



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:05 AM UTC

PDB ID : 6QT0 / pdb_00006qt0
EMDB ID : EMD-4630
Title : Cryo-EM structures of Lsg1-TAP pre-60S ribosomal particles
Authors : Kargas, V.; Warren, A.J.
Deposited on : 2019-02-22
Resolution : 3.40 Å(reported)
Based on initial model : 4V88

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:

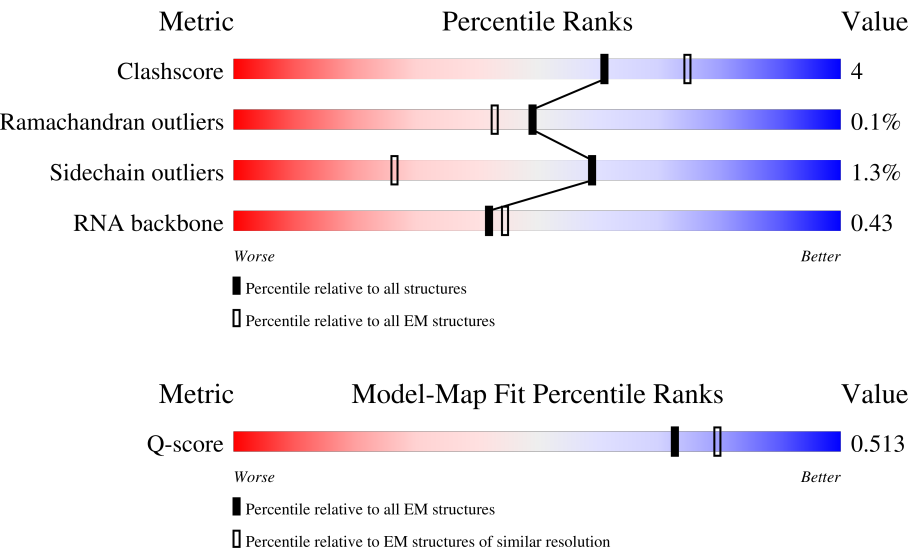
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.40 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.



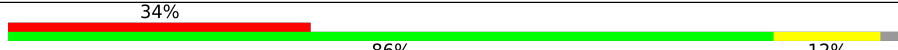
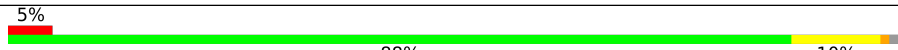
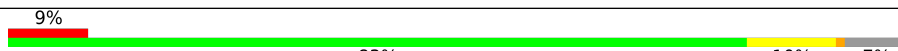
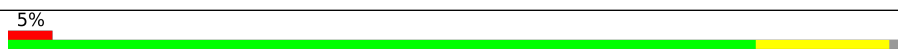
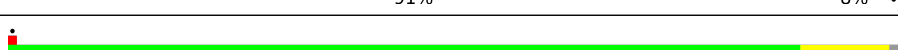
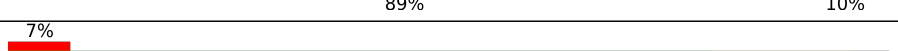
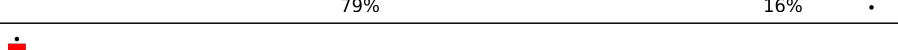
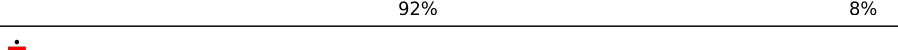
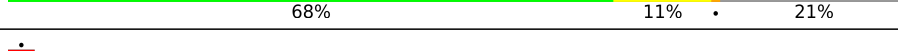
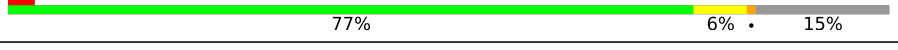
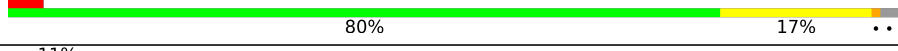
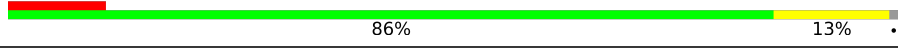
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	A	3396	7% 63% 25% 7%
2	B	254	76% 20% 4%
3	C	387	81% 16% 3%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	362	
5	E	174	
6	F	189	
7	G	176	
8	H	256	
9	q	221	
10	J	198	
11	K	199	
12	L	137	
13	M	138	
14	N	149	
15	O	204	
16	P	297	
17	Q	186	
18	R	189	
19	S	172	
20	T	160	
21	U	184	
22	V	121	
23	W	142	
24	X	127	
25	Y	136	
26	Z	120	
27	a	59	
28	b	244	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	c	105	
30	d	113	
31	e	130	
32	f	107	
33	g	121	
34	h	100	
35	i	88	
36	j	78	
37	k	51	
38	l	106	
39	m	92	
40	n	245	
41	t	128	
42	v	155	
43	z	432	
44	x	121	
45	y	158	

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 124065 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3164	Total	C	N	O	P	0	0
			67663	30231	12203	22069	3160		

- Molecule 2 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	247	Total	C	N	O	S	0	0
			1878	1170	381	326	1		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	381	Total	C	N	O	S	0	0
			3039	1928	577	526	8		

- Molecule 4 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	361	Total	C	N	O	S	0	0
			2748	1730	522	493	3		

- Molecule 5 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	169	Total	C	N	O	S	0	0
			1352	847	253	248	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	189	Total	C	N	O	S	0	0
			1502	953	272	273	4		

- Molecule 7 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1399	902	251	245	1		

- Molecule 8 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	223	Total	C	N	O	S	0	0
			1742	1117	309	313	3		

- Molecule 9 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	q	216	Total	C	N	O	S	0	0
			1754	1111	332	304	7		

- Molecule 10 is a protein called 60S ribosomal protein L16-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	197	Total	C	N	O	S	0	0
			1563	1005	292	265	1		

- Molecule 11 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	186	Total	C	N	O	S	0	0
			1486	929	304	253			

- Molecule 12 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	136	Total	C	N	O	S	0	0
			1002	628	189	178	7		

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	137	Total	C	N	O	S	0	0
			1058	678	200	178	2		

- Molecule 14 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	148	Total	C	N	O	S	0	0
			1172	749	231	189	3		

- Molecule 15 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	203	Total	C	N	O	S	0	0
			1719	1077	361	280	1		

- Molecule 16 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	286	Total	C	N	O	S	0	0
			2298	1453	400	443	2		

- Molecule 17 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	185	Total	C	N	O	S	0	0
			1440	908	290	240	2		

- Molecule 18 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	150	Total	C	N	O	0	0
			1209	752	257	200		

- Molecule 19 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	172	Total	C	N	O	S	0	0
			1444	930	267	243	4		

- Molecule 20 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	159	Total	C	N	O	S	0	0
			1275	805	246	220	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	154	Total	C	N	O	0	0
			1222	761	237	224		

- Molecule 22 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	99	Total	C	N	O	0	0
			786	510	129	147		

- Molecule 23 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	120	Total	C	N	O	S	0	0
			958	617	168	171	2		

- Molecule 24 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 25 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	135	Total	C	N	O	0	0
			1091	710	202	179		

- Molecule 26 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	119	Total	C	N	O	S	0	0
			968	615	186	166	1		

- Molecule 27 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	54	Total	C	N	O	0	0
			430	268	93	69		

- Molecule 28 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	219	Total	C	N	O	S	0	0
			1760	1138	320	301	1		

- Molecule 29 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	97	Total	C	N	O	S	0	0
			741	479	124	137	1		

- Molecule 30 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	107	Total	C	N	O	S	0	0
			872	553	165	153	1		

- Molecule 31 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	121	Total	C	N	O	S	0	0
			976	618	197	160	1		

- Molecule 32 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	106	Total	C	N	O	S	0	0
			849	540	165	143	1		

- Molecule 33 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	103	Total	C	N	O	S	0	0
			812	504	167	137	4		

- Molecule 34 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	98	Total	C	N	O	S	0	0
			763	477	155	129	2		

- Molecule 35 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 36 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	77	Total	C	N	O	S	0	0
			611	391	115	105			

- Molecule 37 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	50	Total	C	N	O	S	0	0
			435	272	97	64	2		

- Molecule 38 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	94	Total	C	N	O	S	0	0
			756	476	153	122	5		

- Molecule 39 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	91	Total	C	N	O	S	0	0
			693	429	138	120	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	224	Total	C	N	O	S	0	0
			1691	1051	293	340	7		

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 42 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	v	60	Total	C	N	O	S	0	0
			500	322	98	79	1		

- Molecule 43 is a protein called Cytoplasmic 60S subunit biogenesis factor REH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	z	53	Total	C	N	O	S	0	0
			445	274	88	80	3		

- Molecule 44 is a RNA chain called 5S rRNA.

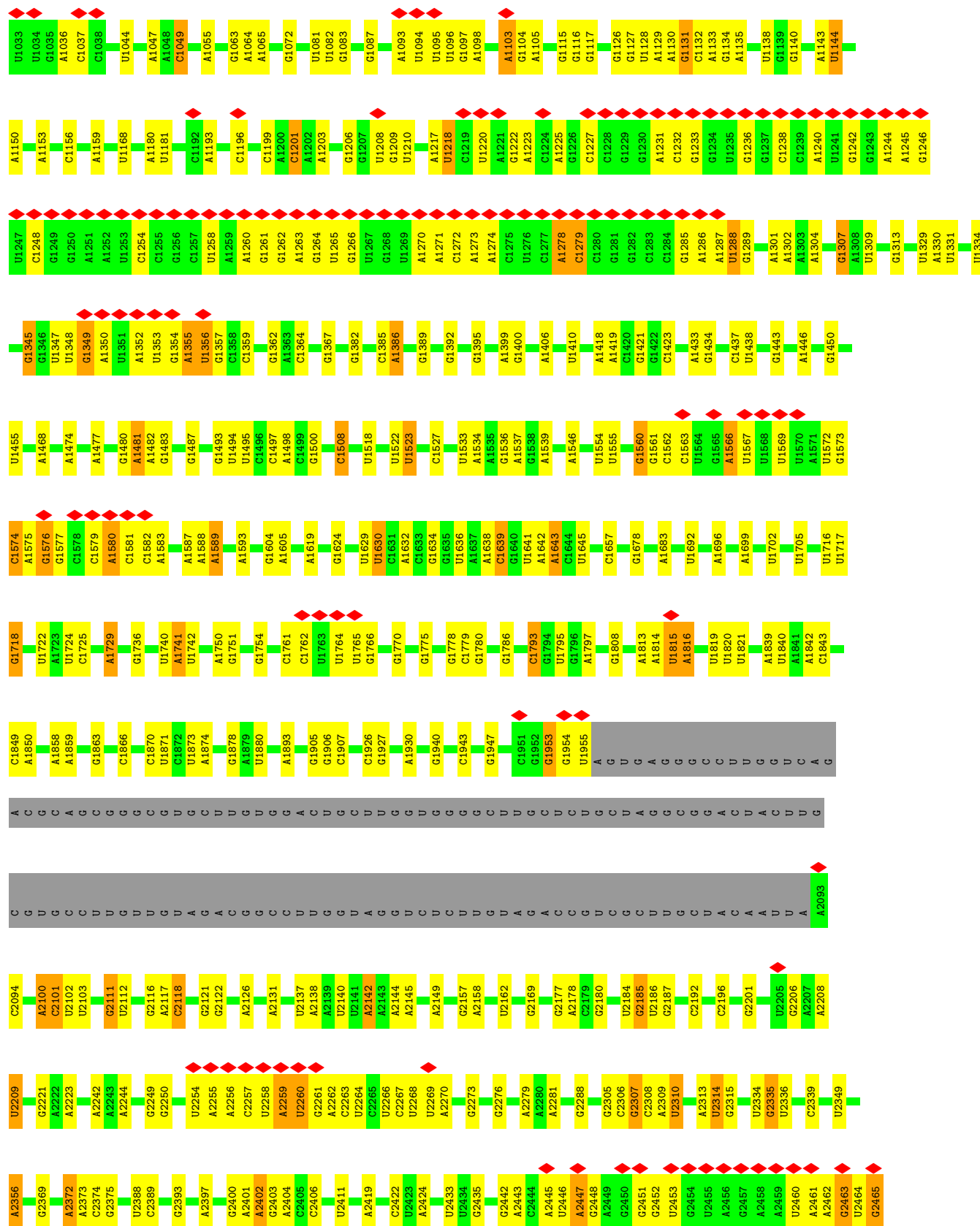
Mol	Chain	Residues	Atoms					AltConf	Trace
44	x	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

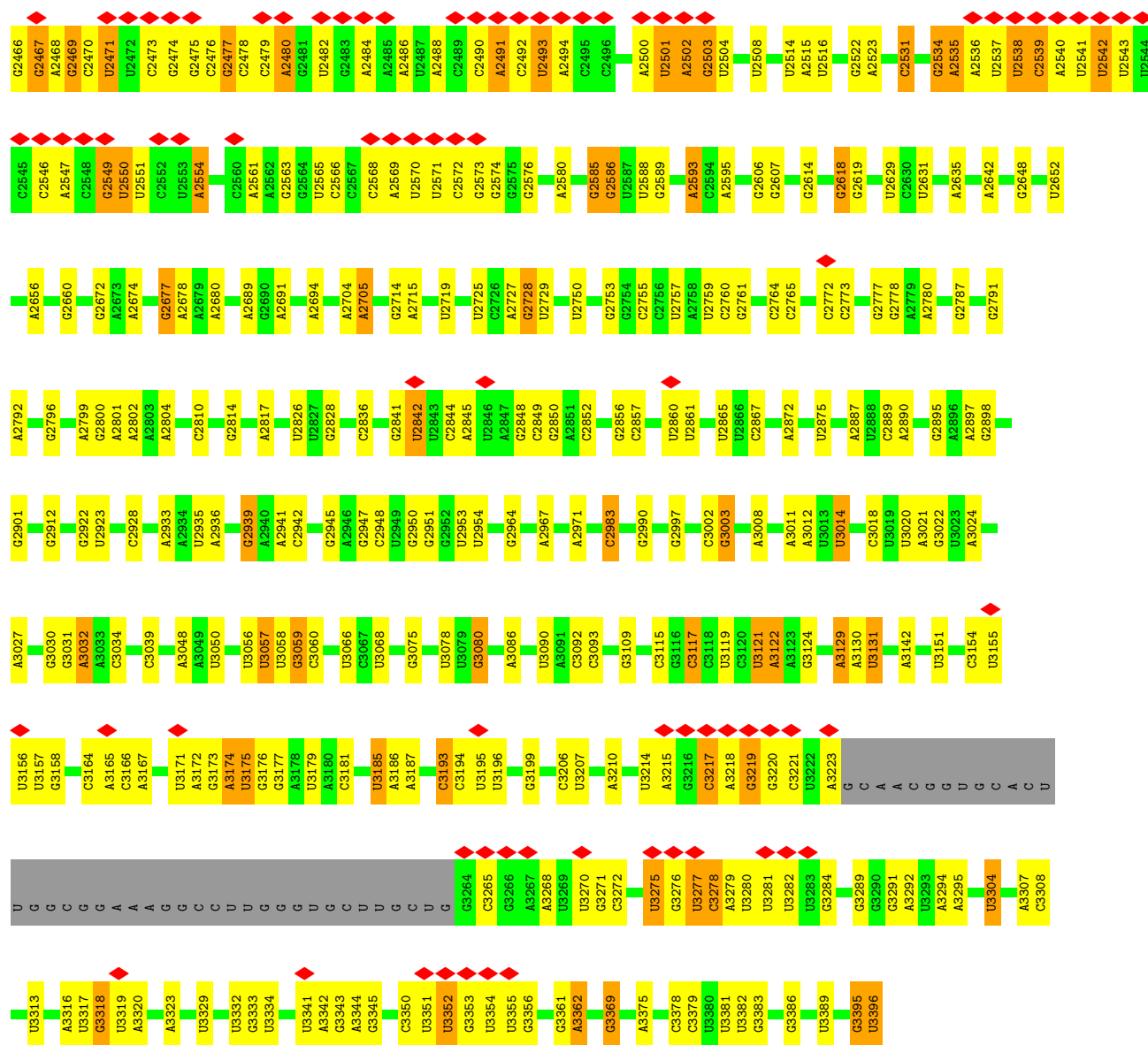
- Molecule 45 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	y	156	Total	C	N	O	P	0	0
			3313	1482	582	1093	156		

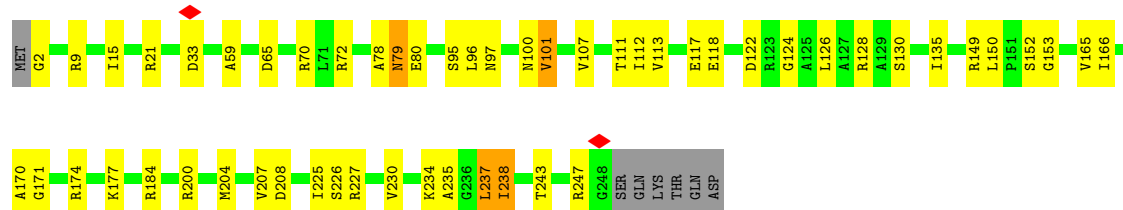
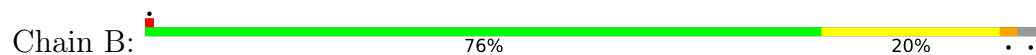
- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
46	g	1	Total	Zn	0
			1	1	
46	i	1	Total	Zn	0
			1	1	
46	l	1	Total	Zn	0
			1	1	
46	m	1	Total	Zn	0
			1	1	
46	t	1	Total	Zn	0
			1	1	

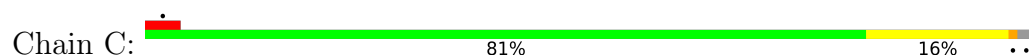


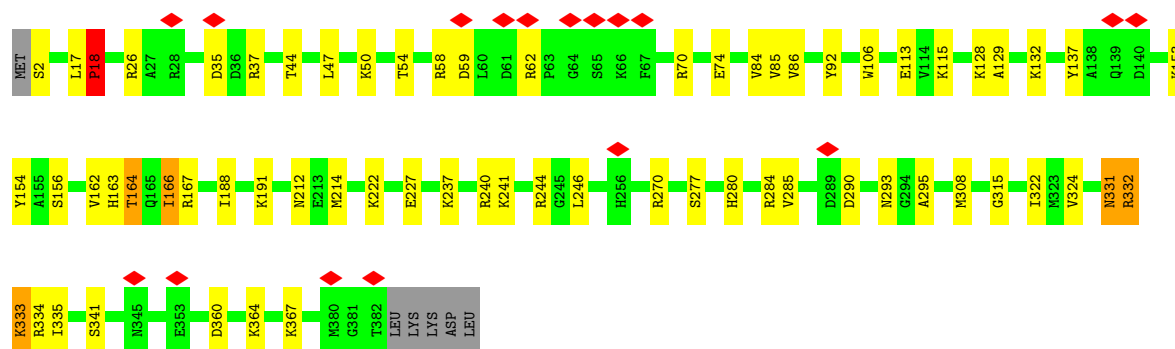


• Molecule 2: 60S ribosomal protein L2-A

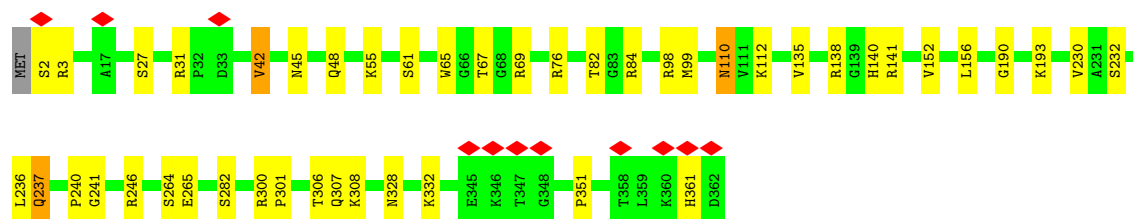
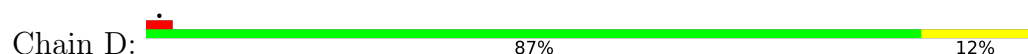


• Molecule 3: 60S ribosomal protein L3

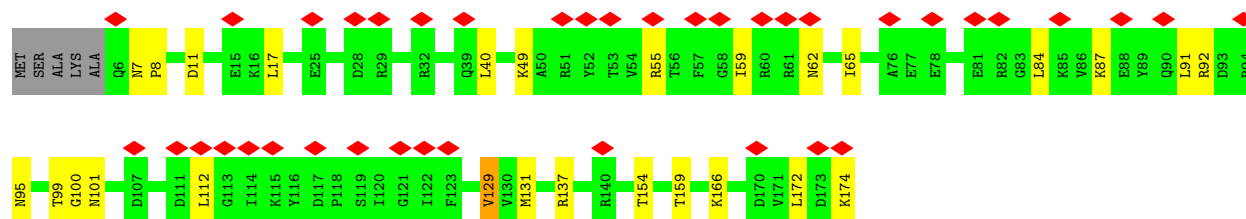
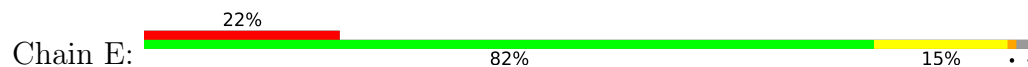




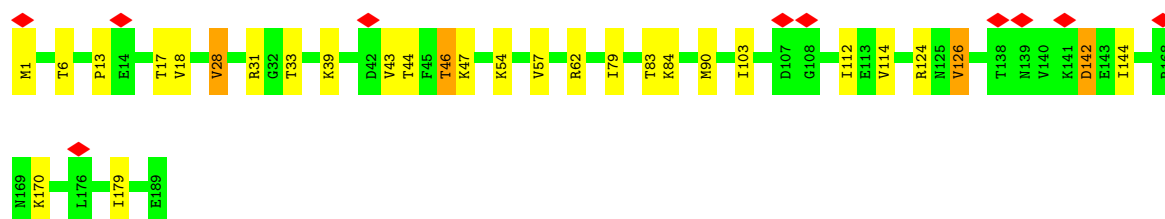
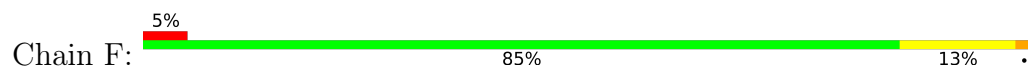
• Molecule 4: 60S ribosomal protein L4-A



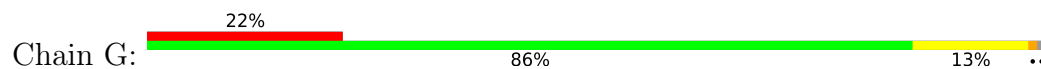
• Molecule 5: 60S ribosomal protein L11-A



• Molecule 6: 60S ribosomal protein L9-A

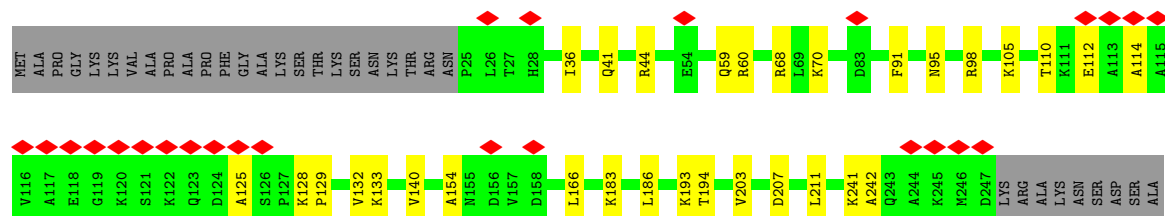
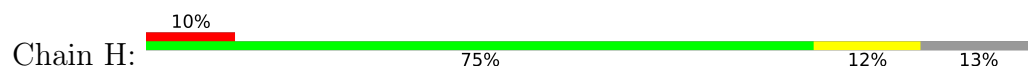


• Molecule 7: 60S ribosomal protein L6-A

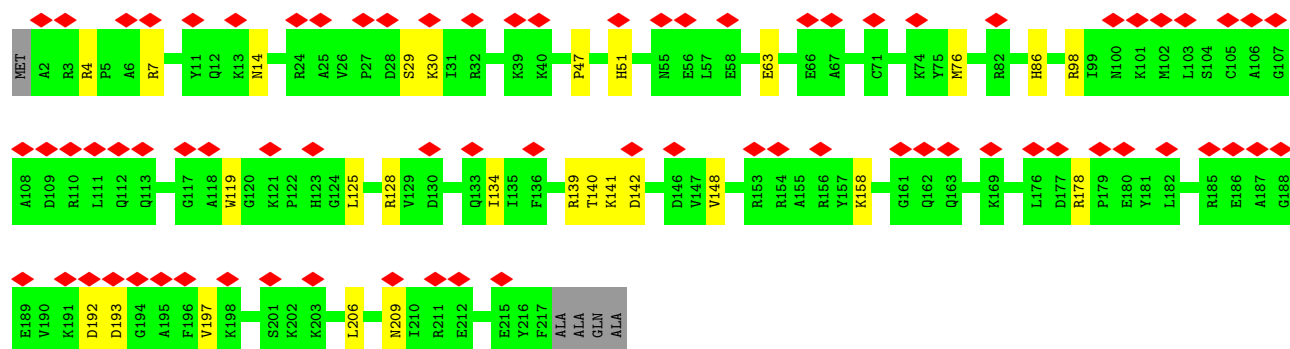
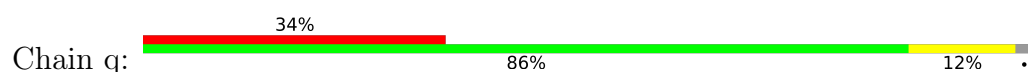




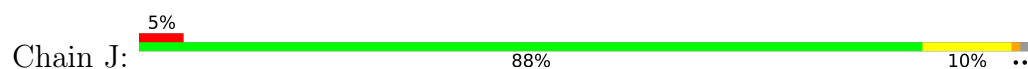
• Molecule 8: 60S ribosomal protein L8-A



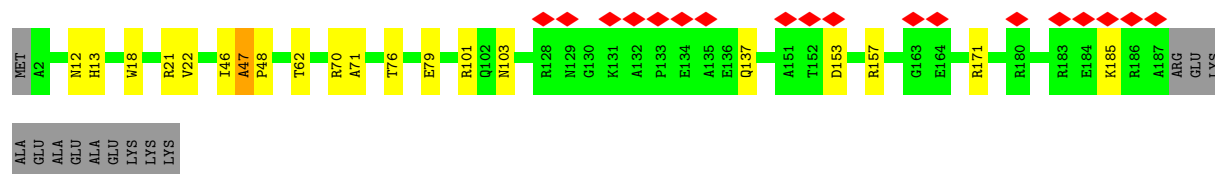
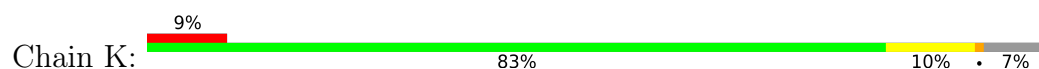
• Molecule 9: 60S ribosomal protein L10



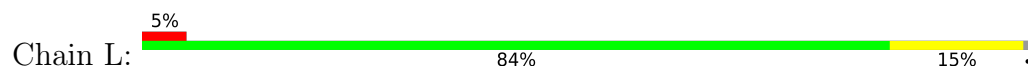
• Molecule 10: 60S ribosomal protein L16-B



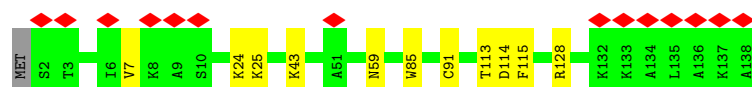
• Molecule 11: 60S ribosomal protein L13-A



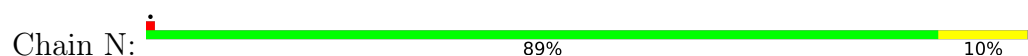
- Molecule 12: 60S ribosomal protein L23-A



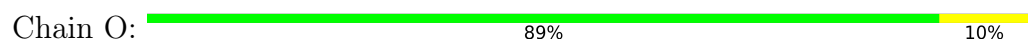
- Molecule 13: 60S ribosomal protein L14-A



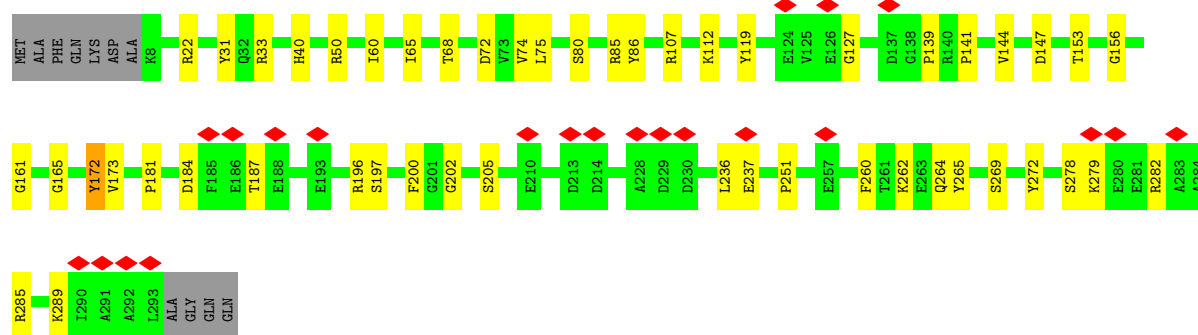
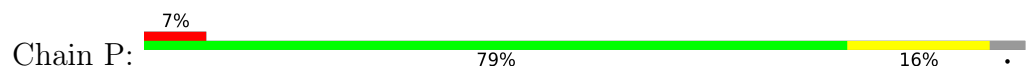
- Molecule 14: 60S ribosomal protein L28



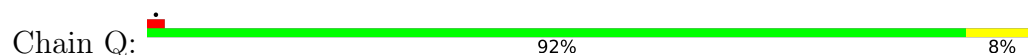
- Molecule 15: 60S ribosomal protein L15-A

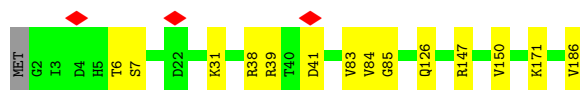


- Molecule 16: 60S ribosomal protein L5



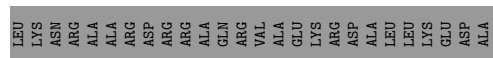
- Molecule 17: 60S ribosomal protein L18-A





- Molecule 18: 60S ribosomal protein L19-A

Chain R: 68% 11% 21%



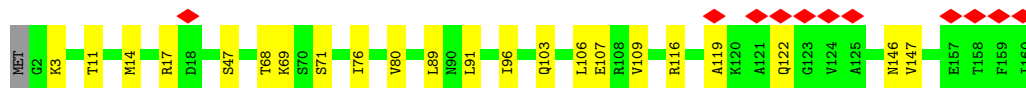
- Molecule 19: 60S ribosomal protein L20-A

Chain S: 80% 20%



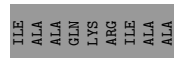
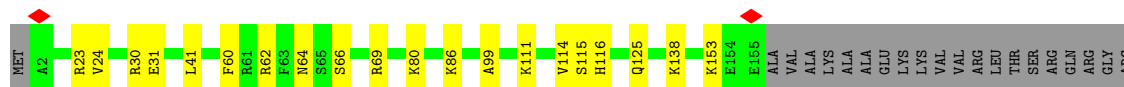
- Molecule 20: 60S ribosomal protein L21-A

Chain T: 7% 86% 14%



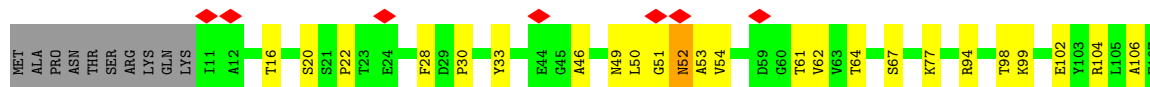
- Molecule 21: 60S ribosomal protein L17-A

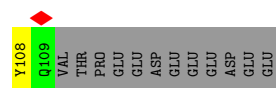
Chain U: 73% 11% 16%



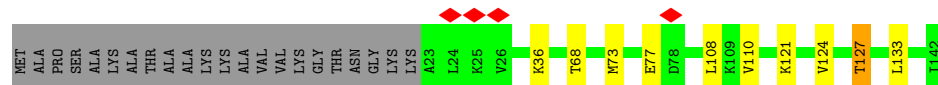
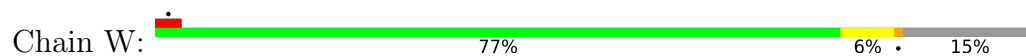
- Molecule 22: 60S ribosomal protein L22-A

Chain V: 7% 61% 20% 18%

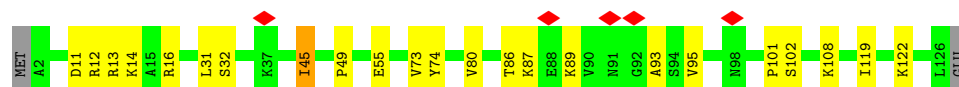
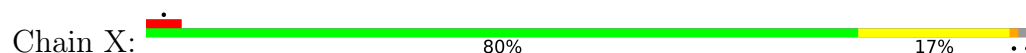




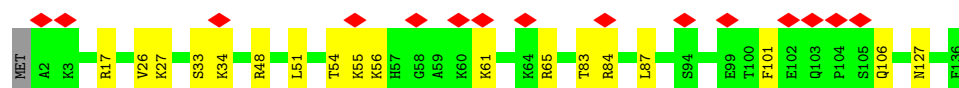
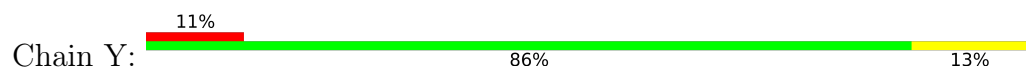
- Molecule 23: 60S ribosomal protein L25



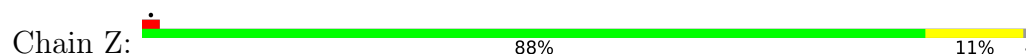
- Molecule 24: 60S ribosomal protein L26-A



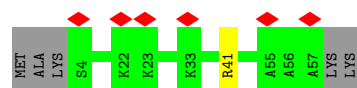
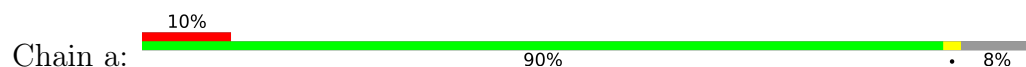
- Molecule 25: 60S ribosomal protein L27-A



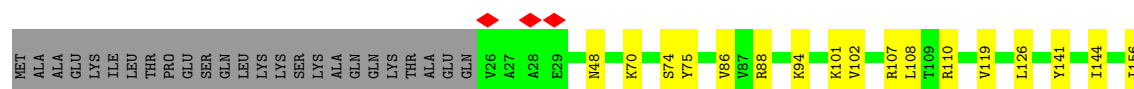
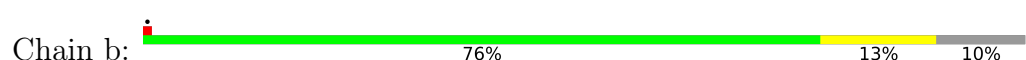
- Molecule 26: 60S ribosomal protein L35-A



- Molecule 27: 60S ribosomal protein L29

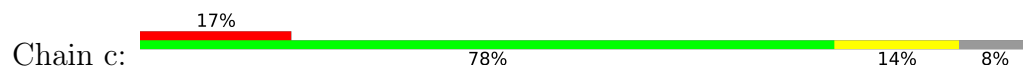


- Molecule 28: 60S ribosomal protein L7-A

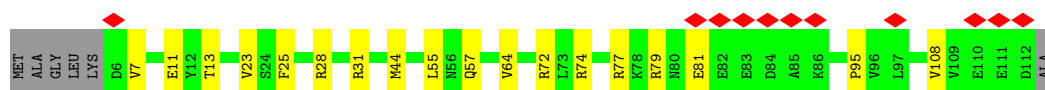
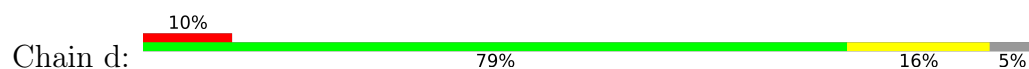




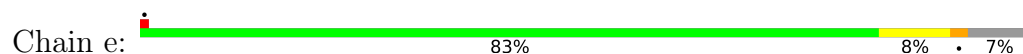
- Molecule 29: 60S ribosomal protein L30



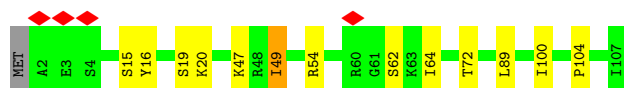
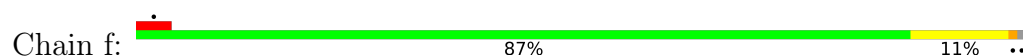
- Molecule 30: 60S ribosomal protein L31-A



- Molecule 31: 60S ribosomal protein L32



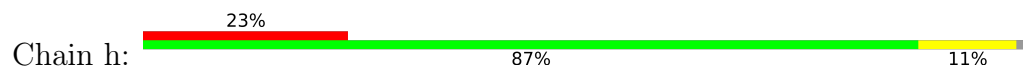
- Molecule 32: 60S ribosomal protein L33-A



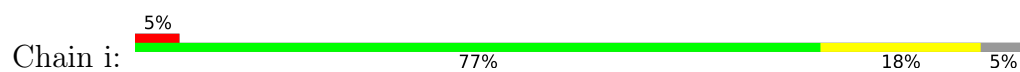
- Molecule 33: 60S ribosomal protein L34-A



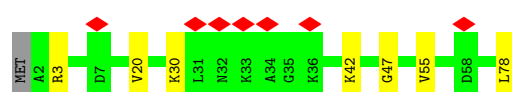
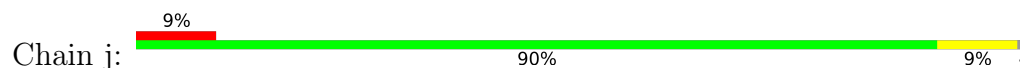
- Molecule 34: 60S ribosomal protein L36-A



- Molecule 35: 60S ribosomal protein L37-A



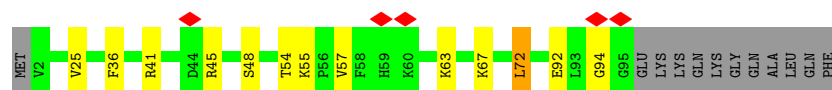
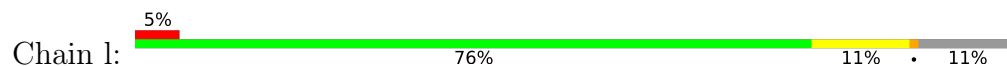
- Molecule 36: 60S ribosomal protein L38



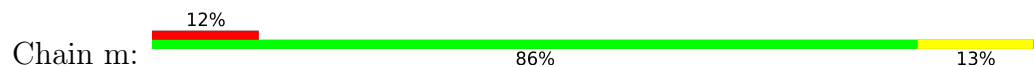
- Molecule 37: 60S ribosomal protein L39



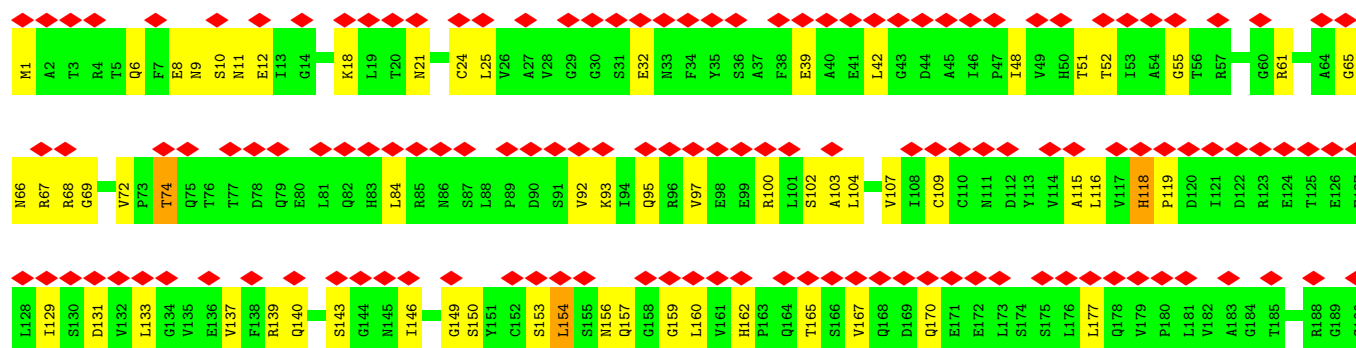
- Molecule 38: 60S ribosomal protein L42-A

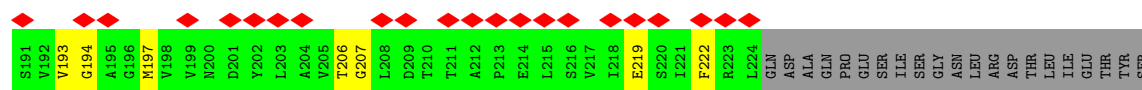


- Molecule 39: 60S ribosomal protein L43-A

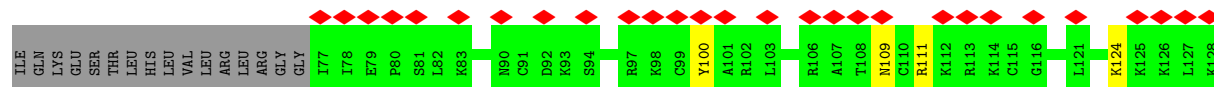
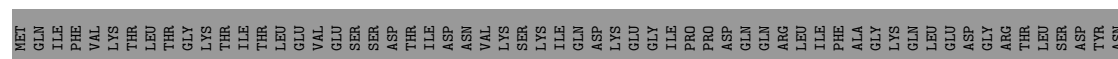


- Molecule 40: Eukaryotic translation initiation factor 6

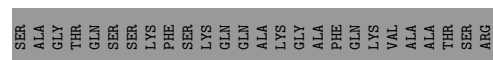
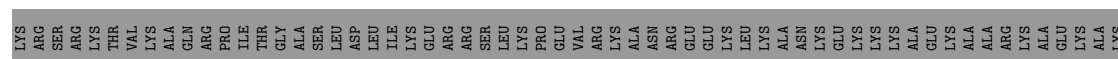
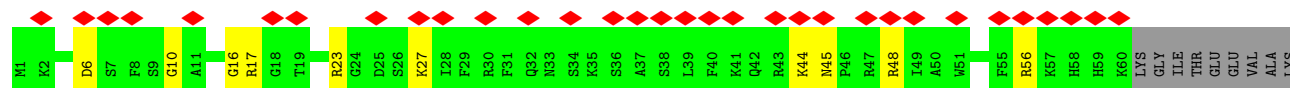




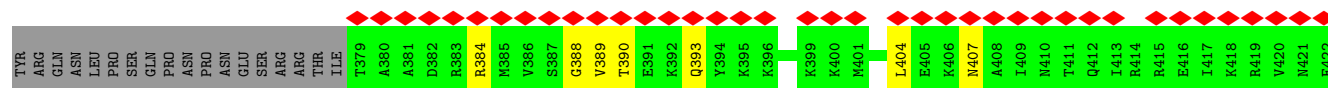
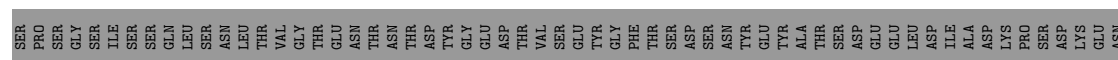
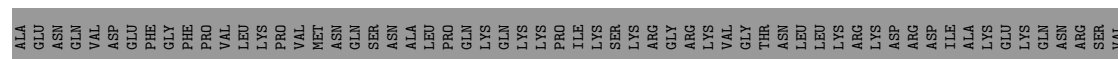
- Molecule 41: Ubiquitin-60S ribosomal protein L40

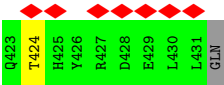


- Molecule 42: 60S ribosomal protein L24-A



- Molecule 43: Cytoplasmic 60S subunit biogenesis factor REH1

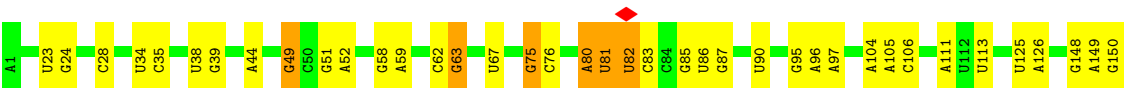




● Molecule 44: 5S rRNA



● Molecule 45: 5.8S rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46734	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 ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.468	Depositor
Minimum map value	-0.255	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	383.40002, 383.40002, 383.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.50	0/75742	0.43	2/118089 (0.0%)
2	B	0.54	0/1912	0.70	1/2569 (0.0%)
3	C	0.50	0/3110	0.69	2/4184 (0.0%)
4	D	0.53	0/2800	0.66	1/3791 (0.0%)
5	E	0.27	0/1373	0.55	0/1841
6	F	0.30	0/1523	0.55	0/2051
7	G	0.35	0/1423	0.58	0/1911
8	H	0.38	0/1774	0.58	0/2395
9	q	0.33	0/1791	0.58	0/2402
10	J	0.48	0/1593	0.57	0/2137
11	K	0.52	0/1511	0.62	0/2031
12	L	0.45	0/1017	0.60	0/1368
13	M	0.37	0/1073	0.55	0/1445
14	N	0.55	0/1203	0.63	0/1611
15	O	0.59	0/1756	0.64	0/2353
16	P	0.35	0/2347	0.56	2/3167 (0.1%)
17	Q	0.51	0/1464	0.62	0/1964
18	R	0.46	0/1226	0.52	0/1637
19	S	0.43	0/1480	0.60	2/1989 (0.1%)
20	T	0.46	0/1299	0.59	1/1742 (0.1%)
21	U	0.53	0/1245	0.60	0/1676
22	V	0.38	0/802	0.77	3/1087 (0.3%)
23	W	0.47	0/973	0.60	0/1313
24	X	0.46	0/995	0.63	0/1329
25	Y	0.32	0/1117	0.61	0/1496
26	Z	0.44	0/977	0.58	0/1300
27	a	0.42	0/441	0.73	0/589
28	b	0.50	0/1797	0.69	1/2419 (0.0%)
29	c	0.35	0/749	0.49	0/1007
30	d	0.46	0/886	0.64	0/1190
31	e	0.51	0/995	0.60	0/1329
32	f	0.53	0/867	0.75	0/1167

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.51	0/822	0.67	0/1099
34	h	0.34	0/770	0.53	0/1023
35	i	0.63	0/680	0.69	0/901
36	j	0.39	0/617	0.54	0/825
37	k	0.53	0/442	0.61	0/587
38	l	0.42	0/768	0.58	0/1016
39	m	0.42	0/700	0.59	0/933
40	n	0.31	0/1712	0.66	1/2330 (0.0%)
41	t	0.27	0/423	0.56	0/562
42	v	0.28	0/512	0.54	0/680
43	z	0.31	0/448	0.63	0/593
44	x	0.39	0/2883	0.36	0/4491
45	y	0.55	0/3702	0.45	0/5764
All	All	0.48	0/133740	0.50	16/197383 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	18	PRO	CB-CA-C	10.54	128.95	111.56
3	C	18	PRO	CA-N-CD	-9.62	98.54	112.00
40	n	193	VAL	N-CA-C	-7.07	106.99	113.71
4	D	42	VAL	N-CA-C	-6.81	105.45	113.42
2	B	238	ILE	N-CA-C	6.50	116.64	110.53
22	V	53	ALA	CA-C-N	-6.04	115.31	123.10
22	V	53	ALA	C-N-CA	-6.04	115.31	123.10
19	S	140	VAL	N-CA-C	-5.80	107.16	112.96
28	b	229	PHE	CA-CB-CG	5.51	119.31	113.80
16	P	172	TYR	CA-C-N	-5.50	118.86	122.60
16	P	172	TYR	C-N-CA	-5.50	118.86	122.60
1	A	1815	U	P-O3'-C3'	5.39	128.28	120.20
22	V	51	GLY	O-C-N	5.11	127.15	122.19
19	S	133	ALA	N-CA-C	-5.09	108.33	114.75
20	T	147	VAL	N-CA-C	-5.01	104.36	109.02
1	A	2101	C	P-O3'-C3'	5.01	127.71	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	A	67663	0	34013	340	0
2	B	1878	0	1946	51	0
3	C	3039	0	3113	61	0
4	D	2748	0	2863	35	0
5	E	1352	0	1383	19	0
6	F	1502	0	1572	18	0
7	G	1399	0	1501	18	0
8	H	1742	0	1834	21	0
9	q	1754	0	1794	18	0
10	J	1563	0	1665	15	0
11	K	1486	0	1554	20	0
12	L	1002	0	1048	12	0
13	M	1058	0	1154	7	0
14	N	1172	0	1215	13	0
15	O	1719	0	1779	19	0
16	P	2298	0	2248	30	0
17	Q	1440	0	1543	9	0
18	R	1209	0	1295	15	0
19	S	1444	0	1487	19	0
20	T	1275	0	1323	14	0
21	U	1222	0	1231	12	0
22	V	786	0	799	22	0
23	W	958	0	1023	6	0
24	X	984	0	1075	16	0
25	Y	1091	0	1155	13	0
26	Z	968	0	1078	12	0
27	a	430	0	447	1	0
28	b	1760	0	1843	22	0
29	c	741	0	797	9	0
30	d	872	0	914	9	0
31	e	976	0	1045	11	0
32	f	849	0	880	8	0
33	g	812	0	875	11	0
34	h	763	0	842	9	0
35	i	665	0	669	14	0
36	j	611	0	682	4	0
37	k	435	0	475	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	l	756	0	818	9	0
39	m	693	0	736	9	0
40	n	1691	0	1689	44	0
41	t	417	0	455	5	0
42	v	500	0	524	7	0
43	z	445	0	466	6	0
44	x	2579	0	1304	17	0
45	y	3313	0	1675	20	0
46	g	1	0	0	0	0
46	i	1	0	0	0	0
46	l	1	0	0	0	0
46	m	1	0	0	0	0
46	t	1	0	0	0	0
All	All	124065	0	89827	828	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 4.

All (828) 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)
11:K:47:ALA:CB	11:K:48:PRO:HD3	1.70	1.19
11:K:47:ALA:HB1	11:K:48:PRO:HD3	1.16	1.14
11:K:47:ALA:CB	11:K:48:PRO:CD	2.35	1.04
3:C:222:LYS:HD3	3:C:331:ASN:HD21	1.24	0.99
3:C:222:LYS:HD3	3:C:331:ASN:ND2	1.77	0.99
1:A:3304:U:OP1	3:C:332:ARG:NH2	2.03	0.92
2:B:234:LYS:HD3	2:B:238:ILE:HD11	1.53	0.90
3:C:332:ARG:HH11	3:C:332:ARG:HG2	1.36	0.86
3:C:50:LYS:O	3:C:332:ARG:O	1.93	0.85
22:V:50:LEU:HB2	22:V:54:VAL:HG12	1.58	0.85
11:K:47:ALA:HB3	11:K:48:PRO:CD	2.06	0.85
2:B:234:LYS:CD	2:B:238:ILE:HD11	2.07	0.84
2:B:126:LEU:HD21	2:B:150:LEU:HD21	1.60	0.82
1:A:2177:G:O2'	2:B:126:LEU:O	2.05	0.74
11:K:47:ALA:HB1	11:K:48:PRO:CD	2.03	0.74
22:V:50:LEU:HB2	22:V:54:VAL:CG1	2.18	0.74
22:V:46:ALA:HB1	22:V:49:ASN:HB2	1.70	0.73
3:C:222:LYS:CD	3:C:331:ASN:HD21	2.00	0.72
3:C:17:LEU:HB3	3:C:18:PRO:HD2	1.71	0.72
25:Y:87:LEU:HD13	25:Y:127:ASN:HD21	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LYS:HD3	2:B:238:ILE:CD1	2.21	0.70
2:B:237:LEU:N	2:B:237:LEU:HD23	2.07	0.69
16:P:260:PHE:HB3	16:P:264:GLN:HB2	1.75	0.69
22:V:46:ALA:HB3	22:V:49:ASN:HB3	1.76	0.67
3:C:222:LYS:CD	3:C:331:ASN:ND2	2.56	0.67
1:A:804:C:OP1	4:D:98:ARG:NH2	2.28	0.67
2:B:225:ILE:HG13	2:B:235:ALA:O	1.95	0.66
1:A:1566:A:HO2'	1:A:1573:G:H1	1.44	0.66
3:C:17:LEU:CB	3:C:18:PRO:HD2	2.26	0.65
22:V:46:ALA:CB	22:V:49:ASN:CB	2.75	0.65
3:C:227:GLU:HG2	3:C:270:ARG:HE	1.61	0.65
11:K:47:ALA:HB3	11:K:48:PRO:HD3	1.66	0.64
1:A:2402:A:H5'	4:D:67:THR:HG22	1.80	0.64
10:J:9:ASP:HB2	10:J:116:ARG:HB3	1.80	0.64
12:L:108:GLU:HA	12:L:128:ARG:HD2	1.80	0.64
22:V:50:LEU:HD12	22:V:50:LEU:O	1.97	0.64
3:C:332:ARG:HH11	3:C:332:ARG:CG	2.07	0.64
1:A:1348:U:OP2	17:Q:38:ARG:NH2	2.32	0.63
1:A:3275:U:H3	32:f:62:SER:HG	1.45	0.63
1:A:2406:C:O2'	1:A:2619:G:N2	2.31	0.62
1:A:155:G:N1	1:A:265:A:OP2	2.31	0.62
16:P:107:ARG:HG3	16:P:251:PRO:HG3	1.80	0.62
2:B:234:LYS:CG	2:B:238:ILE:HD11	2.30	0.62
24:X:11:ASP:HB3	24:X:14:LYS:HB2	1.81	0.62
1:A:1438:U:OP1	4:D:76:ARG:NH2	2.33	0.62
1:A:3308:C:N3	21:U:69:ARG:NH2	2.45	0.62
1:A:2389:C:H5''	21:U:66:SER:HA	1.82	0.61
1:A:2948:C:OP1	3:C:244:ARG:NH2	2.33	0.61
1:A:405:U:O2'	1:A:1395:G:N2	2.32	0.61
6:F:28:VAL:HG12	6:F:33:THR:HG23	1.82	0.61
2:B:101:VAL:HB	2:B:165:VAL:HG12	1.83	0.61
1:A:163:C:H42	1:A:259:C:H42	1.48	0.61
1:A:2117:A:HO2'	1:A:3080:G:HO2'	1.47	0.61
6:F:142:ASP:N	6:F:142:ASP:OD1	2.32	0.61
24:X:55:GLU:HB3	24:X:108:LYS:HB3	1.83	0.61
40:n:18:LYS:HE3	40:n:65:GLY:H	1.65	0.61
1:A:266:A:N6	34:h:29:LYS:O	2.34	0.61
1:A:3115:C:O2	1:A:3117:C:N4	2.34	0.60
1:A:1634:G:N7	25:Y:17:ARG:NH2	2.49	0.60
1:A:116:A:OP1	15:O:2:GLY:N	2.34	0.60
7:G:51:ARG:O	7:G:72:ASN:ND2	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:U:H3	1:A:649:A:H61	1.49	0.60
8:H:112:GLU:HG2	8:H:125:ALA:HB3	1.84	0.60
22:V:16:THR:HG22	22:V:64:THR:HG22	1.83	0.60
29:c:95:ALA:HA	29:c:100:ILE:HD11	1.83	0.60
1:A:901:G:OP1	35:i:13:ASN:ND2	2.34	0.60
1:A:2852:C:N3	9:q:158:LYS:NZ	2.49	0.60
3:C:70:ARG:NH2	40:n:52:THR:OG1	2.35	0.60
4:D:65:TRP:O	4:D:69:ARG:NH1	2.35	0.60
2:B:117:GLU:HB2	2:B:122:ASP:OD1	2.01	0.60
4:D:112:LYS:HG2	15:O:202:TYR:HB3	1.84	0.59
21:U:64:ASN:O	21:U:80:LYS:NZ	2.33	0.59
1:A:1203:A:OP2	1:A:1301:A:N6	2.34	0.59
3:C:47:LEU:HD12	3:C:335:ILE:HD11	1.84	0.59
1:A:2678:A:H62	5:E:55:ARG:HH21	1.50	0.59
2:B:33:ASP:OD1	2:B:33:ASP:N	2.34	0.59
19:S:109:ASP:OD1	19:S:113:ARG:NH1	2.35	0.59
28:b:228:SER:HA	28:b:232:ARG:HH21	1.66	0.59
1:A:3022:G:N2	1:A:3032:A:OP2	2.36	0.59
1:A:3344:A:N6	1:A:3361:G:O2'	2.35	0.59
16:P:205:SER:HB2	16:P:236:LEU:HD22	1.85	0.59
22:V:50:LEU:HD22	22:V:54:VAL:HG13	1.84	0.59
1:A:2953:U:H2'	1:A:2954:U:H2'	1.84	0.59
1:A:763:G:H1	1:A:768:C:H42	1.51	0.58
19:S:71:LYS:O	19:S:73:LYS:NZ	2.36	0.58
20:T:76:ILE:HD12	20:T:89:LEU:HD21	1.84	0.58
1:A:1347:U:O2'	1:A:1349:G:N2	2.35	0.58
1:A:3343:G:H21	1:A:3362:A:H2	1.50	0.58
1:A:981:U:H3	1:A:1105:A:H4'	1.69	0.58
1:A:3329:U:H5''	3:C:308:MET:HE2	1.86	0.58
22:V:46:ALA:HB3	22:V:49:ASN:CB	2.32	0.58
40:n:119:PRO:HA	40:n:139:ARG:HB2	1.85	0.58
9:q:47:PRO:HD2	9:q:141:LYS:HA	1.86	0.58
15:O:110:ALA:HB1	15:O:113:LEU:HD12	1.86	0.57
35:i:34:CYS:SG	35:i:35:SER:N	2.76	0.57
1:A:185:C:OP1	24:X:122:LYS:NZ	2.36	0.57
1:A:799:G:O2'	11:K:18:TRP:NE1	2.28	0.57
6:F:31:ARG:NH1	6:F:84:LYS:O	2.38	0.57
40:n:129:ILE:HG23	40:n:133:LEU:HD12	1.86	0.57
9:q:142:ASP:OD1	9:q:178:ARG:NH2	2.38	0.57
1:A:1027:A:N6	1:A:1029:G:N3	2.51	0.57
1:A:1013:G:O6	1:A:1036:A:N6	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3020:U:O2'	1:A:3034:C:N4	2.37	0.57
22:V:46:ALA:HB1	22:V:49:ASN:CB	2.35	0.57
1:A:439:C:O2'	1:A:494:G:N2	2.37	0.57
6:F:1:MET:SD	19:S:113:ARG:NH2	2.78	0.57
11:K:47:ALA:HB3	11:K:48:PRO:HD2	1.87	0.57
1:A:2435:G:OP1	15:O:20:ARG:NH1	2.38	0.57
30:d:55:LEU:HB2	30:d:95:PRO:HD3	1.87	0.57
2:B:79:ASN:OD1	2:B:79:ASN:N	2.36	0.57
1:A:674:G:OP1	4:D:31:ARG:NH1	2.38	0.57
1:A:1348:U:OP1	17:Q:39:ARG:NH1	2.36	0.57
1:A:2945:G:O2'	1:A:2948:C:OP2	2.20	0.57
16:P:33:ARG:NH1	44:x:7:G:OP1	2.35	0.57
1:A:2842:U:OP1	1:A:2844:C:N4	2.37	0.56
4:D:361:HIS:O	19:S:28:ARG:NH2	2.38	0.56
37:k:29:LEU:HD11	43:z:393:GLN:HE22	1.70	0.56
1:A:824:C:H5''	2:B:21:ARG:HD3	1.86	0.56
1:A:3344:A:H2	1:A:3361:G:H21	1.54	0.56
18:R:21:LYS:HE3	18:R:55:VAL:HA	1.87	0.56
32:f:15:SER:OG	32:f:16:TYR:N	2.38	0.56
1:A:2501:U:N3	1:A:2503:G:N7	2.53	0.56
1:A:3057:U:H5'	1:A:3086:A:H61	1.71	0.56
8:H:95:ASN:OD1	8:H:98:ARG:NH2	2.39	0.56
11:K:79:GLU:OE2	11:K:103:ASN:ND2	2.39	0.56
13:M:113:THR:OG1	13:M:114:ASP:N	2.39	0.56
1:A:776:U:OP1	27:a:41:ARG:NH1	2.38	0.56
1:A:3177:G:N7	7:G:167:ASN:ND2	2.53	0.56
1:A:1468:A:N6	1:A:1508:C:O2	2.39	0.56
28:b:216:VAL:HG11	28:b:227:GLY:HA3	1.86	0.56
1:A:1302:A:N7	1:A:2857:C:O2'	2.38	0.56
2:B:184:ARG:NH2	39:m:14:TYR:OH	2.36	0.56
2:B:234:LYS:HG2	2:B:238:ILE:HD11	1.88	0.56
8:H:207:ASP:OD1	8:H:207:ASP:N	2.38	0.56
11:K:21:ARG:HB3	15:O:196:THR:HG22	1.88	0.56
31:e:78:ASN:N	31:e:78:ASN:OD1	2.39	0.56
40:n:68:ARG:NH2	40:n:131:ASP:O	2.39	0.56
1:A:148:G:OP2	15:O:4:TYR:OH	2.24	0.56
19:S:12:ARG:NH1	19:S:57:GLU:OE2	2.35	0.56
1:A:1355:A:OP1	17:Q:31:LYS:NZ	2.40	0.55
1:A:1953:G:O2'	1:A:2094:C:N3	2.38	0.55
13:M:43:LYS:HA	13:M:59:ASN:HA	1.87	0.55
1:A:1096:U:OP2	20:T:116:ARG:NH2	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:U:O2	11:K:12:ASN:ND2	2.40	0.55
1:A:1128:U:OP1	9:q:4:ARG:NH2	2.37	0.55
1:A:2759:U:H5''	1:A:2760:C:H5'	1.88	0.55
3:C:284:ARG:NH2	3:C:295:ALA:O	2.39	0.55
33:g:11:ASN:O	33:g:18:ASN:ND2	2.39	0.55
2:B:225:ILE:CG1	2:B:235:ALA:O	2.54	0.55
3:C:106:TRP:O	3:C:137:TYR:OH	2.25	0.55
14:N:130:VAL:HG21	14:N:145:VAL:HG11	1.87	0.55
29:c:9:SER:N	29:c:104:LEU:O	2.39	0.55
39:m:79:VAL:HA	39:m:82:THR:HG22	1.89	0.55
1:A:65:A:N1	1:A:109:A:O2'	2.40	0.55
1:A:1261:G:O2'	1:A:1278:A:N6	2.38	0.55
1:A:1345:G:H21	4:D:307:GLN:HE22	1.54	0.55
5:E:59:ILE:HG21	5:E:65:ILE:HD12	1.89	0.55
1:A:785:G:O6	14:N:77:LYS:NZ	2.40	0.55
1:A:1127:G:OP2	9:q:98:ARG:NH1	2.39	0.55
18:R:105:LEU:HD23	18:R:138:LEU:HD23	1.88	0.55
28:b:229:PHE:CD1	28:b:229:PHE:C	2.85	0.55
1:A:1127:G:N2	1:A:1130:A:OP2	2.39	0.55
33:g:38:LEU:O	33:g:58:ARG:NH2	2.40	0.55
1:A:945:C:OP1	31:e:36:LYS:NZ	2.40	0.55
1:A:2180:G:OP1	2:B:174:ARG:NH2	2.40	0.55
1:A:3333:G:N2	1:A:3369:G:O2'	2.39	0.55
6:F:90:MET:HB2	6:F:144:ILE:HG23	1.89	0.55
40:n:24:CYS:HB3	40:n:48:ILE:HG22	1.89	0.55
20:T:106:LEU:HA	20:T:109:VAL:HG12	1.89	0.55
1:A:1150:A:N6	1:A:2369:G:O2'	2.40	0.54
20:T:119:ALA:HA	20:T:122:GLN:HB2	1.89	0.54
1:A:3214:U:OP2	13:M:128:ARG:NH1	2.41	0.54
9:q:30:LYS:HG3	9:q:63:GLU:HB3	1.89	0.54
12:L:18:PRO:HA	12:L:51:ALA:HA	1.87	0.54
1:A:3304:U:P	3:C:332:ARG:NH2	2.80	0.54
1:A:3316:A:OP1	1:A:3318:G:N2	2.40	0.54
1:A:2514:U:O2	1:A:2593:A:N6	2.39	0.54
4:D:61:SER:O	4:D:61:SER:OG	2.24	0.54
12:L:65:GLY:H	12:L:70:ARG:HH21	1.55	0.54
15:O:5:LYS:HG3	34:h:40:VAL:HG11	1.88	0.54
1:A:813:G:O6	1:A:926:A:N6	2.41	0.54
1:A:1307:G:OP1	10:J:59:LYS:NZ	2.39	0.54
1:A:1858:A:H1'	33:g:4:ARG:HD3	1.88	0.54
11:K:70:ARG:NH1	11:K:71:ALA:O	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1632:A:OP1	25:Y:48:ARG:NH2	2.41	0.54
1:A:2588:U:OP1	8:H:241:LYS:NZ	2.38	0.54
1:A:2912:G:N2	1:A:3014:U:OP1	2.41	0.54
8:H:183:LYS:HB3	8:H:194:THR:HG23	1.90	0.54
40:n:119:PRO:HD2	40:n:146:ILE:HG23	1.89	0.54
1:A:1722:U:OP2	18:R:103:ARG:NH1	2.41	0.54
1:A:2157:G:N2	2:B:126:LEU:O	2.40	0.54
4:D:300:ARG:NH1	4:D:301:PRO:O	2.41	0.54
20:T:68:THR:OG1	20:T:71:SER:OG	2.26	0.54
1:A:1156:C:OP2	28:b:94:LYS:NZ	2.41	0.54
1:A:2463:G:H1	1:A:2493:U:H4'	1.72	0.54
1:A:2516:U:O2'	1:A:2595:A:N6	2.41	0.54
3:C:214:MET:O	3:C:341:SER:OG	2.26	0.54
23:W:110:VAL:HG13	23:W:124:VAL:HG12	1.90	0.54
1:A:52:A:N3	1:A:811:U:O2'	2.41	0.54
1:A:860:G:OP1	39:m:17:ARG:NH2	2.39	0.54
28:b:229:PHE:HD1	28:b:230:GLY:N	2.06	0.53
1:A:2550:U:N3	8:H:36:ILE:O	2.38	0.53
3:C:17:LEU:HG	3:C:18:PRO:HD2	1.90	0.53
10:J:187:SER:OG	10:J:188:ASP:N	2.41	0.53
16:P:75:LEU:O	16:P:112:LYS:NZ	2.39	0.53
1:A:2476:C:OP2	1:A:2480:A:N6	2.40	0.53
9:q:192:ASP:HA	9:q:197:VAL:HG23	1.90	0.53
10:J:60:ALA:HA	10:J:69:PRO:HD2	1.91	0.53
38:l:36:PHE:O	38:l:41:ARG:NH1	2.39	0.53
1:A:86:G:O2'	1:A:98:G:O6	2.24	0.53
5:E:137:ARG:NH1	44:x:28:C:OP1	2.42	0.53
8:H:91:PHE:O	8:H:95:ASN:ND2	2.40	0.53
44:x:72:A:O2'	44:x:74:C:OP2	2.26	0.53
1:A:3050:U:O2'	42:v:16:GLY:O	2.27	0.53
6:F:112:ILE:HB	6:F:126:VAL:HG13	1.90	0.53
17:Q:147:ARG:HB2	17:Q:150:VAL:HG23	1.91	0.53
1:A:501:A:OP1	7:G:82:ARG:NH1	2.41	0.53
22:V:98:THR:OG1	22:V:102:GLU:OE2	2.27	0.53
2:B:65:ASP:OD2	2:B:70:ARG:NH2	2.42	0.53
5:E:101:ASN:OD1	5:E:101:ASN:N	2.42	0.53
16:P:184:ASP:OD2	16:P:187:THR:OG1	2.27	0.53
1:A:1874:A:N7	18:R:20:ARG:NH1	2.57	0.53
2:B:80:GLU:HG3	2:B:170:ALA:HA	1.90	0.53
6:F:17:THR:HB	6:F:28:VAL:HG22	1.91	0.53
1:A:713:U:O5'	11:K:171:ARG:NH2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:GLY:HA2	2:B:207:VAL:HG12	1.90	0.53
19:S:13:ARG:NH2	19:S:50:LYS:O	2.42	0.53
38:l:92:GLU:HG2	38:l:94:GLY:H	1.74	0.53
1:A:358:G:N2	1:A:361:A:OP2	2.41	0.52
1:A:1382:G:N2	4:D:241:GLY:O	2.39	0.52
1:A:1410:U:H4'	31:e:75:LEU:HD11	1.90	0.52
3:C:86:VAL:HG22	3:C:162:VAL:HG12	1.90	0.52
4:D:138:ARG:HH21	4:D:240:PRO:HD2	1.73	0.52
9:q:14:ASN:O	9:q:128:ARG:NH2	2.32	0.52
11:K:47:ALA:O	11:K:137:GLN:NE2	2.33	0.52
1:A:1863:G:N1	1:A:1866:C:OP2	2.39	0.52
1:A:2137:U:OP2	1:A:2142:A:N6	2.38	0.52
9:q:206:LEU:HD23	16:P:289:LYS:HD2	1.91	0.52
21:U:24:VAL:HG12	21:U:86:LYS:HG2	1.92	0.52
22:V:61:THR:HG23	22:V:62:VAL:HG22	1.90	0.52
40:n:107:VAL:HB	40:n:118:HIS:HB3	1.91	0.52
1:A:2836:C:H5	1:A:2852:C:H42	1.58	0.52
2:B:126:LEU:HD21	2:B:150:LEU:CD2	2.35	0.52
29:c:40:LYS:HE2	29:c:95:ALA:HB2	1.92	0.52
38:l:25:VAL:HG12	38:l:72:LEU:HB3	1.92	0.52
1:A:2897:A:OP2	41:t:124:LYS:NZ	2.40	0.52
1:A:3186:A:N3	6:F:44:THR:OG1	2.39	0.52
1:A:937:G:N2	1:A:961:C:OP1	2.42	0.52
3:C:17:LEU:CG	3:C:18:PRO:HD2	2.38	0.52
17:Q:83:VAL:HG12	17:Q:85:GLY:H	1.74	0.52
1:A:383:G:N2	1:A:386:A:OP2	2.38	0.52
10:J:35:VAL:HG13	10:J:107:ILE:HG12	1.92	0.52
16:P:22:ARG:HD3	44:x:7:G:H5''	1.91	0.52
1:A:543:C:N4	1:A:548:G:O6	2.43	0.52
1:A:1793:C:OP2	39:m:49:ARG:NH2	2.40	0.52
1:A:2307:G:O2'	1:A:2310:U:OP2	2.28	0.52
1:A:2445:A:OP1	34:h:62:ARG:NH1	2.42	0.52
1:A:3039:C:OP1	3:C:62:ARG:NH2	2.42	0.52
3:C:35:ASP:HB3	3:C:37:ARG:HE	1.73	0.52
3:C:58:ARG:NH1	3:C:74:GLU:OE2	2.43	0.52
14:N:85:ASP:N	14:N:85:ASP:OD1	2.43	0.52
17:Q:6:THR:OG1	17:Q:7:SER:N	2.43	0.52
35:i:28:HIS:HD2	35:i:31:LYS:HB2	1.75	0.52
2:B:225:ILE:O	2:B:238:ILE:O	2.28	0.52
33:g:58:ARG:HD3	33:g:59:PRO:HD2	1.92	0.52
3:C:17:LEU:HG	3:C:18:PRO:CD	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:VAL:O	10:J:100:ARG:NH1	2.43	0.52
30:d:11:GLU:O	30:d:72:ARG:NH2	2.43	0.52
1:A:609:G:N7	4:D:308:LYS:NZ	2.57	0.51
1:A:815:G:OP2	35:i:31:LYS:NZ	2.43	0.51
1:A:1334:U:H5''	28:b:206:LYS:HB3	1.92	0.51
1:A:1364:C:OP1	28:b:110:ARG:NH2	2.44	0.51
2:B:130:SER:OG	2:B:174:ARG:NH1	2.43	0.51
1:A:2162:U:OP1	2:B:234:LYS:NZ	2.41	0.51
1:A:2586:G:O6	8:H:242:ALA:N	2.40	0.51
1:A:2727:A:OP2	1:A:2728:G:N2	2.41	0.51
4:D:328:ASN:OD1	28:b:48:ASN:ND2	2.41	0.51
26:Z:48:ARG:NH2	45:y:49:G:OP2	2.40	0.51
26:Z:63:ARG:NH2	45:y:97:A:OP1	2.41	0.51
30:d:79:ARG:NH1	30:d:81:GLU:OE2	2.42	0.51
40:n:10:SER:OG	40:n:12:GLU:OE1	2.29	0.51
1:A:353:G:O6	35:i:55:ARG:NH2	2.42	0.51
2:B:149:ARG:HH21	2:B:153:GLY:HA2	1.75	0.51
2:B:177:LYS:NZ	39:m:33:GLN:OE1	2.43	0.51
3:C:113:GLU:OE1	3:C:167:ARG:HD2	2.11	0.51
16:P:141:PRO:HB2	16:P:172:TYR:HB2	1.93	0.51
7:G:51:ARG:NH1	7:G:161:ALA:O	2.42	0.51
9:q:29:SER:HB3	9:q:125:LEU:HD12	1.93	0.51
28:b:208:SER:OG	28:b:209:ASN:N	2.42	0.51
1:A:1208:U:O2	41:t:109:ASN:ND2	2.42	0.51
30:d:13:THR:OG1	30:d:72:ARG:NH2	2.43	0.51
36:j:42:LYS:HG2	36:j:55:VAL:HG22	1.93	0.51
1:A:873:C:H3'	1:A:874:U:H4'	1.92	0.51
1:A:1522:U:OP2	23:W:121:LYS:NZ	2.44	0.51
1:A:3003:G:O2'	3:C:92:TYR:OH	2.29	0.51
22:V:30:PRO:HA	22:V:33:TYR:HB3	1.92	0.51
40:n:39:GLU:HA	40:n:42:LEU:HB3	1.92	0.51
1:A:2116:G:OP1	1:A:2118:C:N4	2.44	0.51
1:A:3350:C:N4	1:A:3352:U:O2	2.44	0.51
1:A:2465:G:N7	1:A:2467:G:N2	2.58	0.50
1:A:2677:G:H1	1:A:2680:A:H62	1.59	0.50
24:X:32:SER:HA	24:X:49:PRO:HA	1.92	0.50
40:n:61:ARG:NH2	40:n:194:GLY:O	2.43	0.50
44:x:29:C:O2'	44:x:51:A:N1	2.36	0.50
1:A:439:C:H1'	1:A:495:G:H1'	1.93	0.50
1:A:929:A:OP1	4:D:61:SER:OG	2.23	0.50
1:A:1055:A:N3	44:x:81:U:O2'	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:93:LYS:NZ	40:n:95:GLN:OE1	2.43	0.50
1:A:1474:A:O2'	30:d:57:GLN:OE1	2.29	0.50
1:A:3024:A:N6	1:A:3031:G:O2'	2.44	0.50
1:A:3174:A:N6	1:A:3175:U:O4	2.43	0.50
1:A:3217:C:O2'	1:A:3219:G:OP1	2.28	0.50
16:P:272:TYR:OH	44:x:22:A:N6	2.45	0.50
1:A:2111:G:H1'	42:v:44:LYS:HD2	1.93	0.50
8:H:59:GLN:NE2	45:y:150:G:O2'	2.45	0.50
25:Y:33:SER:OG	25:Y:34:LYS:N	2.43	0.50
1:A:3193:C:H42	1:A:3199:G:H1	1.59	0.50
8:H:128:LYS:HD2	8:H:129:PRO:HD2	1.92	0.50
40:n:66:ASN:HB3	40:n:69:GLY:H	1.76	0.50
18:R:30:SER:O	18:R:34:GLN:NE2	2.43	0.50
24:X:31:LEU:HB3	24:X:101:PRO:HG2	1.94	0.50
45:y:81:U:H4'	45:y:82:U:H5'	1.93	0.50
1:A:577:C:O2'	1:A:579:G:OP1	2.24	0.50
10:J:156:GLU:OE2	10:J:159:ARG:NH1	2.43	0.50
1:A:1518:U:H5'	43:z:384:ARG:HH22	1.76	0.50
1:A:2259:A:OP1	1:A:2260:U:N3	2.44	0.50
26:Z:113:GLN:NE2	26:Z:114:ARG:O	2.45	0.50
35:i:63:ARG:NH2	45:y:58:G:O6	2.45	0.50
1:A:412:G:OP1	21:U:62:ARG:NH1	2.44	0.49
1:A:1231:A:H5''	1:A:1232:C:H5'	1.94	0.49
1:A:1385:C:O2	7:G:2:SER:N	2.44	0.49
1:A:1947:G:O6	1:A:2100:A:N6	2.45	0.49
14:N:101:VAL:HG22	14:N:124:ILE:HD11	1.93	0.49
1:A:911:C:H5''	2:B:15:ILE:HD13	1.94	0.49
5:E:17:LEU:HD13	5:E:129:VAL:HB	1.94	0.49
12:L:109:MET:SD	12:L:132:ASN:ND2	2.83	0.49
16:P:197:SER:O	16:P:202:GLY:N	2.45	0.49
19:S:80:ARG:HG2	19:S:122:HIS:HB2	1.93	0.49
22:V:54:VAL:HG23	22:V:67:SER:HB2	1.93	0.49
1:A:2890:A:O2'	1:A:2933:A:N3	2.42	0.49
3:C:54:THR:OG1	3:C:360:ASP:O	2.31	0.49
25:Y:26:VAL:HG12	25:Y:27:LYS:HG2	1.94	0.49
40:n:21:ASN:OD1	40:n:156:ASN:ND2	2.46	0.49
1:A:1481:A:N3	1:A:1858:A:O2'	2.46	0.49
1:A:1692:U:HO2'	1:A:1754:G:HO2'	1.60	0.49
1:A:1729:A:N6	29:c:47:ASN:O	2.45	0.49
1:A:2356:A:H61	1:A:2983:C:H5	1.60	0.49
1:A:2406:C:HO2'	1:A:2619:G:H21	1.58	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2964:G:N2	1:A:2967:A:OP2	2.46	0.49
4:D:190:GLY:O	4:D:193:LYS:NZ	2.45	0.49
5:E:172:LEU:HD22	5:E:174:LYS:HZ3	1.77	0.49
19:S:8:GLN:HB3	19:S:64:ILE:HD11	1.94	0.49
26:Z:83:LYS:O	35:i:73:ARG:NH2	2.46	0.49
1:A:353:G:O2'	1:A:364:G:O6	2.29	0.49
1:A:3185:U:HO2'	19:S:170:THR:HG1	1.57	0.49
2:B:112:ILE:HG22	2:B:135:ILE:HG12	1.94	0.49
25:Y:101:PHE:HA	25:Y:106:GLN:HG2	1.95	0.49
7:G:89:THR:HG21	13:M:115:PHE:HB2	1.94	0.49
8:H:41:GLN:OE1	8:H:44:ARG:NH2	2.45	0.49
22:V:104:ARG:HH21	22:V:106:ALA:HB2	1.77	0.49
40:n:18:LYS:HB3	40:n:25:LEU:HB2	1.94	0.49
40:n:154:LEU:HA	40:n:159:GLY:HA2	1.95	0.49
43:z:404:LEU:HA	43:z:407:ASN:HD21	1.77	0.49
1:A:158:G:H2'	1:A:159:A:H8	1.78	0.49
1:A:3395:G:N2	1:A:3396:U:O4	2.44	0.49
16:P:200:PHE:HB3	16:P:237:GLU:HG2	1.94	0.49
1:A:1201:C:N4	1:A:2857:C:OP1	2.43	0.49
1:A:1907:C:O2	3:C:240:ARG:NH2	2.45	0.49
18:R:68:GLN:NE2	18:R:72:GLU:OE2	2.45	0.49
28:b:74:SER:OG	28:b:75:TYR:N	2.43	0.49
35:i:21:ARG:HD2	35:i:39:TYR:HD1	1.76	0.49
1:A:1699:A:O2'	36:j:3:ARG:NH1	2.46	0.49
3:C:331:ASN:HB2	3:C:334:ARG:NH2	2.28	0.49
9:q:140:THR:OG1	9:q:141:LYS:N	2.44	0.49
18:R:147:ALA:O	18:R:151:ARG:NH1	2.45	0.49
1:A:679:U:O2'	1:A:788:C:O2	2.29	0.48
1:A:1740:U:H4'	1:A:1741:A:H5'	1.95	0.48
1:A:2841:G:N2	1:A:2898:G:O6	2.45	0.48
1:A:3151:U:OP1	3:C:128:LYS:NZ	2.45	0.48
40:n:116:LEU:HD22	40:n:140:GLN:HE21	1.78	0.48
1:A:1678:G:OP2	22:V:77:LYS:NZ	2.43	0.48
1:A:2335:G:N2	1:A:2339:C:O2'	2.45	0.48
1:A:2433:U:H1'	15:O:125:SER:HB2	1.96	0.48
4:D:42:VAL:HG12	4:D:236:LEU:HD21	1.96	0.48
20:T:91:LEU:HD12	20:T:96:ILE:HD11	1.96	0.48
1:A:26:A:N3	1:A:328:U:O2'	2.42	0.48
1:A:3068:U:OP2	18:R:62:ARG:NH2	2.34	0.48
31:e:23:ASP:OD1	31:e:23:ASP:N	2.39	0.48
1:A:2356:A:H5'	21:U:138:LYS:HE3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2465:G:N2	1:A:2491:A:O2'	2.46	0.48
5:E:99:THR:OG1	5:E:101:ASN:OD1	2.31	0.48
31:e:79:VAL:HG22	31:e:108:ILE:HG22	1.96	0.48
2:B:117:GLU:CB	2:B:122:ASP:OD1	2.61	0.48
5:E:84:LEU:HD23	5:E:87:LYS:HB2	1.95	0.48
21:U:30:ARG:NH1	21:U:31:GLU:OE1	2.47	0.48
33:g:46:ASP:OD2	33:g:88:ARG:NH2	2.39	0.48
44:x:11:A:O2'	44:x:13:A:OP2	2.32	0.48
1:A:901:G:H5''	35:i:13:ASN:HD21	1.79	0.48
1:A:3018:C:OP1	40:n:9:ASN:ND2	2.38	0.48
5:E:49:LYS:HB3	5:E:62:ASN:HA	1.96	0.48
13:M:85:TRP:NE1	13:M:91:CYS:SG	2.71	0.48
16:P:282:ARG:NE	44:x:63:A:OP2	2.46	0.48
1:A:175:C:O2	1:A:244:G:N2	2.47	0.48
1:A:2572:C:O2'	25:Y:61:LYS:NZ	2.46	0.48
25:Y:51:LEU:HD11	25:Y:65:ARG:HH11	1.79	0.48
1:A:348:A:N3	1:A:352:A:O2'	2.46	0.48
1:A:2939:G:H5'	3:C:2:SER:HA	1.96	0.48
2:B:118:GLU:HG2	2:B:126:LEU:HD13	1.96	0.48
20:T:68:THR:HG1	20:T:71:SER:HG	1.53	0.48
40:n:68:ARG:HA	40:n:92:VAL:HG12	1.95	0.48
1:A:351:A:N6	37:k:37:TYR:O	2.46	0.48
1:A:3323:A:N6	1:A:3383:G:O6	2.47	0.48
28:b:156:ILE:HD12	28:b:161:VAL:HG21	1.94	0.48
34:h:34:SER:OG	34:h:35:ASN:N	2.46	0.48
35:i:17:THR:OG1	35:i:18:LEU:N	2.47	0.48
1:A:1493:G:O6	37:k:2:ALA:N	2.47	0.47
4:D:264:SER:OG	4:D:265:GLU:N	2.47	0.47
16:P:72:ASP:H	44:x:115:G:H21	1.60	0.47
40:n:6:GLN:NE2	40:n:11:ASN:OD1	2.39	0.47
1:A:1639:C:OP2	33:g:74:ARG:NH2	2.46	0.47
1:A:1705:U:O2	1:A:1786:G:O2'	2.33	0.47
1:A:3119:U:O3'	41:t:111:ARG:NH2	2.47	0.47
3:C:290:ASP:O	3:C:293:ASN:ND2	2.48	0.47
4:D:3:ARG:HH22	4:D:27:SER:HB3	1.79	0.47
10:J:188:ASP:N	10:J:188:ASP:OD1	2.41	0.47
22:V:20:SER:OG	22:V:61:THR:OG1	2.32	0.47
32:f:49:ILE:HG23	32:f:100:ILE:HG13	1.96	0.47
1:A:286:U:O2'	15:O:179:LYS:O	2.30	0.47
1:A:1134:G:O2'	1:A:2642:A:N3	2.46	0.47
4:D:2:SER:OG	4:D:3:ARG:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:82:THR:HG23	4:D:84:ARG:H	1.80	0.47
1:A:980:A:O2'	1:A:981:U:O4'	2.33	0.47
1:A:2828:G:OP1	9:q:7:ARG:NH1	2.43	0.47
2:B:130:SER:HB2	2:B:171:GLY:HA3	1.96	0.47
3:C:70:ARG:HH21	40:n:55:GLY:HA2	1.79	0.47
3:C:331:ASN:HB2	3:C:334:ARG:HH21	1.79	0.47
12:L:136:VAL:H	40:n:100:ARG:HH12	1.61	0.47
20:T:103:GLN:O	20:T:107:GLU:N	2.47	0.47
30:d:11:GLU:HG2	30:d:74:ARG:HB3	1.95	0.47
1:A:148:G:OP2	15:O:49:ARG:NH1	2.48	0.47
1:A:153:U:OP2	26:Z:103:LYS:NZ	2.42	0.47
2:B:70:ARG:HH21	2:B:72:ARG:HD2	1.78	0.47
16:P:269:SER:CB	44:x:1:G:H21	2.27	0.47
22:V:50:LEU:HD12	22:V:50:LEU:C	2.38	0.47
1:A:2549:G:O2'	1:A:2550:U:O2	2.32	0.47
3:C:237:LYS:HE3	3:C:246:LEU:HD21	1.95	0.47
8:H:140:VAL:HG22	8:H:166:LEU:HD21	1.96	0.47
14:N:149:ALA:HA	34:h:15:LYS:HB2	1.96	0.47
25:Y:54:THR:HG23	25:Y:56:LYS:H	1.79	0.47
29:c:10:ILE:HD12	29:c:13:LYS:HD3	1.95	0.47
1:A:8:C:H42	45:y:149:A:H61	1.61	0.47
1:A:89:A:N7	17:Q:171:LYS:NZ	2.63	0.47
1:A:1356:U:O4	7:G:9:TRP:NE1	2.48	0.47
1:A:1560:G:N2	1:A:1580:A:N1	2.63	0.47
1:A:2177:G:H2'	2:B:128:ARG:HD3	1.95	0.47
1:A:2469:G:H1	1:A:2477:G:H8	1.63	0.47
1:A:3048:A:OP2	3:C:222:LYS:NZ	2.38	0.47
4:D:351:PRO:HB3	28:b:70:LYS:HB3	1.97	0.47
29:c:57:GLU:OE2	29:c:69:TYR:OH	2.32	0.47
40:n:162:HIS:O	40:n:165:THR:OG1	2.32	0.47
1:A:2531:C:H5	1:A:2542:U:H3	1.62	0.47
1:A:2761:G:N7	38:l:63:LYS:NZ	2.50	0.47
40:n:109:CYS:HB2	40:n:149:GLY:HA2	1.97	0.47
16:P:60:ILE:HB	16:P:80:SER:HB3	1.97	0.47
24:X:86:THR:OG1	24:X:95:VAL:O	2.33	0.47
1:A:1566:A:O2'	1:A:1573:G:N1	2.45	0.47
16:P:127:GLY:HA3	16:P:196:ARG:HB2	1.96	0.47
34:h:79:SER:OG	34:h:80:PHE:N	2.48	0.47
1:A:1131:G:N2	1:A:2372:A:OP2	2.44	0.46
2:B:59:ALA:HB2	2:B:78:ALA:HB2	1.96	0.46
8:H:203:VAL:HG21	8:H:211:LEU:HD22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:A:O3'	35:i:45:ARG:NH2	2.49	0.46
1:A:1389:G:H5''	31:e:101:SER:HB3	1.97	0.46
1:A:2516:U:OP1	15:O:31:ARG:NH1	2.47	0.46
5:E:92:ARG:HG2	5:E:95:ASN:HB2	1.98	0.46
7:G:39:VAL:O	7:G:87:THR:OG1	2.25	0.46
16:P:278:SER:OG	16:P:279:LYS:N	2.48	0.46
21:U:115:SER:OG	21:U:116:HIS:N	2.48	0.46
1:A:964:G:OP2	1:A:1115:G:N1	2.45	0.46
40:n:24:CYS:SG	40:n:25:LEU:N	2.88	0.46
40:n:51:THR:HG21	40:n:84:LEU:HD11	1.97	0.46
40:n:116:LEU:HD21	40:n:177:LEU:HD22	1.97	0.46
1:A:38:U:H4'	14:N:32:ARG:HD2	1.96	0.46
1:A:1144:U:OP1	1:A:1367:G:O2'	2.33	0.46
1:A:3057:U:O2'	1:A:3059:G:OP1	2.32	0.46
1:A:107:A:O2'	1:A:324:A:N3	2.41	0.46
1:A:269:G:N2	1:A:295:A:OP2	2.41	0.46
1:A:1063:G:C6	20:T:109:VAL:HG23	2.50	0.46
1:A:2534:G:O2'	1:A:2535:A:N7	2.40	0.46
1:A:2660:G:OP1	1:A:2750:U:O2'	2.33	0.46
2:B:107:VAL:HB	2:B:111:THR:HG21	1.97	0.46
2:B:113:VAL:HG12	2:B:166:ILE:HG12	1.97	0.46
16:P:265:TYR:O	16:P:269:SER:OG	2.29	0.46
44:x:38:U:N3	44:x:41:G:OP2	2.42	0.46
1:A:585:A:H4'	32:f:72:THR:HG22	1.97	0.46
1:A:2349:U:O2'	1:A:3307:A:N3	2.47	0.46
1:A:3277:U:O2'	1:A:3278:C:O4'	2.34	0.46
7:G:110:LYS:HB3	7:G:110:LYS:HE2	1.77	0.46
12:L:74:MET:HE2	12:L:74:MET:HB3	1.78	0.46
35:i:27:PHE:HA	35:i:34:CYS:HA	1.98	0.46
40:n:97:VAL:HG21	40:n:104:LEU:HD11	1.97	0.46
1:A:1940:G:H21	1:A:3362:A:H8	1.64	0.46
1:A:3194:C:O2	1:A:3199:G:N2	2.48	0.46
22:V:50:LEU:CB	22:V:54:VAL:CG1	2.90	0.46
23:W:77:GLU:HA	23:W:133:LEU:HD21	1.97	0.46
24:X:13:ARG:NE	45:y:24:G:OP2	2.49	0.46
1:A:399:A:O2'	1:A:403:C:O2'	2.27	0.46
10:J:136:THR:HG22	10:J:138:GLY:H	1.81	0.46
19:S:66:GLU:OE2	19:S:99:ARG:N	2.45	0.46
1:A:640:U:OP1	14:N:21:ARG:NH2	2.42	0.46
1:A:1210:U:H5''	6:F:62:ARG:HD3	1.98	0.46
1:A:1348:U:H5''	1:A:1355:A:H61	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2185:G:O2'	1:A:2314:U:OP2	2.26	0.46
3:C:360:ASP:OD2	42:v:17:ARG:NH2	2.49	0.46
45:y:80:A:H8	45:y:81:U:H3	1.64	0.46
1:A:2447:A:N6	1:A:2500:A:N7	2.64	0.46
1:A:2470:C:H3'	1:A:2471:U:H4'	1.98	0.45
3:C:115:LYS:NZ	3:C:129:ALA:O	2.49	0.45
31:e:72:LYS:HD2	31:e:92:TYR:HE1	1.81	0.45
1:A:152:U:OP1	26:Z:106:LYS:NZ	2.47	0.45
1:A:224:C:O2	24:X:102:SER:OG	2.33	0.45
1:A:598:A:O3'	4:D:332:LYS:NZ	2.49	0.45
1:A:1638:A:H5''	33:g:74:ARG:HH22	1.81	0.45
1:A:2950:G:OP2	1:A:2950:G:N2	2.43	0.45
4:D:45:ASN:HA	4:D:110:ASN:HB3	1.98	0.45
5:E:7:ASN:ND2	5:E:8:PRO:O	2.50	0.45
5:E:99:THR:O	5:E:154:THR:OG1	2.33	0.45
44:x:1:G:O6	44:x:120:C:N3	2.49	0.45
1:A:1129:A:N3	1:A:2826:U:O2'	2.44	0.45
6:F:46:THR:HG23	6:F:54:LYS:HB3	1.99	0.45
23:W:68:THR:HA	23:W:73:MET:HE3	1.99	0.45
1:A:694:C:H4'	4:D:232:SER:HA	1.98	0.45
1:A:1814:A:H5'	1:A:1816:A:H1'	1.98	0.45
2:B:204:MET:HB3	2:B:208:ASP:HB2	1.98	0.45
3:C:153:LYS:HG2	3:C:154:TYR:HD1	1.82	0.45
7:G:38:THR:HG22	7:G:90:LYS:HG2	1.96	0.45
11:K:185:LYS:HA	11:K:185:LYS:HD2	1.82	0.45
23:W:108:LEU:HB2	23:W:127:THR:HB	1.97	0.45
1:A:69:C:OP1	15:O:178:HIS:ND1	2.43	0.45
1:A:1103:A:H61	1:A:1364:C:H5'	1.82	0.45
1:A:1624:G:O2'	1:A:1643:A:N1	2.43	0.45
2:B:95:SER:OG	2:B:96:LEU:N	2.50	0.45
16:P:161:GLY:O	16:P:165:GLY:N	2.48	0.45
1:A:860:G:OP1	39:m:18:TYR:OH	2.33	0.45
1:A:215:G:H5''	24:X:12:ARG:HE	1.81	0.45
1:A:912:G:N7	2:B:9:ARG:NH1	2.65	0.45
1:A:936:A:OP2	14:N:27:LYS:NZ	2.41	0.45
6:F:114:VAL:HG22	6:F:124:ARG:HB2	1.97	0.45
9:q:209:ASN:ND2	44:x:64:A:N7	2.60	0.45
12:L:29:SER:O	12:L:29:SER:OG	2.30	0.45
16:P:144:VAL:HG23	16:P:173:VAL:HG22	1.99	0.45
1:A:500:C:H4'	7:G:80:ASN:HD21	1.81	0.45
1:A:1718:G:OP1	18:R:118:HIS:ND1	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2157:G:N7	2:B:152:SER:OG	2.45	0.45
12:L:134:GLY:O	40:n:103:ALA:N	2.40	0.45
13:M:24:LYS:HG3	13:M:25:LYS:HG3	1.97	0.45
1:A:544:C:O2'	1:A:548:G:N2	2.50	0.45
1:A:2221:G:O6	34:h:71:LYS:NZ	2.45	0.45
2:B:79:ASN:HA	2:B:170:ALA:H	1.82	0.45
3:C:212:ASN:OD1	3:C:212:ASN:N	2.50	0.45
5:E:166:LYS:HD2	5:E:166:LYS:HA	1.74	0.45
14:N:126:LYS:HB3	14:N:126:LYS:HE2	1.72	0.45
1:A:2208:A:O2'	1:A:2209:U:O2	2.35	0.45
1:A:2895:G:O2'	41:t:100:TYR:O	2.31	0.45
1:A:3121:U:H1'	1:A:3122:A:H5''	1.98	0.45
7:G:18:LEU:H	7:G:18:LEU:HG	1.67	0.45
11:K:76:THR:HG22	11:K:101:ARG:HB3	1.99	0.45
40:n:206:THR:OG1	40:n:207:GLY:N	2.50	0.45
1:A:1132:C:H2'	1:A:1133:A:C8	2.52	0.44
7:G:52:VAL:HG12	7:G:74:VAL:HG11	1.99	0.44
39:m:42:CYS:HB2	39:m:60:CYS:HB2	1.98	0.44
1:A:2563:G:OP2	25:Y:55:LYS:NZ	2.50	0.44
4:D:237:GLN:O	4:D:246:ARG:NH1	2.48	0.44
16:P:285:ARG:NH2	44:x:62:U:O3'	2.50	0.44
19:S:112:ALA:O	19:S:115:ARG:NH1	2.50	0.44
20:T:11:THR:HG22	20:T:14:MET:HE3	1.99	0.44
32:f:54:ARG:HG2	32:f:64:ILE:HG22	1.99	0.44
45:y:44:A:N6	45:y:58:G:O6	2.50	0.44
25:Y:83:THR:OG1	25:Y:84:ARG:N	2.50	0.44
26:Z:83:LYS:NZ	45:y:38:U:O2'	2.33	0.44
33:g:66:SER:O	33:g:70:LYS:NZ	2.47	0.44
40:n:143:SER:OG	40:n:162:HIS:NE2	2.47	0.44
1:A:1307:G:OP1	10:J:58:ARG:NH1	2.49	0.44
1:A:1362:G:H1'	28:b:159:GLN:HG2	1.99	0.44
6:F:90:MET:HE2	6:F:179:ILE:HG22	1.98	0.44
15:O:73:ARG:HA	15:O:74:PRO:HD3	1.85	0.44
1:A:2585:G:H22	45:y:151:C:H3'	1.81	0.44
9:q:76:MET:HE2	9:q:148:VAL:HA	1.99	0.44
17:Q:41:ASP:OD1	17:Q:41:ASP:N	2.50	0.44
37:k:25:GLN:HB3	43:z:389:VAL:HG21	1.99	0.44
1:A:123:A:OP1	8:H:105:LYS:NZ	2.40	0.44
1:A:2103:U:H4'	18:R:85:ARG:HH22	1.83	0.44
1:A:3151:U:OP2	3:C:132:LYS:NZ	2.50	0.44
1:A:3304:U:P	3:C:332:ARG:HH22	2.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:332:ARG:NH1	3:C:333:LYS:HD2	2.32	0.44
19:S:66:GLU:CD	19:S:99:ARG:H	2.25	0.44
28:b:102:VAL:HG13	28:b:126:LEU:HD22	2.00	0.44
1:A:2196:C:H2'	1:A:2242:A:H61	1.83	0.44
5:E:91:LEU:HD23	5:E:91:LEU:HA	1.87	0.44
12:L:75:PRO:HG2	12:L:105:PRO:HD3	1.98	0.44
12:L:80:ARG:HB2	12:L:99:ALA:HB3	2.00	0.44
20:T:3:LYS:HB3	20:T:3:LYS:HE2	1.82	0.44
23:W:36:LYS:HA	23:W:36:LYS:HD3	1.84	0.44
44:x:77:G:O2'	44:x:101:G:O6	2.31	0.44
1:A:196:G:H22	1:A:199:A:H5'	1.83	0.44
1:A:1843:C:OP1	37:k:48:LYS:NZ	2.38	0.44
1:A:2842:U:H5''	1:A:2844:C:H41	1.82	0.44
1:A:3086:A:OP1	3:C:367:LYS:NZ	2.40	0.44
5:E:11:ASP:OD1	5:E:11:ASP:N	2.49	0.44
28:b:48:ASN:ND2	28:b:182:ASP:OD2	2.51	0.44
1:A:1126:G:H5''	9:q:119:TRP:HZ3	1.83	0.43
1:A:3018:C:H4'	40:n:8:GLU:HB3	1.99	0.43
4:D:152:VAL:HG21	4:D:156:LEU:HD22	1.98	0.43
5:E:100:GLY:O	5:E:159:THR:OG1	2.32	0.43
10:J:13:HIS:CE1	10:J:118:VAL:HG23	2.52	0.43
12:L:126:TRP:HB2	12:L:129:VAL:HG22	2.00	0.43
22:V:98:THR:OG1	22:V:99:LYS:N	2.51	0.43
29:c:55:GLU:HB3	33:g:94:LEU:HD11	2.00	0.43
1:A:518:G:OP2	1:A:518:G:N2	2.37	0.43
6:F:13:PRO:HD3	6:F:79:ILE:HD12	2.00	0.43
1:A:2631:U:OP1	1:A:2757:U:O2'	2.36	0.43
1:A:2792:A:OP1	38:l:67:LYS:NZ	2.51	0.43
1:A:3291:G:H2'	1:A:3292:A:C8	2.54	0.43
3:C:92:TYR:O	3:C:156:SER:N	2.42	0.43
5:E:137:ARG:NH2	44:x:44:C:OP2	2.51	0.43
7:G:58:LEU:HD22	7:G:102:ASN:HA	1.99	0.43
29:c:25:LEU:HG	29:c:87:VAL:HG21	2.01	0.43
35:i:84:SER:HB2	45:y:67:U:H4'	2.00	0.43
36:j:30:LYS:HA	36:j:30:LYS:HD3	1.75	0.43
40:n:100:ARG:NE	40:n:102:SER:O	2.51	0.43
1:A:2546:C:H2'	1:A:2547:A:H8	1.83	0.43
1:A:3008:A:OP2	10:J:73:ARG:NH1	2.52	0.43
19:S:129:ILE:HG23	19:S:134:ASP:HB2	2.00	0.43
24:X:74:TYR:OH	45:y:75:G:OP2	2.33	0.43
28:b:144:ILE:HD12	28:b:189:ILE:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:19:SER:OG	32:f:20:LYS:O	2.36	0.43
1:A:170:G:H3'	1:A:171:G:C8	2.54	0.43
1:A:1421:G:N2	7:G:2:SER:O	2.41	0.43
10:J:84:ARG:HE	10:J:84:ARG:HB3	1.65	0.43
20:T:17:ARG:HH11	20:T:47:SER:HB2	1.84	0.43
40:n:115:ALA:HB3	40:n:137:VAL:HG12	2.00	0.43
1:A:292:U:OP2	15:O:68:ARG:NH2	2.52	0.43
1:A:677:A:N1	1:A:703:G:O2'	2.47	0.43
1:A:1874:A:H5''	18:R:18:GLY:HA3	2.00	0.43
2:B:247:ARG:HE	2:B:247:ARG:HB2	1.64	0.43
31:e:71:HIS:ND1	31:e:90:LYS:O	2.44	0.43
38:l:54:THR:OG1	38:l:55:LYS:N	2.51	0.43
2:B:226:SER:OG	2:B:227:ARG:N	2.51	0.43
3:C:285:VAL:HA	3:C:322:ILE:HG22	1.99	0.43
19:S:159:SER:OG	19:S:161:LYS:O	2.36	0.43
24:X:45:ILE:HD11	24:X:119:ILE:HG23	1.99	0.43
32:f:47:LYS:HA	32:f:104:PRO:HD2	2.00	0.43
1:A:439:C:H3'	1:A:440:A:H3'	2.00	0.43
1:A:1575:A:H5'	1:A:1576:G:H2'	2.00	0.43
1:A:2618:G:C8	1:A:2865:U:H5''	2.54	0.43
1:A:2901:G:O2'	1:A:3024:A:N1	2.52	0.43
6:F:39:LYS:HA	6:F:39:LYS:HD2	1.92	0.43
11:K:153:ASP:HB3	11:K:157:ARG:HH22	1.84	0.43
22:V:94:ARG:HB3	22:V:108:TYR:CZ	2.54	0.43
26:Z:68:GLN:HA	26:Z:71:LYS:HB2	2.00	0.43
40:n:18:LYS:HA	40:n:18:LYS:HD3	1.83	0.43
40:n:118:HIS:HB2	40:n:146:ILE:HG22	2.01	0.43
1:A:1573:G:N7	1:A:1574:C:N4	2.66	0.43
1:A:2446:U:O2	1:A:2503:G:N1	2.51	0.43
7:G:55:LEU:HD11	7:G:66:SER:HB3	2.01	0.43
22:V:22:PRO:HB2	22:V:28:PHE:HB2	2.01	0.43
29:c:34:LEU:HD13	29:c:59:TYR:HB3	2.01	0.43
40:n:150:SER:HA	40:n:194:GLY:HA3	2.01	0.43
3:C:17:LEU:HD12	3:C:17:LEU:HA	1.81	0.43
4:D:48:GLN:HE21	4:D:48:GLN:HB3	1.57	0.43
8:H:154:ALA:HB2	8:H:186:LEU:HD12	2.01	0.43
18:R:15:VAL:HG11	18:R:52:LYS:HB2	2.01	0.43
21:U:111:LYS:HE3	21:U:153:LYS:HE2	2.01	0.43
1:A:268:A:N7	15:O:12:ARG:NH1	2.67	0.42
6:F:83:THR:OG1	6:F:84:LYS:N	2.52	0.42
26:Z:24:LEU:HB3	26:Z:51:ILE:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:83:LYS:HZ3	45:y:38:U:HO2'	1.59	0.42
31:e:36:LYS:HE2	31:e:36:LYS:HB2	1.87	0.42
35:i:32:LYS:NZ	45:y:111:A:OP1	2.40	0.42
1:A:2554:A:O5'	33:g:91:ARG:NH1	2.52	0.42
9:q:51:HIS:CD2	9:q:134:ILE:HD13	2.54	0.42
16:P:156:GLY:HA2	16:P:181:PRO:HD3	2.00	0.42
24:X:13:ARG:NH1	45:y:24:G:N7	2.67	0.42
1:A:577:C:H2'	1:A:579:G:H5''	2.02	0.42
1:A:691:A:N1	45:y:28:C:O2'	2.42	0.42
1:A:710:A:H2'	1:A:711:A:C8	2.54	0.42
1:A:2502:A:N1	8:H:70:LYS:NZ	2.66	0.42
2:B:97:ASN:H	2:B:100:ASN:HD22	1.67	0.42
32:f:16:TYR:OH	32:f:89:LEU:O	2.31	0.42
1:A:1481:A:O2'	1:A:1859:A:OP2	2.37	0.42
1:A:2538:U:O2'	1:A:2539:C:O4'	2.33	0.42
18:R:74:ARG:HD3	18:R:74:ARG:HA	1.87	0.42
19:S:99:ARG:NH2	19:S:126:VAL:O	2.53	0.42
40:n:197:MET:HE2	40:n:197:MET:HB2	1.94	0.42
1:A:268:A:C5	15:O:12:ARG:HD2	2.55	0.42
1:A:1003:A:N1	1:A:1049:C:O2'	2.50	0.42
1:A:2463:G:O6	1:A:2493:U:O2'	2.35	0.42
1:A:3304:U:O5'	3:C:332:ARG:NH2	2.53	0.42
28:b:101:LYS:HD2	28:b:101:LYS:HA	1.85	0.42
28:b:141:TYR:HB2	28:b:189:ILE:HG12	2.01	0.42
1:A:93:C:OP2	1:A:2764:C:O2'	2.30	0.42
1:A:269:G:OP1	15:O:47:LYS:NZ	2.37	0.42
1:A:1523:U:OP2	1:A:1604:G:O2'	2.37	0.42
1:A:1630:U:OP2	1:A:1813:A:N6	2.51	0.42
1:A:2424:A:H61	2:B:230:VAL:HG11	1.83	0.42
12:L:104:ASN:OD1	12:L:108:GLU:N	2.52	0.42
21:U:41:LEU:HD21	21:U:99:ALA:HB2	2.02	0.42
24:X:87:LYS:HD3	24:X:87:LYS:HA	1.89	0.42
2:B:237:LEU:HD23	2:B:237:LEU:H	1.82	0.42
40:n:1:MET:HB3	40:n:219:GLU:HG2	2.01	0.42
43:z:388:GLY:N	45:y:76:C:O2'	2.50	0.42
1:A:284:A:H5''	1:A:285:A:H5'	2.01	0.42
1:A:3060:C:O2	1:A:3332:U:O2'	2.29	0.42
19:S:44:PHE:HE1	19:S:122:HIS:HD2	1.68	0.42
1:A:168:U:H2'	1:A:169:U:C2	2.55	0.42
1:A:3002:C:OP1	3:C:26:ARG:NH2	2.52	0.42
1:A:3379:C:H4'	3:C:315:GLY:HA2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:103:ASN:OD1	11:K:103:ASN:N	2.47	0.42
16:P:85:ARG:NH2	16:P:86:TYR:OH	2.52	0.42
18:R:4:LEU:HD11	18:R:29:THR:HG22	2.01	0.42
40:n:167:VAL:HA	40:n:170:GLN:HG2	2.01	0.42
1:A:2186:U:H5	2:B:200:ARG:HD3	1.84	0.42
1:A:3129:A:N6	1:A:3131:U:O2	2.53	0.42
11:K:48:PRO:HB2	26:Z:116:TYR:O	2.20	0.42
14:N:88:ASP:N	14:N:88:ASP:OD1	2.42	0.42
19:S:24:LEU:HD22	19:S:59:VAL:HG21	2.02	0.42
40:n:67:ARG:NH1	40:n:133:LEU:O	2.53	0.42
40:n:153:SER:O	40:n:160:LEU:N	2.53	0.42
42:v:45:ASN:HB3	42:v:48:ARG:HG2	2.00	0.42
1:A:296:A:OP1	34:h:86:LYS:NZ	2.39	0.41
1:A:838:G:N7	39:m:4:ARG:NH2	2.68	0.41
1:A:1010:G:N2	9:q:193:ASP:OD1	2.53	0.41
1:A:1260:A:O2'	1:A:1279:C:O2	2.31	0.41
2:B:117:GLU:HB3	2:B:124:GLY:H	1.84	0.41
3:C:277:SER:OG	3:C:280:HIS:NE2	2.45	0.41
20:T:146:ASN:OD1	20:T:146:ASN:N	2.53	0.41
25:Y:127:ASN:OD1	25:Y:127:ASN:N	2.53	0.41
26:Z:49:LYS:NZ	45:y:63:G:O2'	2.37	0.41
1:A:900:G:H1'	1:A:1589:A:N6	2.35	0.41
1:A:1905:G:O6	3:C:241:LYS:NZ	2.52	0.41
3:C:59:ASP:OD1	3:C:59:ASP:N	2.52	0.41
14:N:133:LEU:HD23	14:N:133:LEU:HA	1.94	0.41
19:S:14:LEU:HA	19:S:15:PRO:HD3	1.94	0.41
30:d:23:VAL:HG11	30:d:31:ARG:HD2	2.02	0.41
1:A:44:U:H1'	38:l:54:THR:HB	2.02	0.41
1:A:964:G:N2	14:N:40:HIS:O	2.48	0.41
1:A:1307:G:OP2	10:J:58:ARG:NH2	2.50	0.41
1:A:2242:A:H5'	2:B:243:THR:HG23	2.01	0.41
3:C:17:LEU:CB	3:C:18:PRO:CD	2.98	0.41
16:P:40:HIS:NE2	20:T:69:LYS:HB2	2.35	0.41
1:A:2424:A:H5'	15:O:89:VAL:HB	2.02	0.41
28:b:107:ARG:NH2	28:b:199:ASN:O	2.52	0.41
1:A:596:C:O2'	28:b:165:ASP:OD1	2.37	0.41
1:A:1563:C:N4	1:A:1575:A:N1	2.68	0.41
8:H:133:LYS:HA	8:H:133:LYS:HD3	1.92	0.41
16:P:119:TYR:OH	16:P:139:PRO:O	2.38	0.41
19:S:146:LYS:HE3	19:S:146:LYS:HB3	1.85	0.41
30:d:25:PHE:HD1	30:d:28:ARG:HD2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:76:ARG:HD3	34:h:76:ARG:HA	1.86	0.41
1:A:1029:G:H2'	1:A:1030:A:C8	2.56	0.41
1:A:1218:U:H3	1:A:1288:U:H3	1.68	0.41
1:A:1406:A:H5'	31:e:17:PHE:HD2	1.86	0.41
3:C:188:ILE:HA	3:C:191:LYS:HD2	2.03	0.41
4:D:99:MET:HE3	4:D:99:MET:HB2	1.98	0.41
7:G:100:LYS:HE2	7:G:100:LYS:HB2	1.89	0.41
9:q:86:HIS:HB3	9:q:139:ARG:HB3	2.01	0.41
28:b:88:ARG:NH1	28:b:108:LEU:O	2.53	0.41
1:A:2514:U:H6	8:H:68:ARG:HB3	1.85	0.41
3:C:222:LYS:CG	3:C:331:ASN:ND2	2.84	0.41
4:D:31:ARG:HE	4:D:31:ARG:HB3	1.63	0.41
5:E:40:LEU:HD11	5:E:112:LEU:HD11	2.03	0.41
15:O:197:LEU:HD23	15:O:197:LEU:HA	1.85	0.41
40:n:157:GLN:NE2	40:n:222:PHE:O	2.35	0.41
1:A:399:A:HO2'	1:A:403:C:HO2'	1.55	0.41
5:E:131:MET:HE3	5:E:131:MET:HB3	1.85	0.41
25:Y:54:THR:OG1	25:Y:55:LYS:N	2.53	0.41
31:e:47:ARG:HE	31:e:47:ARG:HB3	1.59	0.41
33:g:11:ASN:ND2	33:g:18:ASN:HD22	2.19	0.41
38:l:48:SER:O	38:l:48:SER:OG	2.36	0.41
1:A:63:A:N3	1:A:78:U:O2'	2.43	0.41
1:A:144:A:OP1	8:H:193:LYS:NZ	2.42	0.41
1:A:824:C:O2'	1:A:1534:A:N3	2.48	0.41
1:A:1132:C:H2'	1:A:1133:A:H8	1.86	0.41
1:A:2705:A:OP1	16:P:31:TYR:OH	2.32	0.41
2:B:80:GLU:HG2	39:m:66:GLY:HA2	2.03	0.41
3:C:163:HIS:ND1	3:C:164:THR:O	2.52	0.41
4:D:55:LYS:HE2	4:D:55:LYS:HB3	1.88	0.41
6:F:6:THR:HB	6:F:57:VAL:HG12	2.03	0.41
6:F:47:LYS:HB2	13:M:7:VAL:HB	2.02	0.41
8:H:60:ARG:NH2	45:y:151:C:OP1	2.54	0.41
10:J:182:ALA:O	10:J:185:SER:OG	2.36	0.41
16:P:65:ILE:HG12	16:P:74:VAL:HG22	2.01	0.41
28:b:178:ILE:HD11	28:b:187:GLU:HG3	2.03	0.41
43:z:389:VAL:H	43:z:389:VAL:HG23	1.64	0.41
1:A:2848:G:OP1	41:t:100:TYR:OH	2.34	0.41
8:H:110:THR:O	8:H:114:ALA:N	2.44	0.41
24:X:89:LYS:HE3	24:X:93:ALA:HB3	2.02	0.41
1:A:1168:U:O4	1:A:1329:U:O2'	2.37	0.40
1:A:1359:C:O2'	4:D:306:THR:OG1	2.27	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:60:PHE:HB3	21:U:64:ASN:HB3	2.03	0.40
1:A:98:G:N7	11:K:13:HIS:NE2	2.64	0.40
1:A:1560:G:H2'	1:A:1561:G:C8	2.55	0.40
1:A:2305:G:OP2	1:A:2305:G:N2	2.45	0.40
4:D:135:VAL:HG12	4:D:140:HIS:HB2	2.03	0.40
4:D:282:SER:HB3	17:Q:126:GLN:HE21	1.85	0.40
6:F:170:LYS:HB2	6:F:170:LYS:HE2	1.86	0.40
1:A:1423:C:H4'	7:G:5:LYS:HD2	2.02	0.40
1:A:1497:C:H2'	1:A:1498:A:C8	2.57	0.40
1:A:1870:C:O2	1:A:3066:U:O2'	2.34	0.40
1:A:2765:C:OP1	14:N:55:LYS:NZ	2.54	0.40
3:C:84:VAL:HG12	3:C:164:THR:HA	2.04	0.40
16:P:50:ARG:NH1	16:P:147:ASP:OD2	2.55	0.40
16:P:262:LYS:HA	16:P:265:TYR:HB2	2.03	0.40
24:X:73:VAL:HA	24:X:80:VAL:HG23	2.03	0.40
30:d:44:MET:HB2	30:d:77:ARG:HE	1.87	0.40
42:v:23:ARG:HH21	42:v:27:LYS:HD2	1.85	0.40
1:A:216:G:OP1	24:X:16:ARG:NH1	2.53	0.40
1:A:1386:A:H5''	4:D:141:ARG:HH22	1.87	0.40
3:C:166:ILE:HD13	3:C:166:ILE:HA	1.90	0.40
21:U:23:ARG:NH1	21:U:125:GLN:OE1	2.55	0.40
36:j:20:VAL:HG12	36:j:47:GLY:HA2	2.02	0.40
42:v:6:ASP:HB3	42:v:10:GLY:H	1.85	0.40
1:A:68:C:OP2	1:A:301:G:N2	2.52	0.40
1:A:279:U:O4	38:l:45:ARG:NH1	2.40	0.40
1:A:1477:A:OP1	1:A:3075:G:O2'	2.38	0.40
1:A:1873:U:OP2	18:R:20:ARG:NH2	2.55	0.40
1:A:3369:G:O6	42:v:56:ARG:NH1	2.54	0.40
40:n:74:THR:OG1	40:n:97:VAL:O	2.25	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	
2	B	245/254 (96%)	220 (90%)	25 (10%)	0	100	100
3	C	379/387 (98%)	353 (93%)	24 (6%)	2 (0%)	24	54
4	D	359/362 (99%)	332 (92%)	27 (8%)	0	100	100
5	E	167/174 (96%)	155 (93%)	12 (7%)	0	100	100
6	F	187/189 (99%)	176 (94%)	11 (6%)	0	100	100
7	G	173/176 (98%)	151 (87%)	22 (13%)	0	100	100
8	H	221/256 (86%)	207 (94%)	14 (6%)	0	100	100
9	q	214/221 (97%)	193 (90%)	21 (10%)	0	100	100
10	J	195/198 (98%)	189 (97%)	6 (3%)	0	100	100
11	K	184/199 (92%)	168 (91%)	15 (8%)	1 (0%)	24	54
12	L	134/137 (98%)	125 (93%)	9 (7%)	0	100	100
13	M	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
14	N	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
15	O	201/204 (98%)	186 (92%)	15 (8%)	0	100	100
16	P	284/297 (96%)	264 (93%)	20 (7%)	0	100	100
17	Q	183/186 (98%)	177 (97%)	6 (3%)	0	100	100
18	R	148/189 (78%)	145 (98%)	3 (2%)	0	100	100
19	S	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
20	T	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
21	U	152/184 (83%)	146 (96%)	6 (4%)	0	100	100
22	V	97/121 (80%)	88 (91%)	8 (8%)	1 (1%)	12	40
23	W	118/142 (83%)	105 (89%)	13 (11%)	0	100	100
24	X	123/127 (97%)	112 (91%)	11 (9%)	0	100	100
25	Y	133/136 (98%)	119 (90%)	14 (10%)	0	100	100
26	Z	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
27	a	52/59 (88%)	49 (94%)	3 (6%)	0	100	100
28	b	217/244 (89%)	205 (94%)	12 (6%)	0	100	100
29	c	95/105 (90%)	93 (98%)	2 (2%)	0	100	100
30	d	105/113 (93%)	91 (87%)	14 (13%)	0	100	100
31	e	119/130 (92%)	113 (95%)	6 (5%)	0	100	100
32	f	104/107 (97%)	93 (89%)	11 (11%)	0	100	100
33	g	101/121 (84%)	94 (93%)	7 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	h	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
35	i	82/88 (93%)	74 (90%)	8 (10%)	0	100	100
36	j	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
37	k	48/51 (94%)	42 (88%)	6 (12%)	0	100	100
38	l	92/106 (87%)	86 (94%)	6 (6%)	0	100	100
39	m	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
40	n	222/245 (91%)	195 (88%)	27 (12%)	0	100	100
41	t	50/128 (39%)	45 (90%)	5 (10%)	0	100	100
42	v	58/155 (37%)	56 (97%)	2 (3%)	0	100	100
43	z	51/432 (12%)	45 (88%)	6 (12%)	0	100	100
All	All	6278/7232 (87%)	5828 (93%)	446 (7%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	18	PRO
11	K	47	ALA
22	V	52	ASN
3	C	364	LYS

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	
2	B	189/196 (96%)	186 (98%)	3 (2%)	55	68
3	C	317/323 (98%)	308 (97%)	9 (3%)	38	60
4	D	288/289 (100%)	285 (99%)	3 (1%)	68	75
5	E	147/150 (98%)	146 (99%)	1 (1%)	76	78
6	F	169/169 (100%)	162 (96%)	7 (4%)	27	52
7	G	152/153 (99%)	151 (99%)	1 (1%)	76	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	183/208 (88%)	182 (100%)	1 (0%)	81	81
9	q	185/187 (99%)	185 (100%)	0	100	100
10	J	163/164 (99%)	161 (99%)	2 (1%)	63	72
11	K	149/159 (94%)	146 (98%)	3 (2%)	48	65
12	L	104/105 (99%)	102 (98%)	2 (2%)	50	66
13	M	108/109 (99%)	108 (100%)	0	100	100
14	N	118/119 (99%)	118 (100%)	0	100	100
15	O	175/176 (99%)	174 (99%)	1 (1%)	78	80
16	P	237/245 (97%)	235 (99%)	2 (1%)	73	77
17	Q	150/151 (99%)	148 (99%)	2 (1%)	61	71
18	R	124/154 (80%)	122 (98%)	2 (2%)	55	68
19	S	156/156 (100%)	153 (98%)	3 (2%)	50	66
20	T	136/137 (99%)	135 (99%)	1 (1%)	76	78
21	U	125/146 (86%)	124 (99%)	1 (1%)	73	77
22	V	86/107 (80%)	85 (99%)	1 (1%)	63	72
23	W	104/118 (88%)	103 (99%)	1 (1%)	68	75
24	X	108/110 (98%)	107 (99%)	1 (1%)	70	76
25	Y	115/116 (99%)	115 (100%)	0	100	100
26	Z	104/105 (99%)	104 (100%)	0	100	100
27	a	43/47 (92%)	43 (100%)	0	100	100
28	b	184/205 (90%)	180 (98%)	4 (2%)	45	63
29	c	81/88 (92%)	81 (100%)	0	100	100
30	d	94/97 (97%)	91 (97%)	3 (3%)	34	58
31	e	104/111 (94%)	102 (98%)	2 (2%)	50	66
32	f	90/91 (99%)	89 (99%)	1 (1%)	65	74
33	g	88/103 (85%)	87 (99%)	1 (1%)	65	74
34	h	80/82 (98%)	80 (100%)	0	100	100
35	i	69/71 (97%)	69 (100%)	0	100	100
36	j	68/69 (99%)	67 (98%)	1 (2%)	57	69
37	k	45/46 (98%)	45 (100%)	0	100	100
38	l	81/91 (89%)	79 (98%)	2 (2%)	42	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	m	71/72 (99%)	70 (99%)	1 (1%)	59	70
40	n	192/211 (91%)	187 (97%)	5 (3%)	40	61
41	t	47/116 (40%)	47 (100%)	0	100	100
42	v	53/129 (41%)	53 (100%)	0	100	100
43	z	48/392 (12%)	46 (96%)	2 (4%)	26	52
All	All	5330/6073 (88%)	5261 (99%)	69 (1%)	59	71

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	79	ASN
2	B	101	VAL
2	B	237	LEU
3	C	18	PRO
3	C	44	THR
3	C	85	VAL
3	C	164	THR
3	C	166	ILE
3	C	324	VAL
3	C	331	ASN
3	C	332	ARG
3	C	333	LYS
4	D	110	ASN
4	D	230	VAL
4	D	237	GLN
5	E	129	VAL
6	F	18	VAL
6	F	28	VAL
6	F	43	VAL
6	F	46	THR
6	F	103	ILE
6	F	126	VAL
6	F	142	ASP
7	G	18	LEU
8	H	132	VAL
10	J	35	VAL
10	J	118	VAL
11	K	22	VAL
11	K	46	ILE
11	K	62	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	49	LEU
12	L	78	VAL
15	O	165	THR
16	P	68	THR
16	P	153	THR
17	Q	84	VAL
17	Q	186	VAL
18	R	142	ILE
18	R	151	ARG
19	S	16	THR
19	S	135	VAL
19	S	172	TYR
20	T	80	VAL
21	U	114	VAL
22	V	52	ASN
23	W	127	THR
24	X	45	ILE
28	b	86	VAL
28	b	119	VAL
28	b	228	SER
28	b	229	PHE
30	d	7	VAL
30	d	64	VAL
30	d	108	VAL
31	e	78	ASN
31	e	79	VAL
32	f	49	ILE
33	g	40	THR
36	j	78	LEU
38	l	57	VAL
38	l	72	LEU
39	m	64	VAL
40	n	32	GLU
40	n	72	VAL
40	n	74	THR
40	n	118	HIS
40	n	154	LEU
43	z	390	THR
43	z	424	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	8	GLN
3	C	68	HIS
3	C	121	ASN
3	C	243	HIS
3	C	331	ASN
4	D	58	HIS
4	D	296	GLN
5	E	7	ASN
5	E	47	GLN
6	F	51	GLN
6	F	100	ASN
6	F	163	GLN
7	G	167	ASN
8	H	59	GLN
8	H	61	GLN
9	q	113	GLN
10	J	25	GLN
10	J	28	ASN
12	L	4	ASN
12	L	24	ASN
12	L	98	ASN
14	N	39	HIS
14	N	74	ASN
15	O	86	ASN
16	P	39	GLN
16	P	57	ASN
17	Q	23	ASN
17	Q	126	GLN
17	Q	136	ASN
18	R	68	GLN
18	R	75	HIS
20	T	26	HIS
20	T	103	GLN
21	U	50	GLN
21	U	120	ASN
21	U	137	ASN
23	W	85	GLN
25	Y	128	GLN
26	Z	99	GLN
27	a	19	ASN
28	b	93	ASN
31	e	49	ASN
31	e	98	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	f	26	ASN
33	g	11	ASN
33	g	69	HIS
34	h	35	ASN
35	i	13	ASN
35	i	28	HIS
37	k	25	GLN
38	l	23	HIS
38	l	59	HIS
38	l	82	GLN
40	n	140	GLN
40	n	170	GLN
40	n	187	ASN
41	t	90	ASN
41	t	120	GLN
43	z	393	GLN
43	z	407	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3160/3396 (93%)	710 (22%)	19 (0%)
44	x	120/121 (99%)	15 (12%)	0
45	y	155/158 (98%)	29 (18%)	0
All	All	3435/3675 (93%)	754 (21%)	19 (0%)

All (754) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	18	G
1	A	22	G
1	A	26	A
1	A	40	A
1	A	43	A
1	A	48	A
1	A	49	A
1	A	57	A
1	A	59	G
1	A	60	A
1	A	65	A
1	A	66	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	73	C
1	A	74	G
1	A	83	U
1	A	85	A
1	A	92	G
1	A	99	A
1	A	105	C
1	A	108	A
1	A	109	A
1	A	110	G
1	A	116	A
1	A	117	U
1	A	122	A
1	A	130	A
1	A	132	C
1	A	134	U
1	A	135	C
1	A	136	G
1	A	148	G
1	A	154	U
1	A	156	G
1	A	157	A
1	A	164	A
1	A	166	C
1	A	169	U
1	A	170	G
1	A	172	G
1	A	190	U
1	A	191	U
1	A	199	A
1	A	206	G
1	A	211	A
1	A	212	G
1	A	213	A
1	A	218	G
1	A	219	A
1	A	220	G
1	A	230	U
1	A	231	G
1	A	234	G
1	A	237	G
1	A	239	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	240	U
1	A	241	G
1	A	243	G
1	A	244	G
1	A	246	U
1	A	249	U
1	A	250	U
1	A	251	G
1	A	252	U
1	A	253	A
1	A	254	A
1	A	255	A
1	A	257	U
1	A	263	C
1	A	266	A
1	A	269	G
1	A	281	G
1	A	284	A
1	A	286	U
1	A	295	A
1	A	298	U
1	A	305	U
1	A	315	C
1	A	329	U
1	A	352	A
1	A	359	U
1	A	374	A
1	A	375	A
1	A	376	G
1	A	390	G
1	A	395	A
1	A	398	A
1	A	399	A
1	A	401	U
1	A	402	A
1	A	403	C
1	A	404	G
1	A	406	G
1	A	420	G
1	A	421	G
1	A	422	A
1	A	429	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	439	C
1	A	440	A
1	A	503	C
1	A	515	C
1	A	521	A
1	A	523	A
1	A	536	U
1	A	542	G
1	A	546	C
1	A	547	G
1	A	548	G
1	A	550	A
1	A	552	G
1	A	555	U
1	A	556	U
1	A	557	A
1	A	558	U
1	A	559	A
1	A	560	G
1	A	569	A
1	A	578	A
1	A	579	G
1	A	592	A
1	A	600	G
1	A	601	U
1	A	602	A
1	A	604	G
1	A	607	A
1	A	611	A
1	A	612	U
1	A	619	A
1	A	620	U
1	A	621	A
1	A	622	A
1	A	644	G
1	A	645	A
1	A	649	A
1	A	675	C
1	A	677	A
1	A	684	G
1	A	689	U
1	A	690	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	691	A
1	A	698	U
1	A	712	G
1	A	715	A
1	A	716	A
1	A	719	U
1	A	720	A
1	A	725	G
1	A	747	A
1	A	761	A
1	A	765	C
1	A	766	U
1	A	767	U
1	A	768	C
1	A	774	G
1	A	776	U
1	A	777	U
1	A	780	A
1	A	781	G
1	A	785	G
1	A	801	A
1	A	806	A
1	A	808	A
1	A	817	A
1	A	830	A
1	A	849	C
1	A	861	C
1	A	874	U
1	A	879	U
1	A	880	G
1	A	888	A
1	A	890	C
1	A	896	A
1	A	897	U
1	A	907	G
1	A	908	G
1	A	914	A
1	A	915	A
1	A	916	G
1	A	917	A
1	A	923	C
1	A	924	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	932	U
1	A	933	A
1	A	937	G
1	A	944	C
1	A	959	C
1	A	960	U
1	A	963	G
1	A	979	U
1	A	980	A
1	A	981	U
1	A	982	C
1	A	984	G
1	A	991	G
1	A	994	G
1	A	1001	G
1	A	1002	A
1	A	1006	A
1	A	1010	G
1	A	1011	A
1	A	1013	G
1	A	1016	C
1	A	1018	G
1	A	1025	A
1	A	1029	G
1	A	1037	C
1	A	1044	U
1	A	1047	A
1	A	1049	C
1	A	1064	A
1	A	1065	A
1	A	1072	G
1	A	1081	U
1	A	1082	U
1	A	1083	G
1	A	1087	G
1	A	1093	A
1	A	1094	U
1	A	1095	U
1	A	1097	G
1	A	1098	A
1	A	1103	A
1	A	1104	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1116	G
1	A	1117	G
1	A	1131	G
1	A	1135	A
1	A	1138	U
1	A	1140	G
1	A	1143	A
1	A	1144	U
1	A	1153	A
1	A	1159	A
1	A	1180	A
1	A	1181	U
1	A	1193	A
1	A	1196	C
1	A	1199	C
1	A	1201	C
1	A	1206	G
1	A	1209	G
1	A	1217	A
1	A	1218	U
1	A	1220	U
1	A	1222	G
1	A	1223	A
1	A	1225	A
1	A	1227	C
1	A	1233	G
1	A	1236	G
1	A	1238	C
1	A	1240	A
1	A	1242	G
1	A	1244	A
1	A	1245	A
1	A	1246	G
1	A	1248	C
1	A	1254	C
1	A	1258	U
1	A	1262	G
1	A	1263	A
1	A	1264	G
1	A	1265	U
1	A	1266	G
1	A	1270	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1271	A
1	A	1272	C
1	A	1273	A
1	A	1274	A
1	A	1278	A
1	A	1279	C
1	A	1285	G
1	A	1286	A
1	A	1288	U
1	A	1289	G
1	A	1304	A
1	A	1307	G
1	A	1309	U
1	A	1313	G
1	A	1330	A
1	A	1331	U
1	A	1345	G
1	A	1349	G
1	A	1350	A
1	A	1352	A
1	A	1353	U
1	A	1354	G
1	A	1355	A
1	A	1356	U
1	A	1357	G
1	A	1386	A
1	A	1392	G
1	A	1399	A
1	A	1400	G
1	A	1418	A
1	A	1419	A
1	A	1433	A
1	A	1434	G
1	A	1437	C
1	A	1443	G
1	A	1446	A
1	A	1450	G
1	A	1455	U
1	A	1480	G
1	A	1481	A
1	A	1482	A
1	A	1483	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1487	G
1	A	1494	U
1	A	1495	U
1	A	1500	G
1	A	1508	C
1	A	1523	U
1	A	1527	C
1	A	1533	U
1	A	1536	G
1	A	1537	A
1	A	1539	A
1	A	1546	A
1	A	1554	U
1	A	1555	U
1	A	1560	G
1	A	1562	C
1	A	1566	A
1	A	1567	U
1	A	1569	U
1	A	1572	U
1	A	1574	C
1	A	1576	G
1	A	1577	G
1	A	1579	C
1	A	1580	A
1	A	1581	C
1	A	1582	C
1	A	1583	A
1	A	1587	A
1	A	1588	A
1	A	1589	A
1	A	1593	A
1	A	1605	A
1	A	1619	A
1	A	1629	U
1	A	1630	U
1	A	1636	U
1	A	1639	C
1	A	1641	U
1	A	1642	A
1	A	1643	A
1	A	1645	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1657	C
1	A	1683	A
1	A	1696	A
1	A	1702	U
1	A	1716	U
1	A	1717	U
1	A	1718	G
1	A	1724	U
1	A	1725	C
1	A	1729	A
1	A	1736	G
1	A	1741	A
1	A	1742	U
1	A	1750	A
1	A	1751	G
1	A	1761	C
1	A	1762	C
1	A	1764	U
1	A	1765	U
1	A	1766	G
1	A	1770	G
1	A	1775	G
1	A	1778	G
1	A	1779	C
1	A	1780	G
1	A	1793	C
1	A	1795	U
1	A	1797	A
1	A	1808	G
1	A	1816	A
1	A	1819	U
1	A	1820	U
1	A	1821	U
1	A	1839	A
1	A	1840	U
1	A	1842	A
1	A	1849	C
1	A	1850	A
1	A	1871	U
1	A	1878	G
1	A	1880	U
1	A	1893	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1906	G
1	A	1926	C
1	A	1927	G
1	A	1930	A
1	A	1943	C
1	A	1953	G
1	A	1954	G
1	A	1955	U
1	A	2100	A
1	A	2101	C
1	A	2102	U
1	A	2111	G
1	A	2112	U
1	A	2118	C
1	A	2121	G
1	A	2122	G
1	A	2126	A
1	A	2131	A
1	A	2138	A
1	A	2140	U
1	A	2142	A
1	A	2144	A
1	A	2145	A
1	A	2149	A
1	A	2158	A
1	A	2169	G
1	A	2178	A
1	A	2184	U
1	A	2185	G
1	A	2187	G
1	A	2192	C
1	A	2201	G
1	A	2206	G
1	A	2209	U
1	A	2223	A
1	A	2244	A
1	A	2250	G
1	A	2255	A
1	A	2256	A
1	A	2257	C
1	A	2258	U
1	A	2259	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2260	U
1	A	2261	G
1	A	2262	A
1	A	2263	C
1	A	2264	U
1	A	2267	C
1	A	2268	U
1	A	2269	U
1	A	2270	A
1	A	2273	G
1	A	2276	G
1	A	2279	A
1	A	2281	A
1	A	2288	G
1	A	2306	C
1	A	2307	G
1	A	2308	C
1	A	2309	A
1	A	2310	U
1	A	2313	A
1	A	2314	U
1	A	2315	G
1	A	2334	U
1	A	2335	G
1	A	2336	U
1	A	2356	A
1	A	2372	A
1	A	2373	A
1	A	2374	C
1	A	2375	G
1	A	2388	U
1	A	2393	G
1	A	2397	A
1	A	2401	A
1	A	2402	A
1	A	2403	G
1	A	2404	A
1	A	2411	U
1	A	2419	A
1	A	2422	C
1	A	2442	G
1	A	2443	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2447	A
1	A	2448	G
1	A	2451	G
1	A	2452	G
1	A	2453	U
1	A	2460	U
1	A	2461	A
1	A	2462	A
1	A	2463	G
1	A	2464	U
1	A	2465	G
1	A	2466	G
1	A	2467	G
1	A	2468	A
1	A	2469	G
1	A	2471	U
1	A	2473	C
1	A	2474	G
1	A	2475	G
1	A	2477	G
1	A	2478	C
1	A	2479	C
1	A	2480	A
1	A	2482	U
1	A	2484	A
1	A	2486	A
1	A	2488	A
1	A	2490	C
1	A	2491	A
1	A	2492	C
1	A	2494	A
1	A	2501	U
1	A	2502	A
1	A	2503	G
1	A	2504	U
1	A	2508	U
1	A	2515	A
1	A	2522	G
1	A	2523	A
1	A	2531	C
1	A	2534	G
1	A	2535	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2536	A
1	A	2537	U
1	A	2538	U
1	A	2539	C
1	A	2540	A
1	A	2541	U
1	A	2542	U
1	A	2543	U
1	A	2549	G
1	A	2550	U
1	A	2551	U
1	A	2554	A
1	A	2561	A
1	A	2565	U
1	A	2566	C
1	A	2568	C
1	A	2569	A
1	A	2570	U
1	A	2571	U
1	A	2573	G
1	A	2574	G
1	A	2576	G
1	A	2580	A
1	A	2585	G
1	A	2586	G
1	A	2589	G
1	A	2593	A
1	A	2606	G
1	A	2607	G
1	A	2614	G
1	A	2618	G
1	A	2629	U
1	A	2635	A
1	A	2648	G
1	A	2652	U
1	A	2656	A
1	A	2672	G
1	A	2674	A
1	A	2677	G
1	A	2689	A
1	A	2691	A
1	A	2694	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2704	A
1	A	2705	A
1	A	2714	G
1	A	2715	A
1	A	2719	U
1	A	2725	U
1	A	2728	G
1	A	2729	U
1	A	2753	G
1	A	2755	C
1	A	2772	C
1	A	2773	C
1	A	2777	G
1	A	2778	G
1	A	2780	A
1	A	2787	G
1	A	2791	G
1	A	2796	G
1	A	2799	A
1	A	2800	G
1	A	2801	A
1	A	2802	A
1	A	2804	A
1	A	2810	C
1	A	2814	G
1	A	2817	A
1	A	2842	U
1	A	2845	A
1	A	2849	C
1	A	2850	G
1	A	2856	G
1	A	2860	U
1	A	2861	U
1	A	2867	C
1	A	2872	A
1	A	2875	U
1	A	2887	A
1	A	2889	C
1	A	2922	G
1	A	2923	U
1	A	2928	C
1	A	2935	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2936	A
1	A	2939	G
1	A	2941	A
1	A	2942	C
1	A	2947	G
1	A	2951	G
1	A	2971	A
1	A	2983	C
1	A	2990	G
1	A	2997	G
1	A	3003	G
1	A	3011	A
1	A	3012	A
1	A	3014	U
1	A	3021	A
1	A	3027	A
1	A	3030	G
1	A	3032	A
1	A	3056	U
1	A	3057	U
1	A	3058	U
1	A	3059	G
1	A	3078	U
1	A	3080	G
1	A	3090	U
1	A	3092	C
1	A	3093	C
1	A	3109	G
1	A	3117	C
1	A	3122	A
1	A	3124	G
1	A	3129	A
1	A	3130	A
1	A	3131	U
1	A	3142	A
1	A	3154	C
1	A	3155	U
1	A	3156	U
1	A	3157	U
1	A	3158	G
1	A	3164	C
1	A	3165	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3166	C
1	A	3167	A
1	A	3171	U
1	A	3172	A
1	A	3173	G
1	A	3174	A
1	A	3175	U
1	A	3176	G
1	A	3179	U
1	A	3181	C
1	A	3185	U
1	A	3187	A
1	A	3193	C
1	A	3195	U
1	A	3196	U
1	A	3206	C
1	A	3207	U
1	A	3210	A
1	A	3215	A
1	A	3217	C
1	A	3218	A
1	A	3219	G
1	A	3220	G
1	A	3221	C
1	A	3223	A
1	A	3265	C
1	A	3268	A
1	A	3270	U
1	A	3271	G
1	A	3272	C
1	A	3275	U
1	A	3276	G
1	A	3277	U
1	A	3278	C
1	A	3279	A
1	A	3280	U
1	A	3281	U
1	A	3282	U
1	A	3284	G
1	A	3289	G
1	A	3294	A
1	A	3295	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3304	U
1	A	3313	U
1	A	3317	U
1	A	3318	G
1	A	3319	U
1	A	3320	A
1	A	3334	U
1	A	3341	U
1	A	3342	A
1	A	3345	G
1	A	3351	U
1	A	3352	U
1	A	3353	G
1	A	3354	U
1	A	3355	U
1	A	3356	G
1	A	3362	A
1	A	3369	G
1	A	3375	A
1	A	3378	C
1	A	3381	U
1	A	3382	U
1	A	3386	G
1	A	3389	U
1	A	3395	G
1	A	3396	U
44	x	7	G
44	x	10	C
44	x	49	G
44	x	50	U
44	x	63	A
44	x	64	A
44	x	65	G
44	x	74	C
44	x	76	A
44	x	91	G
44	x	99	G
44	x	100	C
44	x	102	A
44	x	112	G
44	x	121	U
45	y	23	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	y	34	U
45	y	35	C
45	y	39	G
45	y	49	G
45	y	51	G
45	y	52	A
45	y	59	A
45	y	62	C
45	y	63	G
45	y	75	G
45	y	80	A
45	y	81	U
45	y	82	U
45	y	83	C
45	y	85	G
45	y	86	U
45	y	87	G
45	y	90	U
45	y	95	G
45	y	96	A
45	y	104	A
45	y	105	A
45	y	106	C
45	y	113	U
45	y	125	U
45	y	126	A
45	y	148	G
45	y	151	C

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	239	G
1	A	916	G
1	A	1064	A
1	A	1103	A
1	A	1217	A
1	A	1287	A
1	A	1288	U
1	A	1355	A
1	A	1716	U
1	A	1815	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2101	C
1	A	2249	G
1	A	2254	U
1	A	2261	G
1	A	2266	U
1	A	2400	G
1	A	2462	A
1	A	2493	U
1	A	3121	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

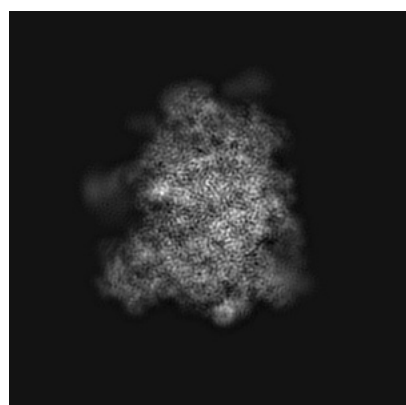
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4630. These allow visual inspection of the internal detail of the map and identification of artifacts.

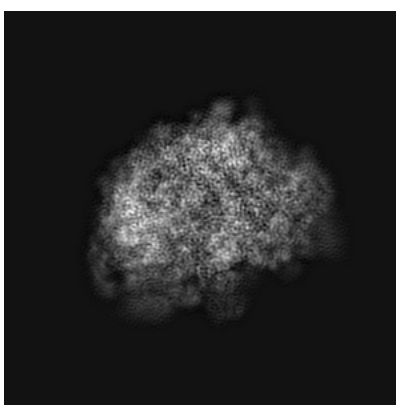
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

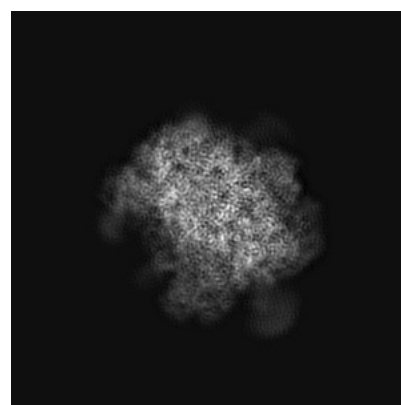
6.1.1 Primary map



X



Y

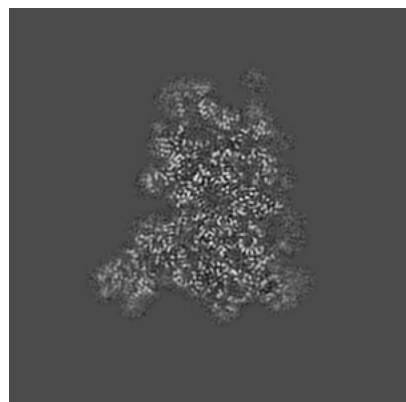


Z

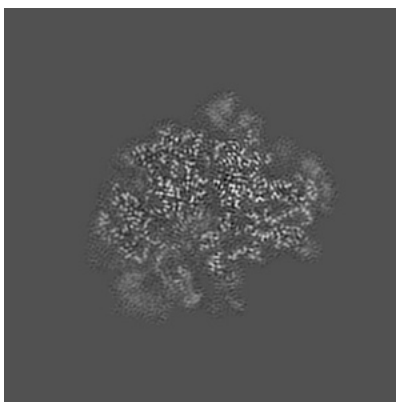
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

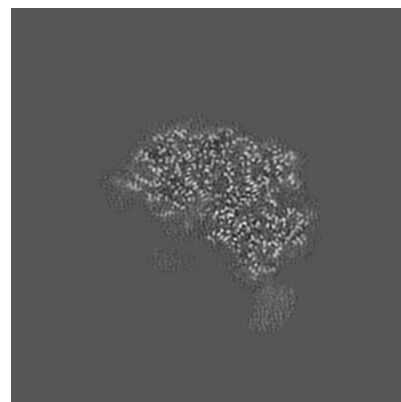
6.2.1 Primary map



X Index: 180



Y Index: 180

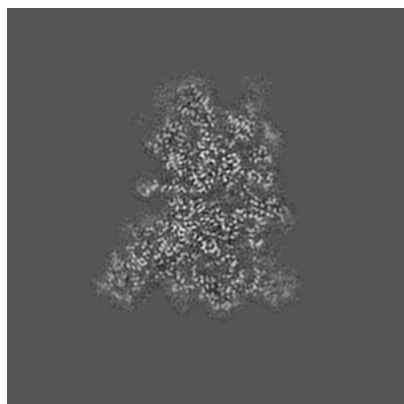


Z Index: 180

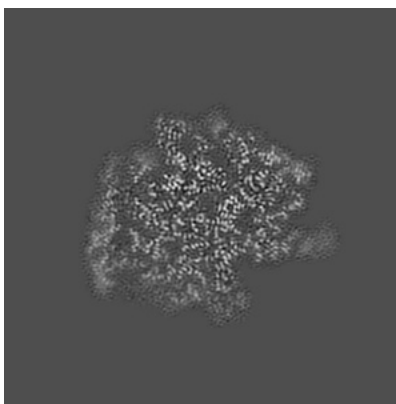
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

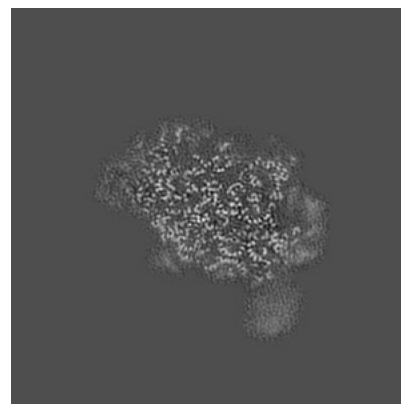
6.3.1 Primary map



X Index: 189



Y Index: 196

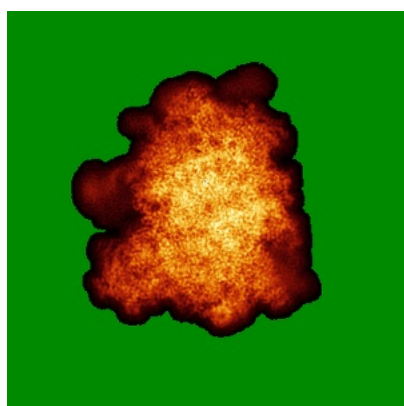


Z Index: 199

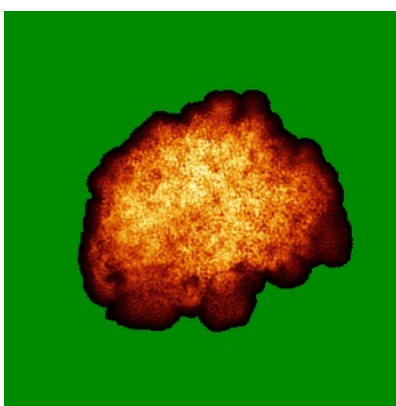
The images above show the largest variance slices of the map in three orthogonal directions.

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

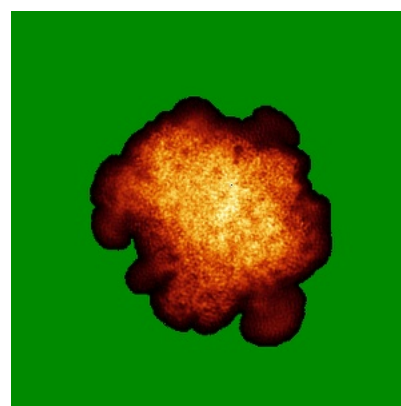
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

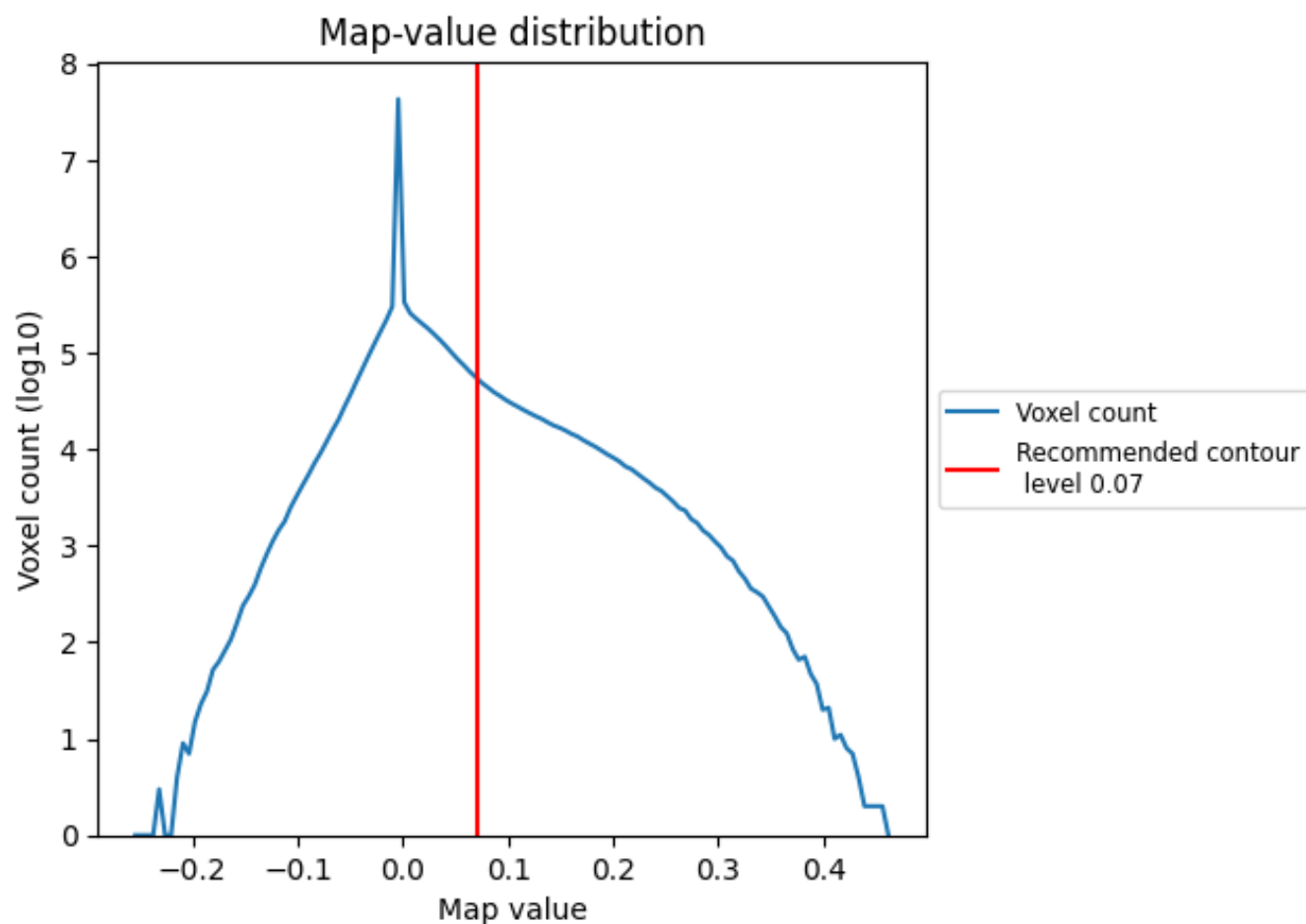
6.6 Mask visualisation

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

7 Map analysis [i](#)

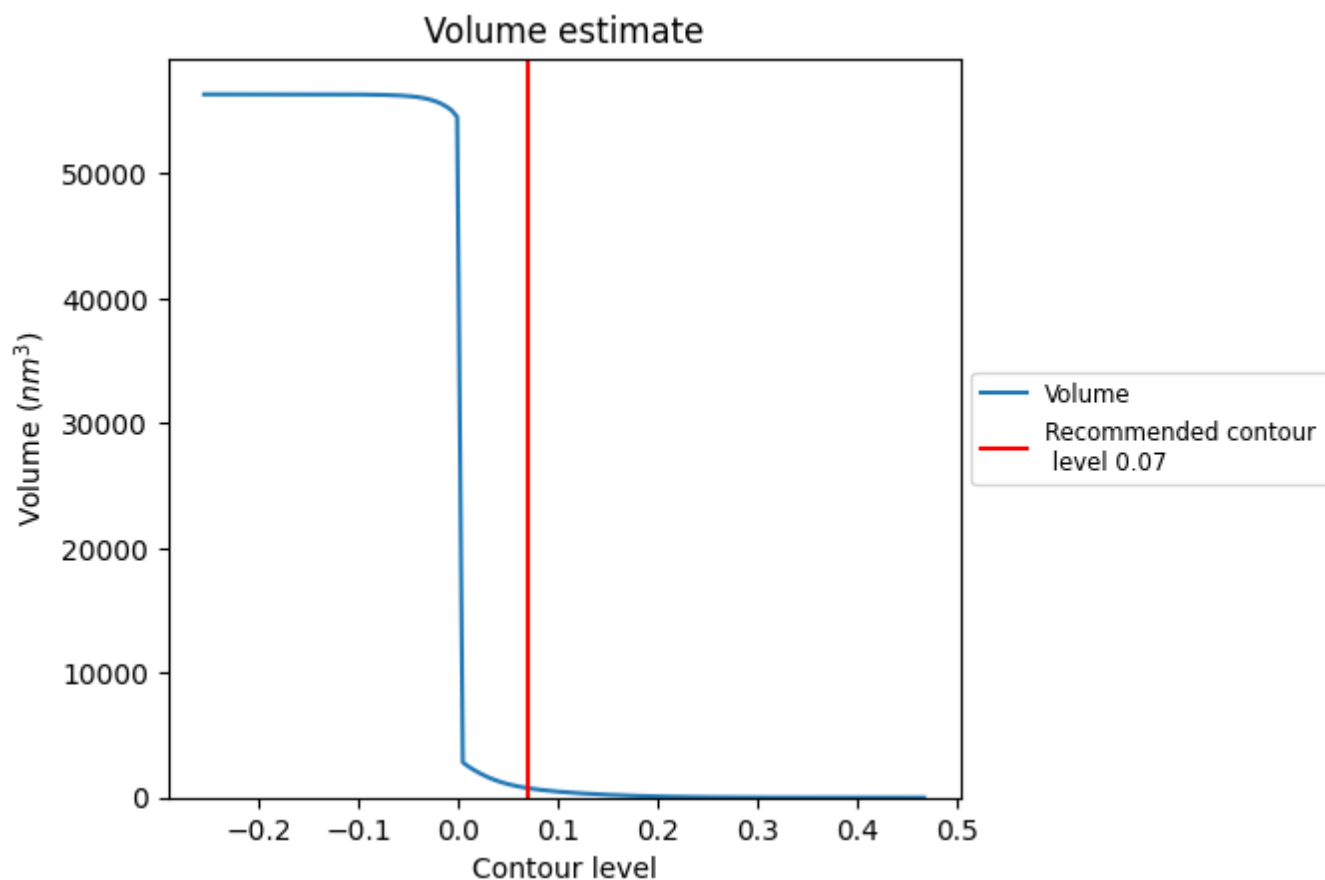
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

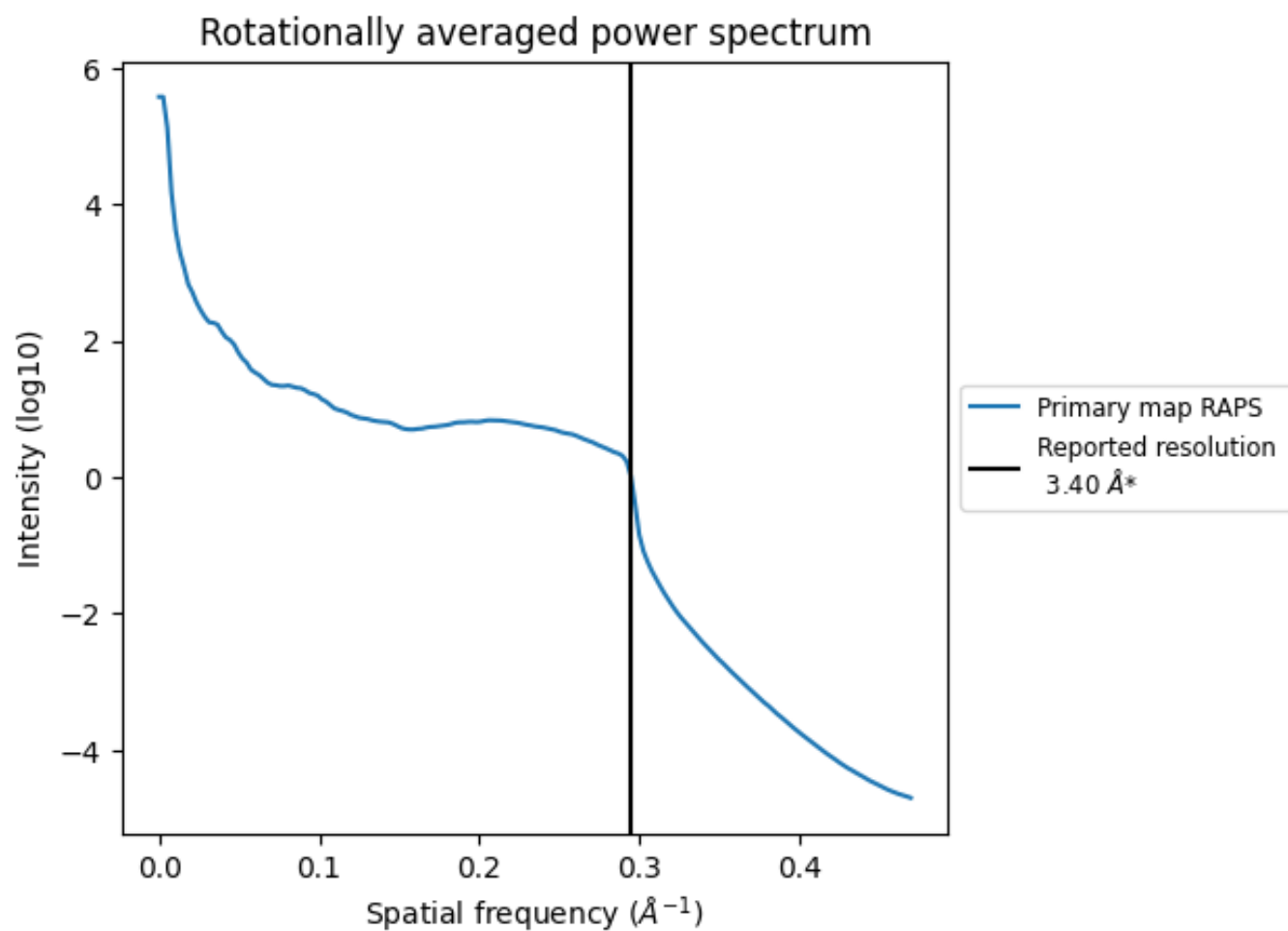
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 759 nm³; this corresponds to an approximate mass of 685 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 0.294 Å⁻¹

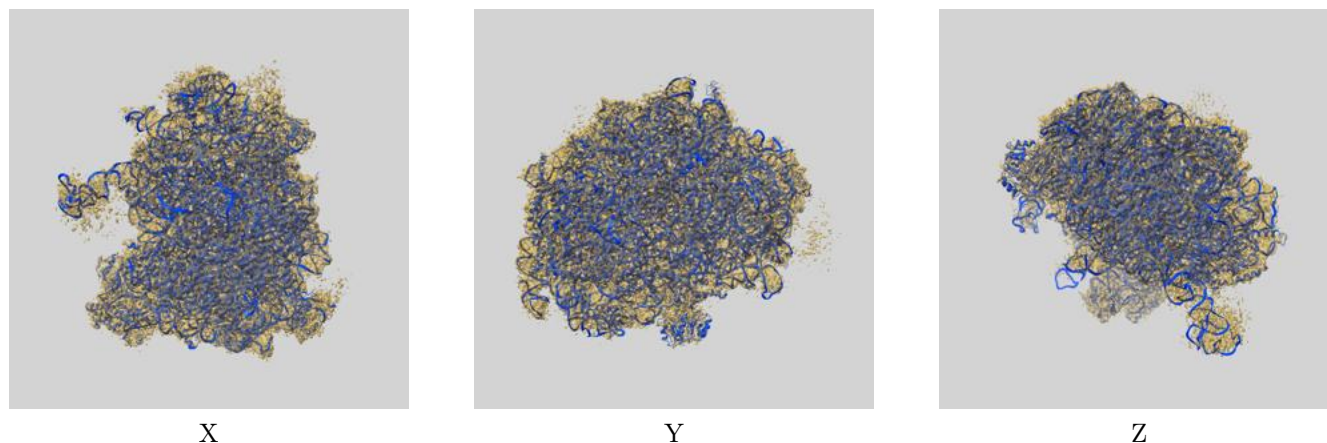
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

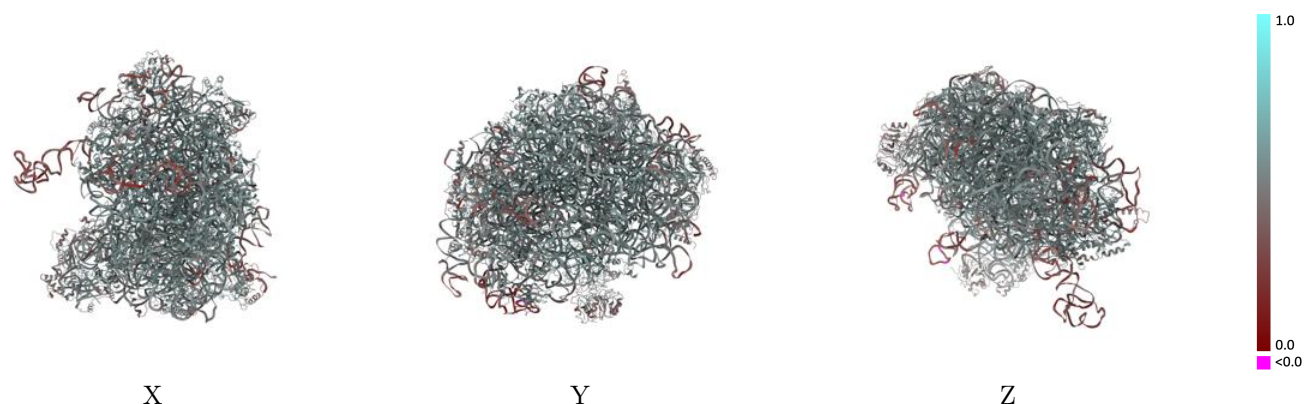
This section contains information regarding the fit between EMDB map EMD-4630 and PDB model 6QT0. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



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

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

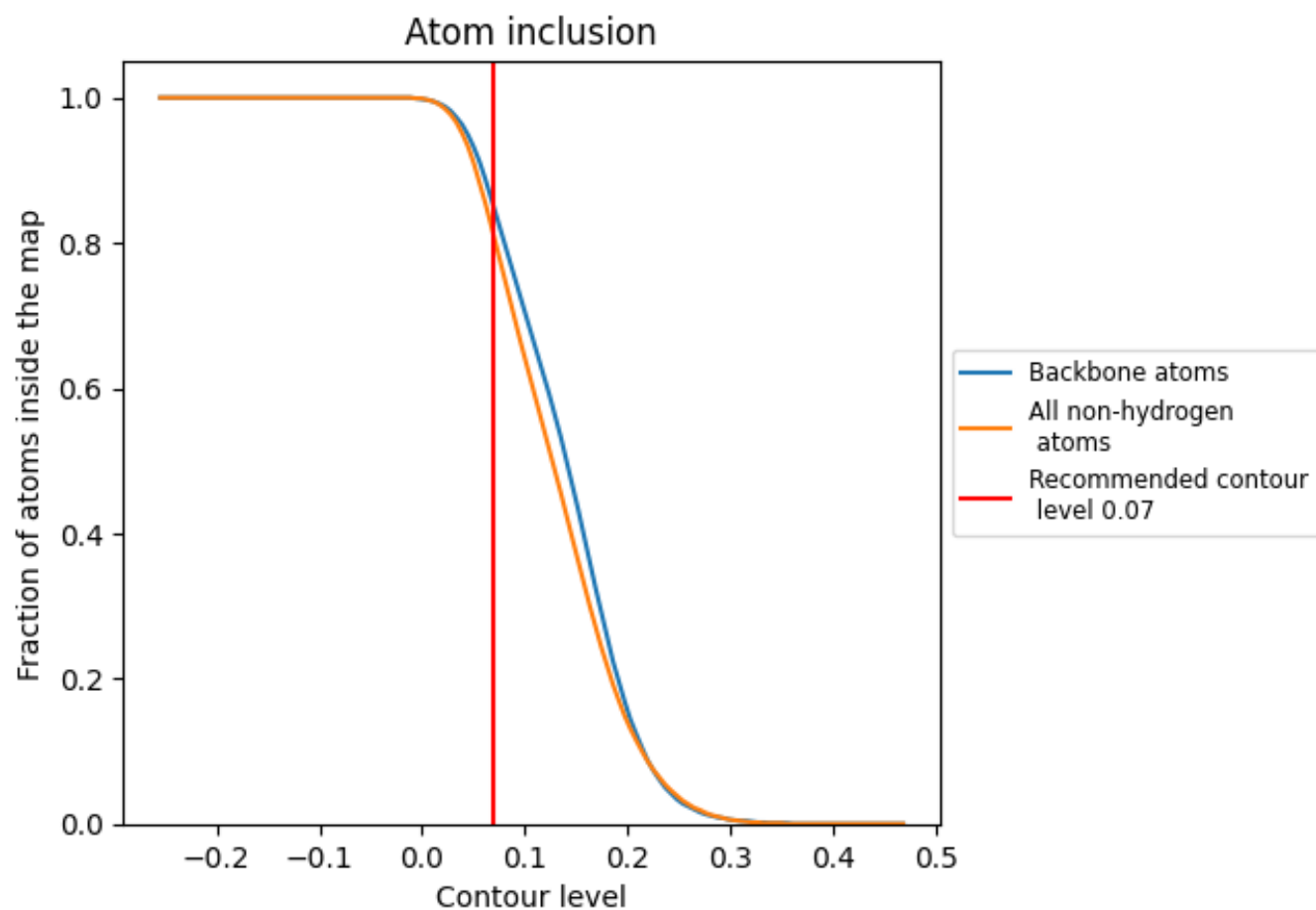


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8080	 0.5130
A	 0.8540	 0.5010
B	 0.8180	 0.5630
C	 0.8050	 0.5470
D	 0.8070	 0.5510
E	 0.5810	 0.4370
F	 0.7000	 0.5080
G	 0.6260	 0.4690
H	 0.7140	 0.5050
J	 0.7710	 0.5410
K	 0.7630	 0.5400
L	 0.7330	 0.5430
M	 0.7270	 0.5050
N	 0.8570	 0.5620
O	 0.8530	 0.5720
P	 0.7550	 0.4950
Q	 0.8490	 0.5650
R	 0.8040	 0.5470
S	 0.7790	 0.5400
T	 0.7620	 0.5410
U	 0.8230	 0.5640
V	 0.6800	 0.4940
W	 0.7960	 0.5500
X	 0.8140	 0.5530
Y	 0.7130	 0.4900
Z	 0.8050	 0.5440
a	 0.7260	 0.5330
b	 0.8060	 0.5470
c	 0.6720	 0.4720
d	 0.7440	 0.5350
e	 0.8130	 0.5670
f	 0.8100	 0.5600
g	 0.7980	 0.5520
h	 0.5940	 0.5050
i	 0.8500	 0.5710



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.7190	 0.5170
k	 0.8240	 0.5720
l	 0.7860	 0.5570
m	 0.7000	 0.5260
n	 0.3040	 0.4410
q	 0.4930	 0.5000
t	 0.4110	 0.5040
v	 0.4360	 0.5080
x	 0.9320	 0.5020
y	 0.9340	 0.5350
z	 0.1530	 0.4430