYS:NZ	44:1:1803:C:O3'	2.46	0.48
32:j:10:LYS:NZ	44:1:900:G:OP1	2.45	0.48
1:B:331:ASN:ND2	44:1:3304:U:O3'	2.47	0.48
29:g:25:THR:OG1	29:g:29:ILE:O	2.31	0.48
30:h:41:LEU:O	30:h:44:ILE:HG22	2.14	0.48
31:i:50:LEU:HD23	31:i:55:ARG:CD	2.44	0.48
36:o:118:LYS:N	36:o:139:PHE:O	2.46	0.48
38:r:155:THR:OG1	38:r:212:LEU:O	2.31	0.48
44:1:196:G:N1	44:1:199:A:OP2	2.45	0.48
44:1:1532:C:O2'	44:1:1799:A:N3	2.37	0.48
14:R:13:SER:OG	14:R:38:ARG:NH2	2.45	0.48
35:n:18:ARG:NH2	35:n:29:LEU:HD11	2.29	0.48
38:r:256:ASN:ND2	44:1:2831:G:N3	2.60	0.48
41:u:82:ASN:ND2	41:u:84:GLU:OE2	2.45	0.48
44:1:835:G:O2'	44:1:836:A:OP2	2.27	0.48
44:1:1237:G:H22	44:1:1251:A:H2	1.62	0.48
45:2:39:G:O2'	45:2:105:A:N1	2.41	0.48
41:u:56:ARG:NE	41:u:62:GLU:OE2	2.45	0.48
44:1:177:U:O2	44:1:241:G:C2	2.66	0.48
10:N:31:ARG:NH2	47:w:702:ASP:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:n:242:LEU:CD1	35:n:264:LEU:HD23	2.42	0.47
38:r:197:ILE:HD11	38:r:199:ALA:O	2.14	0.47
47:w:114:ASP:O	47:w:155:THR:N	2.45	0.47
1:B:317:ILE:HG22	1:B:319:ASN:H	1.79	0.47
43:z:39:GLU:OE1	43:z:43:LYS:NZ	2.25	0.47
44:1:209:A:O2'	44:1:211:A:OP2	2.20	0.47
47:w:269:ILE:HA	47:w:271:MET:HE1	1.96	0.47
18:V:49:LEU:HD13	44:1:2338:C:H1'	1.96	0.47
24:b:31:THR:OG1	24:b:31:THR:O	2.33	0.47
24:b:169:THR:HG23	24:b:217:GLN:HG2	1.95	0.47
27:e:101:SER:OG	27:e:104:ASN:ND2	2.48	0.47
36:o:152:MET:O	36:o:162:LEU:HD11	2.14	0.47
40:t:292:ARG:NH2	46:6:230:A:O5'	2.47	0.47
7:K:218:SER:OG	7:K:221:THR:HG23	2.15	0.47
24:b:270:LEU:O	24:b:273:SER:OG	2.29	0.47
39:s:8:SER:OG	39:s:10:ARG:N	2.46	0.47
40:t:67:ALA:CB	40:t:152:ALA:HB3	2.45	0.47
10:N:53:TYR:CE2	10:N:61:ILE:HD11	2.49	0.47
10:N:122:ASN:OD1	10:N:123:GLN:N	2.48	0.47
14:R:70:LYS:NZ	14:R:75:HIS:O	2.48	0.47
42:y:77:THR:HG23	42:y:80:GLU:H	1.80	0.47
44:1:1142:G:OP1	44:1:1144:U:O2'	2.14	0.47
18:V:13:ILE:HD11	18:V:54:LEU:O	2.15	0.47
35:n:148:THR:HG23	35:n:149:ASN:O	2.14	0.47
40:t:194:VAL:HG13	40:t:196:ILE:HD11	1.96	0.47
45:2:103:G:OP2	45:2:105:A:O2'	2.32	0.47
5:G:185:ARG:O	5:G:188:THR:OG1	2.09	0.47
13:Q:39:ARG:NH1	44:1:1348:U:OP2	2.47	0.47
17:U:84:LEU:HD23	17:U:90:ARG:CD	2.44	0.47
24:b:171:LEU:HD23	24:b:172:ILE:N	2.30	0.47
24:b:370:ASP:OD1	24:b:374:ARG:NH1	2.46	0.47
24:b:423:GLU:OE2	24:b:423:GLU:N	2.46	0.47
31:i:31:GLY:O	44:1:297:G:O2'	2.24	0.47
36:o:130:ASN:N	36:o:130:ASN:OD1	2.44	0.47
36:o:158:MET:HE2	46:6:2:C:N4	2.28	0.47
38:r:19:ASP:OD1	38:r:23:ARG:NH1	2.48	0.47
40:t:176:PHE:CE1	40:t:204:ILE:HD12	2.49	0.47
43:z:9:SER:OG	43:z:10:HIS:N	2.46	0.47
44:1:705:A:N3	44:1:714:G:N2	2.63	0.47
44:1:915:A:O2'	44:1:917:A:OP1	2.16	0.47
44:1:3205:G:OP2	44:1:3206:C:N4	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:697:ASP:HA	47:w:700:LEU:HD12	1.96	0.47
1:B:119:TYR:OH	1:B:128:LYS:N	2.47	0.47
22:Z:17:ARG:NH1	44:1:1634:G:O6	2.44	0.47
29:g:44:CYS:N	29:g:49:SER:O	2.42	0.47
40:t:162:ILE:HG13	40:t:190:ILE:HD11	1.97	0.47
2:C:258:LEU:HA	2:C:261:VAL:HG12	1.97	0.47
22:Z:36:HIS:CE1	22:Z:74:VAL:HG21	2.50	0.47
1:B:119:TYR:OH	1:B:129:ALA:N	2.48	0.47
1:B:252:ILE:HD13	44:1:2393:G:H4'	1.97	0.47
2:C:232:SER:OG	2:C:233:LEU:N	2.48	0.47
5:G:134:TYR:CG	5:G:190:VAL:HG21	2.49	0.47
24:b:34:ARG:NH2	44:1:2825:C:N3	2.61	0.47
35:n:172:LYS:HD2	35:n:264:LEU:HD22	1.96	0.47
44:1:712:G:N2	44:1:754:G:O3'	2.48	0.47
3:E:157:GLN:OE1	3:E:157:GLN:N	2.45	0.46
4:F:108:LEU:HD21	4:F:115:THR:HG22	1.97	0.46
4:F:109:THR:OG1	4:F:110:ARG:N	2.47	0.46
5:G:82:LEU:HD11	5:G:86:THR:HG21	1.96	0.46
24:b:188:THR:HG21	24:b:207:GLY:CA	2.45	0.46
44:1:1392:G:H21	44:1:1418:A:N6	2.02	0.46
4:F:150:LYS:NZ	44:1:507:U:OP2	2.44	0.46
15:S:92:LYS:NZ	15:S:139:TYR:OH	2.41	0.46
19:W:26:ILE:HD13	19:W:29:GLU:OE1	2.14	0.46
37:q:224:GLY:C	37:q:237:LEU:HD11	2.39	0.46
44:1:1189:C:N3	44:1:1315:U:O2'	2.48	0.46
6:H:62:ARG:NH2	19:W:4:SER:HG	2.12	0.46
16:T:108:ARG:NH1	44:1:1097:G:O2'	2.48	0.46
40:t:74:ARG:NH2	40:t:75:ILE:HD11	2.30	0.46
44:1:2841:G:O2'	44:1:2847:A:N6	2.49	0.46
44:1:3112:G:N2	44:1:3113:A:N7	2.63	0.46
47:w:142:ALA:HB1	47:w:156:PHE:HE1	1.80	0.46
24:b:49:LYS:NZ	44:1:2828:G:OP1	2.25	0.46
31:i:45:ARG:NH2	31:i:49:GLY:O	2.49	0.46
40:t:248:GLU:HA	40:t:251:ILE:HD12	1.97	0.46
44:1:3060:C:O2	44:1:3332:U:O2'	2.32	0.46
1:B:8:ALA:HB2	18:V:46:LEU:HD21	1.98	0.46
7:K:154:ILE:O	7:K:155:ILE:HD13	2.15	0.46
26:d:12:TYR:HD2	26:d:75:ILE:HD12	1.81	0.46
38:r:223:VAL:HG11	38:r:243:ALA:HB3	1.97	0.46
11:O:90:HIS:NE2	44:1:2382:G:OP2	2.46	0.46
41:u:45:ASN:ND2	47:w:299:GLU:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:1523:U:OP2	44:1:1604:G:O2'	2.31	0.46
24:b:421:LEU:HD21	42:y:88:LEU:O	2.16	0.46
32:j:25:ARG:NH1	44:1:359:U:O3'	2.48	0.46
44:1:42:C:O2'	44:1:43:A:O5'	2.30	0.46
19:W:165:MET:HB3	19:W:171:ILE:HD11	1.98	0.46
44:1:800:G:O2'	44:1:801:A:O4'	2.32	0.46
44:1:1477:A:OP1	44:1:3075:G:O2'	2.34	0.46
44:1:1523:U:OP1	44:1:1834:U:O2'	2.32	0.46
47:w:802:ASN:HA	47:w:805:LEU:HD12	1.97	0.46
1:B:332:ARG:NH1	44:1:3304:U:O5'	2.46	0.46
3:E:52:VAL:HG13	3:E:67:GLY:HA2	1.98	0.46
9:M:15:VAL:HG22	15:S:150:PHE:O	2.15	0.46
10:N:119:TYR:CE2	10:N:133:ILE:HD11	2.51	0.46
22:Z:107:ARG:NH1	44:1:1634:G:OP1	2.49	0.46
40:t:171:THR:HG21	46:6:64:C:O2	2.16	0.46
46:6:5:C:H41	46:6:23:U:H4'	1.80	0.46
1:B:287:LYS:O	1:B:293:ASN:ND2	2.49	0.46
16:T:126:VAL:O	16:T:127:GLN:NE2	2.48	0.46
16:T:128:LEU:HD11	44:1:1096:U:H5'	1.98	0.46
17:U:36:TYR:O	17:U:40:HIS:ND1	2.45	0.46
42:y:162:HIS:ND1	42:y:164:GLN:OE1	2.46	0.46
47:w:101:ARG:NH2	47:w:141:GLN:OE1	2.49	0.46
3:E:64:LEU:HD11	3:E:76:LEU:HD11	1.98	0.45
11:O:68:ARG:NH2	44:1:2365:C:O2	2.50	0.45
18:V:22:ILE:HD11	18:V:33:ASN:ND2	2.31	0.45
19:W:17:LYS:NZ	44:1:1279:C:OP2	2.33	0.45
19:W:173:THR:O	19:W:173:THR:OG1	2.34	0.45
22:Z:41:ALA:HB2	22:Z:77:TYR:CE1	2.47	0.45
40:t:17:GLU:HA	40:t:20:LEU:HD13	1.97	0.45
41:u:89:THR:O	41:u:93:MET:HE3	2.16	0.45
44:1:91:G:OP2	44:1:93:C:N4	2.44	0.45
44:1:637:C:O2'	44:1:638:C:O5'	2.24	0.45
47:w:713:ILE:HD11	47:w:718:ALA:HB2	1.98	0.45
11:O:171:LYS:NZ	44:1:3180:A:O5'	2.49	0.45
20:X:120:LYS:NZ	44:1:1832:C:OP1	2.43	0.45
47:w:274:GLU:N	47:w:274:GLU:OE1	2.49	0.45
7:K:137:GLU:OE1	7:K:137:GLU:N	2.48	0.45
7:K:247:HIS:NE2	46:6:47:A:O3'	2.46	0.45
38:r:23:ARG:NE	44:1:3109:G:OP1	2.47	0.45
46:6:32:A:N3	46:6:47:A:N6	2.65	0.45
2:C:296:GLN:HA	2:C:299:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:z:8:SER:O	43:z:12:ASN:ND2	2.49	0.45
45:2:79:A:O2'	45:2:80:A:OP1	2.19	0.45
8:L:157:ARG:O	23:a:99:ALA:N	2.46	0.45
12:P:61:ARG:O	12:P:64:ASN:ND2	2.50	0.45
37:q:236:GLU:OE1	37:q:240:LYS:NZ	2.29	0.45
44:1:1201:C:O2'	44:1:1202:A:O5'	2.27	0.45
6:H:22:SER:OG	6:H:23:ARG:N	2.50	0.45
6:H:48:VAL:HG13	6:H:49:ASN:H	1.81	0.45
24:b:254:MET:SD	24:b:255:ASP:N	2.89	0.45
27:e:95:GLU:OE1	44:1:1410:U:O2'	2.34	0.45
37:q:412:GLU:OE1	40:t:24:ARG:NH2	2.50	0.45
44:1:3335:A:OP2	44:1:3368:U:N3	2.48	0.45
1:B:20:LYS:O	1:B:273:HIS:ND1	2.50	0.45
15:S:94:ILE:HD12	15:S:102:ALA:HB1	1.98	0.45
19:W:126:ARG:NH2	44:1:1230:G:OP1	2.49	0.45
21:Y:74:TYR:OH	45:2:75:G:OP2	2.28	0.45
22:Z:26:VAL:O	22:Z:93:LYS:NZ	2.44	0.45
40:t:57:ARG:O	40:t:60:SER:N	2.49	0.45
44:1:345:G:N1	44:1:349:A:OP2	2.50	0.45
44:1:2838:A:N6	44:1:2850:G:O2'	2.50	0.45
44:1:3217:C:O2'	44:1:3218:A:O5'	2.18	0.45
6:H:115:ARG:NH2	6:H:123:ILE:HD11	2.32	0.45
30:h:35:LYS:NZ	30:h:39:PRO:O	2.50	0.45
37:q:250:ASP:OD1	37:q:251:GLU:N	2.50	0.45
44:1:1200:A:H2	44:1:2824:G:H22	1.65	0.45
44:1:1926:C:O4'	44:1:1927:G:N2	2.49	0.45
47:w:95:ILE:HD13	47:w:138:LEU:HD11	1.98	0.45
1:B:162:VAL:HG11	1:B:181:ILE:HD12	1.98	0.45
4:F:190:THR:O	4:F:190:THR:OG1	2.33	0.45
11:O:18:ARG:NH2	44:1:1315:U:OP1	2.48	0.45
32:j:55:ARG:NH1	44:1:353:G:O6	2.49	0.45
41:u:82:ASN:OD1	41:u:85:LEU:N	2.50	0.45
1:B:308:MET:HE3	1:B:308:MET:HA	1.99	0.45
25:c:17:VAL:HG22	25:c:98:SER:HB3	1.99	0.45
10:N:14:LYS:NZ	44:1:268:A:O2'	2.49	0.44
35:n:433:PHE:O	35:n:437:ASN:ND2	2.51	0.44
37:q:405:SER:O	37:q:405:SER:OG	2.33	0.44
40:t:92:HIS:C	40:t:93:ILE:HD12	2.42	0.44
1:B:238:LEU:CD2	1:B:250:ALA:HB2	2.47	0.44
7:K:143:GLN:NE2	7:K:223:THR:HG21	2.32	0.44
7:K:184:ASP:O	46:6:22:G:N2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:21:LYS:NZ	44:1:1873:U:OP1	2.47	0.44
24:b:133:LEU:HA	24:b:136:MET:HE3	1.98	0.44
31:i:59:ASP:O	31:i:63:ASN:ND2	2.50	0.44
44:1:1529:A:P	44:1:1592:G:H22	2.39	0.44
1:B:11:HIS:ND1	1:B:234:GLY:O	2.50	0.44
1:B:339:ARG:NH1	44:1:3137:C:OP1	2.45	0.44
10:N:46:ASP:OD1	10:N:46:ASP:N	2.50	0.44
44:1:405:U:N3	45:2:18:U:O4	2.50	0.44
3:E:102:ASN:OD1	3:E:105:TYR:N	2.46	0.44
4:F:125:GLU:O	4:F:129:LEU:HD23	2.17	0.44
7:K:79:GLN:NE2	7:K:282:LYS:O	2.50	0.44
7:K:126:ILE:C	7:K:127:LEU:HD22	2.42	0.44
10:N:53:TYR:HE2	10:N:61:ILE:HD11	1.81	0.44
11:O:85:ARG:NH2	44:1:2383:C:OP2	2.50	0.44
35:n:216:ARG:O	35:n:220:THR:HG23	2.17	0.44
36:o:113:GLN:OE1	40:t:56:VAL:HG22	2.18	0.44
36:o:157:LEU:HD23	36:o:158:MET:N	2.33	0.44
3:E:62:THR:C	3:E:63:LEU:HD12	2.43	0.44
14:R:110:ARG:NH2	44:1:1720:U:OP2	2.50	0.44
26:d:14:ILE:HD12	26:d:39:PHE:CD1	2.52	0.44
33:k:44:LYS:NZ	44:1:1751:G:O6	2.30	0.44
35:n:84:LYS:NZ	44:1:1574:C:O5'	2.50	0.44
11:O:18:ARG:NH1	44:1:1318:A:N7	2.66	0.44
13:Q:16:ARG:NH2	13:Q:18:ALA:O	2.47	0.44
29:g:105:VAL:O	29:g:109:THR:HG23	2.18	0.44
35:n:380:ILE:HD13	35:n:387:VAL:CG2	2.47	0.44
44:1:1497:C:O2'	44:1:1602:A:N3	2.44	0.44
44:1:2110:G:HO2'	44:1:2111:G:P	2.37	0.44
44:1:2120:A:O2'	44:1:2121:G:N7	2.39	0.44
44:1:2890:A:N6	44:1:2913:C:H42	2.15	0.44
1:B:4:ARG:NH1	1:B:6:TYR:O	2.50	0.44
7:K:32:ILE:HD11	7:K:292:TYR:HB2	1.98	0.44
10:N:97:SER:OG	10:N:99:ARG:N	2.49	0.44
40:t:238:GLN:HB2	40:t:239:LEU:HD12	1.99	0.44
18:V:54:LEU:HD21	18:V:119:GLY:HA3	2.00	0.44
24:b:444:PHE:CE2	41:u:72:ALA:HB2	2.52	0.44
40:t:236:GLU:HG3	40:t:245:ILE:HG23	1.99	0.44
44:1:2950:G:C6	44:1:2952:G:O6	2.70	0.44
1:B:364:LYS:NZ	44:1:3049:A:O2'	2.30	0.44
6:H:128:VAL:HG12	6:H:129:ARG:O	2.18	0.44
8:L:52:ASP:OD1	8:L:52:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:22:PRO:O	15:S:24:LEU:HD12	2.17	0.44
19:W:158:ILE:HG13	19:W:161:LEU:HD23	1.99	0.44
34:l:11:GLN:O	34:l:14:ALA:HB3	2.18	0.44
37:q:228:ASN:OD1	37:q:403:SER:N	2.51	0.44
42:y:173:LEU:HA	42:y:176:LEU:HD12	2.00	0.44
19:W:11:THR:OG1	19:W:12:LEU:N	2.51	0.43
26:d:56:ASN:ND2	44:1:1458:U:O2	2.51	0.43
37:q:264:HIS:O	37:q:268:THR:OG1	2.18	0.43
42:y:124:GLU:O	42:y:128:LEU:HD23	2.18	0.43
44:1:2110:G:O2'	44:1:2111:G:O5'	2.23	0.43
1:B:90:VAL:HG12	1:B:104:THR:CG2	2.45	0.43
26:d:19:ARG:O	26:d:20:LEU:HD23	2.18	0.43
35:n:129:ILE:HA	35:n:132:ILE:HD12	2.00	0.43
36:o:189:ILE:HG23	46:6:37:C:H5''	2.00	0.43
40:t:280:PHE:HB3	46:6:231:A:H62	1.81	0.43
12:P:86:LYS:NZ	44:1:2353:G:O3'	2.48	0.43
19:W:48:VAL:HG13	19:W:53:LEU:HD21	2.00	0.43
44:1:1278:A:HO2'	44:1:1279:C:P	2.38	0.43
47:w:819:VAL:HG11	47:w:824:LYS:NZ	2.33	0.43
1:B:218:ILE:HG22	1:B:276:THR:HG23	1.99	0.43
3:E:35:VAL:O	3:E:38:THR:OG1	2.33	0.43
7:K:114:SER:HA	7:K:117:ALA:HB3	2.00	0.43
11:O:12:LYS:NZ	44:1:3184:A:OP2	2.34	0.43
14:R:72:GLU:N	14:R:72:GLU:OE1	2.51	0.43
35:n:187:TYR:CE2	35:n:200:LEU:HD21	2.53	0.43
44:1:1262:G:H22	44:1:1277:C:H42	1.67	0.43
44:1:1392:G:N2	44:1:1418:A:N6	2.60	0.43
44:1:3005:A:O2'	44:1:3140:G:N2	2.50	0.43
46:6:49:C:HO2'	46:6:50:U:P	2.41	0.43
19:W:123:ASP:OD1	19:W:211:SER:OG	2.37	0.43
24:b:105:VAL:HA	24:b:108:VAL:HG12	2.00	0.43
24:b:172:ILE:HG23	24:b:251:LEU:CD2	2.45	0.43
36:o:110:TYR:CE1	40:t:58:ALA:HB2	2.54	0.43
44:1:1662:G:H22	44:1:1787:A:H2	1.67	0.43
6:H:55:VAL:CG2	6:H:68:LEU:HD11	2.49	0.43
7:K:240:ARG:NH2	46:6:45:U:OP1	2.50	0.43
7:K:256:PRO:O	7:K:260:VAL:HG23	2.19	0.43
7:K:258:GLU:OE2	7:K:262:ASN:ND2	2.52	0.43
9:M:14:LEU:O	9:M:19:ARG:NE	2.51	0.43
18:V:45:ARG:NH1	44:1:3043:C:OP1	2.46	0.43
24:b:300:GLU:OE1	24:b:300:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:q:228:ASN:ND2	37:q:403:SER:O	2.52	0.43
44:1:268:A:N6	44:1:296:A:OP2	2.52	0.43
44:1:396:A:N7	44:1:399:A:N6	2.60	0.43
44:1:1890:U:O4	44:1:1891:A:N6	2.52	0.43
44:1:2950:G:O6	44:1:2952:G:O6	2.36	0.43
6:H:173:ARG:NH1	44:1:2899:C:N3	2.67	0.43
31:i:63:ASN:OD1	31:i:64:SER:N	2.52	0.43
36:o:157:LEU:HD21	40:t:62:VAL:HG11	2.01	0.43
44:1:1863:G:N2	44:1:1867:A:H62	2.16	0.43
44:1:3042:U:OP2	44:1:3092:C:N4	2.51	0.43
5:G:220:ALA:HB3	36:o:154:ASN:ND2	2.34	0.43
8:L:15:ARG:NH1	44:1:799:G:OP1	2.51	0.43
20:X:59:SER:HB3	20:X:98:ALA:HB1	1.99	0.43
22:Z:59:ALA:HA	22:Z:62:VAL:HG22	2.01	0.43
24:b:380:GLU:OE2	24:b:380:GLU:N	2.50	0.43
40:t:264:CYS:O	40:t:268:LEU:HD23	2.18	0.43
47:w:178:GLU:N	47:w:178:GLU:OE1	2.51	0.43
7:K:221:THR:HG22	46:6:16:U:C5'	2.49	0.43
40:t:192:PRO:O	40:t:299:ARG:NH1	2.52	0.43
42:y:24:CYS:SG	42:y:25:LEU:N	2.91	0.43
42:y:212:ALA:HB3	42:y:213:PRO:HD3	2.01	0.43
47:w:258:SER:OG	47:w:259:ILE:N	2.50	0.43
2:C:303:GLY:N	44:1:1347:U:OP1	2.51	0.43
10:N:64:VAL:HG11	10:N:102:ALA:HB1	2.00	0.43
19:W:69:LYS:O	19:W:73:LEU:HD23	2.18	0.43
23:a:96:LYS:NZ	23:a:142:GLY:O	2.52	0.43
29:g:10:ARG:NH1	44:1:1489:A:OP1	2.52	0.43
41:u:114:GLY:O	41:u:118:LYS:NZ	2.41	0.43
42:y:61:ARG:NH1	42:y:194:GLY:O	2.51	0.43
44:1:1176:C:OP2	44:1:1177:G:O2'	2.28	0.43
7:K:96:LYS:C	7:K:97:LEU:HD22	2.44	0.42
8:L:60:ALA:HB1	8:L:61:PRO:HD2	1.99	0.42
24:b:396:ARG:NH2	42:y:39:GLU:O	2.47	0.42
35:n:411:ILE:HG23	35:n:429:PRO:HG3	2.00	0.42
38:r:248:GLU:OE2	38:r:251:ARG:NH2	2.52	0.42
14:R:115:ILE:HG22	14:R:116:ASP:O	2.19	0.42
33:k:73:LEU:HD12	33:k:74:LYS:N	2.34	0.42
37:q:234:TRP:CE2	37:q:238:ILE:HD11	2.54	0.42
44:1:1103:A:OP1	44:1:1104:G:N1	2.51	0.42
44:1:1628:C:O2	44:1:1814:A:O2'	2.33	0.42
7:K:139:ASP:OD1	7:K:140:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:133:LYS:N	13:Q:135:GLN:OE1	2.51	0.42
21:Y:39:LEU:HD11	21:Y:107:THR:C	2.44	0.42
27:e:56:GLY:HA2	44:1:1161:G:H21	1.84	0.42
44:1:34:A:N3	44:1:810:A:O2'	2.47	0.42
45:2:78:G:O2'	45:2:79:A:O5'	2.33	0.42
47:w:278:PHE:CD2	47:w:307:LEU:HD11	2.54	0.42
1:B:187:SER:O	1:B:190:GLU:N	2.51	0.42
2:C:309:ARG:NH1	44:1:590:G:O2'	2.46	0.42
6:H:14:GLU:OE1	6:H:14:GLU:N	2.50	0.42
8:L:110:ASP:HA	8:L:113:VAL:HG22	2.02	0.42
13:Q:83:VAL:HG12	13:Q:85:GLY:H	1.85	0.42
24:b:32:VAL:O	24:b:33:ILE:HD13	2.19	0.42
26:d:29:ALA:HB3	26:d:30:PRO:HD3	2.01	0.42
36:o:211:LEU:O	36:o:216:ILE:N	2.46	0.42
22:Z:111:LYS:HA	22:Z:114:VAL:HG12	2.01	0.42
24:b:203:SER:OG	24:b:204:LEU:N	2.52	0.42
31:i:26:ILE:CG2	44:1:155:G:H21	2.33	0.42
35:n:47:ARG:HE	44:1:1620:U:H5''	1.84	0.42
41:u:83:ARG:O	41:u:86:VAL:HG22	2.19	0.42
44:1:2377:G:P	44:1:2378:C:H41	2.41	0.42
44:1:2857:C:HO2'	44:1:2858:U:P	2.43	0.42
46:6:49:C:O2'	46:6:50:U:O5'	2.30	0.42
6:H:190:ASP:O	6:H:191:LEU:HD23	2.19	0.42
10:N:133:ILE:C	10:N:134:LEU:HD12	2.45	0.42
24:b:264:ILE:HD13	24:b:267:GLN:OE1	2.19	0.42
29:g:74:ARG:CZ	29:g:82:ALA:HB2	2.49	0.42
38:r:54:ARG:NH1	38:r:57:GLU:OE2	2.53	0.42
40:t:141:LEU:O	40:t:142:LEU:HD22	2.18	0.42
40:t:146:ARG:CD	40:t:171:THR:HG22	2.49	0.42
42:y:41:GLU:OE1	42:y:203:LEU:HD21	2.20	0.42
44:1:640:U:O2'	44:1:941:G:OP2	2.35	0.42
1:B:92:TYR:HB2	1:B:157:VAL:HG13	2.02	0.42
2:C:7:THR:HG22	2:C:147:GLU:HG2	2.00	0.42
6:H:70:THR:HG23	44:1:3112:G:O2'	2.20	0.42
12:P:25:SER:OG	44:1:1447:G:N7	2.47	0.42
12:P:36:ILE:HD11	12:P:48:LEU:HD21	2.02	0.42
14:R:31:GLU:OE1	14:R:31:GLU:N	2.44	0.42
17:U:43:VAL:HG12	17:U:44:GLU:OE1	2.20	0.42
19:W:108:ASP:OD1	19:W:109:VAL:N	2.52	0.42
31:i:88:GLU:O	31:i:92:ASN:ND2	2.51	0.42
35:n:82:GLU:O	35:n:85:THR:OG1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:n:209:ILE:HG22	35:n:211:SER:N	2.34	0.42
44:1:2364:G:O2'	44:1:2365:C:O5'	2.27	0.42
6:H:41:ILE:HD11	6:H:67:ALA:HB1	2.02	0.42
6:H:89:LYS:O	6:H:182:SER:N	2.49	0.42
15:S:25:PHE:CD2	16:T:151:LEU:HD21	2.51	0.42
18:V:38:ALA:HB3	18:V:59:MET:HB2	2.02	0.42
19:W:39:TYR:HE2	19:W:109:VAL:HG13	1.85	0.42
24:b:324:LEU:HD21	24:b:327:ASN:ND2	2.34	0.42
26:d:29:ALA:O	26:d:32:ALA:HB3	2.20	0.42
42:y:20:THR:HG21	42:y:23:TYR:CZ	2.55	0.42
44:1:1277:C:HO2'	44:1:1278:A:P	2.43	0.42
5:G:94:PHE:CZ	5:G:152:LEU:HD12	2.54	0.42
11:O:159:LYS:NZ	44:1:3243:A:OP1	2.32	0.42
16:T:110:LYS:NZ	44:1:1067:U:O2'	2.29	0.42
20:X:141:TYR:O	20:X:142:ILE:HD13	2.20	0.42
25:c:30:THR:O	25:c:33:SER:OG	2.20	0.42
31:i:25:LYS:NZ	31:i:28:TYR:OH	2.35	0.42
31:i:88:GLU:OE1	31:i:92:ASN:ND2	2.51	0.42
44:1:1436:U:C4	47:w:822:VAL:HG11	2.54	0.42
46:6:13:U:O2'	46:6:15:C:OP2	2.38	0.42
10:N:17:ASP:OD2	10:N:17:ASP:N	2.53	0.42
12:P:55:GLN:OE1	44:1:3299:A:O2'	2.33	0.42
18:V:94:TYR:HE1	41:u:19:ILE:HD11	1.85	0.42
20:X:67:ILE:HG22	20:X:69:SER:H	1.85	0.42
24:b:9:PRO:O	24:b:10:THR:OG1	2.33	0.42
30:h:59:ASN:ND2	45:2:97:A:O2'	2.53	0.42
42:y:20:THR:OG1	42:y:23:TYR:N	2.51	0.42
1:B:215:ILE:HD12	1:B:338:LEU:HD12	2.02	0.41
2:C:332:LYS:O	2:C:335:ALA:HB3	2.20	0.41
5:G:82:LEU:HD13	5:G:218:ILE:HD13	2.01	0.41
19:W:25:ARG:NH2	19:W:26:ILE:HD11	2.34	0.41
24:b:220:ASP:N	24:b:220:ASP:OD1	2.51	0.41
29:g:101:VAL:O	29:g:105:VAL:HG22	2.20	0.41
38:r:7:ILE:HD12	44:1:2898:G:N3	2.34	0.41
44:1:998:A:N3	44:1:1000:C:N4	2.68	0.41
8:L:106:GLN:OE1	31:i:20:MET:HE3	2.20	0.41
10:N:124:ASP:OD2	10:N:125:SER:N	2.49	0.41
17:U:13:LYS:NZ	44:1:1676:A:OP1	2.53	0.41
19:W:133:LEU:HD12	19:W:134:THR:H	1.85	0.41
21:Y:39:LEU:HD11	21:Y:107:THR:O	2.20	0.41
35:n:187:TYR:CD2	35:n:200:LEU:HD21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:o:157:LEU:HD23	36:o:158:MET:H	1.85	0.41
40:t:260:SER:O	40:t:262:SER:N	2.53	0.41
40:t:276:GLU:HG3	40:t:277:VAL:HG23	2.02	0.41
44:l:980:A:H61	44:l:1104:G:P	2.42	0.41
5:G:144:GLU:OE2	5:G:169:LEU:HD21	2.21	0.41
22:Z:36:HIS:O	22:Z:38:PHE:N	2.50	0.41
24:b:284:MET:HE3	24:b:334:LYS:HD2	2.02	0.41
24:b:419:LYS:NZ	42:y:48:ILE:O	2.48	0.41
44:l:912:G:N2	44:l:915:A:C2	2.80	0.41
3:E:21:THR:HG21	44:l:612:U:H4'	2.03	0.41
8:L:168:ARG:NH1	44:l:769:G:O2'	2.52	0.41
14:R:97:ARG:NH2	44:l:1779:C:O4'	2.53	0.41
24:b:171:LEU:HD13	24:b:243:ILE:CD1	2.47	0.41
28:f:71:VAL:HG13	28:f:81:VAL:HG13	2.03	0.41
38:r:58:LYS:NZ	44:l:1207:G:OP2	2.43	0.41
44:l:69:C:HO2'	44:l:101:G:HO2'	1.47	0.41
44:l:980:A:N6	44:l:1103:A:O3'	2.53	0.41
47:w:172:VAL:O	47:w:176:LEU:HD23	2.21	0.41
2:C:312:VAL:HG23	2:C:313:LEU:CB	2.50	0.41
3:E:54:TYR:HA	3:E:65:ILE:HG22	2.02	0.41
15:S:26:ARG:NH1	16:T:150:THR:OG1	2.53	0.41
26:d:79:ARG:HE	26:d:89:LEU:HD21	1.85	0.41
35:n:104:ARG:NH1	44:l:142:C:OP1	2.49	0.41
38:r:22:GLU:OE2	38:r:25:ARG:NH2	2.54	0.41
40:t:149:GLY:CA	46:6:64:C:H42	2.33	0.41
44:l:1695:U:O2'	44:l:1749:A:N1	2.44	0.41
44:l:3138:U:N3	44:l:3139:A:N7	2.68	0.41
47:w:78:ASP:O	47:w:79:ILE:HD13	2.21	0.41
7:K:221:THR:HG22	46:6:16:U:H5''	2.03	0.41
7:K:302:GLU:OE2	7:K:302:GLU:N	2.53	0.41
18:V:9:THR:OG1	18:V:10:LYS:N	2.53	0.41
18:V:94:TYR:CE1	41:u:19:ILE:HD11	2.55	0.41
19:W:197:VAL:O	19:W:201:LEU:HD23	2.21	0.41
24:b:445:LEU:HD12	41:u:89:THR:HG21	2.01	0.41
27:e:77:ALA:HA	27:e:100:ILE:HD11	2.02	0.41
28:f:85:PHE:CZ	28:f:89:LEU:HD11	2.55	0.41
32:j:31:LYS:O	32:j:33:THR:OG1	2.38	0.41
47:w:259:ILE:HG23	47:w:260:LEU:HD22	2.02	0.41
1:B:137:TYR:O	1:B:139:GLN:N	2.54	0.41
5:G:111:LYS:O	5:G:114:ALA:HB3	2.21	0.41
14:R:117:LYS:NZ	44:l:1715:A:OP1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:83:VAL:HG12	20:X:123:TYR:CD1	2.51	0.41
25:c:22:LYS:O	25:c:92:ILE:HD12	2.21	0.41
26:d:65:LYS:NZ	44:1:3058:U:O4	2.54	0.41
34:l:13:MET:HE2	44:1:1493:G:C4	2.56	0.41
45:2:39:G:H1'	45:2:104:A:H61	1.86	0.41
47:w:819:VAL:HG22	47:w:823:MET:HE1	2.02	0.41
4:F:154:GLY:O	4:F:161:VAL:N	2.50	0.41
6:H:45:PHE:CD2	6:H:55:VAL:HG12	2.56	0.41
6:H:165:CYS:O	6:H:167:VAL:HG23	2.20	0.41
24:b:167:THR:OG1	24:b:217:GLN:NE2	2.50	0.41
24:b:172:ILE:HG22	24:b:180:LYS:HZ1	1.84	0.41
40:t:88:ASN:HA	40:t:90:THR:HG23	2.03	0.41
1:B:244:ARG:O	1:B:248:LYS:NZ	2.22	0.41
2:C:220:ARG:NH2	44:1:211:A:OP1	2.54	0.41
13:Q:58:ASN:O	13:Q:144:ARG:NH2	2.50	0.41
14:R:44:LEU:HB3	14:R:50:ILE:HD12	2.02	0.41
14:R:114:LYS:CB	14:R:115:ILE:HD12	2.51	0.41
15:S:34:GLU:O	15:S:37:ALA:HB3	2.21	0.41
22:Z:51:LEU:HD23	22:Z:52:LYS:N	2.36	0.41
29:g:44:CYS:SG	29:g:81:CYS:N	2.94	0.41
29:g:56:THR:O	29:g:57:LEU:HD23	2.20	0.41
33:k:30:LYS:C	33:k:31:LEU:HD12	2.46	0.41
38:r:3:GLN:NE2	44:1:3027:A:N3	2.69	0.41
42:y:11:ASN:OD1	42:y:208:LEU:N	2.53	0.41
5:G:126:SER:OG	44:1:120:G:N2	2.54	0.41
6:H:55:VAL:HG23	6:H:68:LEU:HD11	2.02	0.41
9:M:20:VAL:CG1	9:M:68:LEU:HB2	2.51	0.41
9:M:34:ALA:HB2	9:M:85:TRP:HZ3	1.85	0.41
18:V:15:LEU:HD12	18:V:51:ALA:HB3	2.02	0.41
19:W:177:ALA:O	19:W:179:LYS:N	2.54	0.41
21:Y:33:ALA:N	21:Y:48:LEU:O	2.52	0.41
24:b:289:LYS:NZ	24:b:323:GLN:OE1	2.44	0.41
35:n:173:GLU:OE1	35:n:173:GLU:N	2.54	0.41
44:1:120:G:H21	44:1:121:A:N6	2.19	0.41
44:1:1931:U:O2'	44:1:1933:A:OP2	2.39	0.41
47:w:72:SER:C	47:w:73:LEU:HD23	2.46	0.41
1:B:249:VAL:HG23	1:B:252:ILE:HD11	2.04	0.40
4:F:60:ARG:HA	4:F:63:ILE:HG22	2.03	0.40
42:y:142:ILE:HG12	42:y:148:VAL:HG12	2.02	0.40
44:1:707:U:O2	44:1:712:G:O6	2.37	0.40
44:1:1483:G:O6	44:1:1873:U:C4	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:1712:G:N1	44:1:1731:A:OP2	2.48	0.40
1:B:8:ALA:CB	18:V:46:LEU:HD21	2.51	0.40
7:K:124:LEU:C	7:K:125:LEU:HD22	2.46	0.40
7:K:282:LYS:NZ	46:6:33:U:O2'	2.54	0.40
14:R:114:LYS:HB2	14:R:115:ILE:HD12	2.04	0.40
18:V:109:MET:SD	18:V:110:LYS:N	2.93	0.40
27:e:23:ASP:OD2	44:1:424:G:O2'	2.27	0.40
36:o:98:LEU:HD23	36:o:134:TYR:HA	2.04	0.40
44:1:297:G:OP2	44:1:297:G:N2	2.35	0.40
44:1:2825:C:O2'	44:1:2826:U:OP1	2.35	0.40
1:B:378:ALA:HB1	41:u:97:GLU:OE2	2.22	0.40
7:K:259:PHE:O	7:K:263:VAL:HG23	2.21	0.40
8:L:21:ARG:O	10:N:196:THR:OG1	2.32	0.40
18:V:83:LYS:NZ	18:V:84:SER:O	2.54	0.40
19:W:144:SER:HA	19:W:157:MET:HE3	2.03	0.40
39:s:11:THR:HG23	44:1:1310:G:OP2	2.21	0.40
43:z:2:ALA:HB3	44:1:3015:G:OP2	2.20	0.40
44:1:1846:C:O2'	44:1:1847:A:O5'	2.36	0.40
19:W:48:VAL:CG1	19:W:53:LEU:HD21	2.52	0.40
24:b:362:HIS:ND1	42:y:170:GLN:OE1	2.52	0.40
24:b:446:ASP:O	24:b:449:ILE:HD12	2.22	0.40
40:t:155:ILE:HD12	40:t:160:PHE:CE1	2.57	0.40
40:t:276:GLU:HB2	40:t:321:LEU:HD21	2.04	0.40
44:1:1093:A:O2'	44:1:1094:U:O5'	2.37	0.40
44:1:1404:G:N2	44:1:1407:A:OP2	2.51	0.40
2:C:304:GLN:N	2:C:304:GLN:OE1	2.55	0.40
2:C:312:VAL:HG23	2:C:313:LEU:HB2	2.02	0.40
3:E:41:ILE:HG22	3:E:51:ARG:HG2	2.03	0.40
7:K:124:LEU:HD21	7:K:173:PHE:CE2	2.56	0.40
14:R:74:ARG:NH1	44:1:1942:U:OP2	2.55	0.40
20:X:4:SER:OG	36:o:143:GLU:OE2	2.39	0.40
36:o:158:MET:O	36:o:160:HIS:N	2.54	0.40
44:1:1392:G:O2'	44:1:1393:A:OP2	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
1	B	384/387 (99%)	363 (94%)	21 (6%)	0	100	100
2	C	359/362 (99%)	338 (94%)	20 (6%)	1 (0%)	36	69
3	E	152/176 (86%)	150 (99%)	2 (1%)	0	100	100
4	F	220/244 (90%)	206 (94%)	14 (6%)	0	100	100
5	G	190/256 (74%)	183 (96%)	7 (4%)	0	100	100
6	H	189/191 (99%)	182 (96%)	6 (3%)	1 (0%)	24	59
7	K	252/376 (67%)	242 (96%)	10 (4%)	0	100	100
8	L	185/199 (93%)	176 (95%)	8 (4%)	1 (0%)	24	59
9	M	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
10	N	176/204 (86%)	167 (95%)	9 (5%)	0	100	100
11	O	195/199 (98%)	191 (98%)	4 (2%)	0	100	100
12	P	172/184 (94%)	167 (97%)	5 (3%)	0	100	100
13	Q	132/186 (71%)	132 (100%)	0	0	100	100
14	R	154/189 (82%)	152 (99%)	2 (1%)	0	100	100
15	S	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
16	T	54/160 (34%)	53 (98%)	1 (2%)	0	100	100
17	U	104/121 (86%)	103 (99%)	1 (1%)	0	100	100
18	V	134/137 (98%)	133 (99%)	1 (1%)	0	100	100
19	W	232/236 (98%)	229 (99%)	3 (1%)	0	100	100
20	X	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
21	Y	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
22	Z	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
23	a	91/149 (61%)	87 (96%)	4 (4%)	0	100	100
24	b	468/647 (72%)	451 (96%)	17 (4%)	0	100	100
25	c	95/105 (90%)	95 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	d	105/113 (93%)	103 (98%)	2 (2%)	0	100	100
27	e	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
28	f	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
29	g	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
30	h	117/120 (98%)	110 (94%)	7 (6%)	0	100	100
31	i	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
32	j	85/88 (97%)	82 (96%)	3 (4%)	0	100	100
33	k	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
34	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
35	n	365/605 (60%)	339 (93%)	26 (7%)	0	100	100
36	o	131/220 (60%)	123 (94%)	8 (6%)	0	100	100
37	q	83/455 (18%)	80 (96%)	3 (4%)	0	100	100
38	r	211/261 (81%)	200 (95%)	11 (5%)	0	100	100
39	s	34/520 (6%)	31 (91%)	3 (9%)	0	100	100
40	t	283/322 (88%)	267 (94%)	16 (6%)	0	100	100
41	u	121/199 (61%)	115 (95%)	6 (5%)	0	100	100
42	y	242/245 (99%)	240 (99%)	2 (1%)	0	100	100
43	z	53/106 (50%)	52 (98%)	1 (2%)	0	100	100
47	w	350/841 (42%)	347 (99%)	3 (1%)	0	100	100
All	All	7377/10105 (73%)	7124 (97%)	250 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	339	LEU
8	L	63	VAL
6	H	50	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	322/323 (100%)	318 (99%)	4 (1%)	63	72
2	C	288/289 (100%)	286 (99%)	2 (1%)	76	78
3	E	134/153 (88%)	132 (98%)	2 (2%)	57	70
4	F	186/205 (91%)	185 (100%)	1 (0%)	81	82
5	G	159/208 (76%)	157 (99%)	2 (1%)	61	71
6	H	171/171 (100%)	171 (100%)	0	100	100
7	K	236/346 (68%)	236 (100%)	0	100	100
8	L	149/159 (94%)	148 (99%)	1 (1%)	76	78
9	M	108/109 (99%)	108 (100%)	0	100	100
10	N	156/176 (89%)	147 (94%)	9 (6%)	18	44
11	O	160/162 (99%)	159 (99%)	1 (1%)	78	80
12	P	142/146 (97%)	140 (99%)	2 (1%)	59	71
13	Q	110/151 (73%)	110 (100%)	0	100	100
14	R	129/154 (84%)	128 (99%)	1 (1%)	73	77
15	S	155/156 (99%)	154 (99%)	1 (1%)	78	80
16	T	45/137 (33%)	45 (100%)	0	100	100
17	U	93/107 (87%)	93 (100%)	0	100	100
18	V	104/105 (99%)	102 (98%)	2 (2%)	50	66
19	W	211/213 (99%)	211 (100%)	0	100	100
20	X	117/118 (99%)	116 (99%)	1 (1%)	70	75
21	Y	109/110 (99%)	109 (100%)	0	100	100
22	Z	115/116 (99%)	114 (99%)	1 (1%)	70	75
23	a	76/119 (64%)	75 (99%)	1 (1%)	61	71
24	b	424/573 (74%)	423 (100%)	1 (0%)	87	87
25	c	81/88 (92%)	81 (100%)	0	100	100
26	d	94/97 (97%)	92 (98%)	2 (2%)	47	65
27	e	109/111 (98%)	107 (98%)	2 (2%)	51	67
28	f	90/91 (99%)	89 (99%)	1 (1%)	65	74
29	g	95/103 (92%)	94 (99%)	1 (1%)	65	74
30	h	104/105 (99%)	104 (100%)	0	100	100
31	i	81/82 (99%)	81 (100%)	0	100	100
32	j	70/71 (99%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	k	68/69 (99%)	68 (100%)	0	100	100
34	l	45/46 (98%)	45 (100%)	0	100	100
35	n	334/548 (61%)	332 (99%)	2 (1%)	78	80
36	o	118/199 (59%)	118 (100%)	0	100	100
37	q	80/420 (19%)	80 (100%)	0	100	100
38	r	191/229 (83%)	191 (100%)	0	100	100
39	s	32/445 (7%)	32 (100%)	0	100	100
40	t	256/287 (89%)	256 (100%)	0	100	100
41	u	108/180 (60%)	107 (99%)	1 (1%)	70	75
42	y	210/211 (100%)	210 (100%)	0	100	100
43	z	48/95 (50%)	48 (100%)	0	100	100
47	w	319/745 (43%)	318 (100%)	1 (0%)	86	85
All	All	6432/8728 (74%)	6390 (99%)	42 (1%)	73	78

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	PHE
1	B	63	PRO
1	B	79	VAL
1	B	162	VAL
2	C	145	ILE
2	C	283	THR
3	E	79	VAL
3	E	91	VAL
4	F	77	VAL
5	G	158	ASP
5	G	180	VAL
8	L	10	LEU
10	N	43	THR
10	N	49	ARG
10	N	96	ARG
10	N	112	ASN
10	N	115	VAL
10	N	121	VAL
10	N	132	VAL
10	N	164	LEU
10	N	183	THR

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Mol	Chain	Res	Type
11	O	143	THR
12	P	119	VAL
12	P	120	ASN
14	R	6	THR
15	S	156	VAL
18	V	58	VAL
18	V	73	VAL
20	X	124	VAL
22	Z	14	VAL
23	a	130	VAL
24	b	367	GLN
26	d	16	LEU
26	d	23	VAL
27	e	14	THR
27	e	63	THR
28	f	72	THR
29	g	51	LEU
35	n	17	THR
35	n	35	LEU
41	u	9	CYS
47	w	816	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	140	HIS
3	E	138	GLN
5	G	123	GLN
6	H	64	HIS
6	H	102	ASN
6	H	156	GLN
7	K	84	ASN
7	K	269	GLN
8	L	37	ASN
8	L	66	ASN
11	O	50	ASN
16	T	127	GLN
17	U	49	ASN
17	U	87	ASN
19	W	148	GLN
19	W	205	GLN
21	Y	42	GLN

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Mol	Chain	Res	Type
21	Y	100	HIS
24	b	26	GLN
24	b	70	ASN
24	b	217	GLN
24	b	359	ASN
24	b	406	ASN
24	b	429	ASN
24	b	454	GLN
26	d	56	ASN
27	e	104	ASN
27	e	121	ASN
30	h	59	ASN
33	k	40	GLN
35	n	7	ASN
35	n	160	GLN
35	n	437	ASN
36	o	154	ASN
36	o	163	GLN
38	r	183	ASN
40	t	233	ASN
40	t	300	GLN
41	u	110	ASN
42	y	9	ASN
47	w	255	HIS
47	w	276	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	1	2523/3396 (74%)	689 (27%)	34 (1%)
45	2	157/158 (99%)	46 (29%)	3 (1%)
46	6	63/232 (27%)	29 (46%)	0
All	All	2743/3786 (72%)	764 (27%)	37 (1%)

All (764) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	1	2	U
44	1	3	U
44	1	7	C
44	1	13	A

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Mol	Chain	Res	Type
44	1	14	U
44	1	15	C
44	1	18	G
44	1	22	G
44	1	26	A
44	1	40	A
44	1	43	A
44	1	44	U
44	1	49	A
44	1	57	A
44	1	59	G
44	1	60	A
44	1	65	A
44	1	66	A
44	1	73	C
44	1	74	G
44	1	77	A
44	1	85	A
44	1	92	G
44	1	96	G
44	1	108	A
44	1	110	G
44	1	111	C
44	1	116	A
44	1	117	U
44	1	121	A
44	1	122	A
44	1	124	U
44	1	133	U
44	1	136	G
44	1	142	C
44	1	145	G
44	1	149	U
44	1	156	G
44	1	157	A
44	1	161	G
44	1	165	A
44	1	166	C
44	1	169	U
44	1	170	G
44	1	172	G
44	1	173	G

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Mol	Chain	Res	Type
44	1	187	A
44	1	189	G
44	1	190	U
44	1	191	U
44	1	200	C
44	1	201	A
44	1	206	G
44	1	210	U
44	1	211	A
44	1	213	A
44	1	218	G
44	1	219	A
44	1	220	G
44	1	221	A
44	1	224	C
44	1	234	G
44	1	237	G
44	1	240	U
44	1	241	G
44	1	243	G
44	1	248	U
44	1	250	U
44	1	251	G
44	1	252	U
44	1	253	A
44	1	268	A
44	1	269	G
44	1	270	U
44	1	283	G
44	1	284	A
44	1	285	A
44	1	286	U
44	1	295	A
44	1	304	G
44	1	307	A
44	1	311	C
44	1	317	A
44	1	323	A
44	1	329	U
44	1	334	A
44	1	337	G
44	1	338	A

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Mol	Chain	Res	Type
44	1	339	C
44	1	341	G
44	1	343	U
44	1	346	C
44	1	347	G
44	1	349	A
44	1	350	C
44	1	351	A
44	1	359	U
44	1	370	U
44	1	373	A
44	1	375	A
44	1	376	G
44	1	390	G
44	1	397	A
44	1	399	A
44	1	401	U
44	1	402	A
44	1	403	C
44	1	404	G
44	1	420	G
44	1	421	G
44	1	422	A
44	1	439	C
44	1	440	A
44	1	495	G
44	1	498	A
44	1	503	C
44	1	515	C
44	1	520	U
44	1	521	A
44	1	523	A
44	1	525	C
44	1	535	G
44	1	542	G
44	1	544	C
44	1	545	U
44	1	546	C
44	1	547	G
44	1	552	G
44	1	555	U
44	1	557	A

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Mol	Chain	Res	Type
44	1	559	A
44	1	560	G
44	1	578	A
44	1	579	G
44	1	591	G
44	1	592	A
44	1	597	G
44	1	604	G
44	1	609	G
44	1	610	G
44	1	611	A
44	1	619	A
44	1	620	U
44	1	636	C
44	1	637	C
44	1	638	C
44	1	641	C
44	1	642	U
44	1	643	U
44	1	644	G
44	1	645	A
44	1	646	A
44	1	647	A
44	1	650	C
44	1	660	A
44	1	661	G
44	1	677	A
44	1	678	G
44	1	681	U
44	1	683	U
44	1	689	U
44	1	691	A
44	1	692	A
44	1	701	G
44	1	705	A
44	1	706	A
44	1	708	G
44	1	709	A
44	1	712	G
44	1	716	A
44	1	719	U
44	1	721	G

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Mol	Chain	Res	Type
44	1	735	A
44	1	742	G
44	1	750	G
44	1	762	U
44	1	765	C
44	1	767	U
44	1	774	G
44	1	776	U
44	1	780	A
44	1	781	G
44	1	784	A
44	1	785	G
44	1	786	A
44	1	794	U
44	1	801	A
44	1	817	A
44	1	818	C
44	1	830	A
44	1	832	G
44	1	837	A
44	1	849	C
44	1	861	C
44	1	865	U
44	1	866	A
44	1	870	G
44	1	873	C
44	1	874	U
44	1	875	G
44	1	879	U
44	1	880	G
44	1	887	G
44	1	888	A
44	1	892	U
44	1	894	G
44	1	907	G
44	1	908	G
44	1	914	A
44	1	916	G
44	1	917	A
44	1	922	U
44	1	924	G
44	1	925	A

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Mol	Chain	Res	Type
44	1	926	A
44	1	932	U
44	1	933	A
44	1	934	G
44	1	938	C
44	1	944	C
44	1	954	U
44	1	960	U
44	1	962	A
44	1	976	U
44	1	977	C
44	1	979	U
44	1	980	A
44	1	981	U
44	1	982	C
44	1	984	G
44	1	986	U
44	1	993	G
44	1	994	G
44	1	995	U
44	1	998	A
44	1	1000	C
44	1	1052	U
44	1	1053	A
44	1	1054	A
44	1	1056	U
44	1	1057	A
44	1	1061	A
44	1	1063	G
44	1	1064	A
44	1	1065	A
44	1	1093	A
44	1	1094	U
44	1	1095	U
44	1	1096	U
44	1	1097	G
44	1	1098	A
44	1	1103	A
44	1	1104	G
44	1	1105	A
44	1	1116	G
44	1	1117	G

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Mol	Chain	Res	Type
44	1	1118	C
44	1	1127	G
44	1	1129	A
44	1	1132	C
44	1	1135	A
44	1	1140	G
44	1	1143	A
44	1	1144	U
44	1	1145	G
44	1	1153	A
44	1	1159	A
44	1	1160	C
44	1	1170	A
44	1	1171	G
44	1	1172	G
44	1	1174	G
44	1	1177	G
44	1	1178	G
44	1	1180	A
44	1	1181	U
44	1	1182	A
44	1	1187	C
44	1	1192	C
44	1	1193	A
44	1	1197	A
44	1	1198	C
44	1	1199	C
44	1	1200	A
44	1	1201	C
44	1	1204	A
44	1	1206	G
44	1	1209	G
44	1	1213	G
44	1	1222	G
44	1	1226	G
44	1	1227	C
44	1	1233	G
44	1	1234	G
44	1	1237	G
44	1	1238	C
44	1	1239	C
44	1	1240	A

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Mol	Chain	Res	Type
44	1	1244	A
44	1	1245	A
44	1	1246	G
44	1	1248	C
44	1	1249	G
44	1	1254	C
44	1	1258	U
44	1	1262	G
44	1	1263	A
44	1	1264	G
44	1	1265	U
44	1	1266	G
44	1	1267	U
44	1	1269	U
44	1	1271	A
44	1	1272	C
44	1	1278	A
44	1	1279	C
44	1	1286	A
44	1	1287	A
44	1	1303	A
44	1	1304	A
44	1	1307	G
44	1	1308	A
44	1	1309	U
44	1	1314	C
44	1	1316	C
44	1	1317	A
44	1	1318	A
44	1	1325	U
44	1	1330	A
44	1	1331	U
44	1	1345	G
44	1	1348	U
44	1	1349	G
44	1	1350	A
44	1	1351	U
44	1	1352	A
44	1	1354	G
44	1	1356	U
44	1	1357	G
44	1	1365	G

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Mol	Chain	Res	Type
44	1	1380	G
44	1	1386	A
44	1	1391	C
44	1	1392	G
44	1	1399	A
44	1	1400	G
44	1	1419	A
44	1	1425	U
44	1	1430	U
44	1	1432	C
44	1	1434	G
44	1	1435	A
44	1	1437	C
44	1	1443	G
44	1	1446	A
44	1	1450	G
44	1	1452	A
44	1	1453	A
44	1	1457	U
44	1	1467	A
44	1	1470	U
44	1	1477	A
44	1	1482	A
44	1	1483	G
44	1	1487	G
44	1	1503	A
44	1	1507	G
44	1	1508	C
44	1	1511	U
44	1	1523	U
44	1	1524	A
44	1	1527	C
44	1	1530	U
44	1	1531	C
44	1	1542	G
44	1	1549	U
44	1	1556	C
44	1	1557	A
44	1	1560	G
44	1	1562	C
44	1	1566	A
44	1	1567	U

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Mol	Chain	Res	Type
44	1	1568	U
44	1	1569	U
44	1	1570	U
44	1	1571	A
44	1	1574	C
44	1	1580	A
44	1	1583	A
44	1	1588	A
44	1	1589	A
44	1	1590	G
44	1	1593	A
44	1	1602	A
44	1	1605	A
44	1	1606	U
44	1	1620	U
44	1	1629	U
44	1	1631	C
44	1	1639	C
44	1	1642	A
44	1	1643	A
44	1	1644	C
44	1	1645	U
44	1	1647	A
44	1	1683	A
44	1	1713	G
44	1	1715	A
44	1	1716	U
44	1	1717	U
44	1	1724	U
44	1	1725	C
44	1	1741	A
44	1	1743	G
44	1	1749	A
44	1	1750	A
44	1	1751	G
44	1	1756	C
44	1	1760	A
44	1	1762	C
44	1	1763	U
44	1	1765	U
44	1	1766	G
44	1	1770	G

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Mol	Chain	Res	Type
44	1	1773	C
44	1	1775	G
44	1	1780	G
44	1	1792	C
44	1	1793	C
44	1	1797	A
44	1	1810	A
44	1	1812	G
44	1	1813	A
44	1	1814	A
44	1	1815	U
44	1	1816	A
44	1	1819	U
44	1	1820	U
44	1	1821	U
44	1	1839	A
44	1	1840	U
44	1	1841	A
44	1	1842	A
44	1	1846	C
44	1	1847	A
44	1	1848	G
44	1	1849	C
44	1	1850	A
44	1	1851	G
44	1	1863	G
44	1	1866	C
44	1	1878	G
44	1	1879	A
44	1	1886	A
44	1	1892	G
44	1	1893	A
44	1	1906	G
44	1	1913	A
44	1	1921	A
44	1	1922	A
44	1	1924	U
44	1	1926	C
44	1	1928	G
44	1	1929	G
44	1	1935	G
44	1	1948	G

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Mol	Chain	Res	Type
44	1	1953	G
44	1	2094	C
44	1	2101	C
44	1	2111	G
44	1	2112	U
44	1	2113	A
44	1	2114	C
44	1	2116	G
44	1	2117	A
44	1	2118	C
44	1	2119	A
44	1	2121	G
44	1	2122	G
44	1	2126	A
44	1	2130	G
44	1	2131	A
44	1	2132	C
44	1	2145	A
44	1	2149	A
44	1	2188	A
44	1	2315	G
44	1	2316	G
44	1	2317	A
44	1	2318	U
44	1	2319	U
44	1	2335	G
44	1	2336	U
44	1	2339	C
44	1	2340	U
44	1	2347	U
44	1	2352	A
44	1	2363	A
44	1	2364	G
44	1	2365	C
44	1	2371	G
44	1	2378	C
44	1	2388	U
44	1	2393	G
44	1	2394	G
44	1	2397	A
44	1	2821	C
44	1	2822	U

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Mol	Chain	Res	Type
44	1	2824	G
44	1	2826	U
44	1	2830	G
44	1	2834	G
44	1	2838	A
44	1	2839	G
44	1	2842	U
44	1	2843	U
44	1	2845	A
44	1	2846	U
44	1	2847	A
44	1	2848	G
44	1	2850	G
44	1	2857	C
44	1	2858	U
44	1	2859	U
44	1	2861	U
44	1	2863	G
44	1	2864	A
44	1	2866	U
44	1	2867	C
44	1	2868	U
44	1	2870	C
44	1	2872	A
44	1	2873	U
44	1	2876	C
44	1	2877	G
44	1	2878	G
44	1	2879	C
44	1	2881	C
44	1	2887	A
44	1	2889	C
44	1	2894	C
44	1	2897	A
44	1	2898	G
44	1	2899	C
44	1	2901	G
44	1	2911	A
44	1	2918	G
44	1	2920	U
44	1	2921	U
44	1	2922	G

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Mol	Chain	Res	Type
44	1	2923	U
44	1	2924	U
44	1	2926	A
44	1	2927	C
44	1	2928	C
44	1	2930	A
44	1	2935	U
44	1	2936	A
44	1	2944	U
44	1	2946	A
44	1	2947	G
44	1	2950	G
44	1	2952	G
44	1	2953	U
44	1	2982	A
44	1	2983	C
44	1	2996	U
44	1	2997	G
44	1	3011	A
44	1	3012	A
44	1	3017	A
44	1	3019	U
44	1	3021	A
44	1	3022	G
44	1	3023	U
44	1	3027	A
44	1	3032	A
44	1	3034	C
44	1	3049	A
44	1	3058	U
44	1	3059	G
44	1	3061	G
44	1	3078	U
44	1	3080	G
44	1	3086	A
44	1	3092	C
44	1	3093	C
44	1	3099	C
44	1	3104	U
44	1	3115	C
44	1	3116	G
44	1	3117	C

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Mol	Chain	Res	Type
44	1	3118	C
44	1	3121	U
44	1	3122	A
44	1	3129	A
44	1	3130	A
44	1	3131	U
44	1	3142	A
44	1	3143	C
44	1	3150	A
44	1	3152	U
44	1	3153	U
44	1	3154	C
44	1	3155	U
44	1	3156	U
44	1	3164	C
44	1	3165	A
44	1	3168	A
44	1	3170	A
44	1	3172	A
44	1	3173	G
44	1	3174	A
44	1	3175	U
44	1	3176	G
44	1	3179	U
44	1	3180	A
44	1	3181	C
44	1	3187	A
44	1	3188	G
44	1	3196	U
44	1	3198	U
44	1	3207	U
44	1	3208	G
44	1	3209	A
44	1	3212	C
44	1	3216	G
44	1	3217	C
44	1	3218	A
44	1	3219	G
44	1	3222	U
44	1	3235	C
44	1	3243	A
44	1	3245	A

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Mol	Chain	Res	Type
44	1	3246	G
44	1	3247	G
44	1	3253	G
44	1	3259	U
44	1	3260	G
44	1	3263	G
44	1	3269	U
44	1	3270	U
44	1	3272	C
44	1	3273	A
44	1	3274	A
44	1	3276	G
44	1	3278	C
44	1	3281	U
44	1	3286	G
44	1	3289	G
44	1	3293	U
44	1	3294	A
44	1	3295	A
44	1	3304	U
44	1	3305	A
44	1	3306	U
44	1	3308	C
44	1	3309	G
44	1	3313	U
44	1	3316	A
44	1	3319	U
44	1	3320	A
44	1	3324	C
44	1	3329	U
44	1	3330	A
44	1	3334	U
44	1	3341	U
44	1	3342	A
44	1	3345	G
44	1	3347	A
44	1	3348	G
44	1	3349	C
44	1	3350	C
44	1	3351	U
44	1	3352	U
44	1	3353	G

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Mol	Chain	Res	Type
44	1	3354	U
44	1	3355	U
44	1	3356	G
44	1	3357	U
44	1	3359	A
44	1	3369	G
44	1	3375	A
44	1	3378	C
44	1	3382	U
44	1	3386	G
44	1	3389	U
44	1	3390	G
44	1	3396	U
45	2	2	A
45	2	23	U
45	2	34	U
45	2	35	C
45	2	37	A
45	2	38	U
45	2	39	G
45	2	40	A
45	2	46	G
45	2	48	A
45	2	49	G
45	2	51	G
45	2	59	A
45	2	61	A
45	2	62	C
45	2	63	G
45	2	70	G
45	2	73	U
45	2	74	U
45	2	78	G
45	2	79	A
45	2	80	A
45	2	81	U
45	2	82	U
45	2	83	C
45	2	84	C
45	2	86	U
45	2	87	G
45	2	90	U

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Mol	Chain	Res	Type
45	2	91	C
45	2	94	C
45	2	95	G
45	2	97	A
45	2	100	U
45	2	104	A
45	2	105	A
45	2	106	C
45	2	111	A
45	2	113	U
45	2	116	G
45	2	125	U
45	2	126	A
45	2	127	U
45	2	136	G
45	2	138	A
45	2	151	C
46	6	4	U
46	6	5	C
46	6	7	C
46	6	9	A
46	6	15	C
46	6	16	U
46	6	23	U
46	6	24	A
46	6	25	G
46	6	26	U
46	6	29	G
46	6	34	A
46	6	40	U
46	6	41	G
46	6	42	G
46	6	43	A
46	6	47	A
46	6	49	C
46	6	52	G
46	6	53	A
46	6	54	A
46	6	56	U
46	6	57	U
46	6	58	G
46	6	59	C

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Mol	Chain	Res	Type
46	6	66	U
46	6	230	A
46	6	231	A
46	6	232	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	1	13	A
44	1	42	C
44	1	121	A
44	1	148	G
44	1	160	G
44	1	282	G
44	1	338	A
44	1	637	C
44	1	645	A
44	1	649	A
44	1	705	A
44	1	720	A
44	1	761	A
44	1	916	G
44	1	1064	A
44	1	1097	G
44	1	1200	A
44	1	1205	A
44	1	1307	G
44	1	1329	U
44	1	1355	A
44	1	1567	U
44	1	1568	U
44	1	1605	A
44	1	1641	U
44	1	1838	G
44	1	2110	G
44	1	2187	G
44	1	2317	A
44	1	2920	U
44	1	3269	U
44	1	3341	U
44	1	3350	C
44	1	3375	A

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Mol	Chain	Res	Type
45	2	39	G
45	2	73	U
45	2	79	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
28	f	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	102:LEU	C	103:TYR	N	1.16

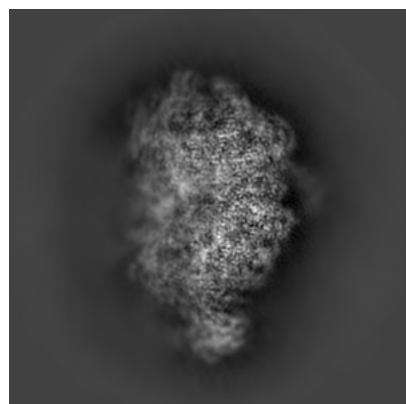
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10841. These allow visual inspection of the internal detail of the map and identification of artifacts.

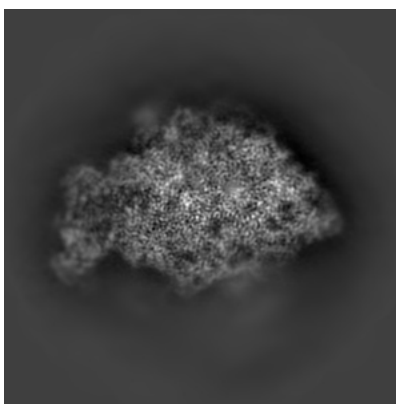
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

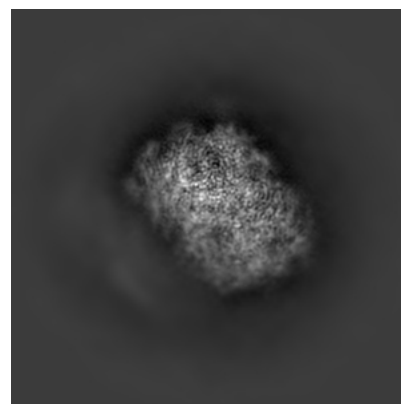
6.1.1 Primary map



X

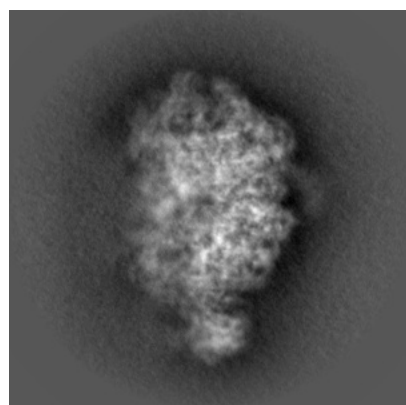


Y

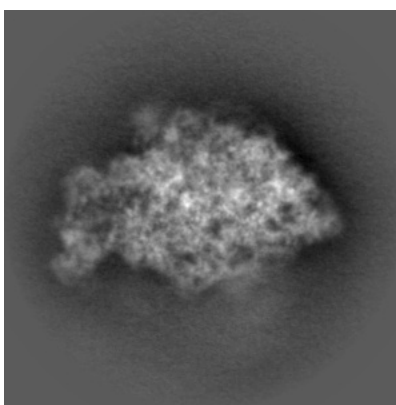


Z

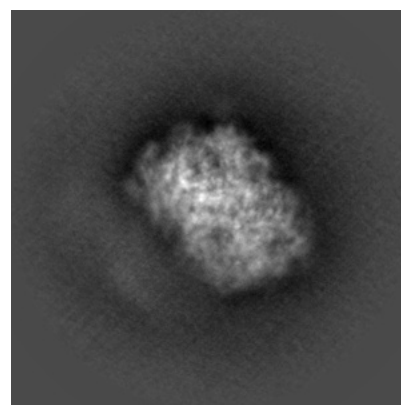
6.1.2 Raw map



X



Y

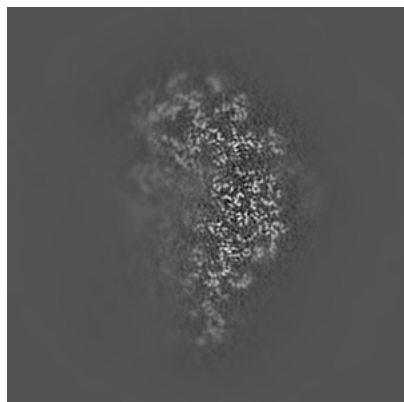


Z

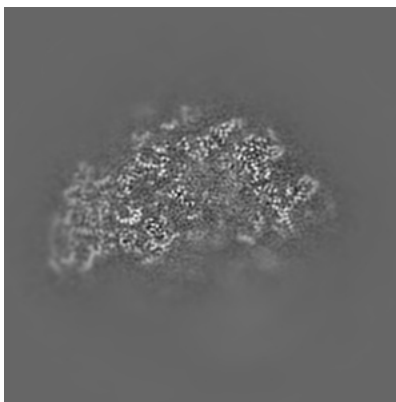
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

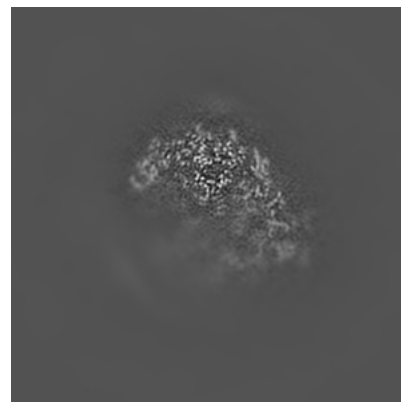
6.2.1 Primary map



X Index: 192

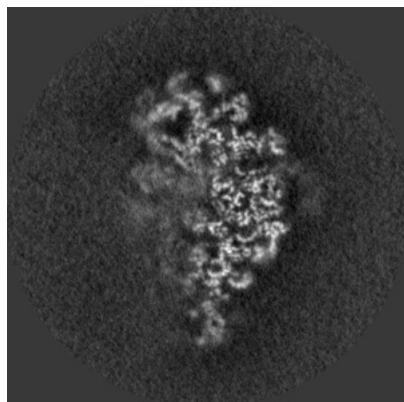


Y Index: 192

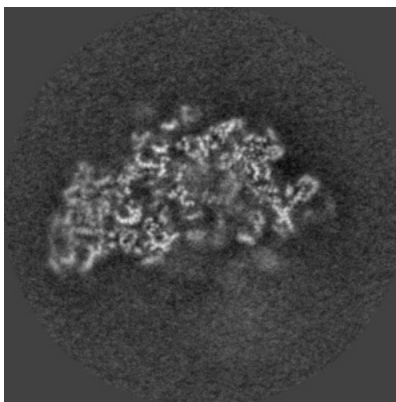


Z Index: 192

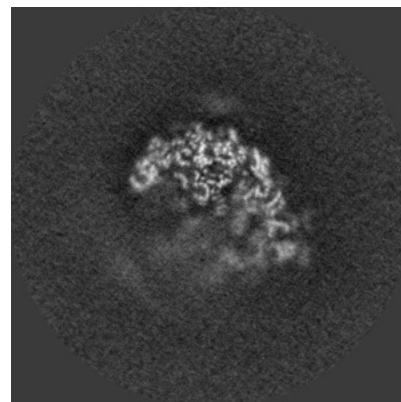
6.2.2 Raw map



X Index: 192



Y Index: 192

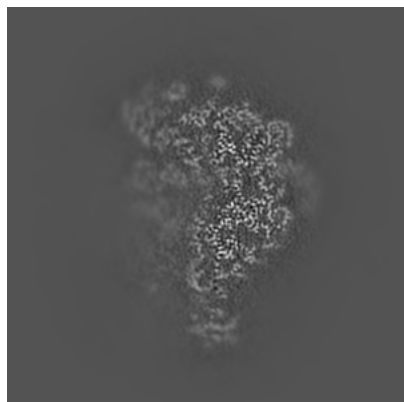


Z Index: 192

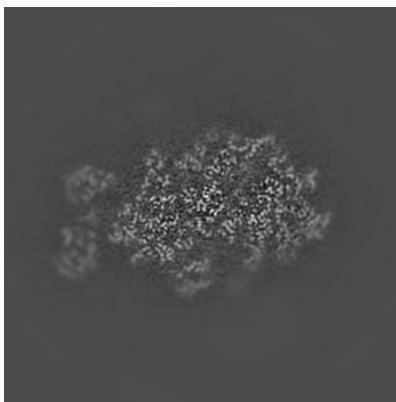
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

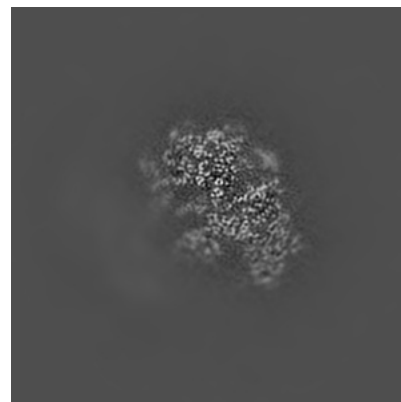
6.3.1 Primary map



X Index: 201

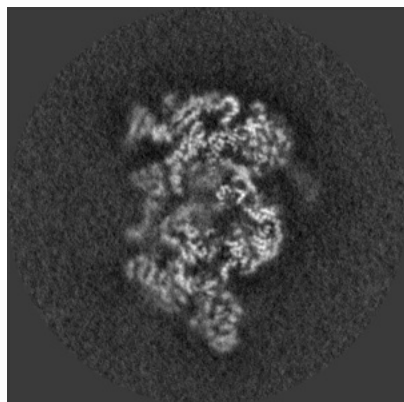


Y Index: 216

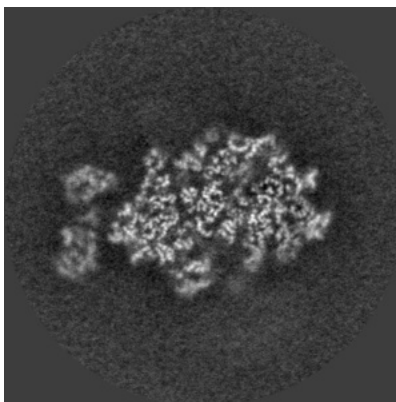


Z Index: 245

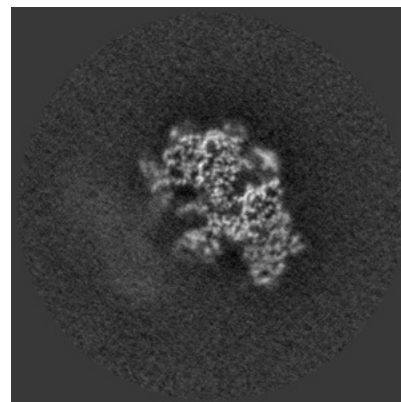
6.3.2 Raw map



X Index: 217



Y Index: 216

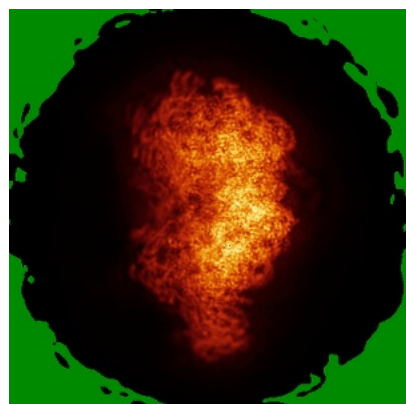


Z Index: 244

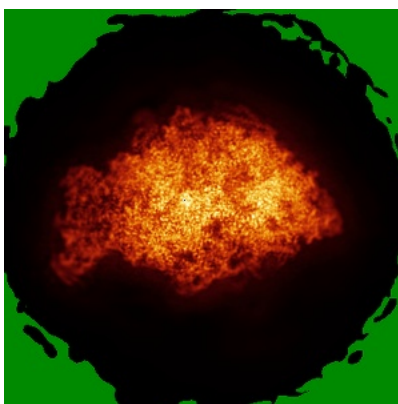
The images above show the largest variance slices of the map in three orthogonal directions.

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

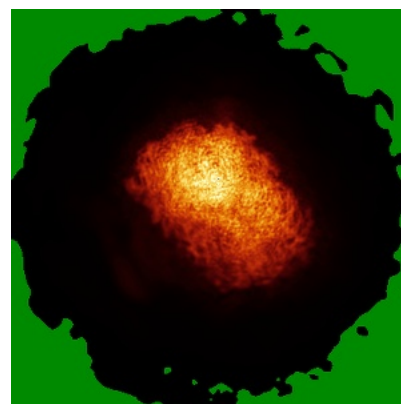
6.4.1 Primary map



X

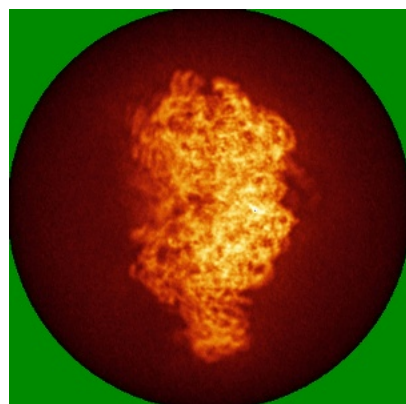


Y

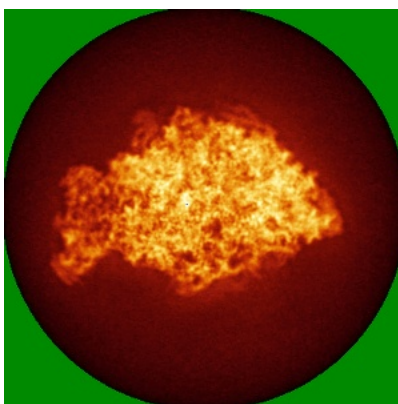


Z

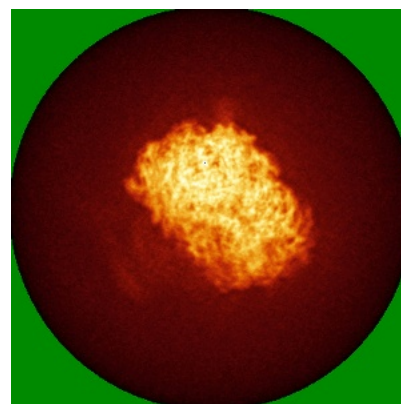
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

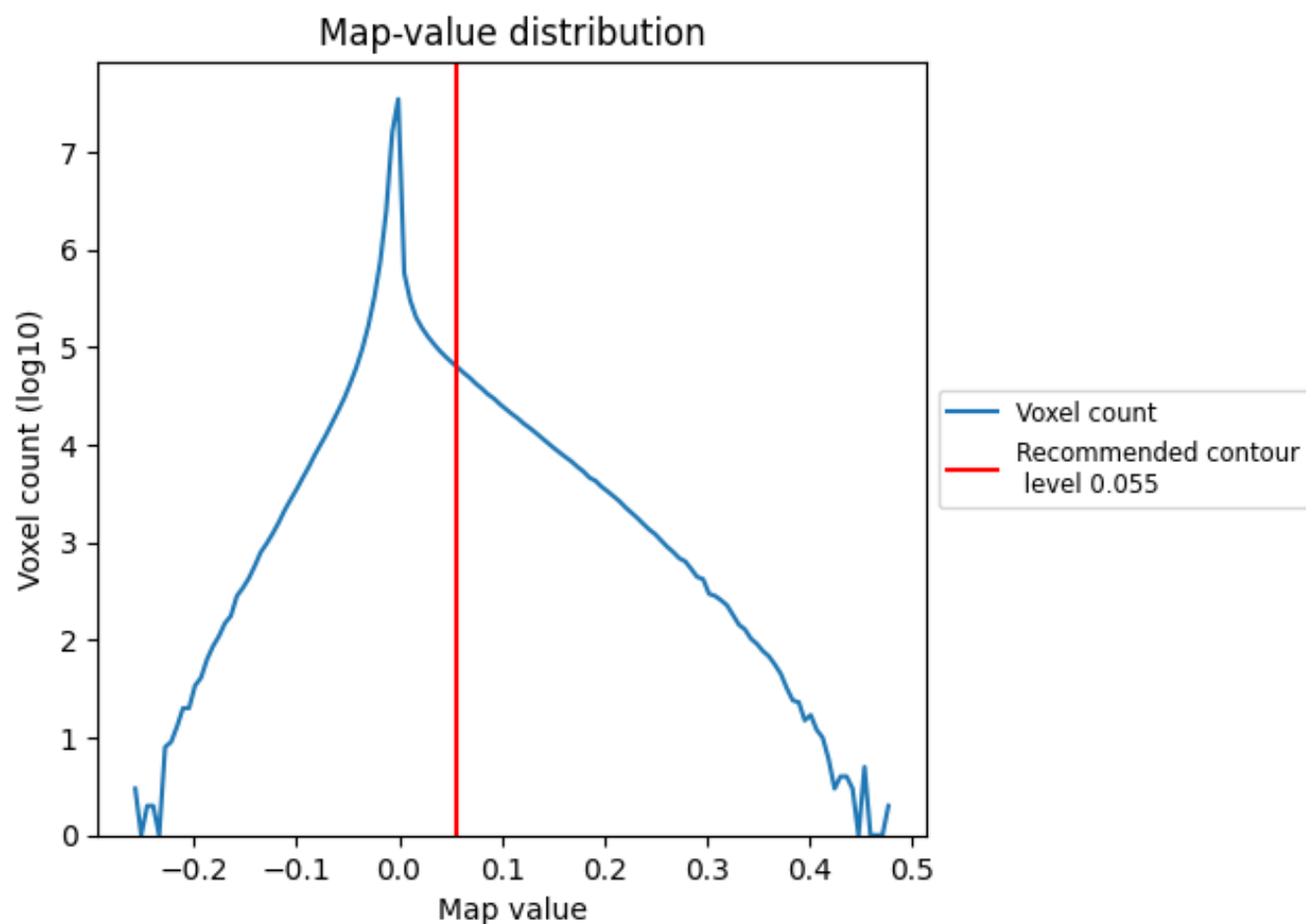
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

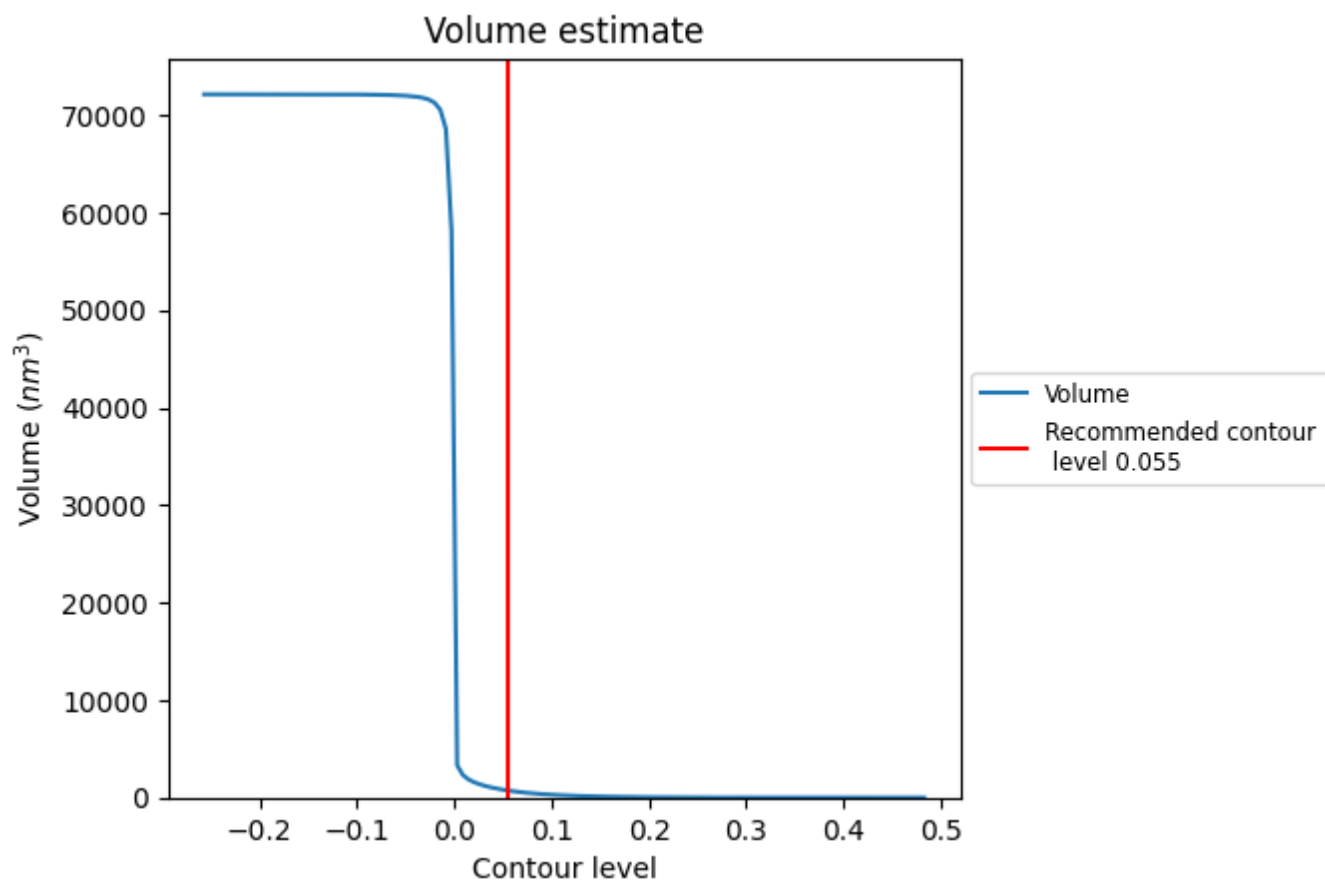
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

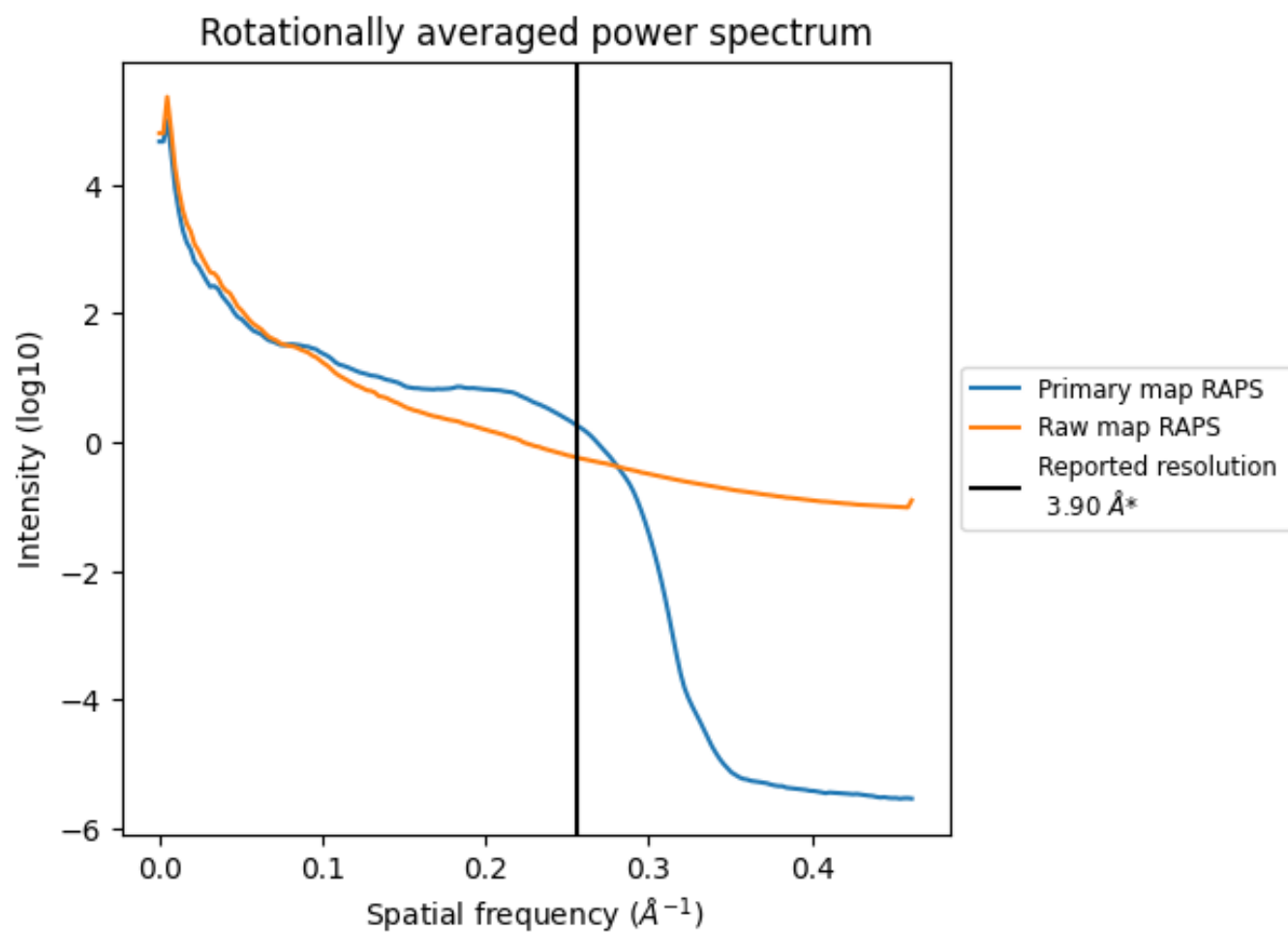
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 727 nm^3 ; this corresponds to an approximate mass of 656 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

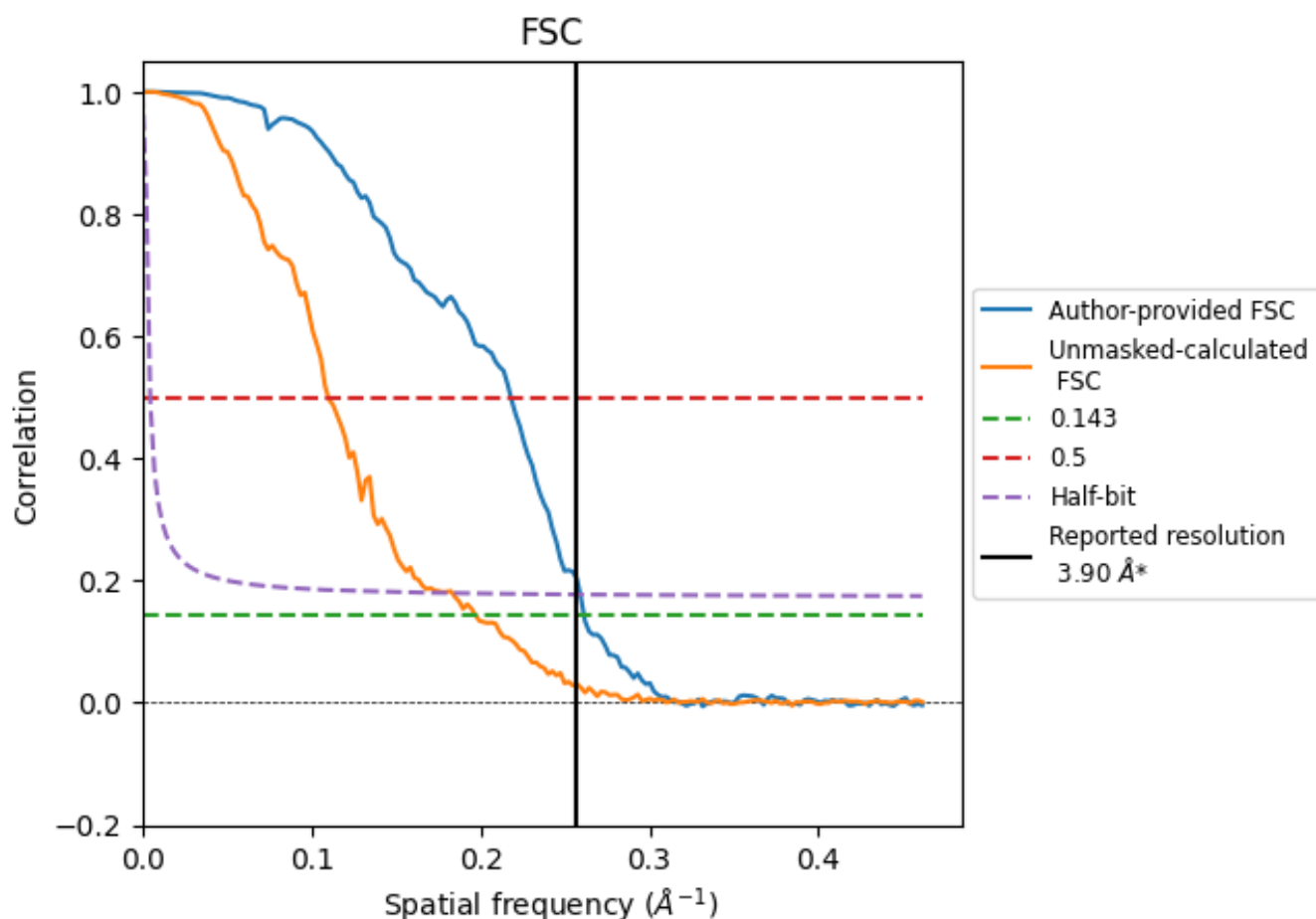


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

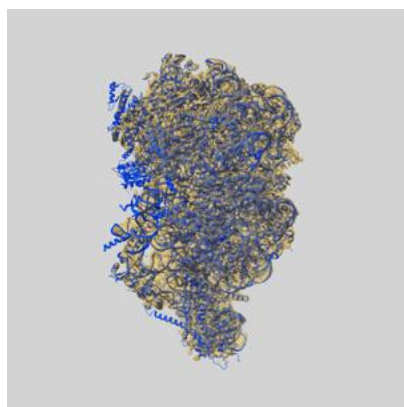
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.83	4.59	3.86
Unmasked-calculated*	5.07	9.08	5.45

*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 5.07 differs from the reported value 3.9 by more than 10 %

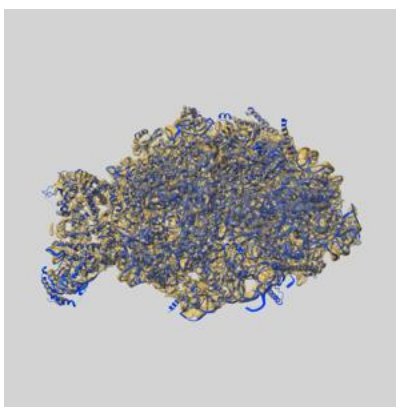
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10841 and PDB model 6YLX. Per-residue inclusion information can be found in section 3 on page 12.

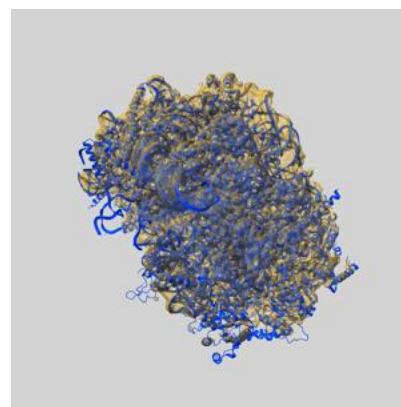
9.1 Map-model overlay [i](#)



X



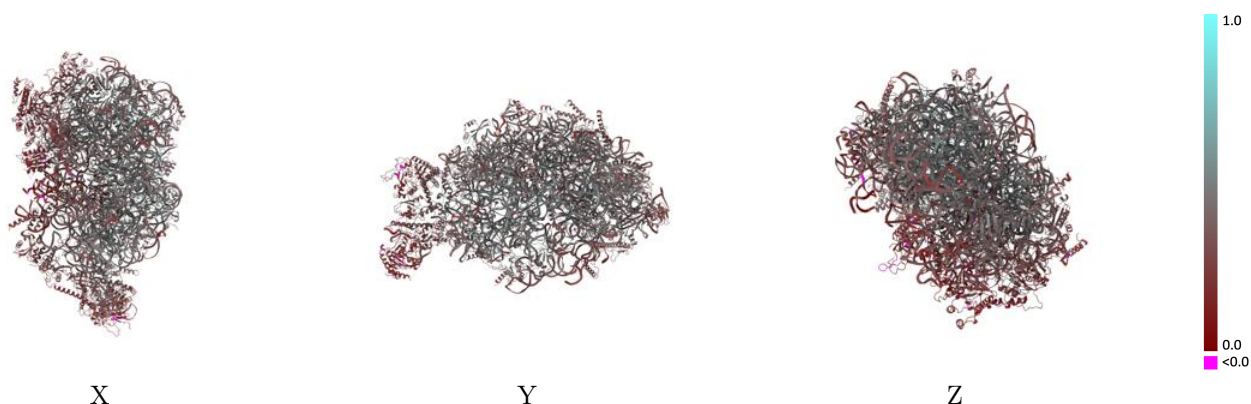
Y



Z

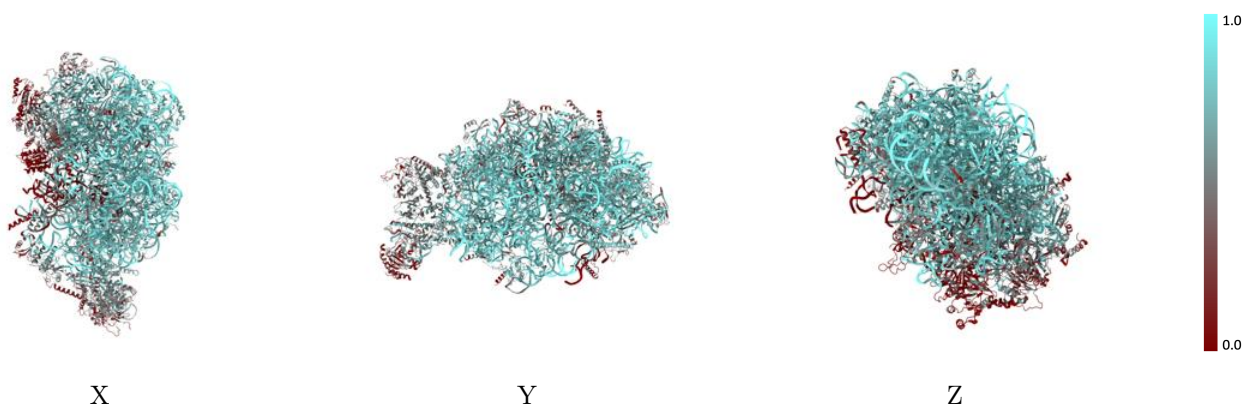
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



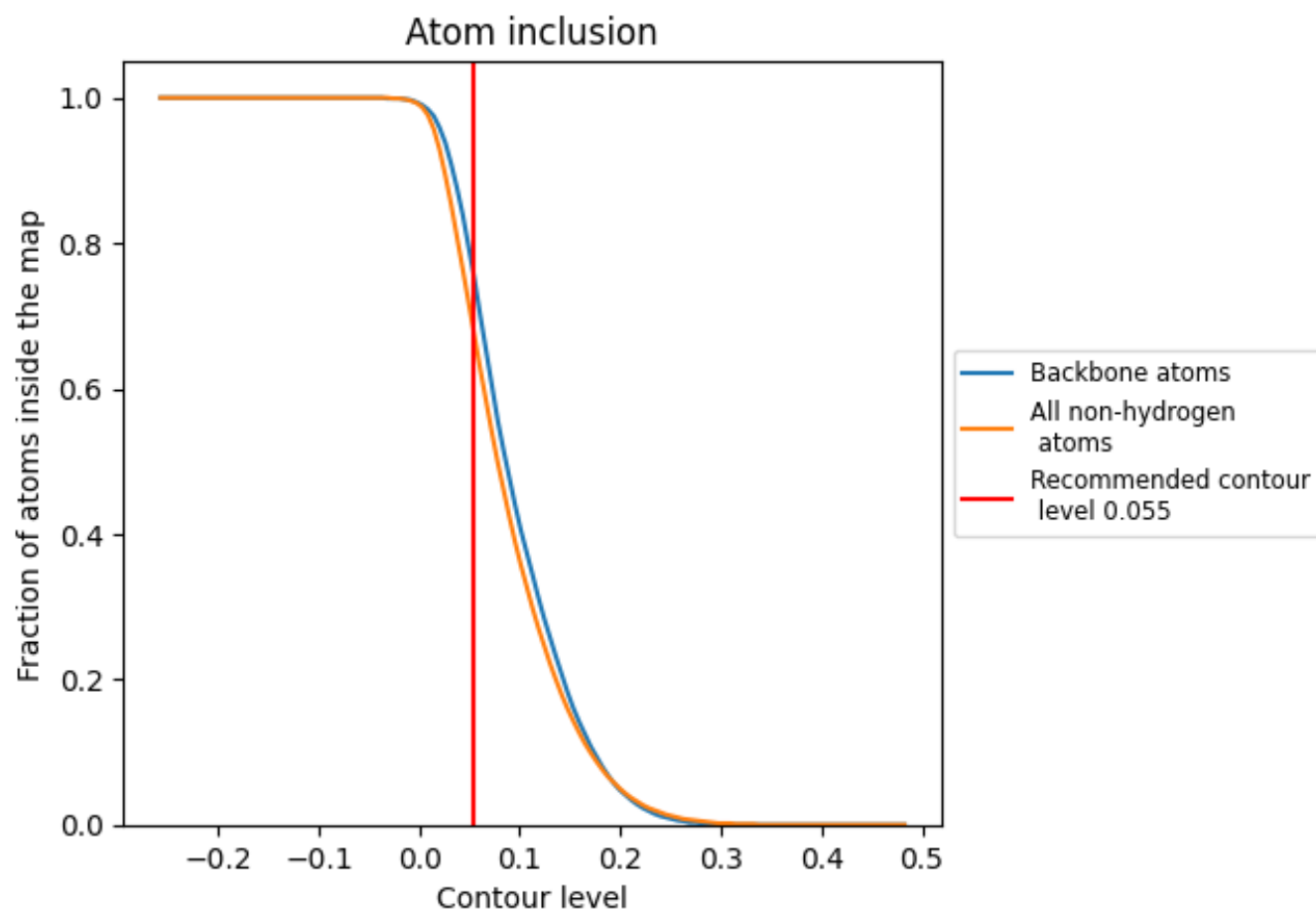
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6730	 0.3840
1	 0.7890	 0.3960
2	 0.8920	 0.4560
6	 0.6830	 0.3070
B	 0.6810	 0.4290
C	 0.7750	 0.4690
E	 0.7250	 0.4280
F	 0.7770	 0.4300
G	 0.6420	 0.3890
H	 0.6870	 0.4150
K	 0.2690	 0.2150
L	 0.6910	 0.4310
M	 0.7610	 0.4410
N	 0.8020	 0.4900
O	 0.8060	 0.4790
P	 0.7620	 0.4590
Q	 0.7510	 0.4440
R	 0.4550	 0.3430
S	 0.7070	 0.4280
T	 0.1880	 0.3110
U	 0.4610	 0.3320
V	 0.5390	 0.3800
W	 0.4070	 0.2770
X	 0.7080	 0.4430
Y	 0.7800	 0.4720
Z	 0.5030	 0.3200
a	 0.6190	 0.3960
b	 0.3230	 0.2730
c	 0.3410	 0.2580
d	 0.7040	 0.4430
e	 0.8010	 0.4980
f	 0.8390	 0.5110
g	 0.5810	 0.3980
h	 0.7410	 0.4570
i	 0.5930	 0.3700



Continued on next page...

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Chain	Atom inclusion	Q-score
j	 0.7500	 0.4660
k	 0.5410	 0.3910
l	 0.2800	 0.3650
n	 0.5320	 0.3380
o	 0.3760	 0.2480
q	 0.1930	 0.2420
r	 0.2480	 0.2720
s	 0.4770	 0.4100
t	 0.4620	 0.3010
u	 0.5330	 0.3480
w	 0.1110	 0.2630
y	 0.4430	 0.2890
z	 0.4560	 0.3770