



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:07 PM UTC

PDB ID : 3J79 / pdb_00003j79
EMDB ID : EMD-2660
Title : Cryo-EM structure of the Plasmodium falciparum 80S ribosome bound to the anti-protozoan drug emetine, large subunit
Authors : Wong, W.; Bai, X.C.; Brown, A.; Fernandez, I.S.; Hanssen, E.; Condrón, M.; Tan, Y.H.; Baum, J.; Scheres, S.H.W.
Deposited on : 2014-06-02
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

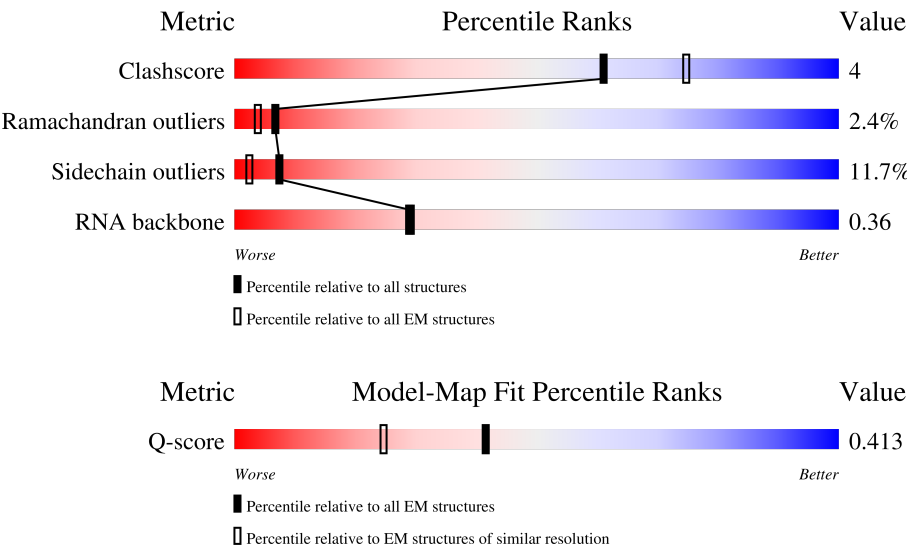
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	3788	
2	B	119	
3	C	159	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	260	
5	E	386	
6	F	411	
7	G	173	
8	H	190	
9	I	221	
10	J	283	
11	K	202	
12	L	215	
13	M	139	
14	N	165	
15	O	148	
16	P	205	
17	Q	219	
18	R	294	
19	S	187	
20	T	182	
21	U	184	
22	V	161	
23	W	203	
24	X	139	
25	Y	190	
26	Z	126	
27	0	162	
28	1	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	2	127	
30	3	124	
31	4	67	
32	5	257	
33	6	108	
34	7	120	
35	8	131	
36	9	140	
37	a	150	
38	b	112	
39	c	92	
40	d	87	
41	e	51	
42	f	128	
43	g	39	
44	h	96	
45	i	104	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	ZN	f	100	-	-	X	-

2 Entry composition [i](#)

There are 47 unique types of molecules in this entry. The entry contains 124514 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3191	Total	C	N	O	P	0	0
			67935	30426	12044	22274	3191		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	P	0	0
			2525	1128	461	818	118		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	151	Total	C	N	O	P	0	0
			3224	1444	589	1040	151		

- Molecule 4 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	247	Total	C	N	O	S	0	0
			1866	1166	374	317	9		

- Molecule 5 is a protein called 60S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	380	Total	C	N	O	S	0	0
			3061	1948	575	521	17		

- Molecule 6 is a protein called 60S ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	390	Total	C	N	O	S	0	0
			3094	1962	594	527	11		

- Molecule 7 is a protein called 60S ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	124	Total	C	N	O	S	0	0
			1010	636	197	171	6		

- Molecule 8 is a protein called 60S ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	185	Total	C	N	O	S	0	0
			1460	938	261	255	6		

- Molecule 9 is a protein called 60S ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	207	Total	C	N	O	S	0	0
			1684	1096	298	285	5		

- Molecule 10 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	229	Total	C	N	O	S	0	0
			1873	1210	337	319	7		

- Molecule 11 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	201	Total	C	N	O	S	0	0
			1659	1064	311	276	8		

- Molecule 12 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	211	Total	C	N	O	S	0	0
			1761	1119	349	290	3		

- Molecule 13 is a protein called 60S ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	132	Total	C	N	O	S	0	0
			996	631	179	178	8		

- Molecule 14 is a protein called 60S ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1197	779	210	202	6		

- Molecule 15 is a protein called 60S ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	147	Total	C	N	O	S	0	0
			1172	747	232	189	4		

- Molecule 16 is a protein called 60S ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1697	1075	351	267	4		

- Molecule 17 is a protein called 60S ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	189	Total	C	N	O	S	0	0
			1544	984	291	261	8		

- Molecule 18 is a protein called 60S ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	252	Total	C	N	O	S	0	0
			2045	1297	384	358	6		

- Molecule 19 is a protein called 60S ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	186	Total	C	N	O	S	0	0
			1502	958	299	240	5		

- Molecule 20 is a protein called 60S ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	181	Total	C	N	O	S	0	0
			1505	949	308	244	4		

- Molecule 21 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	180	Total	C	N	O	S	0	0
			1496	946	289	254	7		

- Molecule 22 is a protein called 60S ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	155	Total	C	N	O	S	0	0
			1275	814	241	214	6		

- Molecule 23 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	170	Total	C	N	O	S	0	0
			1318	824	266	221	7		

- Molecule 24 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	97	Total	C	N	O	S	0	0
			824	548	135	139	2		

- Molecule 25 is a protein called 60S ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	101	Total	C	N	O	S	0	0
			796	502	144	144	6		

- Molecule 26 is a protein called 60S ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	121	Total	C	N	O	S	0	0
			1000	626	206	165	3		

- Molecule 27 is a protein called 60S ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	62	Total	C	N	O	S	0	0
			521	336	97	87	1		

- Molecule 28 is a protein called 60S ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	140	Total	C	N	O	S	0	0
			1134	736	204	191	3		

- Molecule 29 is a protein called 60S ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	104	Total	C	N	O	S	0	0
			830	529	151	147	3		

- Molecule 30 is a protein called 60S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	119	Total	C	N	O	S	0	0
			994	635	194	163	2		

- Molecule 31 is a protein called 60S ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	66	Total	C	N	O	S	0	0
			555	347	116	90	2		

- Molecule 32 is a protein called 60S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	223	Total	C	N	O	S	0	0
			1879	1211	357	306	5		

- Molecule 33 is a protein called 60S ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	98	Total	C	N	O	S	0	0
			740	462	132	139	7		

- Molecule 34 is a protein called 60S ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	96	Total	C	N	O	S	0	0
			793	508	151	129	5		

- Molecule 35 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	125	Total	C	N	O	S	0	0
			1036	660	206	163	7		

- Molecule 36 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	103	Total	C	N	O	S	0	0
			844	543	163	135	3		

- Molecule 37 is a protein called 60S ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	106	Total	C	N	O	S	0	0
			858	530	184	138	6		

- Molecule 38 is a protein called 60S ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	95	Total	C	N	O	S	0	0
			756	477	150	129			

- Molecule 39 is a protein called 60S ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	89	Total	C	N	O	S	0	0
			705	439	150	111	5		

- Molecule 40 is a protein called 60S ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	72	Total	C	N	O	S	0	0
			603	395	107	99	2		

- Molecule 41 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	43	Total	C	N	O	S	0	0
			388	243	92	52	1		

- Molecule 42 is a protein called 60S ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	f	51	Total	C	N	O	S	0	0
			413	255	87	66	5		

- Molecule 43 is a protein called 60S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	37	Total	C	N	O	S	0	0
			342	210	86	44	2		

- Molecule 44 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	h	85	Total	C	N	O	S	0	0
			658	417	127	107	7		

- Molecule 45 is a protein called 60S ribosomal protein eL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	i	95	Total	C	N	O	S	0	0
			778	490	152	127	9		

- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	A	153	Total	Mg	0
			153	153	
46	B	3	Total	Mg	0
			3	3	
46	C	5	Total	Mg	0
			5	5	
46	M	1	Total	Mg	0
			1	1	
46	Q	1	Total	Mg	0
			1	1	

- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
47	a	1	Total	Zn	0
			1	1	
47	c	1	Total	Zn	0
			1	1	

Continued on next page...

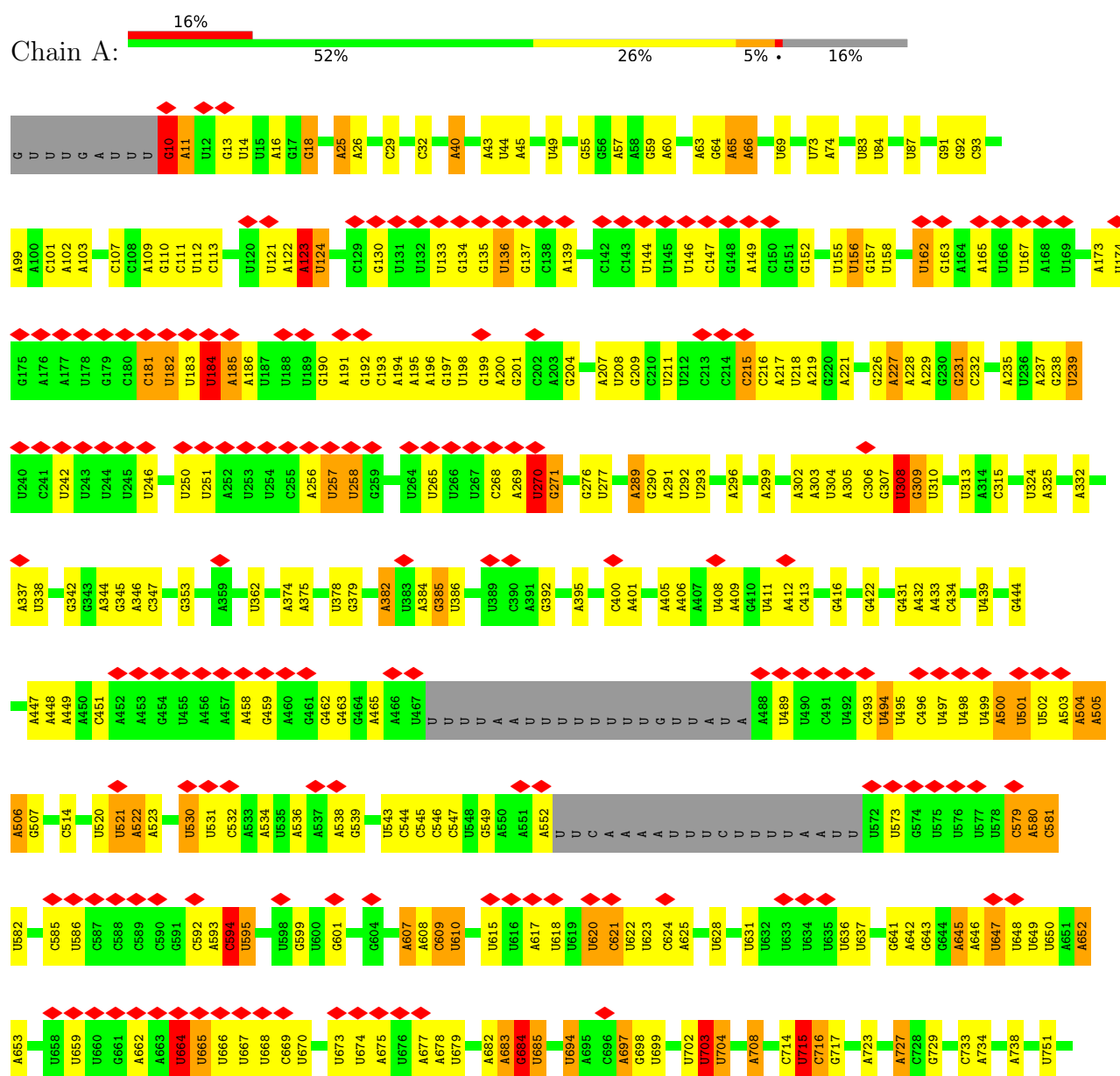
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
47	f	1	Total 1	Zn 1	0
47	h	1	Total 1	Zn 1	0
47	i	1	Total 1	Zn 1	0

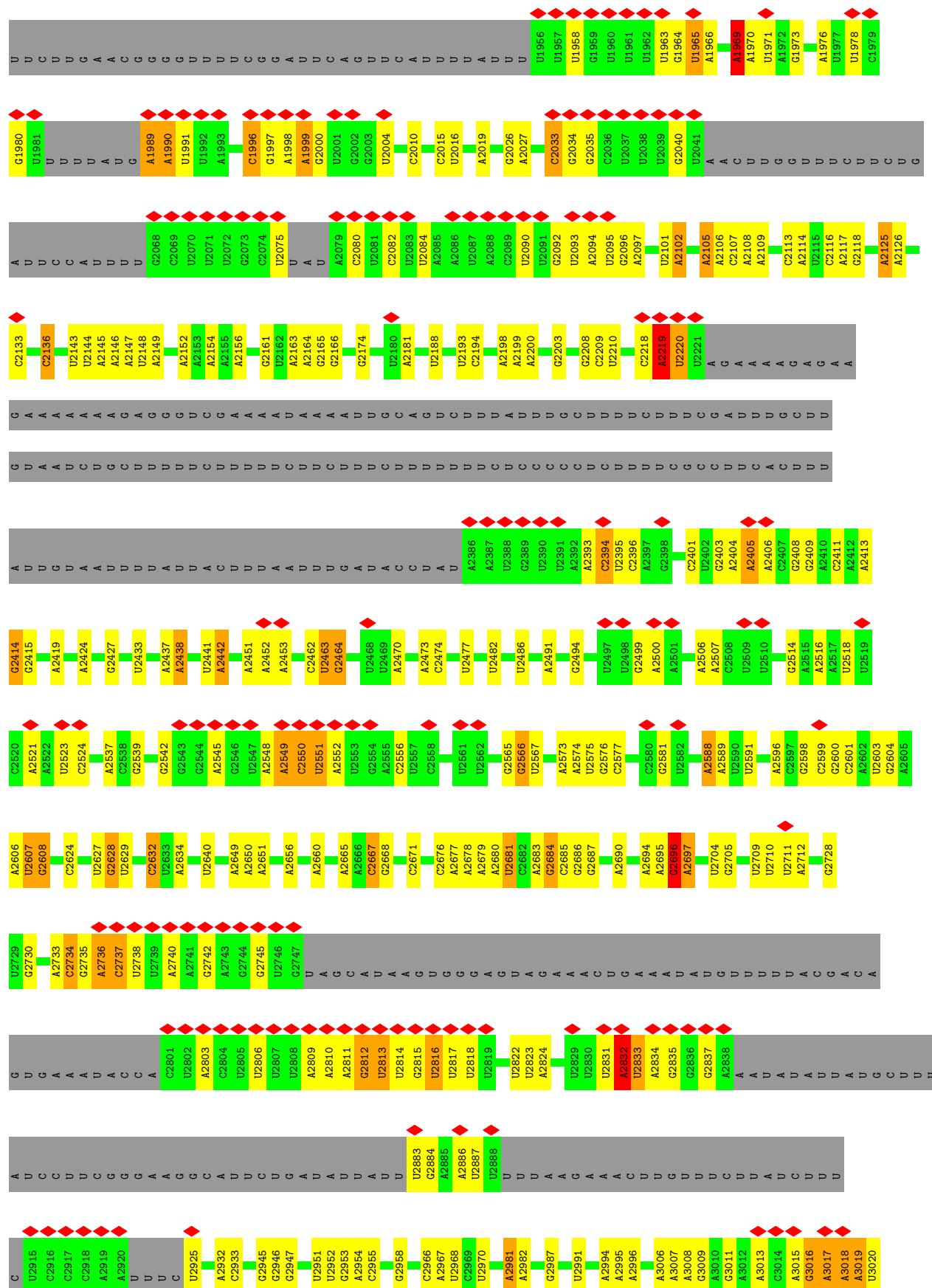
3 Residue-property plots

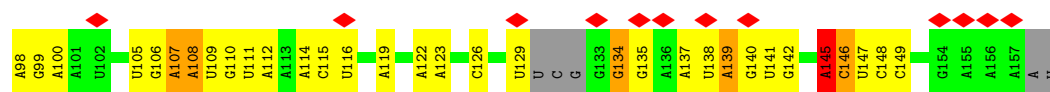
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 28S ribosomal RNA

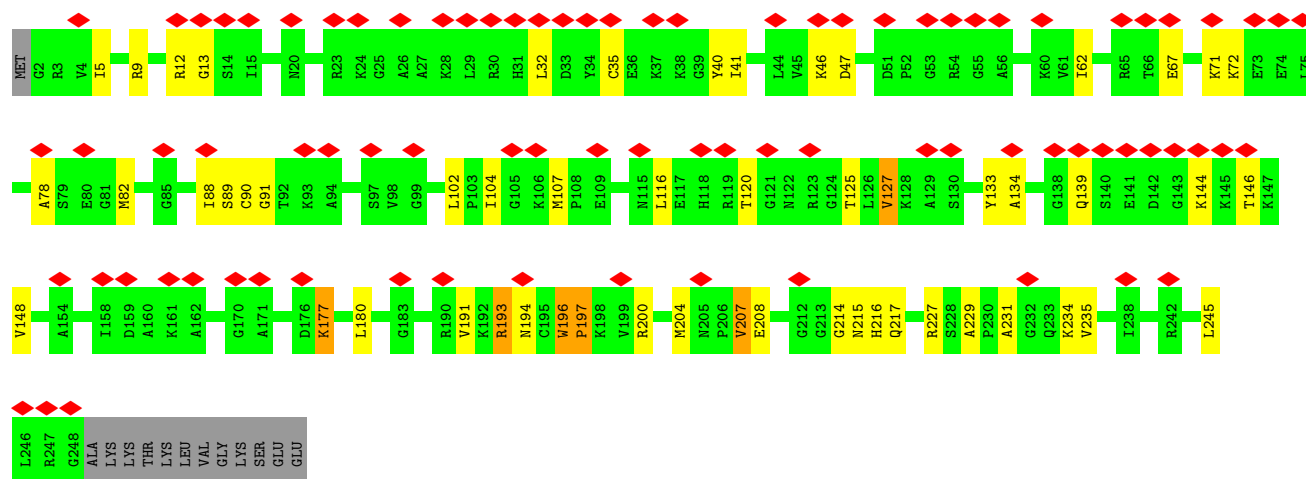
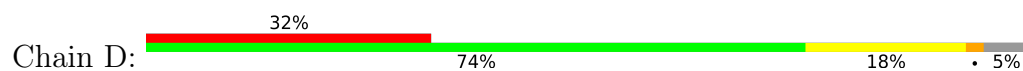




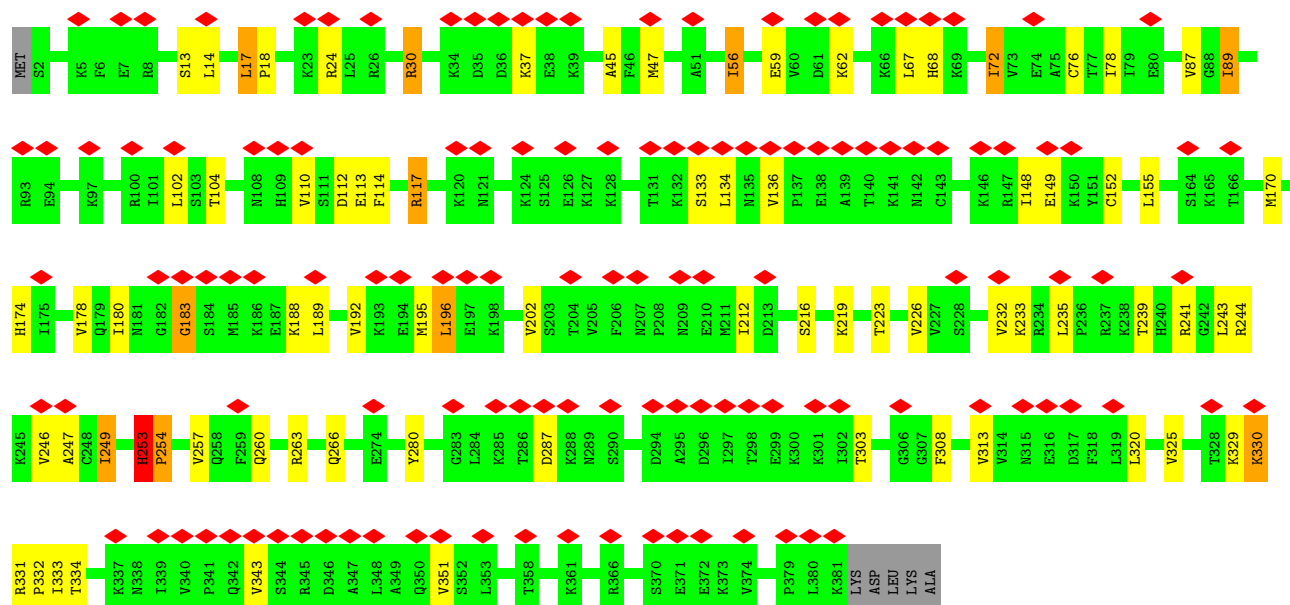
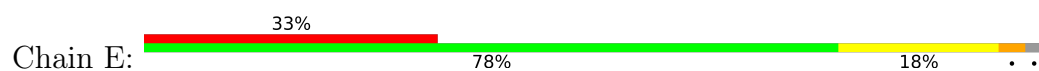




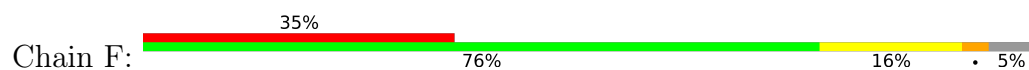
• Molecule 4: 60S ribosomal protein uL2

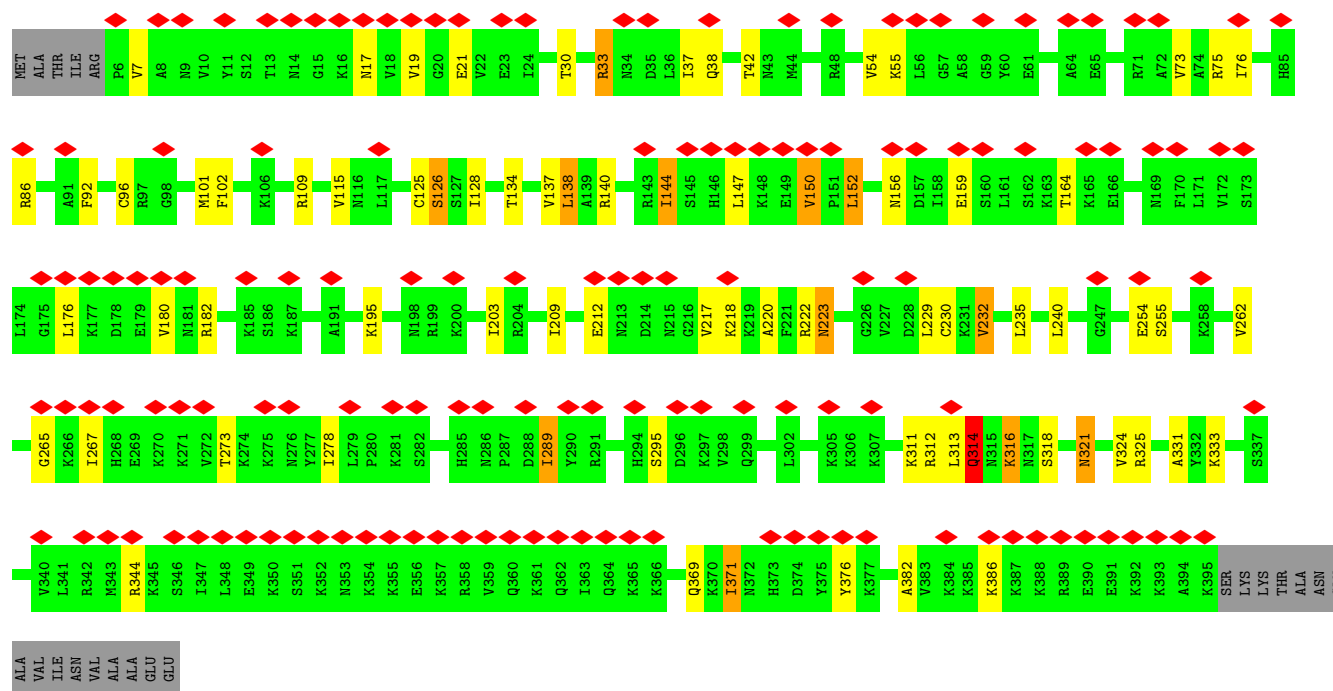


• Molecule 5: 60S ribosomal protein uL3

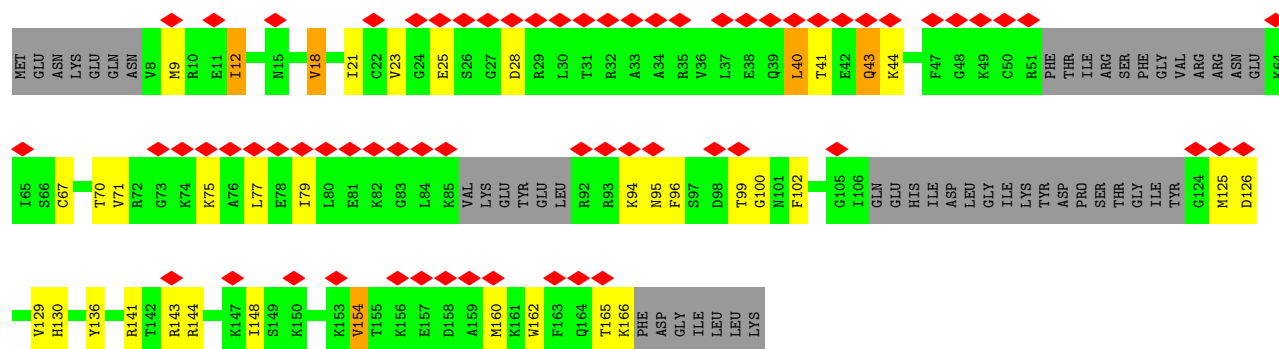


• Molecule 6: 60S ribosomal protein uL4

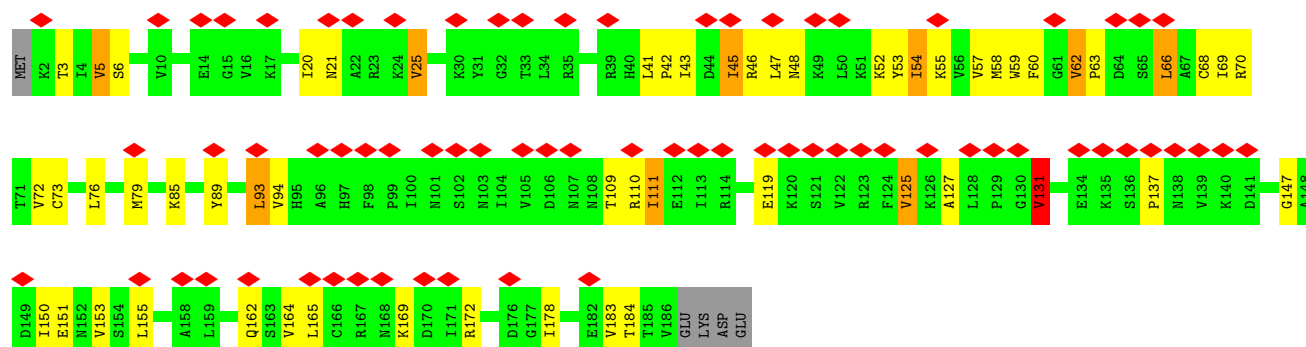




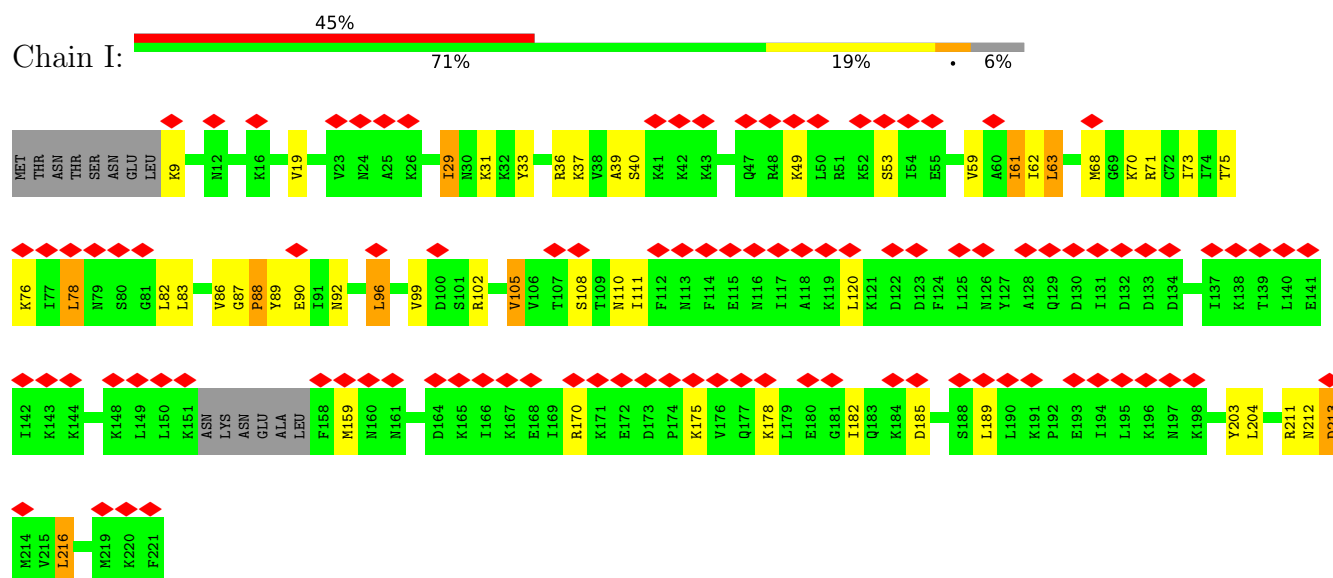
• Molecule 7: 60S ribosomal protein uL5



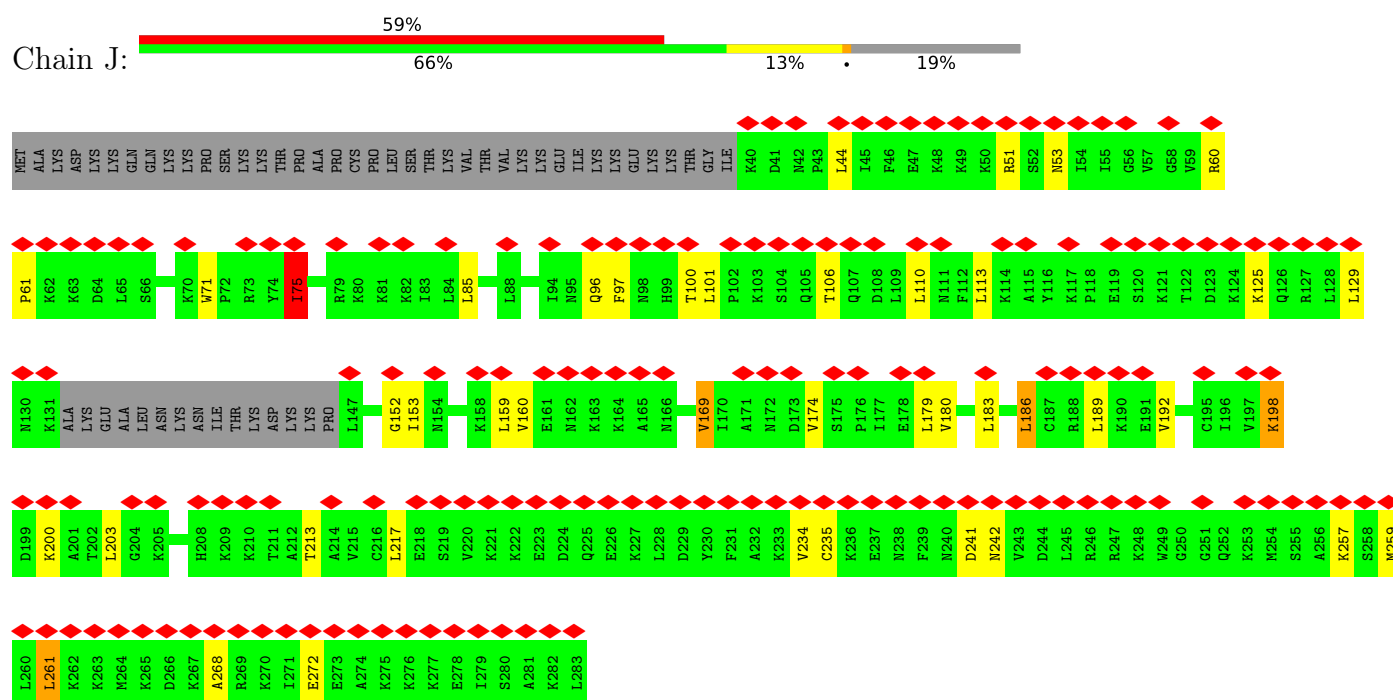
• Molecule 8: 60S ribosomal protein uL6



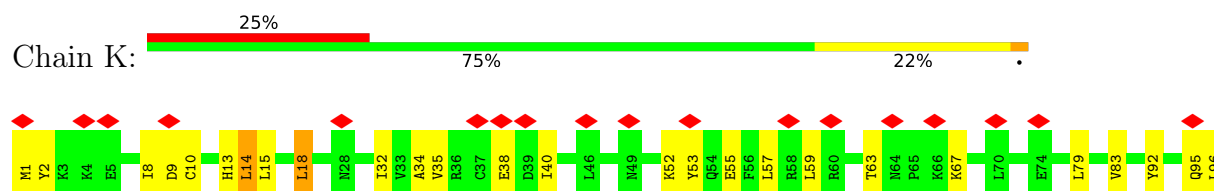
• Molecule 9: 60S ribosomal protein eL6

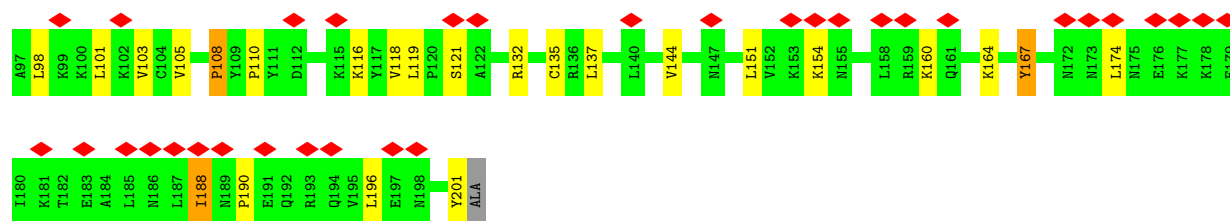


• Molecule 10: 60S ribosomal protein eL8

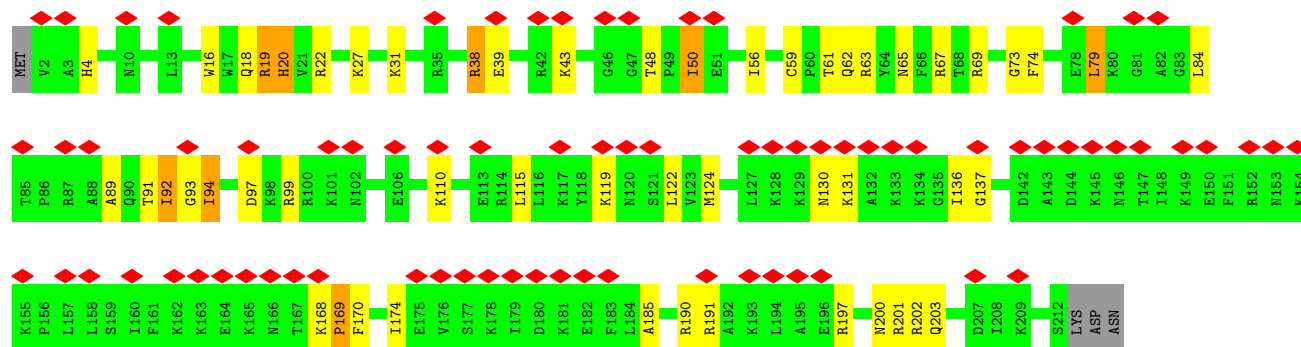
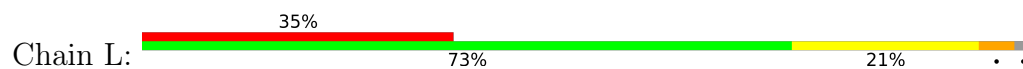


• Molecule 11: 60S ribosomal protein uL13

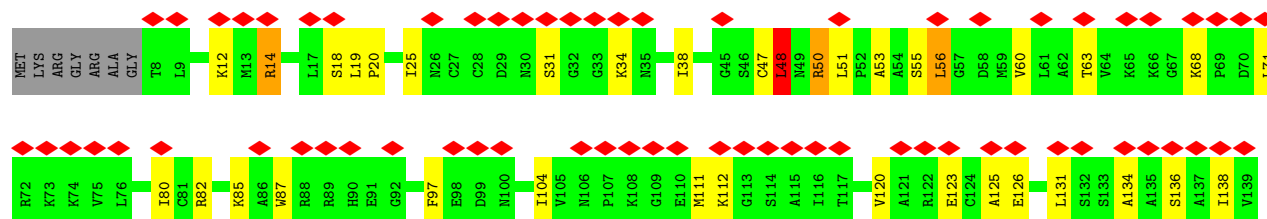




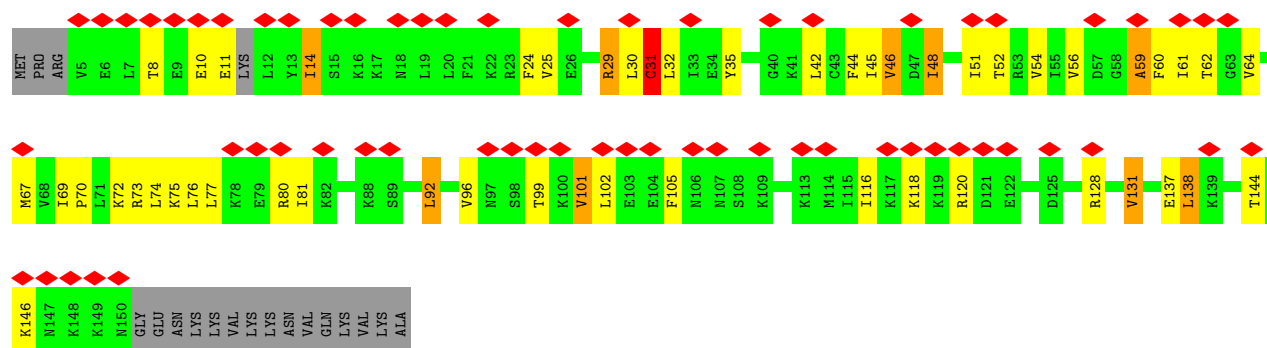
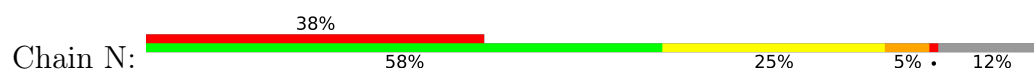
• Molecule 12: 60S ribosomal protein eL13



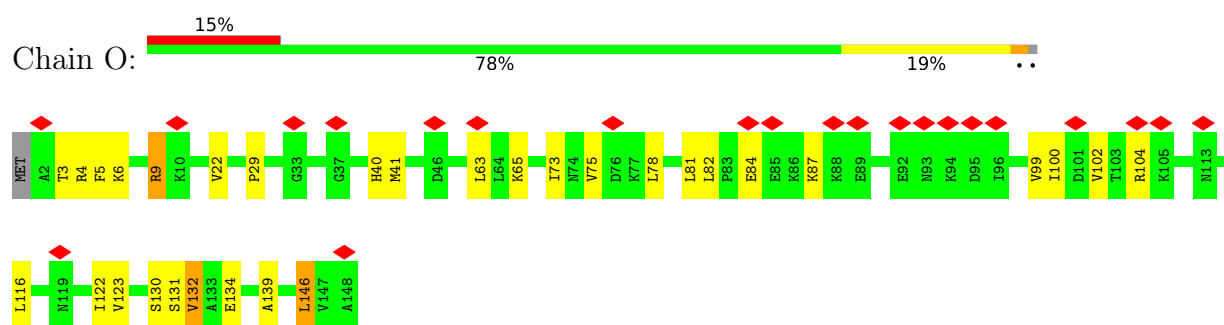
• Molecule 13: 60S ribosomal protein uL14



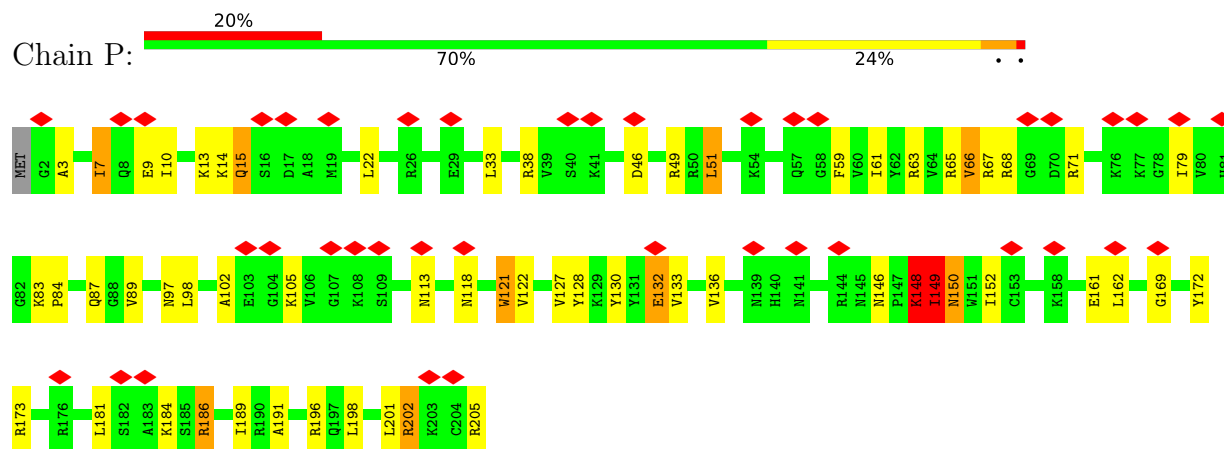
• Molecule 14: 60S ribosomal protein eL14



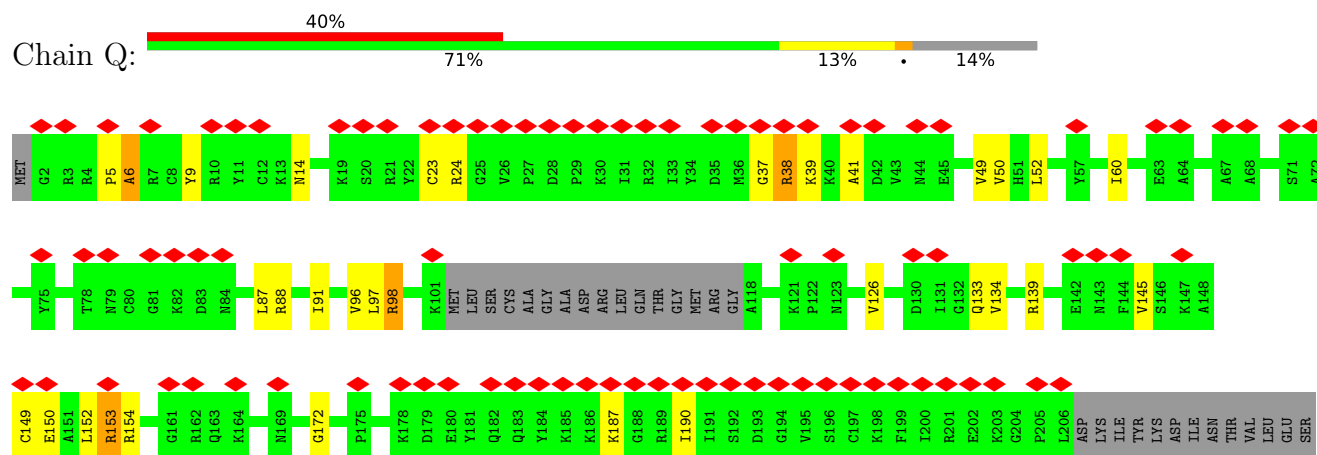
• Molecule 15: 60S ribosomal protein uL15



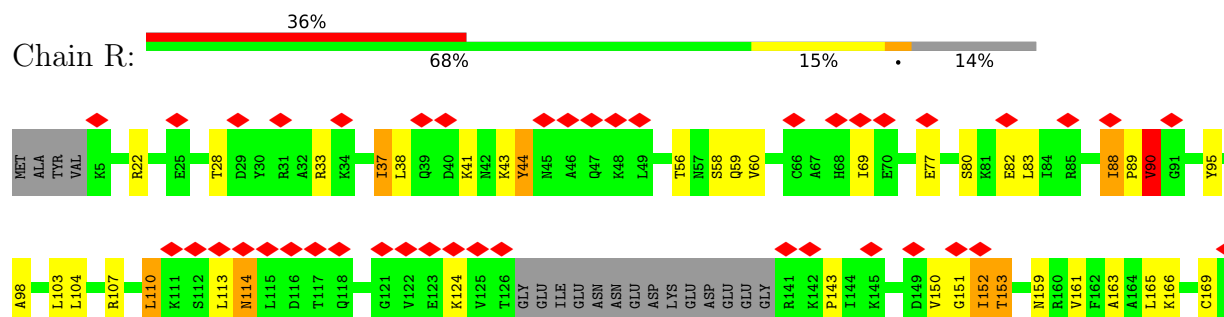
• Molecule 16: 60S ribosomal protein eL15

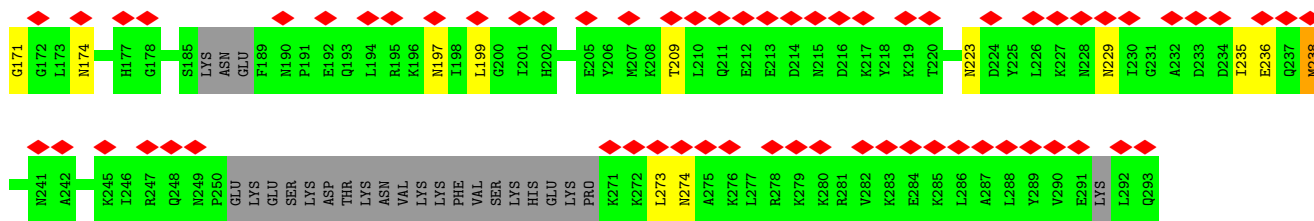


• Molecule 17: 60S ribosomal protein uL16

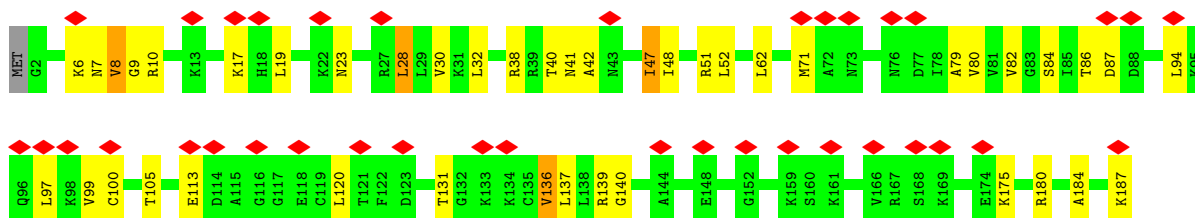
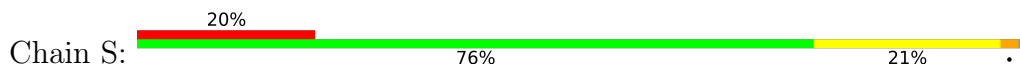


• Molecule 18: 60S ribosomal protein uL18

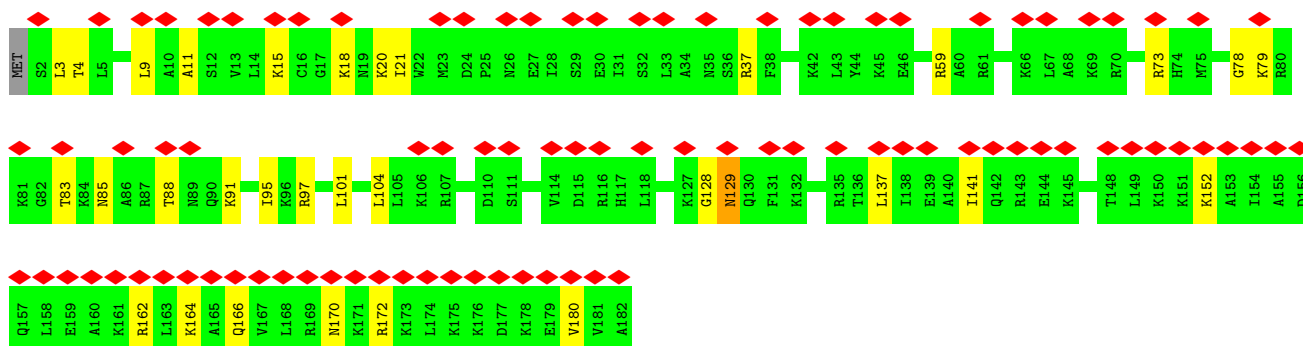
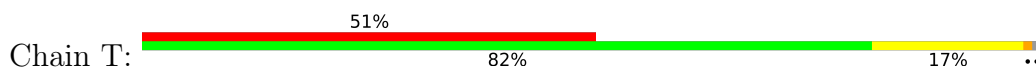




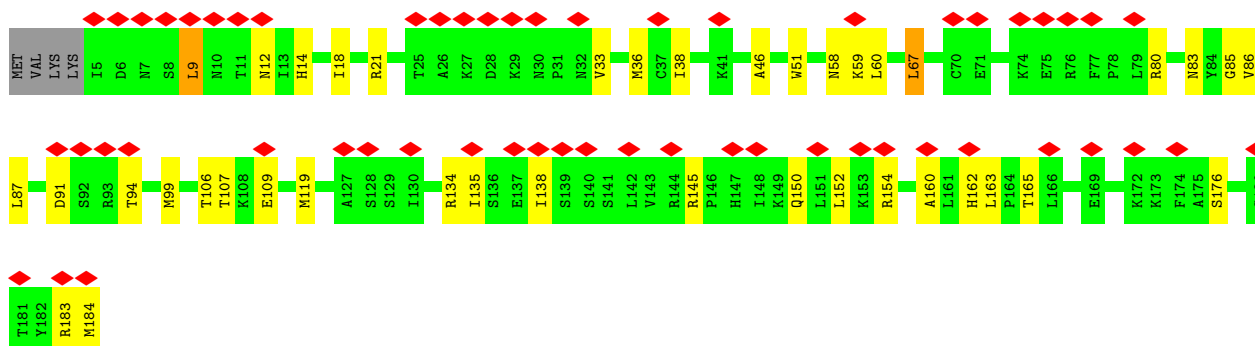
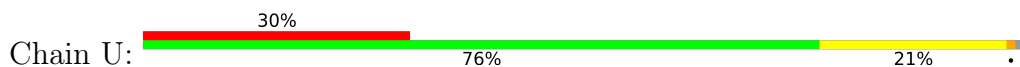
• Molecule 19: 60S ribosomal protein eL18



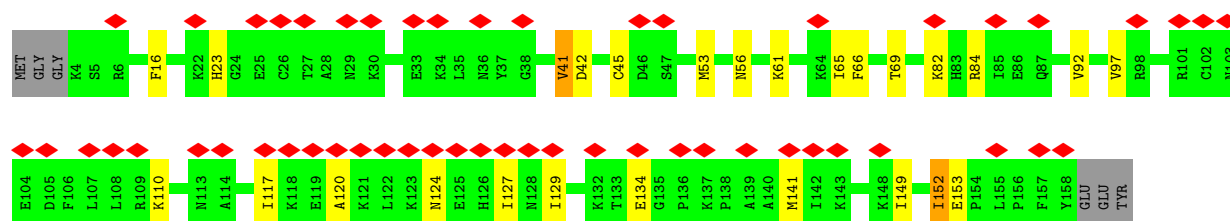
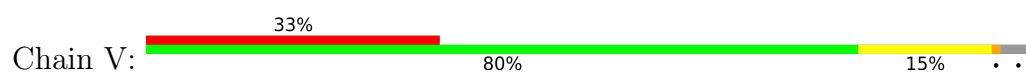
• Molecule 20: 60S ribosomal protein eL19



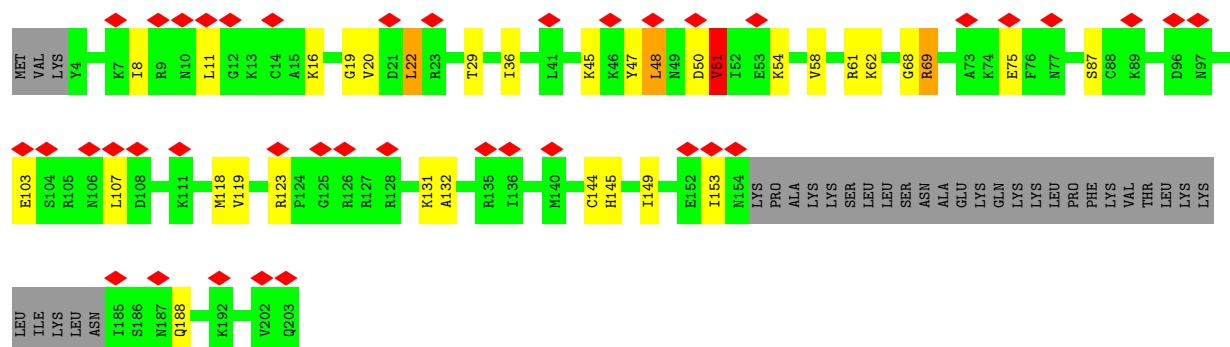
• Molecule 21: 60S ribosomal protein eL20



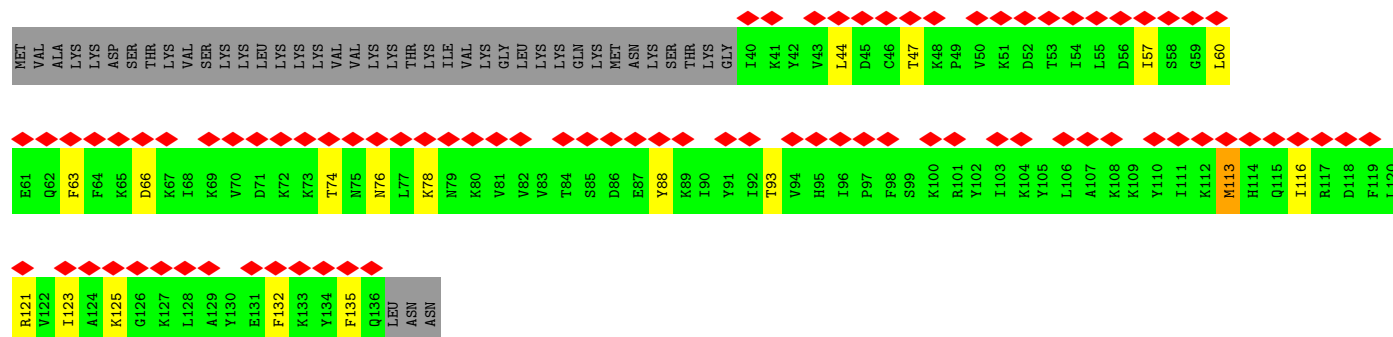
• Molecule 22: 60S ribosomal protein eL21



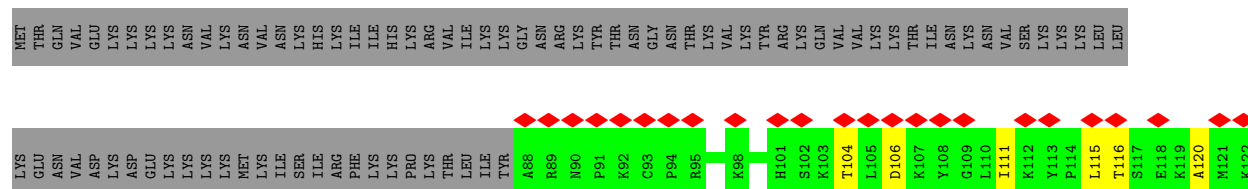
• Molecule 23: 60S ribosomal protein uL22

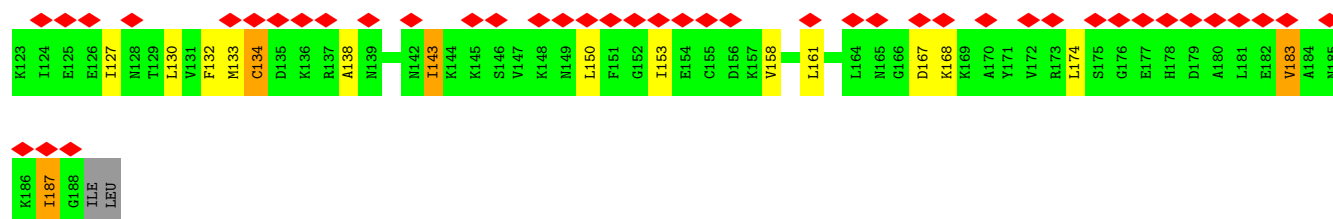


• Molecule 24: 60S ribosomal protein eL22

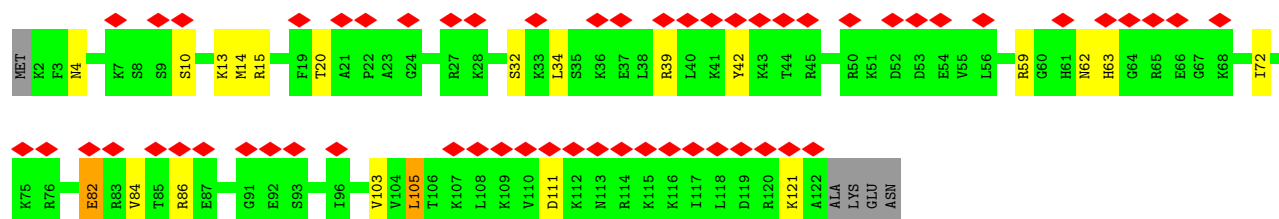
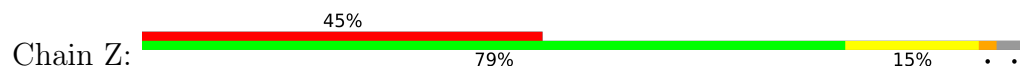


• Molecule 25: 60S ribosomal protein uL23

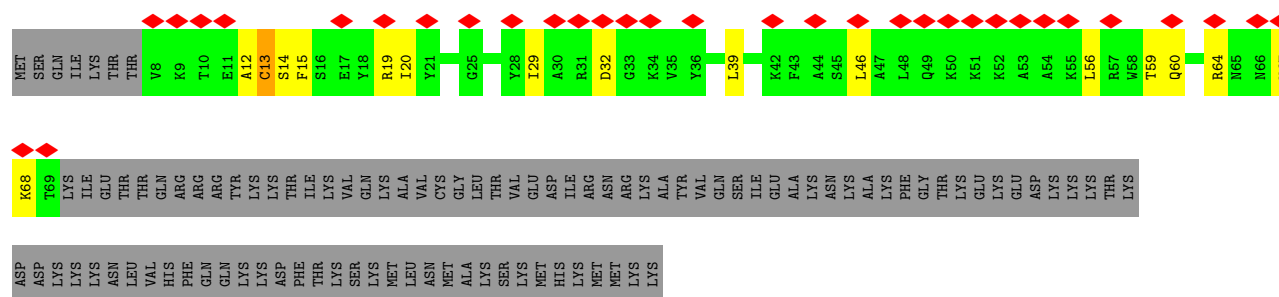




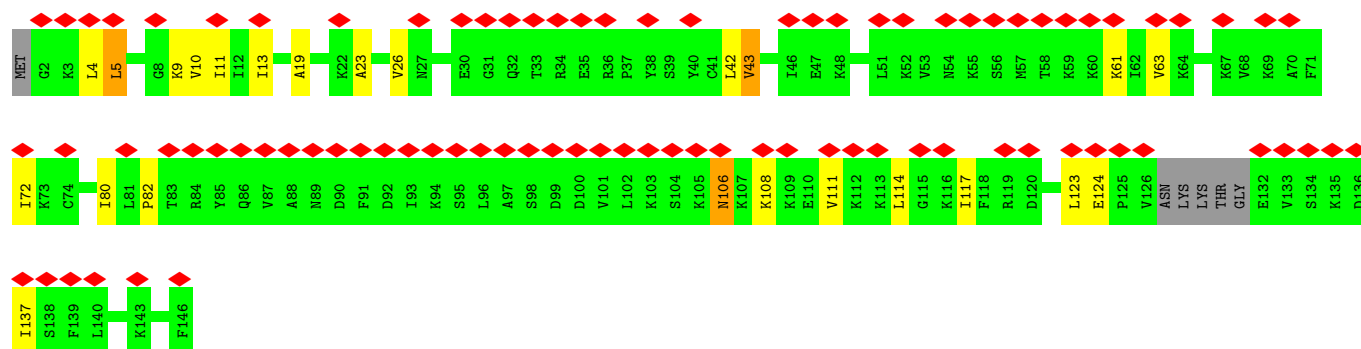
• Molecule 26: 60S ribosomal protein uL24



• Molecule 27: 60S ribosomal protein eL24

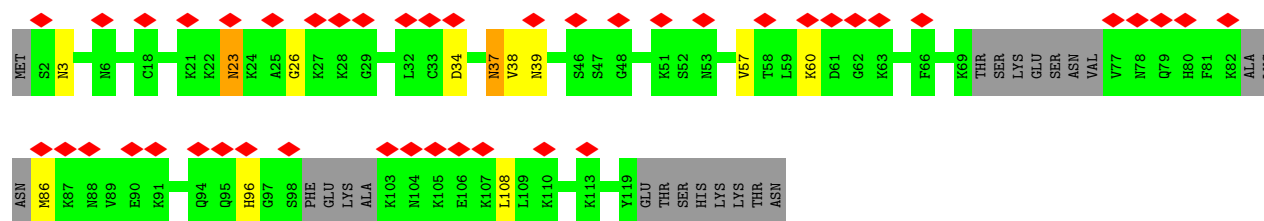


• Molecule 28: 60S ribosomal protein eL27

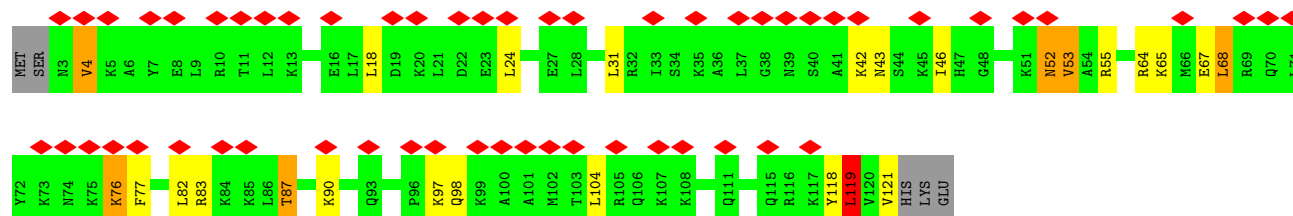
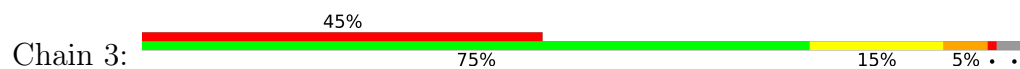


• Molecule 29: 60S ribosomal protein eL28

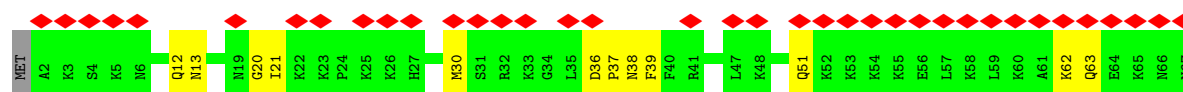
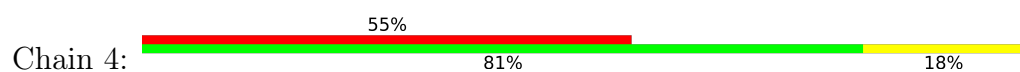




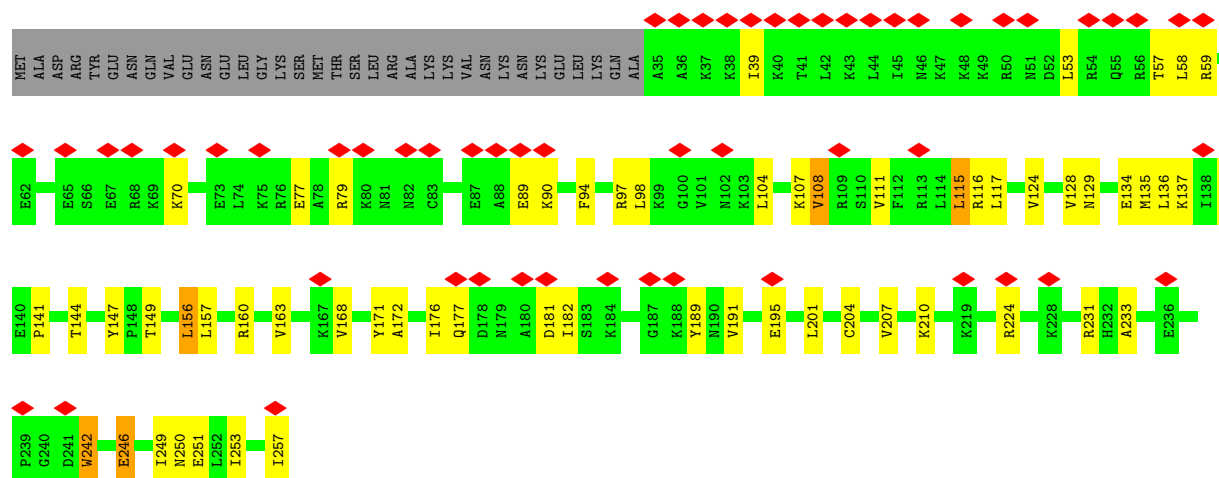
• Molecule 30: 60S ribosomal protein uL29



• Molecule 31: 60S ribosomal protein eL29



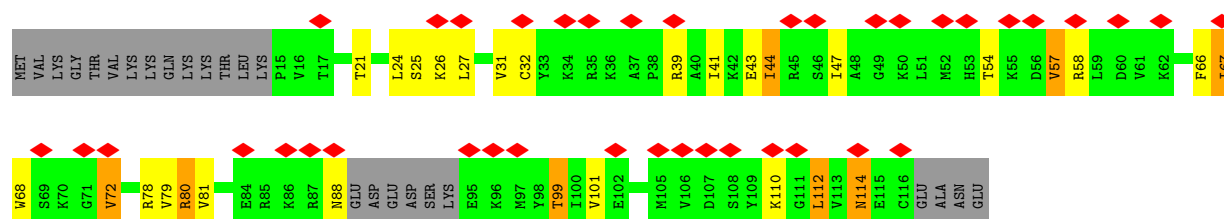
• Molecule 32: 60S ribosomal protein uL30



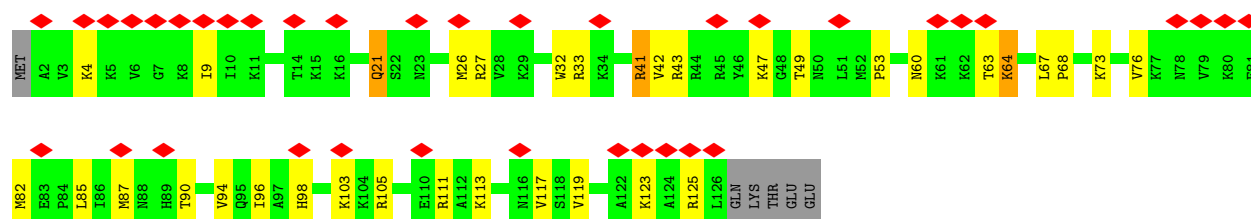
• Molecule 33: 60S ribosomal protein eL30



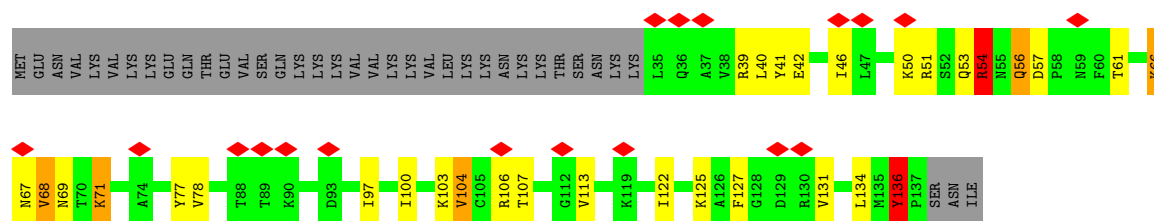
- Molecule 34: 60S ribosomal protein eL31



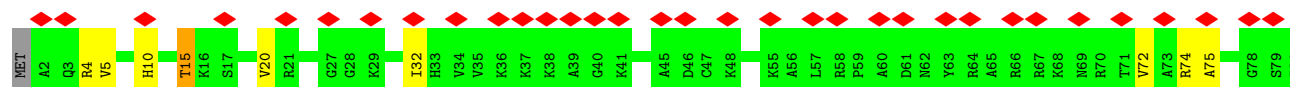
- Molecule 35: 60S ribosomal protein eL32

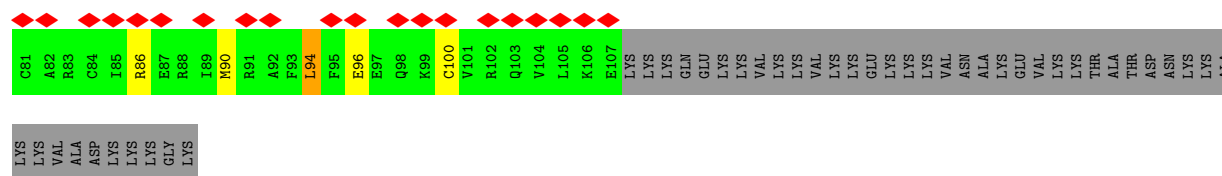


- Molecule 36: 60S ribosomal protein eL33

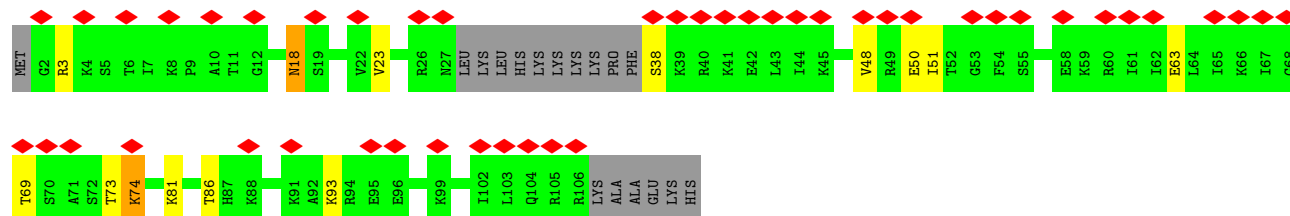
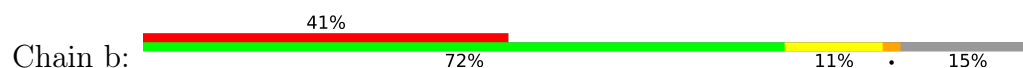


- Molecule 37: 60S ribosomal protein eL34

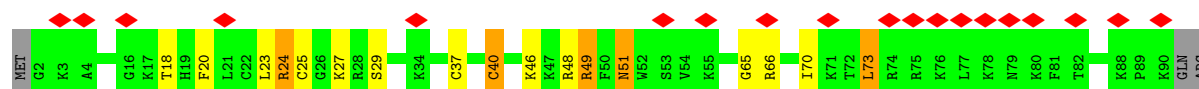
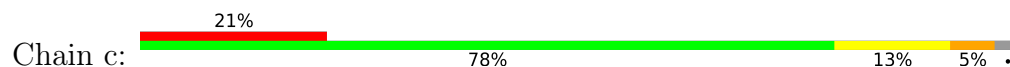




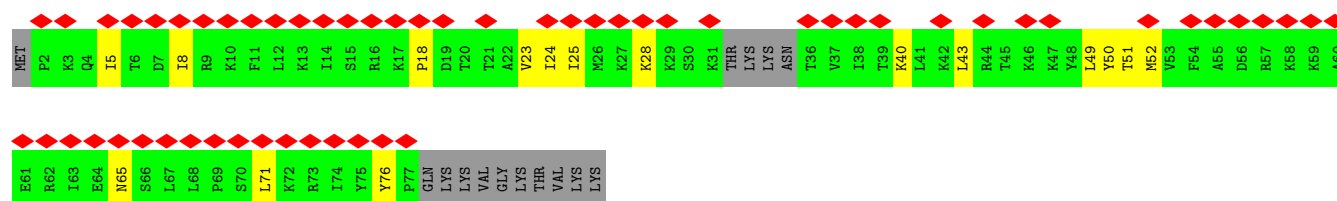
• Molecule 38: 60S ribosomal protein eL36



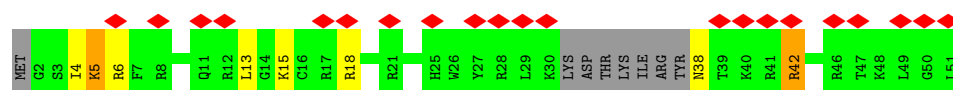
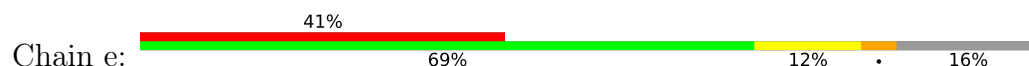
• Molecule 39: 60S ribosomal protein eL37



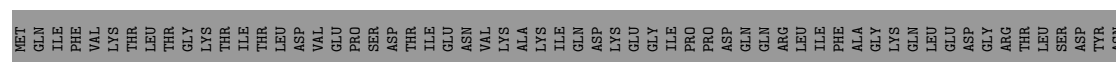
• Molecule 40: 60S ribosomal protein eL38

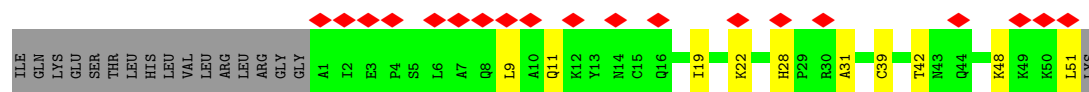


• Molecule 41: 60S ribosomal protein eL39

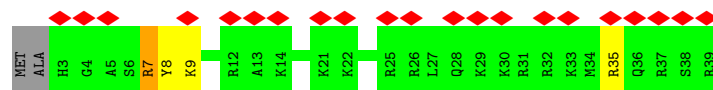
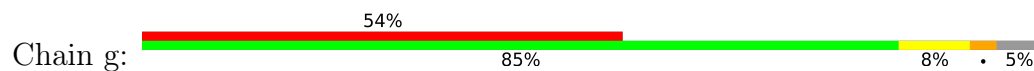


• Molecule 42: 60S ribosomal protein eL40

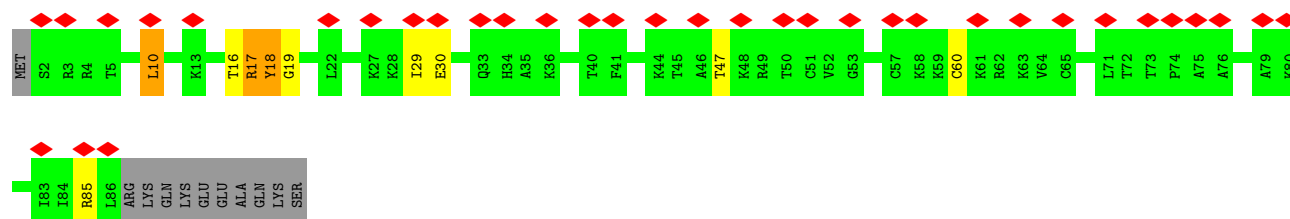
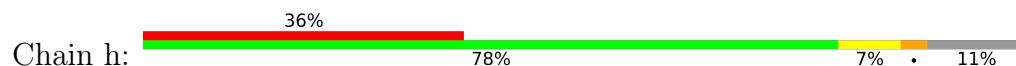




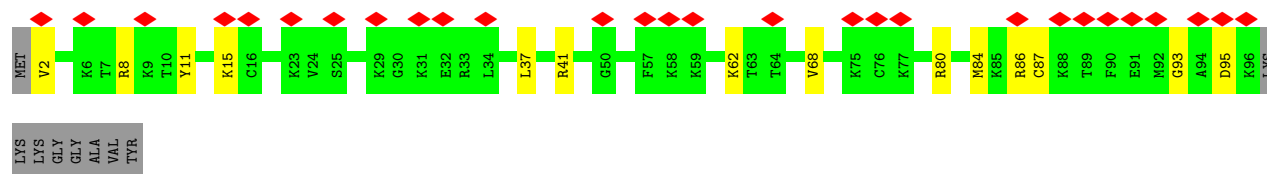
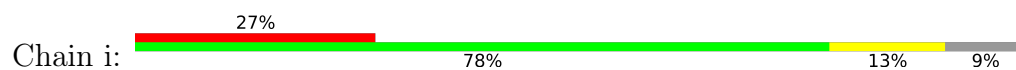
- Molecule 43: 60S ribosomal protein eL41



- Molecule 44: 60S ribosomal protein eL43



- Molecule 45: 60S ribosomal protein eL44



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	104748	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.962	Depositor
Minimum map value	-0.545	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.18	Depositor
Map size ($\text{\AA}$)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.39	0/75991	0.81	121/118299 (0.1%)
2	B	0.39	0/2826	0.73	0/4404
3	C	0.39	0/3608	0.83	8/5615 (0.1%)
4	D	0.67	0/1901	1.00	4/2544 (0.2%)
5	E	0.60	0/3129	0.94	3/4195 (0.1%)
6	F	0.56	0/3144	1.10	3/4205 (0.1%)
7	G	0.57	0/1020	1.04	1/1349 (0.1%)
8	H	0.59	0/1485	0.98	1/2009 (0.0%)
9	I	0.56	0/1707	1.05	0/2274
10	J	0.58	0/1901	1.10	3/2537 (0.1%)
11	K	0.60	0/1689	1.12	2/2260 (0.1%)
12	L	0.57	0/1793	1.07	1/2387 (0.0%)
13	M	0.66	0/1012	0.92	1/1363 (0.1%)
14	N	0.59	0/1213	1.12	2/1616 (0.1%)
15	O	0.60	0/1199	0.96	0/1597
16	P	0.61	0/1735	1.07	3/2320 (0.1%)
17	Q	0.55	0/1579	0.95	0/2113
18	R	0.56	0/2074	1.07	1/2773 (0.0%)
19	S	0.58	0/1530	1.00	0/2040
20	T	0.61	0/1521	1.08	0/2012
21	U	0.60	0/1526	0.91	0/2043
22	V	0.55	0/1300	0.86	0/1732
23	W	0.60	0/1338	1.01	1/1793 (0.1%)
24	X	0.55	0/841	0.96	0/1125
25	Y	0.57	0/805	1.01	1/1074 (0.1%)
26	Z	0.53	0/1012	0.95	0/1339
27	0	0.60	0/533	0.93	1/711 (0.1%)
28	1	0.49	0/1151	0.94	0/1531
29	2	0.52	0/839	0.94	0/1114
30	3	0.58	0/1004	1.16	1/1329 (0.1%)
31	4	0.51	0/564	1.15	0/737
32	5	0.60	0/1917	1.15	6/2562 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.57	0/748	1.26	3/1001 (0.3%)
34	7	0.62	0/805	1.03	0/1073
35	8	0.63	0/1053	1.01	3/1399 (0.2%)
36	9	0.66	0/864	1.00	2/1160 (0.2%)
37	a	0.50	0/871	0.93	0/1161
38	b	0.60	0/762	1.23	1/1008 (0.1%)
39	c	0.63	0/718	0.99	0/946
40	d	0.58	0/611	1.05	1/812 (0.1%)
41	e	0.61	0/396	0.94	0/521
42	f	0.67	0/418	1.07	0/556
43	g	0.58	0/347	1.12	0/448
44	h	0.54	0/667	0.92	0/887
45	i	0.55	0/788	0.84	0/1032
All	All	0.48	0/133935	0.89	174/197006 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
5	E	0	3
6	F	0	1
9	I	0	1
11	K	0	1
14	N	0	1
23	W	0	1
32	5	0	1
33	6	0	1
36	9	0	1
39	c	0	1
All	All	0	13

There are no bond length outliers.

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	A	C4'-C3'-O3'	10.81	125.61	109.40
1	A	1805	U	C2'-C3'-O3'	9.95	128.62	113.70
1	A	289	A	C2'-C3'-O3'	9.52	127.98	113.70
1	A	1574	C	C4'-C3'-O3'	9.41	123.52	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	773	A	C4'-C3'-O3'	9.40	123.49	109.40
3	C	145	A	C2'-C3'-O3'	9.39	127.79	113.70
1	A	664	U	C4'-C3'-O3'	9.23	123.25	109.40
1	A	308	U	C4'-C3'-O3'	9.22	123.23	109.40
33	6	90	ILE	N-CA-C	9.00	119.30	111.56
3	C	37	A	C2'-C3'-O3'	8.97	127.16	113.70
10	J	198	LYS	N-CA-C	8.60	120.65	111.28
1	A	270	U	C2'-C3'-O3'	8.46	122.19	109.50
1	A	652	A	C2'-C3'-O3'	8.23	126.05	113.70
1	A	215	C	C2'-C3'-O3'	8.11	125.86	113.70
1	A	1435	G	C2'-C3'-O3'	7.97	121.45	109.50
1	A	579	C	C4'-C3'-O3'	7.83	121.14	109.40
3	C	38	G	C4'-C3'-O3'	7.75	121.03	109.40
1	A	1536	U	C2'-C3'-O3'	7.60	125.10	113.70
16	P	121	TRP	N-CA-C	7.38	119.11	111.14
1	A	703	U	C2'-C3'-O3'	7.35	124.73	113.70
1	A	1630	A	C2'-C3'-O3'	7.35	120.52	109.50
1	A	3476	A	C4'-C3'-O3'	7.34	120.41	109.40
1	A	3130	U	C2'-C3'-O3'	7.31	120.47	109.50
1	A	505	A	C2'-C3'-O3'	7.30	124.66	113.70
1	A	647	U	C2'-C3'-O3'	7.27	120.41	109.50
1	A	2219	A	C2'-C3'-O3'	7.22	120.33	109.50
6	F	289	ILE	CB-CA-C	-7.17	102.46	112.14
12	L	74	PHE	N-CA-C	7.16	122.02	113.28
1	A	1197	U	C2'-C3'-O3'	7.16	124.43	113.70
1	A	1999	A	C2'-C3'-O3'	7.14	124.41	113.70
1	A	684	G	C4'-C3'-O3'	-7.12	98.72	109.40
1	A	1217	U	C2'-C3'-O3'	7.06	120.09	109.50
1	A	1750	U	C2'-C3'-O3'	7.05	120.08	109.50
1	A	3140	U	C4'-C3'-O3'	7.05	119.98	109.40
1	A	3664	G	C4'-C3'-O3'	7.00	119.91	109.40
1	A	620	U	C2'-C3'-O3'	7.00	120.00	109.50
1	A	3361	U	C2'-C3'-O3'	6.84	119.76	109.50
1	A	2405	A	C2'-C3'-O3'	6.83	119.74	109.50
1	A	1222	U	C4'-C3'-O3'	6.75	119.53	109.40
3	C	134	G	C2'-C3'-O3'	6.68	123.72	113.70
1	A	162	U	C2'-C3'-O3'	6.67	119.50	109.50
1	A	514	C	C4'-C3'-O3'	-6.59	103.11	113.00
1	A	1538	U	C2'-C3'-O3'	6.54	119.30	109.50
1	A	859	C	C2'-C3'-O3'	6.51	123.47	113.70
1	A	992	C	C2'-C3'-O3'	-6.51	103.94	113.70
1	A	581	C	C2'-C3'-O3'	6.50	123.44	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	6	20	VAL	N-CA-CB	6.48	119.35	110.54
36	9	136	TYR	N-CA-CB	6.45	117.93	109.55
14	N	131	VAL	N-CA-CB	6.44	119.30	110.54
1	A	1534	U	C4'-C3'-O3'	6.44	119.06	109.40
1	A	3623	A	C2'-C3'-O3'	6.43	123.34	113.70
1	A	1996	C	C4'-C3'-O3'	6.38	118.97	109.40
1	A	504	A	C2'-C3'-O3'	6.37	123.26	113.70
1	A	1206	U	C4'-C3'-O3'	6.30	118.84	109.40
1	A	1224	A	C4'-C3'-O3'	6.29	118.83	109.40
1	A	1457	G	C4'-C3'-O3'	6.27	122.41	113.00
1	A	1705	A	C2'-C3'-O3'	6.26	118.89	109.50
38	b	23	VAL	N-CA-C	6.25	117.11	109.30
1	A	621	C	C2'-C3'-O3'	6.25	123.08	113.70
8	H	151	GLU	N-CA-C	-6.25	104.16	110.97
36	9	127	PHE	N-CA-C	6.24	120.36	112.87
1	A	91	G	C2'-C3'-O3'	6.18	122.96	113.70
1	A	3414	G	C2'-C3'-O3'	6.17	122.96	113.70
1	A	3381	A	C2'-C3'-O3'	6.17	118.75	109.50
1	A	715	U	C2'-C3'-O3'	6.17	118.75	109.50
1	A	1989	A	C2'-C3'-O3'	6.16	122.94	113.70
1	A	2696	G	C4'-C3'-O3'	6.15	118.63	109.40
32	5	242	TRP	N-CA-C	6.14	120.46	113.15
1	A	505	A	C4'-C3'-O3'	-6.13	103.80	113.00
1	A	1035	G	C4'-C3'-O3'	6.13	122.20	113.00
1	A	1873	U	C2'-C3'-O3'	6.13	118.69	109.50
1	A	2095	U	C2'-C3'-O3'	6.11	118.67	109.50
1	A	514	C	C2'-C3'-O3'	6.10	122.85	113.70
1	A	607	A	C2'-C3'-O3'	6.09	122.83	113.70
1	A	889	U	C2'-C3'-O3'	6.08	118.62	109.50
11	K	167	TYR	CA-C-O	-6.01	114.18	120.55
1	A	1747	U	N1-C1'-C2'	5.97	120.95	112.00
1	A	10	G	C2'-C3'-O3'	5.96	122.64	113.70
1	A	1854	U	C2'-C3'-O3'	-5.93	104.80	113.70
6	F	232	VAL	CB-CA-C	-5.93	104.14	112.14
3	C	37	A	C1'-C2'-O2'	-5.92	99.53	108.40
6	F	344	ARG	N-CA-C	5.91	118.21	111.11
32	5	171	TYR	N-CA-C	5.89	120.77	112.93
1	A	708	A	C4'-C3'-O3'	-5.85	104.23	113.00
1	A	935	A	C2'-C3'-O3'	5.82	118.23	109.50
1	A	2033	C	C4'-C3'-O3'	5.81	121.72	113.00
1	A	2832	A	C2'-C3'-O3'	5.80	118.20	109.50
1	A	1205	U	C2'-C3'-O3'	5.79	118.19	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	715	U	C1'-C2'-O2'	-5.79	103.12	111.80
1	A	889	U	C4'-C3'-O3'	5.78	118.07	109.40
27	0	13	CYS	N-CA-C	5.77	119.85	113.21
1	A	123	A	C2'-C3'-O3'	5.75	118.13	109.50
1	A	3444	G	C2'-C3'-O3'	5.74	122.32	113.70
1	A	888	A	C4'-C3'-O3'	5.73	117.99	109.40
1	A	933	U	C4'-C3'-O3'	-5.68	104.48	113.00
4	D	231	ALA	N-CA-C	5.65	117.89	111.11
1	A	2118	G	C3'-C2'-O2'	5.61	119.12	110.70
1	A	2394	C	C2'-C3'-O3'	5.60	122.10	113.70
1	A	764	G	C2'-C3'-O3'	5.58	122.07	113.70
1	A	3589	U	C4'-C3'-O3'	5.58	117.77	109.40
5	E	253	HIS	N-CA-C	5.52	122.02	109.81
1	A	2105	A	C4'-C3'-O3'	5.52	121.28	113.00
1	A	1540	G	O4'-C1'-C2'	-5.51	100.29	105.80
32	5	108	VAL	N-CA-CB	5.51	118.03	110.54
5	E	254	PRO	N-CA-C	-5.50	101.15	112.47
35	8	42	VAL	N-CA-C	-5.49	105.50	110.82
5	E	249	ILE	N-CA-C	-5.47	104.99	110.30
1	A	1540	G	N9-C1'-C2'	5.47	122.20	114.00
1	A	1881	C	C2'-C3'-O3'	5.46	117.69	109.50
1	A	65	A	C4'-C3'-O3'	5.44	117.56	109.40
13	M	18	SER	N-CA-C	5.44	122.39	110.80
1	A	684	G	C2'-C3'-O3'	5.44	117.66	109.50
3	C	35	A	C2'-C3'-O3'	5.43	121.85	113.70
1	A	2816	U	C2'-C3'-O3'	5.43	121.84	113.70
1	A	594	C	N1-C1'-C2'	5.42	120.14	112.00
1	A	500	A	C4'-C3'-O3'	5.41	117.52	109.40
1	A	3166	U	C4'-C3'-O3'	-5.39	104.91	113.00
1	A	3782	A	C2'-C3'-O3'	5.39	117.58	109.50
4	D	214	GLY	N-CA-C	-5.37	106.85	111.95
1	A	580	A	C2'-C3'-O3'	5.36	121.75	113.70
33	6	101	SER	N-CA-C	5.33	117.42	110.43
1	A	1594	A	C2'-C3'-O3'	-5.33	105.71	113.70
23	W	51	VAL	N-CA-CB	5.33	118.57	110.58
1	A	91	G	C4'-C3'-O3'	-5.32	105.02	113.00
1	A	1704	U	C2'-C3'-O3'	5.32	121.68	113.70
1	A	697	A	C3'-C2'-O2'	5.31	118.67	110.70
1	A	3476	A	C2'-C3'-O3'	5.30	117.45	109.50
1	A	580	A	C3'-C2'-O2'	5.29	118.64	110.70
10	J	53	ASN	N-CA-C	5.27	117.30	108.23
32	5	70	LYS	CA-C-O	-5.25	114.99	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3526	U	C4'-C3'-O3'	5.24	117.27	109.40
16	P	122	VAL	N-CA-C	5.23	120.22	109.34
1	A	184	U	C2'-C3'-O3'	5.23	121.54	113.70
11	K	160	LYS	CA-C-O	-5.22	115.01	120.55
1	A	2588	A	C4'-C3'-O3'	-5.21	105.19	113.00
1	A	3306	G	C3'-C2'-O2'	5.21	118.51	110.70
1	A	501	U	C2'-C3'-O3'	5.19	121.48	113.70
1	A	1226	A	C4'-C3'-O3'	-5.18	105.23	113.00
1	A	3590	A	C2'-C3'-O3'	5.18	117.26	109.50
32	5	90	LYS	N-CA-C	5.17	119.30	113.15
1	A	903	C	C2'-C3'-O3'	5.16	117.24	109.50
25	Y	187	ILE	N-CA-CB	5.15	118.30	110.58
1	A	231	G	C4'-C3'-O3'	-5.14	105.28	113.00
3	C	139	A	C2'-C3'-O3'	5.13	117.20	109.50
16	P	148	LYS	N-CA-C	-5.13	102.09	110.20
1	A	1055	A	C4'-C3'-O3'	-5.13	105.31	113.00
14	N	31	CYS	N-CA-C	5.13	121.72	110.80
1	A	1101	A	C2'-C3'-O3'	5.12	121.39	113.70
30	3	53	VAL	CB-CA-C	-5.12	105.42	111.97
1	A	1990	A	C2'-C3'-O3'	5.12	121.38	113.70
7	G	154	VAL	N-CA-C	5.11	115.33	110.53
3	C	37	A	C3'-C2'-O2'	5.09	118.33	110.70
1	A	2709	U	C4'-C3'-O3'	-5.08	105.37	113.00
4	D	91	GLY	N-CA-C	5.07	116.99	110.96
1	A	2105	A	C2'-C3'-O3'	-5.07	106.10	113.70
1	A	3627	C	O4'-C1'-C2'	-5.06	102.54	107.60
32	5	246	GLU	N-CA-C	5.06	117.53	111.71
1	A	1071	A	C4'-C3'-O3'	-5.06	105.41	113.00
1	A	1779	A	C4'-C3'-O3'	5.06	116.99	109.40
1	A	3299	A	C4'-C3'-O3'	-5.05	105.42	113.00
1	A	3333	U	C1'-C2'-O2'	5.05	115.98	108.40
35	8	68	PRO	CA-C-N	5.05	127.55	120.28
35	8	68	PRO	C-N-CA	5.05	127.55	120.28
1	A	2136	C	C3'-C2'-O2'	5.04	118.27	110.70
1	A	3475	U	C3'-C2'-O2'	5.04	118.27	110.70
4	D	216	HIS	N-CA-C	5.04	122.29	114.64
10	J	268	ALA	N-CA-C	-5.03	104.75	111.24
18	R	37	ILE	N-CA-C	5.03	115.15	110.42
1	A	3782	A	C4'-C3'-O3'	5.03	116.94	109.40
1	A	1969	A	C2'-C3'-O3'	-5.03	101.96	109.50
1	A	3623	A	C3'-C2'-O2'	5.02	118.23	110.70
1	A	1243	G	C4'-C3'-O3'	-5.02	105.47	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	d	18	PRO	N-CA-C	5.01	120.21	114.20
1	A	1881	C	C4'-C3'-O3'	5.00	116.90	109.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	5	89	GLU	Peptide
33	6	52	PRO	Peptide
36	9	136	TYR	Peptide
4	D	196	TRP	Peptide
5	E	17	LEU	Peptide
5	E	195	MET	Peptide
5	E	253	HIS	Peptide
6	F	150	VAL	Peptide
9	I	87	GLY	Peptide
11	K	108	PRO	Peptide
14	N	59	ALA	Peptide
23	W	131	LYS	Peptide
39	c	20	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	67935	0	34190	472	0
2	B	2525	0	1274	7	0
3	C	3224	0	1630	22	0
4	D	1866	0	1964	22	0
5	E	3061	0	3205	42	0
6	F	3094	0	3333	38	0
7	G	1010	0	1073	15	0
8	H	1460	0	1532	21	0
9	I	1684	0	1849	16	0
10	J	1873	0	2055	10	0
11	K	1659	0	1782	18	0
12	L	1761	0	1895	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	996	0	1044	20	0
14	N	1197	0	1312	27	0
15	O	1172	0	1230	17	0
16	P	1697	0	1802	33	0
17	Q	1544	0	1582	12	0
18	R	2045	0	2129	17	0
19	S	1502	0	1636	18	0
20	T	1505	0	1671	14	0
21	U	1496	0	1556	21	0
22	V	1275	0	1355	10	0
23	W	1318	0	1319	11	0
24	X	824	0	882	5	0
25	Y	796	0	850	14	0
26	Z	1000	0	1099	4	0
27	0	521	0	539	6	0
28	1	1134	0	1245	10	0
29	2	830	0	887	3	0
30	3	994	0	1121	10	0
31	4	555	0	599	3	0
32	5	1879	0	2005	24	0
33	6	740	0	763	10	0
34	7	793	0	869	10	0
35	8	1036	0	1139	12	0
36	9	844	0	886	14	0
37	a	858	0	911	2	0
38	b	756	0	842	7	0
39	c	705	0	754	7	0
40	d	603	0	686	6	0
41	e	388	0	421	3	0
42	f	413	0	449	5	0
43	g	342	0	388	1	0
44	h	658	0	724	6	0
45	i	778	0	857	2	0
46	A	153	0	0	0	0
46	B	3	0	0	0	0
46	C	5	0	0	0	0
46	M	1	0	0	0	0
46	Q	1	0	0	0	0
47	a	1	0	0	0	0
47	c	1	0	0	0	0
47	f	1	0	0	2	0
47	h	1	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	i	1	0	0	0	0
All	All	124514	0	91334	940	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 (940) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3626:A:C6	1:A:3660:A:C6	2.12	1.37
1:A:3626:A:C2	1:A:3660:A:C2	2.31	1.19
1:A:3123:C:O2	12:L:202:ARG:NH2	1.80	1.14
1:A:3626:A:C5	1:A:3660:A:C6	2.38	1.12
1:A:3016:G:O6	1:A:3019:A:N6	1.87	1.07
1:A:2737:C:H2'	1:A:2738:U:C6	1.90	1.06
1:A:3626:A:C4	1:A:3660:A:N1	2.29	1.01
1:A:3626:A:C5	1:A:3660:A:N6	2.29	1.00
1:A:2733:A:C2'	1:A:2734:C:H5'	1.91	1.00
1:A:2812:G:C2	1:A:2813:U:C2	2.49	1.00
44:h:60:CYS:SG	47:h:100:ZN:ZN	1.49	0.99
1:A:308:U:HO2'	1:A:309:G:H8	1.04	0.98
42:f:39:CYS:SG	47:f:100:ZN:ZN	1.53	0.98
1:A:1574:C:O2'	1:A:1575:C:O5'	1.80	0.96
1:A:3654:C:C4	1:A:3655:U:O4	2.19	0.94
1:A:3626:A:C5	1:A:3660:A:N1	2.36	0.94
1:A:2733:A:H2'	1:A:2734:C:H5'	1.51	0.93
1:A:3629:U:H2'	1:A:3630:U:C6	2.03	0.93
1:A:3654:C:C5	1:A:3655:U:O4	2.21	0.93
1:A:3654:C:C4	1:A:3655:U:C4	2.59	0.90
1:A:2813:U:H2'	1:A:2814:U:C5	2.07	0.90
1:A:3626:A:C6	1:A:3660:A:N6	2.39	0.89
1:A:1630:A:O2'	1:A:2125:A:H1'	1.72	0.89
1:A:3630:U:H2'	1:A:3631:U:H5'	1.55	0.88
1:A:3632:U:O2'	1:A:3633:U:H5'	1.74	0.88
42:f:39:CYS:HG	47:f:100:ZN:ZN	0.57	0.88
1:A:3626:A:N6	1:A:3659:C:N3	2.21	0.87
12:L:94:ILE:HD12	12:L:115:LEU:HD21	1.57	0.87
1:A:3626:A:C6	1:A:3660:A:C5	2.62	0.87
1:A:3629:U:H3	1:A:3656:A:H2	1.20	0.86
1:A:1910:C:H2'	1:A:1911:A:C8	2.11	0.85
1:A:3018:A:C8	1:A:3018:A:H5''	2.11	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3629:U:O2'	1:A:3630:U:H5'	1.77	0.85
1:A:1534:U:O2'	1:A:1535:G:O5'	1.93	0.85
1:A:3016:G:H3'	1:A:3017:A:H5''	1.56	0.85
1:A:3628:C:O2	1:A:3657:G:N2	2.09	0.84
1:A:3655:U:O2'	1:A:3656:A:H5'	1.79	0.83
1:A:2734:C:H2'	1:A:2735:G:O4'	1.80	0.82
1:A:1574:C:HO2'	1:A:1575:C:P	2.02	0.81
36:9:50:LYS:O	36:9:56:GLN:O	1.99	0.81
1:A:3626:A:N3	1:A:3660:A:C2	2.49	0.80
1:A:3018:A:H5''	1:A:3018:A:H8	1.44	0.80
1:A:3660:A:H2'	1:A:3661:A:C8	2.16	0.80
1:A:3655:U:H2'	1:A:3656:A:C8	2.17	0.80
1:A:2737:C:C5'	1:A:2737:C:H6	1.95	0.79
1:A:3629:U:N3	1:A:3656:A:H2	1.81	0.78
1:A:2812:G:O2'	1:A:2813:U:O5'	2.01	0.77
1:A:3629:U:H2'	1:A:3630:U:H6	1.45	0.77
22:V:120:ALA:HB2	22:V:127:ILE:HD12	1.65	0.77
1:A:3628:C:H2'	1:A:3629:U:C6	2.19	0.77
11:K:34:ALA:HB3	11:K:103:VAL:HG12	1.67	0.76
1:A:3628:C:H2'	1:A:3629:U:C5	2.19	0.76
1:A:3629:U:C2	1:A:3630:U:C5	2.74	0.76
1:A:2813:U:H2'	1:A:2814:U:C6	2.20	0.75
19:S:51:ARG:HB3	19:S:82:VAL:HG21	1.67	0.75
1:A:257:U:O2'	1:A:258:U:O4'	2.03	0.75
1:A:3629:U:N3	1:A:3630:U:C4	2.55	0.74
7:G:41:THR:HG21	7:G:71:VAL:HG11	1.69	0.74
1:A:257:U:H2'	1:A:258:U:C6	2.23	0.73
1:A:3626:A:C2	1:A:3660:A:N1	2.57	0.73
1:A:3629:U:N3	1:A:3656:A:C2	2.51	0.73
1:A:2736:A:N6	1:A:2813:U:O4	2.19	0.73
1:A:2685:C:O2'	5:E:263:ARG:NH2	2.21	0.73
1:A:3626:A:C6	1:A:3660:A:N1	2.56	0.73
1:A:3626:A:N6	1:A:3660:A:C6	2.58	0.72
1:A:3654:C:C5	1:A:3655:U:C4	2.77	0.72
36:9:78:VAL:O	36:9:104:VAL:O	2.08	0.72
19:S:51:ARG:HB2	19:S:82:VAL:HG11	1.71	0.71
1:A:2736:A:H2'	1:A:2737:C:C6	2.25	0.71
16:P:9:GLU:HB3	38:b:48:VAL:HG21	1.72	0.71
1:A:3626:A:N1	1:A:3660:A:C6	2.59	0.71
1:A:63:A:OP1	16:P:173:ARG:NH2	2.24	0.70
19:S:71:MET:HE1	19:S:136:VAL:HG21	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:U:H4'	1:A:258:U:OP1	1.90	0.70
13:M:125:ALA:HB2	13:M:138:ILE:HD11	1.72	0.70
1:A:3631:U:H2'	1:A:3632:U:O4'	1.91	0.70
25:Y:143:ILE:HG21	25:Y:158:VAL:HG21	1.74	0.70
1:A:3660:A:O2'	1:A:3661:A:O4'	2.10	0.69
1:A:107:C:OP1	12:L:38:ARG:NH1	2.25	0.69
1:A:2736:A:C2'	1:A:2737:C:H5'	2.22	0.69
45:i:2:VAL:HG11	45:i:84:MET:HE1	1.74	0.69
1:A:3658:G:N2	1:A:3659:C:H1'	2.08	0.68
1:A:998:U:H4'	23:W:132:ALA:HB2	1.76	0.68
1:A:2812:G:C6	1:A:2813:U:C4	2.81	0.68
1:A:3630:U:C2'	1:A:3631:U:H5'	2.24	0.68
16:P:121:TRP:O	16:P:130:TYR:O	2.12	0.68
1:A:3628:C:H3'	1:A:3629:U:C5	2.29	0.67
1:A:3656:A:O2'	1:A:3657:G:H5'	1.94	0.67
1:A:3613:A:N6	1:A:3614:A:N1	2.43	0.67
1:A:2812:G:N1	1:A:2813:U:C2	2.62	0.66
1:A:3658:G:H1'	1:A:3659:C:O5'	1.96	0.66
6:F:128:ILE:HD11	6:F:235:LEU:HD13	1.77	0.66
8:H:66:LEU:O	8:H:69:ILE:HG22	1.95	0.66
12:L:79:LEU:HD11	12:L:94:ILE:HD11	1.78	0.65
1:A:3655:U:H2'	1:A:3656:A:H8	1.60	0.65
1:A:1216:C:H2'	1:A:1217:U:H5'	1.78	0.65
1:A:3626:A:N1	1:A:3660:A:C5	2.64	0.65
28:1:11:ILE:HG21	28:1:80:ILE:HD13	1.78	0.65
8:H:3:THR:HG21	8:H:66:LEU:HD11	1.78	0.65
5:E:149:GLU:HG3	5:E:189:LEU:HD13	1.79	0.64
1:A:1262:G:O2'	1:A:2981:A:N3	2.25	0.64
1:A:3654:C:N4	1:A:3655:U:O4	2.29	0.64
5:E:89:ILE:HG22	5:E:155:LEU:HD22	1.78	0.64
1:A:3656:A:H2'	1:A:3657:G:C8	2.32	0.64
5:E:249:ILE:HG21	5:E:257:VAL:HG22	1.80	0.64
12:L:20:HIS:HB2	16:P:198:LEU:HD23	1.79	0.64
13:M:111:MET:HE1	13:M:134:ALA:CB	2.28	0.64
1:A:3018:A:H8	1:A:3018:A:C5'	2.10	0.63
1:A:3669:U:C2	9:I:68:MET:HE1	2.33	0.63
14:N:96:VAL:HG23	14:N:101:VAL:HG12	1.80	0.63
1:A:2814:U:O2'	1:A:2815:G:O4'	2.16	0.63
5:E:67:LEU:HD21	5:E:72:ILE:HD12	1.79	0.63
14:N:31:CYS:SG	14:N:45:ILE:HD11	2.39	0.63
1:A:257:U:C2'	1:A:258:U:C6	2.82	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:303:THR:HG21	5:E:313:VAL:HG13	1.80	0.63
1:A:2814:U:O2'	1:A:2815:G:O5'	2.17	0.63
6:F:147:LEU:HD13	6:F:152:LEU:HD12	1.80	0.63
1:A:3626:A:N6	1:A:3660:A:N6	2.48	0.62
1:A:10:G:O2'	1:A:11:A:OP1	2.12	0.62
1:A:3613:A:N6	1:A:3614:A:C6	2.66	0.62
1:A:3628:C:C3'	1:A:3629:U:C6	2.83	0.62
32:5:57:THR:HG23	32:5:195:GLU:HG2	1.81	0.62
1:A:2463:U:H2'	1:A:2464:G:O4'	2.00	0.62
1:A:3632:U:H6	1:A:3632:U:O5'	1.82	0.62
16:P:169:GLY:HA2	16:P:172:TYR:CE2	2.34	0.62
30:3:87:THR:HG23	30:3:90:LYS:HB2	1.82	0.62
1:A:755:A:OP2	19:S:105:THR:HG21	1.99	0.62
1:A:2733:A:H2'	1:A:2734:C:C6	2.35	0.62
4:D:196:TRP:CE3	4:D:197:PRO:HD3	2.35	0.62
27:0:13:CYS:O	27:0:15:PHE:N	2.33	0.62
1:A:2812:G:O2'	1:A:2813:U:O4'	2.17	0.61
1:A:3016:G:H2'	1:A:3016:G:N3	2.14	0.61
19:S:71:MET:SD	19:S:79:ALA:HB2	2.40	0.61
34:7:27:LEU:HD13	34:7:43:GLU:HB3	1.82	0.61
1:A:1480:G:O6	1:A:1502:G:O6	2.17	0.61
1:A:3018:A:H4'	1:A:3018:A:OP1	1.99	0.61
1:A:2733:A:O2'	1:A:2734:C:H5'	2.00	0.61
1:A:1908:U:H2'	1:A:1909:U:H5'	1.83	0.61
35:8:94:VAL:CG2	35:8:119:VAL:HG22	2.31	0.61
1:A:257:U:H2'	1:A:258:U:C5	2.34	0.60
1:A:1444:A:C5	21:U:163:LEU:HD11	2.36	0.60
8:H:127:ALA:HB1	8:H:131:VAL:HG13	1.83	0.60
21:U:36:MET:HE2	21:U:38:ILE:HD11	1.83	0.60
12:L:200:ASN:OD1	38:b:3:ARG:HB3	2.02	0.60
32:5:189:TYR:HB3	32:5:207:VAL:HG21	1.82	0.60
36:9:56:GLN:HA	36:9:56:GLN:HE21	1.67	0.60
40:d:23:VAL:HG23	40:d:71:LEU:HD12	1.84	0.60
1:A:3626:A:N3	1:A:3660:A:N1	2.49	0.60
24:X:47:THR:HG22	24:X:88:TYR:HB3	1.84	0.60
1:A:1542:A:OP1	35:8:98:HIS:NE2	2.34	0.59
1:A:3626:A:N6	1:A:3659:C:C2	2.70	0.59
5:E:226:VAL:HG11	5:E:246:VAL:HG23	1.84	0.59
13:M:47:CYS:SG	13:M:50:ARG:NH1	2.74	0.59
1:A:2736:A:N6	1:A:2813:U:H3	2.01	0.59
1:A:257:U:O2'	1:A:258:U:C6	2.52	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3628:C:C2'	1:A:3629:U:C5	2.85	0.59
21:U:160:ALA:HB1	21:U:162:HIS:CE1	2.37	0.59
1:A:257:U:O2'	1:A:258:U:OP1	2.21	0.59
1:A:2812:G:N1	1:A:2813:U:N3	2.51	0.59
1:A:3626:A:N6	1:A:3660:A:C5	2.70	0.59
16:P:161:GLU:HG2	16:P:162:LEU:HD22	1.83	0.59
1:A:1462:C:O2'	32:5:160:ARG:NH1	2.36	0.59
1:A:2812:G:C6	1:A:2813:U:N3	2.71	0.59
7:G:102:PHE:CE2	7:G:129:VAL:HG21	2.37	0.59
1:A:3629:U:OP2	1:A:3629:U:H3'	2.03	0.59
14:N:69:ILE:HD11	14:N:74:LEU:HD21	1.85	0.58
18:R:150:VAL:HG23	18:R:161:VAL:HG21	1.85	0.58
1:A:2463:U:C2	1:A:2464:G:C8	2.91	0.58
1:A:2736:A:H2'	1:A:2737:C:H5'	1.85	0.58
1:A:3658:G:HO2'	1:A:3659:C:C5'	2.15	0.58
18:R:89:PRO:O	18:R:90:VAL:HG22	2.02	0.58
33:6:45:VAL:HG22	33:6:94:VAL:HG22	1.85	0.58
1:A:99:A:OP1	16:P:196:ARG:HD2	2.03	0.58
16:P:10:ILE:HD11	38:b:51:ILE:HD13	1.84	0.58
19:S:40:THR:O	19:S:42:ALA:N	2.36	0.58
34:7:24:LEU:HD23	34:7:27:LEU:HD12	1.85	0.58
1:A:3654:C:C6	1:A:3655:U:C5	2.92	0.58
1:A:3613:A:C6	1:A:3614:A:N1	2.71	0.58
12:L:92:ILE:HG22	12:L:93:GLY:H	1.66	0.58
1:A:3657:G:O5'	1:A:3657:G:H8	1.86	0.58
1:A:3524:G:N7	5:E:30:ARG:NH2	2.51	0.58
1:A:3628:C:C2'	1:A:3629:U:C6	2.85	0.58
1:A:3306:G:C2	5:E:247:ALA:HB1	2.37	0.58
3:C:35:A:H2'	3:C:36:C:O4'	2.04	0.58
17:Q:150:GLU:O	17:Q:153:ARG:HG3	2.04	0.58
1:A:25:A:OP2	39:c:49:ARG:NH1	2.37	0.57
1:A:645:A:OP1	9:I:31:LYS:HG3	2.05	0.57
1:A:685:U:H2'	1:A:685:U:O2	2.03	0.57
13:M:68:LYS:HB3	13:M:71:LEU:HD23	1.86	0.57
5:E:102:LEU:HD12	5:E:152:CYS:SG	2.45	0.57
1:A:3658:G:H1'	1:A:3659:C:P	2.44	0.57
1:A:1909:U:H2'	1:A:1910:C:C2	2.39	0.57
1:A:1910:C:H2'	1:A:1911:A:H8	1.68	0.57
1:A:2812:G:N2	1:A:2813:U:C2	2.73	0.57
1:A:2736:A:O2'	1:A:2737:C:H5'	2.03	0.57
1:A:2737:C:H2'	1:A:2738:U:H6	1.59	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:14:LEU:HD23	5:E:17:LEU:HD11	1.85	0.57
6:F:316:LYS:HB3	6:F:324:VAL:HG21	1.86	0.57
1:A:2812:G:C2	1:A:2813:U:N1	2.73	0.57
1:A:2813:U:C2'	1:A:2814:U:C6	2.87	0.57
1:A:308:U:O2'	1:A:309:G:P	2.63	0.56
12:L:92:ILE:HG23	12:L:124:MET:HE1	1.87	0.56
24:X:121:ARG:NE	24:X:123:ILE:HD11	2.20	0.56
6:F:371:ILE:HD13	32:5:79:ARG:HH11	1.70	0.56
8:H:89:TYR:CE1	8:H:183:VAL:HG13	2.40	0.56
1:A:2551:U:O5'	1:A:2551:U:H6	1.87	0.56
1:A:3629:U:C2'	1:A:3630:U:H5'	2.34	0.56
1:A:1643:U:OP1	41:e:42:ARG:NH2	2.39	0.56
1:A:3350:A:N3	23:W:69:ARG:NH2	2.53	0.56
1:A:3658:G:O2'	1:A:3659:C:O5'	2.23	0.56
14:N:81:ILE:HG22	14:N:99:THR:HG21	1.86	0.56
22:V:66:PHE:CD2	31:4:30:MET:HE1	2.41	0.56
39:c:25:CYS:HB2	39:c:40:CYS:SG	2.46	0.56
1:A:1630:A:HO2'	1:A:2125:A:H1'	1.71	0.56
35:8:85:LEU:HD21	35:8:94:VAL:HG12	1.87	0.56
1:A:101:C:H2'	1:A:102:A:O4'	2.05	0.56
5:E:170:MET:HE1	5:E:174:HIS:CD2	2.40	0.56
1:A:3629:U:C2	1:A:3630:U:C6	2.93	0.56
13:M:111:MET:HE1	13:M:134:ALA:HB3	1.88	0.56
1:A:2812:G:N2	1:A:2813:U:O2	2.38	0.56
1:A:18:G:OP1	30:3:83:ARG:NH2	2.39	0.56
1:A:181:C:O2'	1:A:182:U:OP2	2.23	0.56
1:A:3018:A:C8	1:A:3018:A:C5'	2.85	0.56
23:W:19:GLY:HA3	23:W:22:LEU:HD21	1.88	0.56
1:A:773:A:O2'	1:A:774:A:O5'	2.24	0.56
1:A:2696:G:H4'	1:A:2697:A:OP1	2.06	0.56
16:P:33:LEU:O	16:P:65:ARG:NH2	2.39	0.56
32:5:97:ARG:HB2	32:5:117:LEU:HD23	1.87	0.56
1:A:2812:G:C5	1:A:2813:U:C4	2.94	0.55
5:E:188:LYS:O	5:E:192:VAL:HG23	2.06	0.55
6:F:316:LYS:HG2	6:F:324:VAL:HG21	1.88	0.55
1:A:1552:G:OP1	35:8:64:LYS:O	2.24	0.55
1:A:1572:U:O2	1:A:1572:U:O5'	2.23	0.55
1:A:2679:A:C4	1:A:3353:A:C2	2.93	0.55
1:A:3628:C:C3'	1:A:3629:U:C5	2.89	0.55
4:D:104:ILE:HG22	4:D:146:THR:HG21	1.87	0.55
32:5:147:TYR:CE2	32:5:246:GLU:HB2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:A:C4	21:U:163:LEU:HD11	2.42	0.55
1:A:2577:C:O4'	1:A:2577:C:O2	2.25	0.55
13:M:56:LEU:O	13:M:80:ILE:O	2.24	0.55
1:A:256:A:C2	1:A:257:U:O2	2.59	0.55
1:A:3628:C:H3'	1:A:3629:U:H5	1.72	0.55
6:F:38:GLN:O	6:F:42:THR:HG23	2.07	0.55
1:A:1454:A:H2'	1:A:1455:C:O4'	2.07	0.55
1:A:3626:A:N1	1:A:3660:A:C2	2.74	0.55
14:N:30:LEU:HD12	14:N:44:PHE:CE2	2.42	0.55
1:A:3699:A:O2'	1:A:3704:A:N1	2.39	0.55
1:A:3700:G:H2'	1:A:3701:A:H5''	1.88	0.55
20:T:128:GLY:O	20:T:129:ASN:CB	2.55	0.55
1:A:914:G:H2'	1:A:915:G:C8	2.41	0.55
1:A:2947:G:O2'	16:P:79:ILE:HG12	2.07	0.55
30:3:4:VAL:HB	30:3:52:ASN:HD21	1.72	0.55
1:A:1572:U:C5	1:A:1573:C:C5	2.95	0.55
1:A:2181:A:N3	1:A:2413:A:H2'	2.21	0.55
4:D:196:TRP:CE3	4:D:197:PRO:CD	2.90	0.55
5:E:180:ILE:HD13	5:E:192:VAL:HG22	1.89	0.55
29:2:23:ASN:ND2	29:2:26:GLY:O	2.40	0.54
1:A:3629:U:C2	1:A:3630:U:C4	2.94	0.54
1:A:773:A:O2'	1:A:774:A:C8	2.61	0.54
1:A:3626:A:N1	1:A:3660:A:C4	2.75	0.54
4:D:200:ARG:NH1	4:D:217:GLN:OE1	2.40	0.54
9:I:61:ILE:HD12	9:I:71:ARG:HG2	1.89	0.54
1:A:684:G:H1'	6:F:314:GLN:HG2	1.90	0.54
1:A:3626:A:C2	1:A:3660:A:N3	2.73	0.54
7:G:18:VAL:CG1	7:G:70:THR:HG22	2.37	0.54
32:5:156:LEU:HD12	32:5:257:ILE:HD13	1.90	0.54
1:A:3613:A:C6	1:A:3614:A:C6	2.96	0.54
1:A:3628:C:C3'	1:A:3629:U:H6	2.20	0.54
1:A:3630:U:C2'	1:A:3631:U:C5'	2.86	0.54
5:E:47:MET:HE1	5:E:332:PRO:HB3	1.90	0.54
18:R:150:VAL:HG22	18:R:153:THR:HG23	1.89	0.54
36:9:61:THR:HG21	36:9:122:ILE:HG12	1.90	0.54
1:A:979:G:OP1	44:h:17:ARG:NH1	2.40	0.54
1:A:2737:C:H6	1:A:2737:C:H5'	1.69	0.54
23:W:36:ILE:HD11	23:W:48:LEU:HD21	1.90	0.54
6:F:159:GLU:HA	6:F:217:VAL:HG13	1.90	0.54
1:A:64:G:OP1	16:P:186:ARG:NH2	2.42	0.53
1:A:1794:U:O2	1:A:1794:U:C2'	2.55	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:47:ILE:HG21	19:S:137:LEU:HD13	1.89	0.53
7:G:136:TYR:HA	7:G:148:ILE:HD11	1.90	0.53
16:P:13:LYS:O	16:P:15:GLN:N	2.38	0.53
33:6:84:CYS:SG	33:6:85:GLY:N	2.81	0.53
1:A:123:A:H3'	1:A:124:U:H5''	1.91	0.53
1:A:1549:U:O2	1:A:1549:U:O4'	2.27	0.53
27:0:13:CYS:O	27:0:13:CYS:SG	2.67	0.53
28:1:5:LEU:HD23	28:1:80:ILE:HD11	1.91	0.53
1:A:3735:A:N6	1:A:3753:G:C6	2.77	0.53
4:D:177:LYS:HB2	44:h:29:ILE:HG21	1.91	0.53
1:A:257:U:O2'	1:A:258:U:H5''	2.09	0.53
1:A:521:U:O2'	1:A:522:A:O5'	2.23	0.53
1:A:1203:A:N1	18:R:113:LEU:HD21	2.24	0.53
1:A:2737:C:C5'	1:A:2737:C:C6	2.85	0.53
1:A:3726:U:H4'	1:A:3727:A:H5''	1.90	0.53
6:F:138:LEU:HG	6:F:144:ILE:HG22	1.91	0.53
6:F:314:GLN:HE21	6:F:314:GLN:HA	1.74	0.53
10:J:174:VAL:HG11	10:J:213:THR:HG23	1.89	0.53
18:R:143:PRO:HB2	18:R:174:ASN:HB2	1.91	0.53
1:A:2188:U:O2'	1:A:2200:A:N7	2.41	0.52
13:M:82:ARG:HG2	13:M:97:PHE:CD2	2.45	0.52
23:W:29:THR:HG21	23:W:144:CYS:SG	2.49	0.52
1:A:773:A:O2'	1:A:774:A:H8	1.93	0.52
1:A:3306:G:N3	5:E:247:ALA:HB1	2.24	0.52
23:W:20:VAL:O	23:W:145:HIS:ND1	2.43	0.52
25:Y:115:LEU:HD21	25:Y:133:MET:HE2	1.91	0.52
6:F:30:THR:HG21	6:F:125:CYS:HB3	1.92	0.52
15:O:82:LEU:HD21	15:O:100:ILE:HD11	1.92	0.52
40:d:23:VAL:HG22	40:d:43:LEU:HD23	1.92	0.52
1:A:29:C:OP1	16:P:191:ALA:HB2	2.10	0.52
11:K:53:TYR:CD2	11:K:144:VAL:HG11	2.45	0.52
32:5:115:LEU:HB3	32:5:117:LEU:CD1	2.40	0.52
1:A:3258:C:O2'	1:A:3260:G:OP2	2.28	0.52
14:N:70:PRO:HD3	21:U:9:LEU:HD21	1.92	0.52
25:Y:111:ILE:HD11	25:Y:132:PHE:CG	2.44	0.52
32:5:191:VAL:HG23	32:5:191:VAL:O	2.10	0.52
34:7:44:ILE:HD12	34:7:67:ILE:HD11	1.92	0.52
6:F:134:THR:HG22	6:F:150:VAL:CG2	2.39	0.52
6:F:156:ASN:HD21	6:F:255:SER:H	1.58	0.52
9:I:76:LYS:HD3	9:I:78:LEU:HD12	1.90	0.52
28:1:11:ILE:HG22	28:1:82:PRO:HA	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:289:ILE:HD11	19:S:28:LEU:HG	1.92	0.52
32:5:98:LEU:HD11	32:5:144:THR:CG2	2.39	0.52
34:7:66:PHE:HE2	34:7:79:VAL:HG12	1.75	0.52
1:A:544:C:O2	1:A:544:C:O4'	2.23	0.51
1:A:2737:C:H6	1:A:2737:C:O5'	1.92	0.51
3:C:141:U:H5'	25:Y:104:THR:HG21	1.90	0.51
10:J:160:VAL:HG13	10:J:192:VAL:HG11	1.91	0.51
14:N:69:ILE:CD1	14:N:74:LEU:HD21	2.40	0.51
16:P:10:ILE:HD11	38:b:51:ILE:CD1	2.40	0.51
1:A:1644:U:H5	1:A:2102:A:N1	2.08	0.51
1:A:1753:U:H2'	1:A:1754:G:O4'	2.11	0.51
1:A:2814:U:OP1	38:b:63:GLU:OE1	2.28	0.51
1:A:3015:A:O4'	1:A:3016:G:C6	2.63	0.51
1:A:3247:U:C6	1:A:3270:A:N6	2.79	0.51
8:H:42:PRO:O	8:H:58:MET:HE3	2.11	0.51
20:T:128:GLY:O	20:T:129:ASN:HB2	2.09	0.51
4:D:5:ILE:HG22	4:D:208:GLU:O	2.10	0.51
4:D:104:ILE:HA	4:D:107:MET:HE3	1.91	0.51
8:H:62:VAL:HB	8:H:63:PRO:CD	2.40	0.51
1:A:771:U:O2	1:A:771:U:O4'	2.28	0.51
1:A:3627:C:C6	1:A:3627:C:C5'	2.94	0.51
1:A:2832:A:N3	1:A:2832:A:H2'	2.26	0.51
1:A:3458:A:H2'	1:A:3459:A:O4'	2.10	0.51
6:F:147:LEU:HD11	6:F:176:LEU:HD21	1.93	0.51
8:H:5:VAL:HG22	8:H:59:TRP:CZ3	2.46	0.51
42:f:28:HIS:CD2	42:f:31:ALA:HB2	2.46	0.51
1:A:3699:A:H2'	1:A:3700:G:O4'	2.11	0.51
4:D:104:ILE:HD11	4:D:116:LEU:HD21	1.93	0.51
19:S:175:LYS:O	19:S:180:ARG:NH1	2.42	0.51
1:A:1092:A:H2'	1:A:1093:G:O4'	2.10	0.51
1:A:1133:A:C2	1:A:1163:A:C2	2.99	0.51
1:A:3016:G:C3'	1:A:3017:A:H5''	2.36	0.51
1:A:3629:U:C4	1:A:3630:U:C4	2.99	0.51
4:D:127:VAL:HG11	4:D:133:TYR:HA	1.93	0.51
5:E:148:ILE:HG22	5:E:189:LEU:HD11	1.92	0.51
6:F:137:VAL:HG11	6:F:144:ILE:HD12	1.91	0.51
11:K:83:VAL:HG11	11:K:101:LEU:HD22	1.93	0.51
12:L:94:ILE:CD1	12:L:115:LEU:HD21	2.37	0.51
15:O:73:ILE:HD12	15:O:78:LEU:HD12	1.93	0.51
22:V:41:VAL:HG21	22:V:65:ILE:HD11	1.92	0.51
1:A:3615:A:C2	14:N:32:LEU:HD11	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3627:C:H2'	1:A:3627:C:O2	2.10	0.51
1:A:3657:G:C2	1:A:3658:G:C6	2.99	0.51
8:H:111:ILE:HG23	8:H:125:VAL:HG13	1.93	0.51
13:M:47:CYS:O	13:M:48:LEU:C	2.54	0.51
25:Y:143:ILE:CG2	25:Y:158:VAL:HG21	2.40	0.51
7:G:18:VAL:HG12	7:G:70:THR:HG22	1.93	0.50
22:V:141:MET:HE1	32:5:77:GLU:HB3	1.93	0.50
8:H:62:VAL:HB	8:H:63:PRO:HD2	1.93	0.50
16:P:63:ARG:NH1	16:P:132:GLU:OE2	2.45	0.50
26:Z:32:SER:HB2	26:Z:105:LEU:HD12	1.92	0.50
1:A:1822:A:N1	1:A:2004:U:H5	2.08	0.50
14:N:116:ILE:HG22	14:N:120:ARG:HE	1.76	0.50
1:A:2814:U:H2'	1:A:2815:G:H8	1.76	0.50
1:A:3675:A:H2'	1:A:3676:C:O4'	2.12	0.50
5:E:133:SER:O	5:E:136:VAL:HG22	2.12	0.50
17:Q:9:TYR:CD2	17:Q:97:LEU:HD13	2.46	0.50
1:A:1473:A:H8	1:A:1473:A:H5''	1.75	0.50
1:A:1878:U:O2'	1:A:1880:A:N7	2.38	0.50
12:L:197:ARG:O	12:L:200:ASN:HB2	2.12	0.50
1:A:2677:A:H61	11:K:95:GLN:HE22	1.60	0.50
11:K:144:VAL:HG12	11:K:144:VAL:O	2.12	0.50
18:R:60:VAL:HG21	18:R:98:ALA:HA	1.93	0.50
1:A:976:G:OP2	20:T:91:LYS:NZ	2.44	0.50
1:A:3658:G:C1'	1:A:3659:C:P	3.00	0.50
4:D:196:TRP:C	4:D:197:PRO:O	2.55	0.50
39:c:27:LYS:O	39:c:29:SER:N	2.45	0.50
1:A:609:C:H3'	1:A:610:U:H5'	1.93	0.49
1:A:703:U:H2'	1:A:704:U:C6	2.46	0.49
1:A:2588:A:OP1	13:M:63:THR:HG21	2.11	0.49
1:A:3657:G:N2	1:A:3658:G:N1	2.60	0.49
9:I:88:PRO:O	9:I:90:GLU:N	2.46	0.49
27:0:12:ALA:HB2	27:0:19:ARG:HH12	1.77	0.49
32:5:141:PRO:HA	32:5:242:TRP:CD2	2.47	0.49
1:A:66:A:OP2	12:L:99:ARG:NH2	2.45	0.49
10:J:100:THR:HG21	10:J:198:LYS:HA	1.93	0.49
14:N:11:GLU:O	14:N:14:ILE:HG13	2.12	0.49
1:A:257:U:C4'	1:A:258:U:OP1	2.60	0.49
1:A:1523:A:H2'	1:A:1524:U:O4'	2.13	0.49
1:A:3426:G:H5''	13:M:14:ARG:HB3	1.95	0.49
7:G:21:ILE:HD11	7:G:125:MET:SD	2.51	0.49
19:S:23:ASN:C	19:S:23:ASN:HD22	2.21	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1908:U:C2'	1:A:1909:U:H5'	2.42	0.49
33:6:58:VAL:HG22	37:a:94:LEU:HD21	1.95	0.49
1:A:723:A:N6	1:A:3228:U:OP1	2.43	0.49
1:A:3111:U:O2	1:A:3111:U:O4'	2.31	0.49
1:A:3239:U:O2	5:E:247:ALA:HB3	2.13	0.49
3:C:105:U:C4	3:C:106:G:C6	3.01	0.49
1:A:217:A:H2'	6:F:164:THR:HG21	1.95	0.49
1:A:237:A:H2'	1:A:238:G:O4'	2.12	0.49
3:C:37:A:H2'	3:C:38:G:H5''	1.95	0.49
14:N:31:CYS:SG	14:N:74:LEU:HB3	2.52	0.49
14:N:59:ALA:O	14:N:61:ILE:N	2.46	0.49
1:A:1881:C:O2'	1:A:1882:U:O5'	2.29	0.49
18:R:83:LEU:HB3	18:R:88:ILE:HG23	1.94	0.49
25:Y:153:ILE:HG23	25:Y:174:LEU:HD22	1.94	0.49
35:8:96:ILE:HG21	35:8:105:ARG:HG2	1.95	0.49
15:O:73:ILE:HD11	15:O:102:VAL:HG13	1.94	0.48
22:V:16:PHE:CD2	22:V:53:MET:HE1	2.48	0.48
23:W:8:ILE:HG21	23:W:11:LEU:HG	1.95	0.48
23:W:29:THR:HG23	23:W:119:VAL:HG11	1.94	0.48
1:A:374:A:H2'	1:A:375:A:O4'	2.13	0.48
1:A:3387:U:H2'	1:A:3388:U:O4'	2.13	0.48
4:D:104:ILE:CG2	4:D:146:THR:HG21	2.43	0.48
7:G:102:PHE:CZ	7:G:129:VAL:HG21	2.48	0.48
9:I:29:ILE:HD12	9:I:39:ALA:HB2	1.95	0.48
13:M:31:SER:HB2	13:M:104:ILE:HD11	1.95	0.48
31:4:37:PRO:O	31:4:39:PHE:N	2.44	0.48
32:5:249:ILE:O	32:5:253:ILE:HG13	2.13	0.48
1:A:2954:A:H2'	1:A:2955:C:O4'	2.13	0.48
8:H:20:ILE:HG22	8:H:25:VAL:HG12	1.96	0.48
9:I:61:ILE:HG12	9:I:105:VAL:HG23	1.94	0.48
18:R:88:ILE:HD13	18:R:238:MET:HE3	1.96	0.48
36:9:53:GLN:O	36:9:54:ARG:HG2	2.14	0.48
1:A:2814:U:C2'	1:A:2815:G:H8	2.27	0.48
1:A:2401:C:H1'	1:A:3736:A:C8	2.48	0.48
2:B:22:G:N7	2:B:53:U:H2'	2.28	0.48
3:C:100:A:H5''	30:3:65:LYS:HG3	1.94	0.48
8:H:58:MET:HB2	8:H:69:ILE:HD12	1.96	0.48
12:L:16:TRP:CZ3	12:L:19:ARG:HD3	2.48	0.48
16:P:67:ARG:O	16:P:71:ARG:NH2	2.46	0.48
5:E:67:LEU:HD21	5:E:72:ILE:CD1	2.43	0.48
10:J:257:LYS:O	10:J:261:LEU:HD22	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:100:ILE:HD12	15:O:122:ILE:HD11	1.94	0.48
18:R:60:VAL:HG22	18:R:80:SER:HB2	1.95	0.48
27:O:56:LEU:O	27:O:59:THR:HG22	2.14	0.48
1:A:40:A:N7	15:O:29:PRO:O	2.47	0.48
1:A:3627:C:O5'	1:A:3627:C:H6	1.97	0.48
25:Y:130:LEU:HD11	25:Y:183:VAL:CG2	2.44	0.48
33:6:17:LEU:O	33:6:20:VAL:HG22	2.14	0.48
1:A:2925:U:O4'	1:A:2925:U:O2	2.29	0.47
1:A:3711:U:O2	1:A:3711:U:O4'	2.29	0.47
44:h:17:ARG:HG3	44:h:18:TYR:CE2	2.49	0.47
1:A:239:U:O4'	1:A:239:U:O2	2.29	0.47
1:A:3119:A:H5'	12:L:200:ASN:HB3	1.95	0.47
16:P:84:PRO:HA	16:P:87:GLN:HB2	1.96	0.47
18:R:95:TYR:CE1	18:R:163:ALA:HB2	2.50	0.47
40:d:8:ILE:HG13	40:d:52:MET:HE1	1.97	0.47
1:A:1511:U:H2'	1:A:1512:A:C8	2.50	0.47
1:A:1733:G:H5''	37:a:15:THR:HG21	1.95	0.47
1:A:3623:A:H4'	1:A:3623:A:OP1	2.14	0.47
8:H:54:ILE:HD11	8:H:76:LEU:HD13	1.96	0.47
19:S:30:VAL:HG12	19:S:52:LEU:HB3	1.96	0.47
25:Y:134:CYS:HB3	25:Y:143:ILE:HD11	1.96	0.47
27:O:20:ILE:HG12	27:O:39:LEU:HD23	1.95	0.47
1:A:257:U:HO2'	1:A:258:U:C1'	2.27	0.47
1:A:858:C:H3'	1:A:859:C:H5''	1.96	0.47
1:A:1756:G:OP1	40:d:49:LEU:N	2.48	0.47
1:A:2812:G:C4	1:A:2813:U:C6	3.03	0.47
8:H:66:LEU:N	8:H:66:LEU:HD23	2.29	0.47
14:N:35:TYR:HB3	14:N:73:ARG:HG2	1.97	0.47
34:7:80:ARG:HD3	34:7:112:LEU:HD23	1.96	0.47
1:A:1747:U:H4'	1:A:2102:A:H4'	1.96	0.47
1:A:2549:A:N3	1:A:2549:A:C2'	2.77	0.47
1:A:2566:G:O2'	1:A:2604:G:O6	2.31	0.47
8:H:3:THR:HA	21:U:150:GLN:HE22	1.78	0.47
25:Y:116:THR:O	25:Y:120:ALA:HB3	2.14	0.47
1:A:3631:U:H3'	1:A:3631:U:H6	1.79	0.47
6:F:235:LEU:HD22	6:F:240:LEU:HD11	1.96	0.47
11:K:8:ILE:HD12	11:K:32:ILE:HG23	1.95	0.47
14:N:30:LEU:HD23	14:N:77:LEU:HD23	1.96	0.47
1:A:1572:U:O2	1:A:1572:U:O4'	2.30	0.47
1:A:1575:C:C5'	6:F:42:THR:HG21	2.45	0.47
1:A:1598:A:C2	1:A:2649:A:C4	3.03	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1794:U:O2	1:A:1794:U:H2'	2.14	0.47
1:A:2634:A:OP2	5:E:244:ARG:NH2	2.48	0.47
1:A:3629:U:C4	1:A:3630:U:O4	2.67	0.47
3:C:20:G:O2'	3:C:21:A:OP2	2.32	0.47
3:C:110:G:H4'	3:C:145:A:H5'	1.96	0.47
6:F:218:LYS:HA	6:F:229:LEU:HD13	1.96	0.47
16:P:136:VAL:HG11	16:P:152:ILE:HG21	1.97	0.47
25:Y:115:LEU:HD21	25:Y:133:MET:CE	2.44	0.47
42:f:19:ILE:HD12	42:f:48:LYS:HA	1.97	0.47
1:A:755:A:N1	1:A:797:A:O2'	2.45	0.47
1:A:3347:C:O2	5:E:263:ARG:NH1	2.48	0.47
14:N:10:GLU:O	14:N:14:ILE:HG23	2.14	0.47
1:A:1444:A:H3'	1:A:1445:A:C5'	2.44	0.47
1:A:3707:U:OP1	5:E:117:ARG:NH1	2.48	0.47
3:C:37:A:C2'	3:C:38:G:H5''	2.45	0.47
6:F:134:THR:HG22	6:F:150:VAL:HG21	1.97	0.47
11:K:92:TYR:CE2	11:K:96:LEU:HD11	2.49	0.47
14:N:128:ARG:O	14:N:131:VAL:HG22	2.14	0.47
1:A:2812:G:N2	1:A:2813:U:H1'	2.30	0.47
14:N:48:ILE:C	14:N:48:ILE:HD12	2.39	0.47
14:N:81:ILE:CG2	14:N:99:THR:HG21	2.45	0.47
16:P:148:LYS:O	16:P:149:ILE:HG12	2.15	0.47
1:A:694:U:OP1	23:W:188:GLN:HA	2.14	0.46
1:A:751:U:O3'	6:F:33:ARG:NH1	2.48	0.46
1:A:1580:G:OP2	15:O:9:ARG:NH2	2.49	0.46
1:A:1642:G:C5	41:e:13:LEU:HD21	2.49	0.46
1:A:1644:U:C5	1:A:2102:A:N1	2.83	0.46
1:A:2219:A:O2'	1:A:2220:U:O5'	2.30	0.46
5:E:226:VAL:HG11	5:E:246:VAL:CG2	2.44	0.46
17:Q:38:ARG:HG2	17:Q:41:ALA:HB2	1.97	0.46
25:Y:130:LEU:HD12	25:Y:174:LEU:HD21	1.97	0.46
1:A:3654:C:C5	1:A:3655:U:C5	3.03	0.46
4:D:82:MET:SD	4:D:88:ILE:HD11	2.55	0.46
11:K:18:LEU:HD23	11:K:119:LEU:HD12	1.97	0.46
13:M:120:VAL:HB	13:M:138:ILE:HD12	1.96	0.46
21:U:14:HIS:HA	21:U:109:GLU:HG2	1.97	0.46
1:A:227:A:N7	1:A:1538:U:H2'	2.29	0.46
5:E:78:ILE:HD13	5:E:308:PHE:HZ	1.81	0.46
20:T:18:LYS:HA	20:T:21:ILE:HD12	1.97	0.46
1:A:3016:G:H4'	1:A:3017:A:OP2	2.15	0.46
16:P:127:VAL:HG23	16:P:128:TYR:CD2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:50:VAL:HG11	17:Q:149:CYS:SG	2.55	0.46
32:5:107:LYS:O	32:5:111:VAL:HG23	2.16	0.46
6:F:76:ILE:HG21	6:F:96:CYS:SG	2.55	0.46
15:O:100:ILE:CD1	15:O:122:ILE:HD11	2.45	0.46
1:A:107:C:O2'	1:A:332:A:N3	2.44	0.46
1:A:664:U:H4'	1:A:665:U:OP1	2.16	0.46
1:A:1070:A:C4	1:A:1518:A:C2	3.03	0.46
1:A:1086:C:H6	1:A:1086:C:H5''	1.81	0.46
1:A:1322:G:H2'	1:A:1323:A:C8	2.50	0.46
1:A:1536:U:C2'	1:A:1537:G:OP1	2.64	0.46
2:B:5:U:OP1	7:G:144:ARG:NH2	2.47	0.46
45:i:11:TYR:O	45:i:80:ARG:NH2	2.49	0.46
1:A:3627:C:C6	1:A:3627:C:O5'	2.69	0.46
1:A:3629:U:O2	1:A:3630:U:C6	2.69	0.46
1:A:3654:C:C6	1:A:3655:U:H5	2.34	0.46
11:K:8:ILE:HD12	11:K:32:ILE:CG2	2.46	0.46
13:M:111:MET:HE1	13:M:134:ALA:HB2	1.98	0.46
1:A:1118:A:C2	1:A:1177:A:C4	3.04	0.46
1:A:1881:C:O2'	1:A:1882:U:C6	2.64	0.46
1:A:3613:A:C6	1:A:3614:A:C2	3.04	0.46
1:A:733:C:H2'	1:A:734:A:C8	2.51	0.46
1:A:3028:A:N3	1:A:3028:A:H2'	2.31	0.46
4:D:78:ALA:HA	4:D:82:MET:HE2	1.98	0.46
6:F:222:ARG:O	6:F:223:ASN:CB	2.64	0.46
26:Z:63:HIS:ND1	26:Z:63:HIS:O	2.48	0.46
1:A:1470:A:H2'	1:A:1471:A:O4'	2.16	0.46
1:A:2628:G:N2	1:A:2632:C:O2'	2.49	0.46
1:A:3594:G:C2	1:A:3611:A:C2	3.04	0.46
2:B:26:C:H5'	2:B:27:A:OP2	2.16	0.46
3:C:42:U:H3'	3:C:43:G:H5'	1.98	0.46
7:G:43:GLN:HE21	7:G:43:GLN:N	2.14	0.46
8:H:20:ILE:C	8:H:20:ILE:HD12	2.41	0.46
11:K:9:ASP:HB2	11:K:116:LYS:HB3	1.96	0.46
14:N:72:LYS:O	21:U:165:THR:HG22	2.16	0.46
16:P:146:ASN:O	16:P:150:ASN:HB2	2.16	0.46
26:Z:39:ARG:O	26:Z:42:TYR:O	2.34	0.46
1:A:103:A:O3'	12:L:67:ARG:NH2	2.49	0.45
1:A:136:U:O4'	1:A:136:U:O2	2.33	0.45
1:A:270:U:O2'	1:A:271:G:OP2	2.31	0.45
1:A:422:G:H21	23:W:118:MET:HE1	1.80	0.45
1:A:809:A:N1	1:A:900:G:O2'	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3613:A:N1	1:A:3614:A:C2	2.84	0.45
1:A:3658:G:C2	1:A:3659:C:C2	3.04	0.45
10:J:169:VAL:HG22	10:J:203:LEU:HD21	1.97	0.45
11:K:10:CYS:HA	11:K:13:HIS:HD2	1.81	0.45
11:K:10:CYS:SG	11:K:34:ALA:HB1	2.56	0.45
17:Q:91:ILE:HD13	17:Q:133:GLN:OE1	2.16	0.45
18:R:95:TYR:CZ	18:R:163:ALA:HB2	2.51	0.45
28:1:23:ALA:HB1	28:1:43:VAL:HG12	1.99	0.45
1:A:3656:A:N1	1:A:3657:G:C6	2.84	0.45
21:U:86:VAL:HB	21:U:135:ILE:HG22	1.97	0.45
32:5:117:LEU:HD11	32:5:124:VAL:HG12	1.97	0.45
25:Y:138:ALA:HB1	25:Y:143:ILE:HD13	1.97	0.45
34:7:24:LEU:HD21	34:7:44:ILE:HG13	1.99	0.45
1:A:1216:C:N4	1:A:1217:U:C4	2.85	0.45
5:E:325:VAL:HG11	5:E:333:ILE:CD1	2.46	0.45
35:8:82:MET:SD	35:8:94:VAL:HG11	2.56	0.45
1:A:809:A:OP1	15:O:132:VAL:HG13	2.17	0.45
1:A:2408:G:H4'	20:T:78:GLY:O	2.16	0.45
1:A:2737:C:C6	1:A:2737:C:O5'	2.70	0.45
1:A:3698:U:O3'	5:E:331:ARG:NH2	2.50	0.45
7:G:100:GLY:HA3	7:G:154:VAL:HG23	1.99	0.45
25:Y:130:LEU:HD11	25:Y:183:VAL:HG21	1.99	0.45
38:b:69:THR:O	38:b:73:THR:HG23	2.16	0.45
1:A:702:U:O2	1:A:702:U:O4'	2.34	0.45
1:A:2101:U:H3'	1:A:2102:A:H5'	1.99	0.45
1:A:3344:C:H2'	1:A:3345:U:O4'	2.17	0.45
16:P:3:ALA:O	16:P:7:ILE:HG23	2.16	0.45
1:A:2163:A:O2'	1:A:3439:G:H4'	2.17	0.45
1:A:3524:G:H2'	1:A:3525:A:O4'	2.16	0.45
1:A:3632:U:C2'	1:A:3633:U:H5'	2.44	0.45
11:K:10:CYS:HB3	11:K:40:ILE:HG12	1.99	0.45
33:6:77:ASN:ND2	33:6:91:SER:OG	2.41	0.45
1:A:10:G:C2'	1:A:11:A:OP1	2.64	0.45
1:A:379:G:H4'	1:A:406:A:N1	2.32	0.45
3:C:149:C:OP1	16:P:38:ARG:HD3	2.17	0.45
6:F:314:GLN:HE21	6:F:314:GLN:CA	2.28	0.45
9:I:86:VAL:CG1	9:I:96:LEU:HD22	2.46	0.45
10:J:160:VAL:HG11	10:J:186:LEU:HD13	1.98	0.45
12:L:59:CYS:SG	12:L:69:ARG:HG2	2.57	0.45
13:M:19:LEU:HD21	13:M:25:ILE:HG21	1.99	0.45
1:A:3629:U:C6	1:A:3629:U:OP2	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:VAL:HG23	8:H:79:MET:HE1	1.99	0.45
19:S:51:ARG:CB	19:S:82:VAL:HG11	2.44	0.45
20:T:9:LEU:HD22	20:T:37:ARG:HD3	1.99	0.45
24:X:63:PHE:CE1	24:X:113:MET:HE2	2.52	0.45
28:1:72:ILE:HD12	28:1:111:VAL:HG22	1.99	0.45
2:B:23:A:C2	2:B:118:A:O2'	2.70	0.45
8:H:93:LEU:HD12	8:H:178:ILE:HD12	1.99	0.45
17:Q:5:PRO:O	17:Q:6:ALA:HB3	2.17	0.45
32:5:157:LEU:HD21	32:5:201:LEU:HD13	1.98	0.45
1:A:594:C:C2'	1:A:594:C:O2	2.65	0.44
1:A:1103:A:C5	1:A:1231:A:C2	3.05	0.44
9:I:63:LEU:HD12	36:9:40:LEU:HD22	2.00	0.44
13:M:31:SER:CB	13:M:104:ILE:HD11	2.46	0.44
15:O:73:ILE:HD11	15:O:102:VAL:CG1	2.47	0.44
28:1:4:LEU:HD22	33:6:65:LEU:HB3	1.98	0.44
1:A:812:U:H2'	15:O:139:ALA:HB1	1.99	0.44
1:A:3656:A:C6	1:A:3657:G:C6	3.05	0.44
5:E:249:ILE:CG2	5:E:257:VAL:HG13	2.46	0.44
1:A:433:A:H2'	1:A:434:C:O4'	2.17	0.44
1:A:2208:G:H21	1:A:3754:A:H8	1.65	0.44
2:B:74:A:N3	21:U:59:LYS:NZ	2.55	0.44
9:I:75:THR:OG1	9:I:86:VAL:HG22	2.18	0.44
13:M:125:ALA:HB2	13:M:138:ILE:CD1	2.44	0.44
44:h:10:LEU:HD12	44:h:30:GLU:HB3	1.98	0.44
1:A:1568:C:OP2	6:F:195:LYS:NZ	2.49	0.44
1:A:3123:C:O2	12:L:202:ARG:CZ	2.58	0.44
23:W:47:TYR:O	23:W:51:VAL:HG12	2.17	0.44
43:g:7:ARG:O	43:g:8:TYR:CG	2.70	0.44
1:A:1897:G:H2'	1:A:1898:U:O4'	2.18	0.44
1:A:2734:C:OP2	1:A:2734:C:C5	2.70	0.44
1:A:3628:C:O3'	1:A:3629:U:H6	2.01	0.44
1:A:3660:A:H4'	1:A:3661:A:OP1	2.17	0.44
40:d:5:ILE:HD11	40:d:50:TYR:CD1	2.53	0.44
42:f:22:LYS:HE3	42:f:42:THR:HG21	1.98	0.44
1:A:3585:A:H1'	11:K:167:TYR:HB2	2.00	0.44
5:E:235:LEU:HB3	5:E:239:THR:HG21	1.98	0.44
15:O:75:VAL:HB	15:O:116:LEU:HD21	2.00	0.44
22:V:117:ILE:HG13	22:V:129:ILE:HD11	1.99	0.44
1:A:1057:C:O2'	1:A:3173:G:O2'	2.34	0.44
1:A:1850:U:O2'	1:A:1969:A:N6	2.50	0.44
1:A:3459:A:H2'	1:A:3460:C:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:A:H2'	3:C:146:C:C6	2.53	0.44
6:F:316:LYS:CB	6:F:324:VAL:HG21	2.48	0.44
27:0:12:ALA:HB2	27:0:19:ARG:NH1	2.33	0.44
1:A:3726:U:H4'	1:A:3727:A:C5'	2.48	0.44
4:D:127:VAL:HG21	4:D:134:ALA:HB2	1.99	0.44
8:H:45:ILE:HD11	8:H:54:ILE:HD12	1.98	0.44
33:6:54:ILE:O	33:6:58:VAL:HG23	2.18	0.44
1:A:299:A:P	16:P:68:ARG:HH22	2.41	0.44
1:A:975:G:C6	1:A:976:G:N1	2.86	0.44
1:A:1035:G:N1	4:D:207:VAL:HG11	2.33	0.44
1:A:1207:U:H2'	1:A:1208:G:O4'	2.18	0.44
1:A:1462:C:HO2'	32:5:160:ARG:HH12	1.66	0.44
1:A:2441:U:H2'	1:A:2442:A:C5	2.53	0.44
1:A:3006:A:H2'	1:A:3007:A:O4'	2.18	0.44
1:A:3008:A:H2'	1:A:3009:G:O4'	2.18	0.44
17:Q:37:GLY:O	17:Q:38:ARG:C	2.60	0.44
33:6:44:LEU:HD12	33:6:95:ILE:HD11	1.99	0.44
1:A:1299:G:H2'	1:A:1300:G:O4'	2.18	0.43
1:A:3630:U:H6	1:A:3630:U:O5'	2.01	0.43
16:P:201:LEU:O	16:P:202:ARG:CB	2.66	0.43
32:5:115:LEU:HB3	32:5:117:LEU:HD13	2.00	0.43
1:A:93:C:OP2	1:A:3103:C:O2'	2.29	0.43
1:A:2833:U:O2'	10:J:60:ARG:NH1	2.49	0.43
1:A:3328:A:N7	4:D:215:ASN:ND2	2.65	0.43
1:A:979:G:N3	1:A:979:G:H3'	2.33	0.43
1:A:2550:C:H3'	1:A:2550:C:O2	2.18	0.43
1:A:3526:U:O2	1:A:3526:U:O4'	2.34	0.43
1:A:3658:G:N2	1:A:3659:C:C1'	2.80	0.43
9:I:212:ASN:O	9:I:213:ASP:CB	2.66	0.43
21:U:21:ARG:HB3	21:U:33:VAL:HG12	2.01	0.43
1:A:715:U:O2'	1:A:716:C:C6	2.71	0.43
1:A:1578:G:OP2	6:F:109:ARG:NH1	2.52	0.43
1:A:1648:U:H2'	1:A:1649:G:O4'	2.18	0.43
1:A:1910:C:O5'	1:A:1910:C:C6	2.72	0.43
1:A:3667:C:H5''	1:A:3669:U:OP2	2.19	0.43
4:D:46:LYS:HG3	4:D:62:ILE:HD12	2.00	0.43
32:5:115:LEU:CD1	32:5:135:MET:HE2	2.48	0.43
1:A:1121:G:C6	1:A:1122:A:N1	2.86	0.43
1:A:1818:C:H5''	20:T:95:ILE:HD13	2.00	0.43
1:A:2951:U:H2'	1:A:2952:U:O4'	2.19	0.43
1:A:3035:A:H3'	1:A:3036:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3628:C:H3'	1:A:3629:U:C6	2.50	0.43
6:F:262:VAL:O	6:F:273:THR:HG22	2.18	0.43
6:F:331:ALA:HB3	32:5:57:THR:HG21	2.00	0.43
14:N:59:ALA:HB2	14:N:92:LEU:HD22	2.01	0.43
34:7:57:VAL:HG13	34:7:99:THR:HG23	2.00	0.43
35:8:85:LEU:HD13	35:8:117:VAL:HG21	2.00	0.43
39:c:51:ASN:N	39:c:51:ASN:HD22	2.17	0.43
1:A:296:A:OP1	16:P:97:ASN:ND2	2.48	0.43
1:A:493:C:H2'	1:A:494:U:O4'	2.19	0.43
1:A:1435:G:C2	1:A:1436:A:C2	3.07	0.43
1:A:2144:U:H5''	1:A:2145:A:O4'	2.18	0.43
1:A:3025:U:H2'	1:A:3026:G:O4'	2.18	0.43
2:B:7:G:OP2	18:R:28:THR:HG22	2.19	0.43
3:C:19:G:C6	3:C:20:G:N1	2.87	0.43
5:E:47:MET:HE2	5:E:174:HIS:HB3	2.00	0.43
11:K:14:LEU:HD12	11:K:14:LEU:HA	1.93	0.43
18:R:33:ARG:HG2	18:R:37:ILE:HD12	2.00	0.43
29:2:57:VAL:HG23	29:2:108:LEU:HD22	2.01	0.43
1:A:195:A:N1	1:A:196:A:N6	2.67	0.43
1:A:2650:A:H2'	1:A:2651:A:C8	2.53	0.43
1:A:3340:U:OP2	5:E:241:ARG:NH1	2.46	0.43
1:A:3572:A:N3	1:A:3572:A:H2'	2.33	0.43
19:S:8:VAL:O	19:S:10:ARG:N	2.51	0.43
19:S:8:VAL:O	19:S:8:VAL:HG13	2.19	0.43
1:A:1222:U:O2'	1:A:1223:U:O5'	2.34	0.43
1:A:2551:U:O5'	1:A:2551:U:C6	2.70	0.43
1:A:3752:C:N4	1:A:3753:G:C6	2.86	0.43
2:B:102:C:H2'	2:B:103:A:O4'	2.19	0.43
5:E:180:ILE:CD1	5:E:192:VAL:HG22	2.48	0.43
5:E:280:TYR:CE1	5:E:351:VAL:HG21	2.53	0.43
6:F:37:ILE:HD11	6:F:126:SER:HB2	2.00	0.43
9:I:120:LEU:HB3	9:I:189:LEU:HD11	2.00	0.43
39:c:23:LEU:O	39:c:24:ARG:CB	2.66	0.43
1:A:84:U:O2'	1:A:101:C:N4	2.51	0.43
1:A:530:U:OP1	32:5:79:ARG:NH2	2.52	0.43
1:A:3615:A:N1	14:N:32:LEU:HD11	2.33	0.43
6:F:164:THR:HG22	6:F:220:ALA:O	2.19	0.43
36:9:71:LYS:HD2	36:9:107:THR:HG21	2.01	0.43
1:A:382:A:N3	1:A:385:G:H5'	2.33	0.43
1:A:3669:U:O4	36:9:39:ARG:O	2.37	0.43
14:N:32:LEU:HB2	14:N:77:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:235:ILE:HG13	18:R:238:MET:HE2	2.01	0.43
1:A:2667:C:N4	1:A:3300:A:O4'	2.52	0.42
1:A:2733:A:H2'	1:A:2734:C:H6	1.80	0.42
5:E:110:VAL:HG11	5:E:114:PHE:CD1	2.53	0.42
14:N:24:PHE:O	14:N:29:ARG:HG3	2.18	0.42
28:1:11:ILE:HD11	28:1:43:VAL:HG11	2.01	0.42
1:A:643:G:H1'	1:A:684:G:N2	2.34	0.42
1:A:1024:U:O2'	4:D:12:ARG:NH2	2.52	0.42
1:A:2683:A:H2'	1:A:2684:G:O4'	2.19	0.42
3:C:126:C:OP1	30:3:64:ARG:NH2	2.52	0.42
3:C:147:U:H2'	3:C:148:C:O4'	2.19	0.42
10:J:71:TRP:HB3	10:J:75:ILE:HD11	2.00	0.42
12:L:73:GLY:HA3	12:L:97:ASP:HB2	2.01	0.42
16:P:201:LEU:HD12	16:P:205:ARG:NH1	2.34	0.42
21:U:165:THR:HG23	21:U:165:THR:O	2.19	0.42
22:V:117:ILE:CG1	22:V:129:ILE:HD11	2.49	0.42
30:3:24:LEU:HB3	30:3:53:VAL:HG22	2.01	0.42
30:3:118:TYR:O	30:3:119:LEU:C	2.61	0.42
1:A:952:U:OP1	20:T:85:ASN:HB2	2.19	0.42
1:A:1272:U:OP2	35:8:43:ARG:NH2	2.52	0.42
1:A:2026:G:H2'	1:A:2027:A:O4'	2.19	0.42
3:C:78:U:O2	3:C:78:U:O4'	2.37	0.42
7:G:12:ILE:HG23	7:G:162:TRP:CD1	2.54	0.42
8:H:60:PHE:CE1	14:N:51:ILE:HD11	2.54	0.42
19:S:100:CYS:HA	19:S:120:LEU:O	2.20	0.42
32:5:233:ALA:HB2	32:5:242:TRP:CZ2	2.54	0.42
36:9:46:ILE:HD11	36:9:122:ILE:HG12	2.00	0.42
1:A:184:U:C2'	1:A:185:A:OP1	2.68	0.42
1:A:258:U:H5''	1:A:258:U:H6	1.84	0.42
1:A:1030:C:O2	1:A:1036:A:N1	2.52	0.42
1:A:2470:A:H4'	1:A:2473:A:H1'	2.01	0.42
1:A:3474:C:OP1	5:E:219:LYS:HD2	2.19	0.42
1:A:3662:U:H3'	1:A:3663:A:H5'	2.01	0.42
6:F:7:VAL:HG12	6:F:21:GLU:HB3	2.01	0.42
16:P:201:LEU:HD12	16:P:205:ARG:CZ	2.50	0.42
1:A:546:C:N3	21:U:80:ARG:NH2	2.64	0.42
1:A:2514:G:N7	38:b:74:LYS:NZ	2.67	0.42
13:M:20:PRO:HA	13:M:53:ALA:HA	2.01	0.42
19:S:86:THR:HA	19:S:105:THR:CG2	2.49	0.42
21:U:86:VAL:CB	21:U:135:ILE:HG22	2.50	0.42
1:A:1254:G:OP1	17:Q:98:ARG:NH1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1537:G:H8	1:A:1537:G:H5''	1.84	0.42
1:A:1575:C:H5''	6:F:42:THR:HG21	2.02	0.42
1:A:2199:A:N6	1:A:2414:G:O4'	2.52	0.42
17:Q:41:ALA:HB3	17:Q:139:ARG:NH2	2.35	0.42
35:8:32:TRP:CZ2	35:8:53:PRO:HD2	2.54	0.42
1:A:256:A:C2	1:A:257:U:C2	3.08	0.42
1:A:595:U:O2	1:A:595:U:O4'	2.38	0.42
1:A:2474:C:OP1	4:D:193:ARG:NH2	2.53	0.42
1:A:3585:A:N6	1:A:3593:U:O2'	2.52	0.42
3:C:27:U:OP1	26:Z:15:ARG:NH1	2.53	0.42
11:K:2:TYR:CZ	36:9:66:LYS:HA	2.54	0.42
11:K:188:ILE:HD11	14:N:138:LEU:HG	2.00	0.42
12:L:89:ALA:HB1	12:L:94:ILE:HG12	2.01	0.42
15:O:63:LEU:HD12	15:O:65:LYS:HG2	2.02	0.42
34:7:68:TRP:HZ3	34:7:72:VAL:HG13	1.83	0.42
1:A:3632:U:H2'	1:A:3633:U:H6	1.85	0.42
4:D:191:VAL:HG12	4:D:191:VAL:O	2.19	0.42
5:E:329:LYS:O	5:E:330:LYS:HB2	2.19	0.42
29:2:37:ASN:ND2	29:2:39:ASN:O	2.53	0.42
1:A:101:C:O2	1:A:101:C:O4'	2.36	0.42
1:A:1121:G:C2	1:A:1122:A:C2	3.07	0.42
1:A:1560:U:OP1	35:8:105:ARG:NH2	2.52	0.42
1:A:1895:U:H2'	1:A:1896:C:C6	2.55	0.42
1:A:1911:A:H8	1:A:1911:A:O5'	2.02	0.42
1:A:3585:A:H2'	1:A:3586:U:O4'	2.19	0.42
10:J:97:PHE:CZ	10:J:180:VAL:HG13	2.55	0.42
21:U:51:TRP:CE3	21:U:51:TRP:HA	2.55	0.42
30:3:121:VAL:HG12	30:3:121:VAL:O	2.20	0.42
36:9:41:TYR:HB3	36:9:134:LEU:HD13	2.01	0.42
39:c:37:CYS:SG	39:c:40:CYS:HB2	2.59	0.42
1:A:112:U:O2'	1:A:113:C:H5''	2.20	0.42
1:A:2482:U:H4'	44:h:19:GLY:HA3	2.02	0.42
1:A:2506:A:H2'	1:A:2507:A:C8	2.54	0.42
3:C:38:G:O2'	3:C:39:C:P	2.78	0.42
7:G:9:MET:HA	7:G:9:MET:HE2	2.01	0.42
12:L:56:ILE:HD11	12:L:110:LYS:HD2	2.02	0.42
15:O:3:THR:HA	15:O:6:LYS:HG3	2.01	0.42
16:P:66:VAL:HG21	16:P:102:ALA:HB2	2.02	0.42
21:U:18:ILE:HD11	21:U:46:ALA:HB1	2.02	0.42
21:U:83:ASN:HD21	21:U:152:LEU:HD21	1.84	0.42
32:5:94:PHE:CD2	32:5:253:ILE:HD11	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:U:O2'	1:A:258:U:C5'	2.69	0.41
1:A:717:G:H4'	1:A:1583:G:C6	2.55	0.41
1:A:1098:U:H4'	32:5:168:VAL:HG13	2.01	0.41
1:A:1908:U:C4	1:A:1909:U:O4	2.73	0.41
1:A:950:G:H2'	1:A:951:A:O4'	2.20	0.41
1:A:2210:U:OP2	20:T:73:ARG:NH1	2.54	0.41
12:L:185:ALA:HB1	15:O:146:LEU:HD13	2.02	0.41
13:M:138:ILE:O	13:M:138:ILE:HG23	2.20	0.41
14:N:31:CYS:SG	14:N:76:LEU:HD23	2.60	0.41
21:U:58:ASN:HD21	22:V:152:ILE:CD1	2.33	0.41
1:A:123:A:N3	1:A:123:A:C2'	2.83	0.41
1:A:723:A:C8	1:A:727:A:C6	3.09	0.41
1:A:2549:A:N3	1:A:2549:A:H2'	2.35	0.41
1:A:2736:A:N6	1:A:2813:U:N3	2.60	0.41
1:A:2814:U:O2'	1:A:2815:G:C5'	2.68	0.41
3:C:69:A:C2	3:C:99:G:C5	3.07	0.41
5:E:110:VAL:CG1	5:E:114:PHE:CD1	3.03	0.41
6:F:382:ALA:HB1	6:F:386:LYS:NZ	2.35	0.41
17:Q:190:ILE:O	17:Q:190:ILE:HG23	2.19	0.41
36:9:56:GLN:HA	36:9:56:GLN:NE2	2.34	0.41
1:A:1024:U:O2'	1:A:1029:G:O3'	2.34	0.41
1:A:1186:A:C6	22:V:110:LYS:HG2	2.56	0.41
1:A:3629:U:C2'	1:A:3630:U:C5'	2.97	0.41
1:A:3776:U:O2	34:7:114:ASN:ND2	2.53	0.41
9:I:59:VAL:HG21	9:I:203:TYR:HE2	1.86	0.41
21:U:85:GLY:CA	21:U:138:ILE:HD11	2.50	0.41
1:A:2156:A:OP1	5:E:244:ARG:NH1	2.52	0.41
1:A:2438:A:O4'	1:A:3317:A:H4'	2.19	0.41
1:A:2981:A:H2'	1:A:2982:A:C8	2.55	0.41
3:C:60:G:H2'	3:C:61:C:O4'	2.21	0.41
16:P:169:GLY:O	16:P:173:ARG:HG3	2.20	0.41
20:T:11:ALA:HA	20:T:21:ILE:HD11	2.01	0.41
33:6:33:CYS:SG	33:6:59:ILE:HD12	2.59	0.41
1:A:123:A:O2'	1:A:124:U:OP1	2.30	0.41
1:A:889:U:OP2	12:L:191:ARG:NH2	2.53	0.41
1:A:1073:G:H1'	31:4:12:GLN:CD	2.46	0.41
6:F:209:ILE:HD12	6:F:209:ILE:N	2.36	0.41
7:G:94:LYS:O	7:G:96:PHE:N	2.53	0.41
15:O:40:HIS:CD2	15:O:41:MET:HG3	2.55	0.41
17:Q:152:LEU:HD23	17:Q:152:LEU:HA	1.96	0.41
18:R:199:LEU:HD12	18:R:236:GLU:HG2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:97:ARG:O	20:T:101:LEU:HG	2.19	0.41
28:1:106:ASN:C	28:1:106:ASN:HD22	2.29	0.41
30:3:68:LEU:HD23	30:3:82:LEU:HD21	2.03	0.41
1:A:3272:U:H2'	1:A:3273:G:O4'	2.21	0.41
1:A:3443:A:H2'	1:A:3444:G:H5'	2.02	0.41
1:A:3671:A:OP1	36:9:97:ILE:HD11	2.21	0.41
3:C:39:C:H4'	39:c:73:LEU:HD21	2.02	0.41
5:E:37:LYS:O	5:E:183:GLY:HA2	2.21	0.41
7:G:40:LEU:HD12	7:G:79:ILE:HD12	2.03	0.41
14:N:42:LEU:HD21	14:N:105:PHE:CE2	2.55	0.41
18:R:88:ILE:CD1	18:R:238:MET:HE3	2.51	0.41
33:6:37:LEU:HD13	33:6:62:TYR:HB3	2.03	0.41
1:A:3623:A:N7	9:I:211:ARG:HD2	2.36	0.41
1:A:3629:U:HO2'	1:A:3630:U:H5'	1.81	0.41
1:A:3631:U:N3	1:A:3655:U:C2	2.89	0.41
11:K:79:LEU:HD12	11:K:103:VAL:HG11	2.02	0.41
21:U:18:ILE:HG23	21:U:67:LEU:HD21	2.01	0.41
36:9:68:VAL:HG11	36:9:77:TYR:CE1	2.56	0.41
1:A:63:A:H4'	16:P:186:ARG:O	2.21	0.41
1:A:353:G:O2'	3:C:29:G:N3	2.53	0.41
1:A:1540:G:C8	1:A:1565:G:C2	3.09	0.41
1:A:1646:C:H2'	1:A:1647:U:C6	2.56	0.41
1:A:1759:A:H2'	1:A:1760:A:O4'	2.21	0.41
1:A:2004:U:O2	1:A:2004:U:O4'	2.37	0.41
1:A:2736:A:N1	1:A:2813:U:C2	2.88	0.41
1:A:2737:C:C6	1:A:2737:C:C4'	3.04	0.41
3:C:107:A:C8	3:C:108:A:C8	3.09	0.41
6:F:147:LEU:HD13	6:F:152:LEU:CD1	2.49	0.41
8:H:21:ASN:HD22	8:H:21:ASN:HA	1.70	0.41
13:M:56:LEU:HD21	13:M:87:TRP:CZ3	2.56	0.41
13:M:104:ILE:HD12	13:M:112:LYS:HD3	2.03	0.41
19:S:6:LYS:O	19:S:8:VAL:N	2.53	0.41
19:S:62:LEU:HD23	19:S:140:GLY:HA2	2.02	0.41
24:X:44:LEU:HD22	24:X:132:PHE:CE1	2.55	0.41
28:1:13:ILE:O	28:1:19:ALA:O	2.39	0.41
40:d:8:ILE:CG1	40:d:52:MET:HE1	2.50	0.41
1:A:156:U:OP2	10:J:152:GLY:HA2	2.21	0.41
1:A:1642:G:N7	41:e:5:LYS:NZ	2.69	0.41
1:A:1745:G:H4'	20:T:9:LEU:HD21	2.02	0.41
1:A:2208:G:H2'	1:A:2209:C:O4'	2.20	0.41
1:A:2970:U:OP1	1:A:3096:U:O2'	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:LYS:C	4:D:72:LYS:HD2	2.46	0.41
4:D:229:ALA:HB3	4:D:234:LYS:HG3	2.01	0.41
5:E:45:ALA:HB3	5:E:178:VAL:HG13	2.03	0.41
5:E:56:ILE:HB	5:E:76:CYS:SG	2.61	0.41
6:F:54:VAL:HG21	6:F:101:MET:SD	2.61	0.41
9:I:178:LYS:HE2	9:I:182:ILE:HD11	2.02	0.41
20:T:137:LEU:HD23	20:T:137:LEU:O	2.21	0.41
22:V:41:VAL:HG13	22:V:97:VAL:HG13	2.02	0.41
34:7:27:LEU:HD11	34:7:47:ILE:HD12	2.02	0.41
1:A:716:C:OP1	35:8:21:GLN:NE2	2.54	0.40
1:A:3353:A:N7	1:A:3526:U:H5	2.19	0.40
17:Q:38:ARG:CG	17:Q:41:ALA:HB2	2.50	0.40
1:A:972:G:N2	20:T:128:GLY:O	2.53	0.40
1:A:1008:U:H2'	1:A:1009:C:O4'	2.22	0.40
1:A:2409:G:OP1	1:A:2411:C:N4	2.54	0.40
1:A:3195:C:O2	1:A:3195:C:O5'	2.40	0.40
1:A:3631:U:C3'	1:A:3631:U:C6	3.04	0.40
28:1:72:ILE:CD1	28:1:111:VAL:HG22	2.51	0.40
1:A:506:A:H2'	1:A:507:G:C8	2.56	0.40
1:A:1206:U:H4'	1:A:1207:U:OP1	2.21	0.40
1:A:1244:G:N2	1:A:3176:A:O4'	2.54	0.40
1:A:1965:U:O2	1:A:1965:U:O4'	2.39	0.40
1:A:2607:U:HO2'	1:A:2608:G:P	2.45	0.40
1:A:3016:G:N3	1:A:3016:G:C2'	2.84	0.40
1:A:3075:A:H2'	1:A:3076:G:O4'	2.21	0.40
7:G:40:LEU:CD1	7:G:79:ILE:HD12	2.52	0.40
9:I:71:ARG:O	9:I:92:ASN:ND2	2.54	0.40
15:O:99:VAL:HA	15:O:123:VAL:HB	2.03	0.40
15:O:130:SER:O	15:O:131:SER:C	2.64	0.40
16:P:59:PHE:HE1	16:P:149:ILE:HD12	1.86	0.40
25:Y:161:LEU:HD12	25:Y:161:LEU:C	2.46	0.40
1:A:193:C:H2'	1:A:194:A:O4'	2.21	0.40
1:A:715:U:H2'	1:A:716:C:C5	2.56	0.40
1:A:824:U:H2'	1:A:825:G:O4'	2.21	0.40
1:A:1020:C:H2'	1:A:1021:G:O4'	2.22	0.40
1:A:2680:A:H2'	1:A:2681:U:O4'	2.22	0.40
1:A:2813:U:O2'	1:A:2814:U:C6	2.70	0.40
30:3:68:LEU:HD23	30:3:82:LEU:HD11	2.04	0.40
1:A:1467:C:H5'	35:8:60:ASN:HA	2.04	0.40
1:A:2165:G:H2'	1:A:2166:G:O4'	2.21	0.40
1:A:3630:U:O2'	1:A:3631:U:H5''	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:325:VAL:HG11	5:E:333:ILE:HD13	2.03	0.40
8:H:68:CYS:O	8:H:72:VAL:HG23	2.21	0.40
12:L:22:ARG:HG3	16:P:198:LEU:HD22	2.04	0.40
18:R:110:LEU:HD13	18:R:110:LEU:HA	1.97	0.40
21:U:99:MET:SD	21:U:119:MET:HE1	2.62	0.40
24:X:66:ASP:O	24:X:74:THR:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	245/260 (94%)	225 (92%)	15 (6%)	5 (2%)	6	31
5	E	378/386 (98%)	345 (91%)	26 (7%)	7 (2%)	6	33
6	F	388/411 (94%)	359 (92%)	20 (5%)	9 (2%)	5	29
7	G	116/173 (67%)	106 (91%)	7 (6%)	3 (3%)	4	26
8	H	183/190 (96%)	150 (82%)	26 (14%)	7 (4%)	2	18
9	I	203/221 (92%)	179 (88%)	15 (7%)	9 (4%)	2	15
10	J	225/283 (80%)	203 (90%)	16 (7%)	6 (3%)	4	25
11	K	199/202 (98%)	185 (93%)	10 (5%)	4 (2%)	6	31
12	L	209/215 (97%)	183 (88%)	17 (8%)	9 (4%)	2	16
13	M	130/139 (94%)	119 (92%)	8 (6%)	3 (2%)	5	29
14	N	144/165 (87%)	135 (94%)	5 (4%)	4 (3%)	4	25
15	O	145/148 (98%)	133 (92%)	12 (8%)	0	100	100
16	P	202/205 (98%)	185 (92%)	11 (5%)	6 (3%)	3	23
17	Q	185/219 (84%)	157 (85%)	22 (12%)	6 (3%)	3	21
18	R	244/294 (83%)	218 (89%)	17 (7%)	9 (4%)	2	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	184/187 (98%)	167 (91%)	12 (6%)	5 (3%)	4	25
20	T	179/182 (98%)	172 (96%)	4 (2%)	3 (2%)	7	35
21	U	178/184 (97%)	166 (93%)	9 (5%)	3 (2%)	7	35
22	V	153/161 (95%)	134 (88%)	13 (8%)	6 (4%)	2	18
23	W	166/203 (82%)	152 (92%)	13 (8%)	1 (1%)	21	56
24	X	95/139 (68%)	86 (90%)	6 (6%)	3 (3%)	3	21
25	Y	99/190 (52%)	93 (94%)	6 (6%)	0	100	100
26	Z	119/126 (94%)	102 (86%)	14 (12%)	3 (2%)	4	27
27	0	60/162 (37%)	55 (92%)	3 (5%)	2 (3%)	3	21
28	1	136/146 (93%)	125 (92%)	10 (7%)	1 (1%)	18	52
29	2	96/127 (76%)	85 (88%)	9 (9%)	2 (2%)	5	31
30	3	117/124 (94%)	104 (89%)	10 (8%)	3 (3%)	4	26
31	4	64/67 (96%)	56 (88%)	5 (8%)	3 (5%)	2	14
32	5	221/257 (86%)	197 (89%)	20 (9%)	4 (2%)	6	34
33	6	96/108 (89%)	92 (96%)	2 (2%)	2 (2%)	5	31
34	7	92/120 (77%)	88 (96%)	4 (4%)	0	100	100
35	8	123/131 (94%)	109 (89%)	10 (8%)	4 (3%)	3	21
36	9	101/140 (72%)	86 (85%)	12 (12%)	3 (3%)	3	23
37	a	104/150 (69%)	98 (94%)	4 (4%)	2 (2%)	6	33
38	b	91/112 (81%)	86 (94%)	3 (3%)	2 (2%)	5	29
39	c	87/92 (95%)	68 (78%)	15 (17%)	4 (5%)	2	15
40	d	68/87 (78%)	65 (96%)	3 (4%)	0	100	100
41	e	39/51 (76%)	38 (97%)	1 (3%)	0	100	100
42	f	49/128 (38%)	45 (92%)	4 (8%)	0	100	100
43	g	35/39 (90%)	31 (89%)	4 (11%)	0	100	100
44	h	83/96 (86%)	74 (89%)	8 (10%)	1 (1%)	10	42
45	i	93/104 (89%)	82 (88%)	7 (8%)	4 (4%)	2	16
All	All	6124/7124 (86%)	5538 (90%)	438 (7%)	148 (2%)	7	28

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	197	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	18	PRO
6	F	102	PHE
7	G	130	HIS
7	G	143	ARG
8	H	53	TYR
8	H	110	ARG
9	I	88	PRO
9	I	89	TYR
9	I	213	ASP
10	J	61	PRO
10	J	241	ASP
11	K	108	PRO
11	K	188	ILE
12	L	65	ASN
12	L	131	LYS
12	L	168	LYS
12	L	169	PRO
13	M	12	LYS
13	M	48	LEU
16	P	51	LEU
18	R	58	SER
18	R	90	VAL
18	R	152	ILE
19	S	7	ASN
19	S	8	VAL
20	T	129	ASN
27	0	32	ASP
30	3	4	VAL
30	3	119	LEU
32	5	116	ARG
33	6	71	HIS
35	8	123	LYS
37	a	10	HIS
37	a	75	ALA
39	c	24	ARG
4	D	13	GLY
5	E	183	GLY
5	E	196	LEU
6	F	267	ILE
6	F	321	ASN
8	H	147	GLY
9	I	53	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	216	LEU
10	J	242	ASN
12	L	92	ILE
14	N	8	THR
16	P	150	ASN
17	Q	172	GLY
18	R	114	ASN
18	R	151	GLY
18	R	171	GLY
19	S	9	GLY
20	T	15	LYS
21	U	154	ARG
22	V	23	HIS
22	V	45	CYS
22	V	56	ASN
23	W	68	GLY
24	X	76	ASN
24	X	78	LYS
24	X	135	PHE
27	0	14	SER
28	1	42	LEU
30	3	76	LYS
31	4	20	GLY
32	5	204	CYS
38	b	18	ASN
39	c	40	CYS
45	i	68	VAL
45	i	93	GLY
45	i	95	ASP
5	E	62	LYS
5	E	254	PRO
6	F	265	GLY
6	F	295	SER
6	F	314	GLN
7	G	95	ASN
9	I	36	ARG
9	I	159	MET
10	J	75	ILE
11	K	110	PRO
12	L	130	ASN
13	M	136	SER
14	N	31	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	14	LYS
16	P	186	ARG
17	Q	14	ASN
18	R	44	TYR
18	R	229	ASN
19	S	41	ASN
19	S	184	ALA
20	T	4	THR
22	V	82	LYS
22	V	124	ASN
22	V	134	GLU
26	Z	10	SER
26	Z	82	GLU
29	2	38	VAL
29	2	60	LYS
32	5	177	GLN
36	9	54	ARG
45	i	15	LYS
4	D	180	LEU
5	E	68	HIS
6	F	17	ASN
9	I	19	VAL
9	I	49	LYS
14	N	60	PHE
16	P	202	ARG
17	Q	6	ALA
17	Q	24	ARG
18	R	124	LYS
21	U	134	ARG
21	U	183	ARG
32	5	172	ALA
35	8	64	LYS
36	9	66	LYS
36	9	104	VAL
39	c	46	LYS
4	D	144	LYS
5	E	330	LYS
8	H	52	LYS
8	H	137	PRO
10	J	51	ARG
12	L	4	HIS
17	Q	23	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	60	ILE
35	8	27	ARG
35	8	41	ARG
38	b	86	THR
44	h	18	TYR
6	F	223	ASN
8	H	62	VAL
12	L	50	ILE
31	4	38	ASN
8	H	131	VAL
10	J	101	LEU
4	D	127	VAL
31	4	36	ASP
6	F	19	VAL
12	L	137	GLY
16	P	149	ILE
33	6	103	ILE
14	N	46	VAL
39	c	65	GLY
11	K	190	PRO
26	Z	84	VAL

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	
4	D	191/202 (95%)	169 (88%)	22 (12%)	5	24
5	E	335/340 (98%)	307 (92%)	28 (8%)	10	38
6	F	336/352 (96%)	304 (90%)	32 (10%)	8	32
7	G	110/155 (71%)	93 (84%)	17 (16%)	2	14
8	H	164/173 (95%)	132 (80%)	32 (20%)	1	8
9	I	189/203 (93%)	164 (87%)	25 (13%)	4	19
10	J	211/260 (81%)	188 (89%)	23 (11%)	6	26
11	K	181/182 (100%)	156 (86%)	25 (14%)	3	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	190/194 (98%)	164 (86%)	26 (14%)	3	18
13	M	106/110 (96%)	93 (88%)	13 (12%)	4	22
14	N	134/152 (88%)	112 (84%)	22 (16%)	2	12
15	O	121/122 (99%)	110 (91%)	11 (9%)	9	34
16	P	179/180 (99%)	158 (88%)	21 (12%)	5	23
17	Q	165/190 (87%)	151 (92%)	14 (8%)	10	37
18	R	214/254 (84%)	185 (86%)	29 (14%)	3	18
19	S	158/159 (99%)	140 (89%)	18 (11%)	5	24
20	T	161/163 (99%)	146 (91%)	15 (9%)	8	33
21	U	162/166 (98%)	150 (93%)	12 (7%)	13	43
22	V	140/144 (97%)	131 (94%)	9 (6%)	16	48
23	W	128/178 (72%)	110 (86%)	18 (14%)	3	17
24	X	92/131 (70%)	86 (94%)	6 (6%)	15	47
25	Y	90/177 (51%)	81 (90%)	9 (10%)	7	30
26	Z	111/115 (96%)	97 (87%)	14 (13%)	4	21
27	0	53/146 (36%)	47 (89%)	6 (11%)	5	24
28	1	127/132 (96%)	113 (89%)	14 (11%)	6	26
29	2	97/118 (82%)	91 (94%)	6 (6%)	16	49
30	3	110/115 (96%)	94 (86%)	16 (14%)	3	16
31	4	60/61 (98%)	55 (92%)	5 (8%)	10	38
32	5	201/231 (87%)	177 (88%)	24 (12%)	5	23
33	6	83/92 (90%)	68 (82%)	15 (18%)	2	9
34	7	90/112 (80%)	68 (76%)	22 (24%)	1	4
35	8	114/120 (95%)	96 (84%)	18 (16%)	2	13
36	9	90/127 (71%)	74 (82%)	16 (18%)	2	10
37	a	89/128 (70%)	77 (86%)	12 (14%)	4	19
38	b	82/97 (84%)	76 (93%)	6 (7%)	13	43
39	c	73/77 (95%)	66 (90%)	7 (10%)	8	32
40	d	69/83 (83%)	62 (90%)	7 (10%)	7	30
41	e	40/48 (83%)	33 (82%)	7 (18%)	2	10
42	f	45/114 (40%)	42 (93%)	3 (7%)	15	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	g	34/35 (97%)	31 (91%)	3 (9%)	9	35
44	h	70/80 (88%)	65 (93%)	5 (7%)	13	44
45	i	87/93 (94%)	81 (93%)	6 (7%)	14	45
All	All	5482/6311 (87%)	4843 (88%)	639 (12%)	7	23

All (639) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	9	ARG
4	D	32	LEU
4	D	35	CYS
4	D	40	TYR
4	D	41	ILE
4	D	47	ASP
4	D	67	GLU
4	D	89	SER
4	D	90	CYS
4	D	102	LEU
4	D	120	THR
4	D	125	THR
4	D	139	GLN
4	D	148	VAL
4	D	177	LYS
4	D	193	ARG
4	D	194	ASN
4	D	204	MET
4	D	207	VAL
4	D	227	ARG
4	D	235	VAL
4	D	245	LEU
5	E	13	SER
5	E	24	ARG
5	E	30	ARG
5	E	56	ILE
5	E	59	GLU
5	E	72	ILE
5	E	87	VAL
5	E	89	ILE
5	E	104	THR
5	E	112	ASP
5	E	113	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	117	ARG
5	E	134	LEU
5	E	196	LEU
5	E	202	VAL
5	E	212	ILE
5	E	216	SER
5	E	223	THR
5	E	232	VAL
5	E	233	LYS
5	E	243	LEU
5	E	253	HIS
5	E	260	GLN
5	E	266	GLN
5	E	287	ASP
5	E	320	LEU
5	E	334	THR
5	E	343	VAL
6	F	33	ARG
6	F	55	LYS
6	F	73	VAL
6	F	75	ARG
6	F	86	ARG
6	F	92	PHE
6	F	115	VAL
6	F	126	SER
6	F	138	LEU
6	F	140	ARG
6	F	144	ILE
6	F	152	LEU
6	F	180	VAL
6	F	182	ARG
6	F	203	ILE
6	F	212	GLU
6	F	230	CYS
6	F	232	VAL
6	F	254	GLU
6	F	278	ILE
6	F	311	LYS
6	F	312	ARG
6	F	313	LEU
6	F	314	GLN
6	F	316	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	318	SER
6	F	321	ASN
6	F	325	ARG
6	F	333	LYS
6	F	369	GLN
6	F	371	ILE
6	F	376	TYR
7	G	12	ILE
7	G	18	VAL
7	G	23	VAL
7	G	25	GLU
7	G	28	ASP
7	G	40	LEU
7	G	43	GLN
7	G	44	LYS
7	G	67	CYS
7	G	75	LYS
7	G	77	LEU
7	G	99	THR
7	G	126	ASP
7	G	141	ARG
7	G	160	MET
7	G	165	THR
7	G	166	LYS
8	H	5	VAL
8	H	6	SER
8	H	25	VAL
8	H	41	LEU
8	H	43	ILE
8	H	45	ILE
8	H	46	ARG
8	H	47	LEU
8	H	48	ASN
8	H	54	ILE
8	H	55	LYS
8	H	57	VAL
8	H	66	LEU
8	H	70	ARG
8	H	73	CYS
8	H	85	LYS
8	H	93	LEU
8	H	94	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	109	THR
8	H	111	ILE
8	H	119	GLU
8	H	125	VAL
8	H	131	VAL
8	H	150	ILE
8	H	153	VAL
8	H	155	LEU
8	H	162	GLN
8	H	164	VAL
8	H	165	LEU
8	H	169	LYS
8	H	172	ARG
8	H	184	THR
9	I	9	LYS
9	I	29	ILE
9	I	33	TYR
9	I	37	LYS
9	I	40	SER
9	I	61	ILE
9	I	62	ILE
9	I	63	LEU
9	I	70	LYS
9	I	73	ILE
9	I	78	LEU
9	I	82	LEU
9	I	83	LEU
9	I	96	LEU
9	I	99	VAL
9	I	102	ARG
9	I	105	VAL
9	I	108	SER
9	I	110	ASN
9	I	111	ILE
9	I	170	ARG
9	I	175	LYS
9	I	185	ASP
9	I	204	LEU
9	I	216	LEU
10	J	44	LEU
10	J	75	ILE
10	J	85	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	96	GLN
10	J	106	THR
10	J	110	LEU
10	J	113	LEU
10	J	125	LYS
10	J	129	LEU
10	J	153	ILE
10	J	159	LEU
10	J	169	VAL
10	J	179	LEU
10	J	183	LEU
10	J	186	LEU
10	J	189	LEU
10	J	200	LYS
10	J	217	LEU
10	J	234	VAL
10	J	235	CYS
10	J	259	MET
10	J	261	LEU
10	J	272	GLU
11	K	1	MET
11	K	14	LEU
11	K	15	LEU
11	K	18	LEU
11	K	35	VAL
11	K	38	GLU
11	K	52	LYS
11	K	55	GLU
11	K	57	LEU
11	K	59	LEU
11	K	63	THR
11	K	67	LYS
11	K	98	LEU
11	K	105	VAL
11	K	118	VAL
11	K	121	SER
11	K	132	ARG
11	K	135	CYS
11	K	137	LEU
11	K	151	LEU
11	K	154	LYS
11	K	164	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	174	LEU
11	K	196	LEU
11	K	201	TYR
12	L	18	GLN
12	L	19	ARG
12	L	20	HIS
12	L	27	LYS
12	L	31	LYS
12	L	38	ARG
12	L	39	GLU
12	L	43	LYS
12	L	48	THR
12	L	50	ILE
12	L	61	THR
12	L	62	GLN
12	L	63	ARG
12	L	79	LEU
12	L	84	LEU
12	L	91	THR
12	L	94	ILE
12	L	119	LYS
12	L	122	LEU
12	L	136	ILE
12	L	169	PRO
12	L	170	PHE
12	L	174	ILE
12	L	190	ARG
12	L	201	ARG
12	L	203	GLN
13	M	14	ARG
13	M	34	LYS
13	M	38	ILE
13	M	48	LEU
13	M	50	ARG
13	M	51	LEU
13	M	55	SER
13	M	56	LEU
13	M	60	VAL
13	M	85	LYS
13	M	123	GLU
13	M	126	GLU
13	M	131	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	14	ILE
14	N	25	VAL
14	N	29	ARG
14	N	31	CYS
14	N	46	VAL
14	N	48	ILE
14	N	52	THR
14	N	54	VAL
14	N	56	VAL
14	N	62	THR
14	N	64	VAL
14	N	67	MET
14	N	75	LYS
14	N	80	ARG
14	N	92	LEU
14	N	101	VAL
14	N	102	LEU
14	N	118	LYS
14	N	137	GLU
14	N	138	LEU
14	N	144	THR
14	N	146	LYS
15	O	4	ARG
15	O	5	PHE
15	O	9	ARG
15	O	22	VAL
15	O	81	LEU
15	O	84	GLU
15	O	87	LYS
15	O	104	ARG
15	O	132	VAL
15	O	134	GLU
15	O	146	LEU
16	P	7	ILE
16	P	15	GLN
16	P	22	LEU
16	P	46	ASP
16	P	49	ARG
16	P	51	LEU
16	P	61	ILE
16	P	66	VAL
16	P	83	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	89	VAL
16	P	98	LEU
16	P	105	LYS
16	P	113	ASN
16	P	118	ASN
16	P	132	GLU
16	P	133	VAL
16	P	148	LYS
16	P	149	ILE
16	P	181	LEU
16	P	184	LYS
16	P	189	ILE
17	Q	38	ARG
17	Q	39	LYS
17	Q	49	VAL
17	Q	52	LEU
17	Q	87	LEU
17	Q	88	ARG
17	Q	96	VAL
17	Q	98	ARG
17	Q	126	VAL
17	Q	134	VAL
17	Q	145	VAL
17	Q	153	ARG
17	Q	154	ARG
17	Q	187	LYS
18	R	22	ARG
18	R	38	LEU
18	R	41	LYS
18	R	43	LYS
18	R	44	TYR
18	R	56	THR
18	R	59	GLN
18	R	69	ILE
18	R	77	GLU
18	R	82	GLU
18	R	88	ILE
18	R	90	VAL
18	R	103	LEU
18	R	104	LEU
18	R	107	ARG
18	R	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	114	ASN
18	R	152	ILE
18	R	153	THR
18	R	159	ASN
18	R	165	LEU
18	R	166	LYS
18	R	169	CYS
18	R	197	ASN
18	R	209	THR
18	R	223	ASN
18	R	238	MET
18	R	273	LEU
18	R	274	ASN
19	S	17	LYS
19	S	19	LEU
19	S	28	LEU
19	S	32	LEU
19	S	38	ARG
19	S	47	ILE
19	S	48	ILE
19	S	80	VAL
19	S	84	SER
19	S	87	ASP
19	S	94	LEU
19	S	97	LEU
19	S	99	VAL
19	S	113	GLU
19	S	131	THR
19	S	136	VAL
19	S	139	ARG
19	S	187	LYS
20	T	3	LEU
20	T	20	LYS
20	T	59	ARG
20	T	79	LYS
20	T	83	THR
20	T	88	THR
20	T	104	LEU
20	T	141	ILE
20	T	152	LYS
20	T	162	ARG
20	T	164	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	T	166	GLN
20	T	170	ASN
20	T	172	ARG
20	T	180	VAL
21	U	9	LEU
21	U	12	ASN
21	U	60	LEU
21	U	67	LEU
21	U	87	LEU
21	U	91	ASP
21	U	94	THR
21	U	106	THR
21	U	107	THR
21	U	145	ARG
21	U	176	SER
21	U	184	MET
22	V	41	VAL
22	V	42	ASP
22	V	61	LYS
22	V	69	THR
22	V	84	ARG
22	V	92	VAL
22	V	149	ILE
22	V	152	ILE
22	V	153	GLU
23	W	16	LYS
23	W	22	LEU
23	W	45	LYS
23	W	48	LEU
23	W	50	ASP
23	W	51	VAL
23	W	54	LYS
23	W	58	VAL
23	W	61	ARG
23	W	62	LYS
23	W	69	ARG
23	W	75	GLU
23	W	87	SER
23	W	103	GLU
23	W	107	LEU
23	W	123	ARG
23	W	149	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	W	153	ILE
24	X	57	ILE
24	X	60	LEU
24	X	93	THR
24	X	113	MET
24	X	116	ILE
24	X	125	LYS
25	Y	106	ASP
25	Y	127	ILE
25	Y	134	CYS
25	Y	143	ILE
25	Y	150	LEU
25	Y	167	ASP
25	Y	168	LYS
25	Y	183	VAL
25	Y	187	ILE
26	Z	4	ASN
26	Z	13	LYS
26	Z	14	MET
26	Z	20	THR
26	Z	34	LEU
26	Z	59	ARG
26	Z	62	ASN
26	Z	72	ILE
26	Z	82	GLU
26	Z	86	ARG
26	Z	103	VAL
26	Z	105	LEU
26	Z	111	ASP
26	Z	121	LYS
27	0	29	ILE
27	0	46	LEU
27	0	60	GLN
27	0	64	ARG
27	0	67	LYS
27	0	68	LYS
28	1	5	LEU
28	1	9	LYS
28	1	10	VAL
28	1	26	VAL
28	1	43	VAL
28	1	61	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	1	63	VAL
28	1	106	ASN
28	1	108	LYS
28	1	114	LEU
28	1	117	ILE
28	1	123	LEU
28	1	124	GLU
28	1	137	ILE
29	2	3	ASN
29	2	23	ASN
29	2	34	ASP
29	2	37	ASN
29	2	86	MET
29	2	96	HIS
30	3	18	LEU
30	3	31	LEU
30	3	42	LYS
30	3	43	ASN
30	3	46	ILE
30	3	52	ASN
30	3	55	ARG
30	3	67	GLU
30	3	68	LEU
30	3	76	LYS
30	3	77	PHE
30	3	87	THR
30	3	97	LYS
30	3	98	GLN
30	3	104	LEU
30	3	119	LEU
31	4	13	ASN
31	4	21	ILE
31	4	51	GLN
31	4	62	LYS
31	4	63	GLN
32	5	39	ILE
32	5	53	LEU
32	5	58	LEU
32	5	59	ARG
32	5	104	LEU
32	5	108	VAL
32	5	115	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	5	128	VAL
32	5	129	ASN
32	5	134	GLU
32	5	136	LEU
32	5	137	LYS
32	5	139	VAL
32	5	149	THR
32	5	156	LEU
32	5	163	VAL
32	5	176	ILE
32	5	181	ASP
32	5	182	ILE
32	5	210	LYS
32	5	224	ARG
32	5	231	ARG
32	5	250	ASN
32	5	251	GLU
33	6	19	LEU
33	6	21	MET
33	6	22	LYS
33	6	28	PHE
33	6	33	CYS
33	6	44	LEU
33	6	46	ILE
33	6	50	ASN
33	6	54	ILE
33	6	55	GLN
33	6	67	LYS
33	6	77	ASN
33	6	80	LEU
33	6	89	ARG
33	6	101	SER
34	7	21	THR
34	7	25	SER
34	7	26	LYS
34	7	31	VAL
34	7	32	CYS
34	7	39	ARG
34	7	41	ILE
34	7	44	ILE
34	7	54	THR
34	7	57	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	7	58	ARG
34	7	67	ILE
34	7	72	VAL
34	7	78	ARG
34	7	80	ARG
34	7	81	VAL
34	7	88	ASN
34	7	99	THR
34	7	101	VAL
34	7	110	LYS
34	7	112	LEU
34	7	114	ASN
35	8	4	LYS
35	8	9	ILE
35	8	21	GLN
35	8	26	MET
35	8	33	ARG
35	8	41	ARG
35	8	47	LYS
35	8	49	THR
35	8	63	THR
35	8	67	LEU
35	8	73	LYS
35	8	76	VAL
35	8	87	MET
35	8	90	THR
35	8	103	LYS
35	8	111	ARG
35	8	113	LYS
35	8	125	ARG
36	9	42	GLU
36	9	51	ARG
36	9	54	ARG
36	9	56	GLN
36	9	57	ASP
36	9	67	ASN
36	9	68	VAL
36	9	69	ASN
36	9	71	LYS
36	9	100	ILE
36	9	103	LYS
36	9	106	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	9	113	VAL
36	9	125	LYS
36	9	131	VAL
36	9	136	TYR
37	a	4	ARG
37	a	5	VAL
37	a	15	THR
37	a	20	VAL
37	a	32	ILE
37	a	72	VAL
37	a	74	ARG
37	a	86	ARG
37	a	90	MET
37	a	94	LEU
37	a	96	GLU
37	a	100	CYS
38	b	18	ASN
38	b	38	SER
38	b	50	GLU
38	b	74	LYS
38	b	81	LYS
38	b	93	LYS
39	c	18	THR
39	c	48	ARG
39	c	49	ARG
39	c	51	ASN
39	c	66	ARG
39	c	70	ILE
39	c	73	LEU
40	d	24	ILE
40	d	25	ILE
40	d	28	LYS
40	d	40	LYS
40	d	51	THR
40	d	65	ASN
40	d	76	TYR
41	e	4	ILE
41	e	5	LYS
41	e	6	ARG
41	e	15	LYS
41	e	18	ARG
41	e	38	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	e	42	ARG
42	f	9	LEU
42	f	11	GLN
42	f	51	LEU
43	g	7	ARG
43	g	9	LYS
43	g	35	ARG
44	h	10	LEU
44	h	16	THR
44	h	17	ARG
44	h	47	THR
44	h	85	ARG
45	i	8	ARG
45	i	37	LEU
45	i	41	ARG
45	i	62	LYS
45	i	86	ARG
45	i	87	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	22	HIS
4	D	194	ASN
4	D	221	HIS
4	D	233	GLN
5	E	162	GLN
5	E	207	ASN
5	E	342	GLN
5	E	364	HIS
6	F	9	ASN
6	F	156	ASN
6	F	169	ASN
6	F	215	ASN
6	F	285	HIS
6	F	314	GLN
6	F	317	ASN
7	G	43	GLN
8	H	21	ASN
8	H	115	ASN
8	H	162	GLN
9	I	12	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	47	GLN
9	I	92	ASN
9	I	110	ASN
9	I	146	GLN
9	I	177	GLN
9	I	202	HIS
10	J	53	ASN
10	J	95	ASN
10	J	99	HIS
11	K	13	HIS
11	K	54	GLN
11	K	95	GLN
11	K	147	ASN
11	K	173	ASN
12	L	24	ASN
12	L	54	HIS
12	L	65	ASN
12	L	111	ASN
12	L	153	ASN
13	M	30	ASN
13	M	35	ASN
13	M	77	ASN
14	N	130	GLN
15	O	8	ASN
15	O	39	HIS
15	O	44	ASN
15	O	74	ASN
15	O	118	HIS
16	P	15	GLN
16	P	32	GLN
16	P	81	HIS
16	P	118	ASN
16	P	139	ASN
16	P	141	ASN
16	P	145	ASN
16	P	180	HIS
17	Q	73	ASN
17	Q	163	GLN
17	Q	169	ASN
17	Q	183	GLN
18	R	45	ASN
18	R	47	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	68	HIS
18	R	179	ASN
18	R	180	ASN
18	R	221	HIS
18	R	223	ASN
18	R	249	ASN
18	R	274	ASN
19	S	23	ASN
19	S	43	ASN
19	S	45	ASN
19	S	150	HIS
20	T	35	ASN
20	T	54	GLN
20	T	129	ASN
20	T	133	ASN
20	T	166	GLN
21	U	12	ASN
21	U	15	GLN
21	U	58	ASN
21	U	114	GLN
21	U	123	HIS
21	U	131	ASN
21	U	162	HIS
22	V	36	ASN
22	V	56	ASN
22	V	103	ASN
23	W	49	ASN
23	W	137	ASN
23	W	154	ASN
25	Y	149	ASN
25	Y	185	ASN
26	Z	99	HIS
26	Z	102	ASN
27	0	66	ASN
28	1	49	HIS
28	1	79	HIS
28	1	106	ASN
29	2	79	GLN
30	3	39	ASN
30	3	52	ASN
30	3	98	GLN
30	3	112	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	4	6	ASN
31	4	12	GLN
32	5	51	ASN
32	5	213	ASN
32	5	250	ASN
32	5	254	ASN
33	6	27	GLN
33	6	50	ASN
33	6	55	GLN
34	7	64	ASN
34	7	74	ASN
34	7	88	ASN
34	7	114	ASN
35	8	70	ASN
35	8	78	ASN
36	9	56	GLN
37	a	11	ASN
38	b	18	ASN
38	b	21	HIS
38	b	98	GLN
39	c	51	ASN
39	c	79	ASN
40	d	4	GLN
41	e	43	HIS
42	f	11	GLN
42	f	14	ASN
42	f	33	ASN
42	f	43	ASN
43	g	3	HIS
45	i	3	ASN
45	i	14	ASN
45	i	46	GLN
45	i	52	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3164/3788 (83%)	954 (30%)	167 (5%)
2	B	117/119 (98%)	23 (19%)	1 (0%)
3	C	148/159 (93%)	44 (29%)	8 (5%)
All	All	3429/4066 (84%)	1021 (29%)	176 (5%)

All (1021) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	13	G
1	A	14	U
1	A	16	A
1	A	18	G
1	A	26	A
1	A	32	C
1	A	40	A
1	A	43	A
1	A	44	U
1	A	45	A
1	A	49	U
1	A	55	G
1	A	57	A
1	A	59	G
1	A	60	A
1	A	66	A
1	A	69	U
1	A	73	U
1	A	74	A
1	A	83	U
1	A	87	U
1	A	92	G
1	A	109	A
1	A	110	G
1	A	111	C
1	A	121	U
1	A	122	A
1	A	123	A
1	A	124	U
1	A	130	G
1	A	133	U
1	A	134	G
1	A	135	G
1	A	136	U
1	A	137	G
1	A	139	A
1	A	144	U
1	A	146	U
1	A	147	C
1	A	149	A
1	A	152	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	155	U
1	A	156	U
1	A	157	G
1	A	158	U
1	A	162	U
1	A	163	G
1	A	165	A
1	A	167	U
1	A	173	A
1	A	174	U
1	A	181	C
1	A	182	U
1	A	183	U
1	A	184	U
1	A	185	A
1	A	186	A
1	A	190	G
1	A	191	A
1	A	192	G
1	A	197	G
1	A	198	U
1	A	199	G
1	A	200	A
1	A	201	G
1	A	204	G
1	A	207	A
1	A	208	U
1	A	209	G
1	A	211	U
1	A	215	C
1	A	216	C
1	A	218	U
1	A	219	A
1	A	221	A
1	A	226	G
1	A	227	A
1	A	228	A
1	A	229	A
1	A	231	G
1	A	232	C
1	A	235	A
1	A	239	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	242	U
1	A	246	U
1	A	250	U
1	A	251	U
1	A	257	U
1	A	258	U
1	A	265	U
1	A	268	C
1	A	269	A
1	A	271	G
1	A	276	G
1	A	277	U
1	A	289	A
1	A	290	G
1	A	291	A
1	A	292	U
1	A	293	U
1	A	302	A
1	A	303	A
1	A	304	U
1	A	305	A
1	A	306	C
1	A	307	G
1	A	308	U
1	A	309	G
1	A	310	U
1	A	313	U
1	A	315	C
1	A	324	U
1	A	325	A
1	A	337	A
1	A	338	U
1	A	342	G
1	A	344	A
1	A	345	G
1	A	346	A
1	A	347	C
1	A	362	U
1	A	378	U
1	A	382	A
1	A	384	A
1	A	385	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	386	U
1	A	392	G
1	A	395	A
1	A	400	C
1	A	401	A
1	A	405	A
1	A	408	U
1	A	409	A
1	A	411	U
1	A	412	A
1	A	413	C
1	A	431	G
1	A	432	A
1	A	439	U
1	A	444	G
1	A	447	A
1	A	448	A
1	A	449	A
1	A	451	C
1	A	458	A
1	A	459	G
1	A	462	G
1	A	463	G
1	A	465	A
1	A	489	U
1	A	494	U
1	A	495	U
1	A	496	C
1	A	497	U
1	A	498	U
1	A	499	U
1	A	500	A
1	A	501	U
1	A	502	U
1	A	503	A
1	A	505	A
1	A	506	A
1	A	520	U
1	A	521	U
1	A	522	A
1	A	523	A
1	A	530	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	531	U
1	A	532	C
1	A	534	A
1	A	536	A
1	A	538	A
1	A	539	G
1	A	543	U
1	A	545	C
1	A	547	C
1	A	549	G
1	A	552	A
1	A	573	U
1	A	579	C
1	A	580	A
1	A	581	C
1	A	582	U
1	A	585	C
1	A	586	U
1	A	592	C
1	A	593	A
1	A	594	C
1	A	595	U
1	A	599	G
1	A	601	G
1	A	608	A
1	A	609	C
1	A	610	U
1	A	615	U
1	A	617	A
1	A	618	U
1	A	620	U
1	A	621	C
1	A	622	U
1	A	623	U
1	A	624	C
1	A	625	A
1	A	628	U
1	A	631	U
1	A	636	U
1	A	637	U
1	A	641	G
1	A	642	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	645	A
1	A	646	A
1	A	647	U
1	A	648	U
1	A	649	U
1	A	650	U
1	A	653	A
1	A	659	U
1	A	662	A
1	A	664	U
1	A	665	U
1	A	666	U
1	A	667	U
1	A	668	U
1	A	669	C
1	A	670	U
1	A	674	U
1	A	675	A
1	A	677	A
1	A	678	A
1	A	679	U
1	A	682	A
1	A	683	A
1	A	684	G
1	A	685	U
1	A	694	U
1	A	697	A
1	A	698	G
1	A	699	U
1	A	704	U
1	A	708	A
1	A	714	C
1	A	715	U
1	A	716	C
1	A	727	A
1	A	729	G
1	A	738	A
1	A	755	A
1	A	759	U
1	A	760	A
1	A	761	U
1	A	763	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	765	A
1	A	767	U
1	A	769	U
1	A	771	U
1	A	772	A
1	A	773	A
1	A	774	A
1	A	778	U
1	A	779	U
1	A	794	C
1	A	799	A
1	A	806	G
1	A	809	A
1	A	812	U
1	A	813	G
1	A	825	G
1	A	831	U
1	A	833	G
1	A	834	U
1	A	835	G
1	A	858	C
1	A	859	C
1	A	860	A
1	A	862	U
1	A	866	C
1	A	874	A
1	A	880	A
1	A	885	A
1	A	889	U
1	A	890	G
1	A	891	C
1	A	893	U
1	A	896	U
1	A	899	A
1	A	900	G
1	A	903	C
1	A	904	G
1	A	905	A
1	A	918	G
1	A	925	A
1	A	936	A
1	A	945	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	951	A
1	A	955	A
1	A	956	A
1	A	965	A
1	A	968	G
1	A	976	G
1	A	980	A
1	A	984	A
1	A	988	G
1	A	993	U
1	A	998	U
1	A	999	G
1	A	1013	U
1	A	1014	C
1	A	1015	A
1	A	1016	A
1	A	1026	G
1	A	1027	G
1	A	1033	A
1	A	1035	G
1	A	1036	A
1	A	1040	A
1	A	1042	C
1	A	1043	G
1	A	1044	A
1	A	1053	U
1	A	1056	G
1	A	1063	A
1	A	1070	A
1	A	1073	G
1	A	1078	C
1	A	1079	U
1	A	1080	C
1	A	1081	A
1	A	1086	C
1	A	1096	G
1	A	1100	A
1	A	1101	A
1	A	1102	U
1	A	1106	A
1	A	1107	U
1	A	1111	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1113	C
1	A	1115	G
1	A	1116	G
1	A	1121	G
1	A	1122	A
1	A	1123	U
1	A	1124	A
1	A	1128	A
1	A	1132	G
1	A	1136	A
1	A	1141	G
1	A	1158	G
1	A	1164	U
1	A	1168	C
1	A	1170	A
1	A	1172	C
1	A	1174	C
1	A	1186	A
1	A	1187	A
1	A	1188	A
1	A	1193	G
1	A	1194	A
1	A	1197	U
1	A	1198	A
1	A	1199	A
1	A	1203	A
1	A	1204	A
1	A	1205	U
1	A	1206	U
1	A	1207	U
1	A	1215	A
1	A	1217	U
1	A	1218	C
1	A	1219	A
1	A	1221	A
1	A	1222	U
1	A	1223	U
1	A	1224	A
1	A	1225	A
1	A	1229	A
1	A	1230	A
1	A	1231	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1233	A
1	A	1234	A
1	A	1245	G
1	A	1257	A
1	A	1259	G
1	A	1272	U
1	A	1273	G
1	A	1276	G
1	A	1281	C
1	A	1283	C
1	A	1287	A
1	A	1295	A
1	A	1300	G
1	A	1309	U
1	A	1310	A
1	A	1314	G
1	A	1320	G
1	A	1324	U
1	A	1325	C
1	A	1326	C
1	A	1329	U
1	A	1330	A
1	A	1336	U
1	A	1337	G
1	A	1340	G
1	A	1341	G
1	A	1344	C
1	A	1345	A
1	A	1418	A
1	A	1420	C
1	A	1435	G
1	A	1436	A
1	A	1437	U
1	A	1441	G
1	A	1444	A
1	A	1445	A
1	A	1450	G
1	A	1453	U
1	A	1458	A
1	A	1459	U
1	A	1460	A
1	A	1473	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1476	A
1	A	1480	G
1	A	1481	A
1	A	1482	A
1	A	1486	A
1	A	1498	U
1	A	1499	U
1	A	1503	A
1	A	1504	A
1	A	1505	U
1	A	1506	C
1	A	1529	G
1	A	1534	U
1	A	1535	G
1	A	1537	G
1	A	1538	U
1	A	1539	U
1	A	1540	G
1	A	1549	U
1	A	1550	A
1	A	1556	G
1	A	1565	G
1	A	1566	A
1	A	1567	A
1	A	1572	U
1	A	1575	C
1	A	1583	G
1	A	1586	C
1	A	1592	G
1	A	1595	A
1	A	1602	A
1	A	1604	U
1	A	1619	U
1	A	1630	A
1	A	1631	A
1	A	1632	G
1	A	1633	U
1	A	1635	G
1	A	1636	A
1	A	1637	G
1	A	1643	U
1	A	1644	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1649	G
1	A	1651	C
1	A	1657	U
1	A	1668	G
1	A	1669	A
1	A	1676	C
1	A	1677	G
1	A	1685	G
1	A	1688	A
1	A	1691	G
1	A	1696	A
1	A	1702	U
1	A	1703	U
1	A	1704	U
1	A	1705	A
1	A	1706	A
1	A	1707	A
1	A	1711	G
1	A	1713	G
1	A	1721	C
1	A	1723	C
1	A	1725	U
1	A	1730	A
1	A	1732	A
1	A	1736	A
1	A	1739	C
1	A	1745	G
1	A	1748	A
1	A	1750	U
1	A	1751	C
1	A	1760	A
1	A	1762	A
1	A	1763	G
1	A	1767	U
1	A	1768	A
1	A	1769	U
1	A	1770	G
1	A	1771	A
1	A	1774	U
1	A	1780	G
1	A	1781	A
1	A	1782	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1783	G
1	A	1788	C
1	A	1792	U
1	A	1794	U
1	A	1795	A
1	A	1796	U
1	A	1797	A
1	A	1800	U
1	A	1801	G
1	A	1805	U
1	A	1806	C
1	A	1812	C
1	A	1817	G
1	A	1832	U
1	A	1838	U
1	A	1850	U
1	A	1852	C
1	A	1855	U
1	A	1856	U
1	A	1857	A
1	A	1871	A
1	A	1872	A
1	A	1873	U
1	A	1874	C
1	A	1881	C
1	A	1882	U
1	A	1886	A
1	A	1888	A
1	A	1898	U
1	A	1899	U
1	A	1900	G
1	A	1901	A
1	A	1902	A
1	A	1903	C
1	A	1904	U
1	A	1905	C
1	A	1907	A
1	A	1909	U
1	A	1912	A
1	A	1958	U
1	A	1963	U
1	A	1964	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1965	U
1	A	1966	A
1	A	1969	A
1	A	1970	A
1	A	1971	U
1	A	1973	G
1	A	1976	A
1	A	1978	U
1	A	1980	G
1	A	1990	A
1	A	1991	U
1	A	1996	C
1	A	1997	G
1	A	1998	A
1	A	1999	A
1	A	2000	G
1	A	2010	C
1	A	2015	C
1	A	2016	U
1	A	2019	A
1	A	2034	G
1	A	2035	G
1	A	2040	G
1	A	2075	U
1	A	2080	C
1	A	2082	C
1	A	2084	U
1	A	2090	U
1	A	2092	G
1	A	2093	U
1	A	2094	A
1	A	2096	G
1	A	2097	A
1	A	2102	A
1	A	2106	A
1	A	2107	C
1	A	2108	A
1	A	2109	A
1	A	2113	C
1	A	2114	A
1	A	2116	C
1	A	2117	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2125	A
1	A	2126	A
1	A	2133	C
1	A	2136	C
1	A	2143	U
1	A	2146	A
1	A	2147	A
1	A	2148	U
1	A	2149	A
1	A	2152	A
1	A	2154	A
1	A	2161	G
1	A	2164	A
1	A	2174	G
1	A	2193	U
1	A	2194	C
1	A	2198	A
1	A	2203	G
1	A	2218	C
1	A	2219	A
1	A	2220	U
1	A	2393	A
1	A	2394	C
1	A	2395	U
1	A	2396	C
1	A	2403	G
1	A	2404	A
1	A	2405	A
1	A	2406	A
1	A	2414	G
1	A	2415	G
1	A	2419	A
1	A	2424	A
1	A	2427	G
1	A	2433	U
1	A	2437	A
1	A	2438	A
1	A	2442	A
1	A	2451	A
1	A	2452	A
1	A	2453	A
1	A	2462	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2463	U
1	A	2464	G
1	A	2477	U
1	A	2486	U
1	A	2491	A
1	A	2494	G
1	A	2499	G
1	A	2500	A
1	A	2516	A
1	A	2518	U
1	A	2521	A
1	A	2524	C
1	A	2537	A
1	A	2539	G
1	A	2542	G
1	A	2545	A
1	A	2548	A
1	A	2549	A
1	A	2550	C
1	A	2551	U
1	A	2552	A
1	A	2556	C
1	A	2565	G
1	A	2566	G
1	A	2567	U
1	A	2573	A
1	A	2574	A
1	A	2575	U
1	A	2576	G
1	A	2581	G
1	A	2589	A
1	A	2591	U
1	A	2596	A
1	A	2598	G
1	A	2599	C
1	A	2600	G
1	A	2601	C
1	A	2603	U
1	A	2606	A
1	A	2607	U
1	A	2608	G
1	A	2624	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2627	U
1	A	2628	G
1	A	2629	U
1	A	2632	C
1	A	2640	U
1	A	2656	A
1	A	2660	A
1	A	2667	C
1	A	2668	G
1	A	2671	C
1	A	2676	C
1	A	2678	A
1	A	2681	U
1	A	2684	G
1	A	2686	G
1	A	2687	G
1	A	2690	A
1	A	2694	A
1	A	2695	A
1	A	2696	G
1	A	2697	A
1	A	2704	U
1	A	2705	G
1	A	2710	U
1	A	2711	U
1	A	2712	A
1	A	2728	G
1	A	2730	G
1	A	2734	C
1	A	2736	A
1	A	2737	C
1	A	2740	A
1	A	2742	G
1	A	2745	G
1	A	2803	A
1	A	2806	U
1	A	2809	A
1	A	2810	A
1	A	2811	A
1	A	2812	G
1	A	2813	U
1	A	2817	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2818	U
1	A	2822	U
1	A	2823	U
1	A	2824	A
1	A	2831	U
1	A	2832	A
1	A	2833	U
1	A	2834	A
1	A	2835	G
1	A	2837	G
1	A	2884	G
1	A	2887	U
1	A	2932	A
1	A	2933	C
1	A	2945	G
1	A	2946	G
1	A	2953	G
1	A	2958	G
1	A	2967	A
1	A	2968	U
1	A	2981	A
1	A	2987	G
1	A	2991	U
1	A	2994	A
1	A	2995	A
1	A	2996	A
1	A	3011	G
1	A	3013	A
1	A	3016	G
1	A	3017	A
1	A	3018	A
1	A	3019	A
1	A	3020	U
1	A	3028	A
1	A	3029	G
1	A	3030	A
1	A	3033	A
1	A	3038	G
1	A	3042	A
1	A	3065	C
1	A	3067	G
1	A	3068	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3073	G
1	A	3076	G
1	A	3079	A
1	A	3086	A
1	A	3088	G
1	A	3091	U
1	A	3092	G
1	A	3094	C
1	A	3100	G
1	A	3108	A
1	A	3111	U
1	A	3112	U
1	A	3113	U
1	A	3116	A
1	A	3118	A
1	A	3123	C
1	A	3124	G
1	A	3126	A
1	A	3127	A
1	A	3130	U
1	A	3131	A
1	A	3138	A
1	A	3139	C
1	A	3140	U
1	A	3141	G
1	A	3146	U
1	A	3155	G
1	A	3158	U
1	A	3159	G
1	A	3160	A
1	A	3161	A
1	A	3162	A
1	A	3169	C
1	A	3173	G
1	A	3175	G
1	A	3176	A
1	A	3180	C
1	A	3193	G
1	A	3201	C
1	A	3202	U
1	A	3204	C
1	A	3208	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3212	G
1	A	3219	U
1	A	3220	U
1	A	3230	G
1	A	3231	A
1	A	3246	A
1	A	3248	C
1	A	3253	G
1	A	3257	G
1	A	3258	C
1	A	3263	G
1	A	3269	A
1	A	3277	G
1	A	3282	U
1	A	3287	C
1	A	3292	A
1	A	3294	U
1	A	3295	A
1	A	3297	G
1	A	3301	C
1	A	3304	G
1	A	3306	G
1	A	3309	G
1	A	3310	G
1	A	3313	U
1	A	3314	U
1	A	3316	G
1	A	3330	A
1	A	3334	U
1	A	3342	C
1	A	3343	C
1	A	3349	G
1	A	3353	A
1	A	3354	A
1	A	3356	U
1	A	3357	U
1	A	3358	U
1	A	3359	A
1	A	3361	U
1	A	3362	A
1	A	3363	U
1	A	3365	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3375	A
1	A	3378	C
1	A	3379	A
1	A	3380	U
1	A	3381	A
1	A	3382	U
1	A	3383	A
1	A	3389	G
1	A	3398	A
1	A	3415	A
1	A	3416	G
1	A	3418	A
1	A	3421	A
1	A	3434	A
1	A	3435	A
1	A	3442	C
1	A	3443	A
1	A	3445	C
1	A	3459	A
1	A	3463	G
1	A	3464	U
1	A	3471	A
1	A	3476	A
1	A	3477	A
1	A	3478	G
1	A	3483	U
1	A	3488	U
1	A	3493	G
1	A	3500	G
1	A	3502	C
1	A	3507	A
1	A	3510	C
1	A	3515	A
1	A	3516	A
1	A	3526	U
1	A	3527	U
1	A	3529	A
1	A	3530	A
1	A	3537	U
1	A	3553	G
1	A	3568	G
1	A	3571	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3572	A
1	A	3573	U
1	A	3575	U
1	A	3576	A
1	A	3577	A
1	A	3580	G
1	A	3581	A
1	A	3582	G
1	A	3583	A
1	A	3584	A
1	A	3585	A
1	A	3590	A
1	A	3591	U
1	A	3594	G
1	A	3615	A
1	A	3616	U
1	A	3617	A
1	A	3618	A
1	A	3619	U
1	A	3623	A
1	A	3624	U
1	A	3626	A
1	A	3627	C
1	A	3628	C
1	A	3629	U
1	A	3631	U
1	A	3632	U
1	A	3635	G
1	A	3655	U
1	A	3658	G
1	A	3659	C
1	A	3660	A
1	A	3661	A
1	A	3662	U
1	A	3663	A
1	A	3664	G
1	A	3665	U
1	A	3667	C
1	A	3668	U
1	A	3670	U
1	A	3671	A
1	A	3677	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3680	A
1	A	3683	G
1	A	3689	C
1	A	3690	A
1	A	3697	G
1	A	3698	U
1	A	3707	U
1	A	3710	U
1	A	3711	U
1	A	3712	G
1	A	3716	C
1	A	3727	A
1	A	3728	A
1	A	3732	U
1	A	3733	G
1	A	3736	A
1	A	3737	G
1	A	3739	A
1	A	3740	A
1	A	3741	A
1	A	3752	C
1	A	3761	G
1	A	3767	U
1	A	3770	C
1	A	3774	A
1	A	3775	G
1	A	3778	G
1	A	3779	U
1	A	3780	A
1	A	3783	G
2	B	3	A
2	B	13	A
2	B	18	A
2	B	22	G
2	B	26	C
2	B	27	A
2	B	31	G
2	B	33	U
2	B	38	U
2	B	51	G
2	B	53	U
2	B	54	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	55	A
2	B	63	A
2	B	64	A
2	B	71	G
2	B	73	U
2	B	74	A
2	B	76	U
2	B	89	G
2	B	97	G
2	B	100	A
2	B	110	G
3	C	3	G
3	C	5	A
3	C	6	C
3	C	16	G
3	C	17	A
3	C	27	U
3	C	35	A
3	C	36	C
3	C	37	A
3	C	38	G
3	C	39	C
3	C	43	G
3	C	50	G
3	C	53	G
3	C	63	A
3	C	64	U
3	C	66	C
3	C	67	G
3	C	75	A
3	C	79	G
3	C	85	A
3	C	86	C
3	C	90	G
3	C	92	A
3	C	98	A
3	C	107	A
3	C	108	A
3	C	109	U
3	C	111	U
3	C	112	A
3	C	114	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	115	C
3	C	116	U
3	C	119	A
3	C	122	A
3	C	123	A
3	C	129	U
3	C	135	G
3	C	137	A
3	C	138	U
3	C	139	A
3	C	140	G
3	C	142	G
3	C	146	C

All (176) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	13	G
1	A	25	A
1	A	43	A
1	A	65	A
1	A	123	A
1	A	124	U
1	A	155	U
1	A	162	U
1	A	173	A
1	A	181	C
1	A	184	U
1	A	208	U
1	A	215	C
1	A	218	U
1	A	251	U
1	A	257	U
1	A	270	U
1	A	289	A
1	A	290	G
1	A	306	C
1	A	337	A
1	A	345	G
1	A	416	G
1	A	500	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	501	U
1	A	504	A
1	A	579	C
1	A	580	A
1	A	581	C
1	A	594	C
1	A	607	A
1	A	608	A
1	A	620	U
1	A	621	C
1	A	641	G
1	A	645	A
1	A	647	U
1	A	648	U
1	A	652	A
1	A	664	U
1	A	666	U
1	A	673	U
1	A	674	U
1	A	683	A
1	A	697	A
1	A	698	G
1	A	703	U
1	A	715	U
1	A	764	G
1	A	771	U
1	A	778	U
1	A	799	A
1	A	859	C
1	A	888	A
1	A	889	U
1	A	899	A
1	A	935	A
1	A	998	U
1	A	1013	U
1	A	1035	G
1	A	1042	C
1	A	1080	C
1	A	1101	A
1	A	1115	G
1	A	1197	U
1	A	1205	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1206	U
1	A	1217	U
1	A	1221	A
1	A	1222	U
1	A	1224	A
1	A	1272	U
1	A	1324	U
1	A	1336	U
1	A	1435	G
1	A	1457	G
1	A	1481	A
1	A	1503	A
1	A	1536	U
1	A	1537	G
1	A	1538	U
1	A	1539	U
1	A	1566	A
1	A	1574	C
1	A	1632	G
1	A	1643	U
1	A	1704	U
1	A	1705	A
1	A	1750	U
1	A	1762	A
1	A	1779	A
1	A	1805	U
1	A	1873	U
1	A	1881	C
1	A	1904	U
1	A	1970	A
1	A	1989	A
1	A	1990	A
1	A	1996	C
1	A	1999	A
1	A	2015	C
1	A	2033	C
1	A	2034	G
1	A	2096	G
1	A	2105	A
1	A	2107	C
1	A	2108	A
1	A	2113	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2125	A
1	A	2193	U
1	A	2219	A
1	A	2394	C
1	A	2403	G
1	A	2405	A
1	A	2437	A
1	A	2451	A
1	A	2452	A
1	A	2499	G
1	A	2523	U
1	A	2575	U
1	A	2598	G
1	A	2665	A
1	A	2696	G
1	A	2737	C
1	A	2813	U
1	A	2816	U
1	A	2822	U
1	A	2832	A
1	A	2883	U
1	A	2886	A
1	A	2966	C
1	A	3018	A
1	A	3067	G
1	A	3123	C
1	A	3130	U
1	A	3137	U
1	A	3140	U
1	A	3257	G
1	A	3309	G
1	A	3313	U
1	A	3342	C
1	A	3361	U
1	A	3381	A
1	A	3382	U
1	A	3391	G
1	A	3414	G
1	A	3434	A
1	A	3471	A
1	A	3476	A
1	A	3477	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3526	U
1	A	3529	A
1	A	3575	U
1	A	3576	A
1	A	3590	A
1	A	3617	A
1	A	3623	A
1	A	3627	C
1	A	3658	G
1	A	3660	A
1	A	3661	A
1	A	3664	G
1	A	3667	C
1	A	3697	G
1	A	3711	U
1	A	3782	A
2	B	63	A
3	C	35	A
3	C	37	A
3	C	64	U
3	C	98	A
3	C	108	A
3	C	134	G
3	C	139	A
3	C	145	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 168 ligands modelled in this entry, 168 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

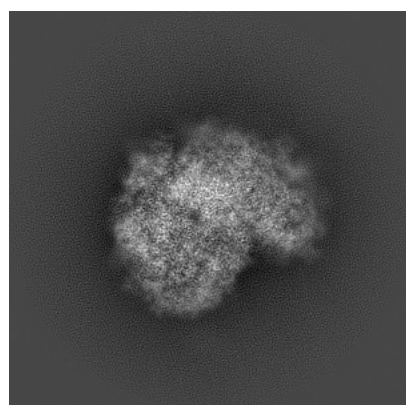
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2660. These allow visual inspection of the internal detail of the map and identification of artifacts.

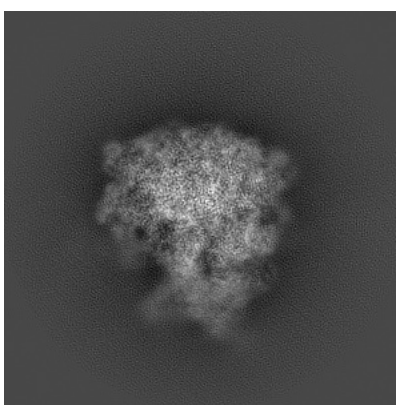
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

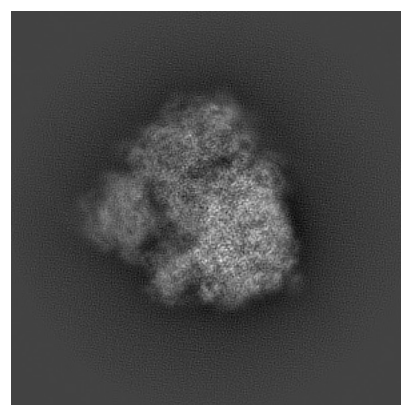
6.1.1 Primary map



X



Y

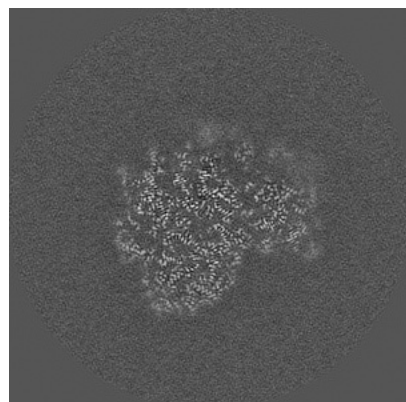


Z

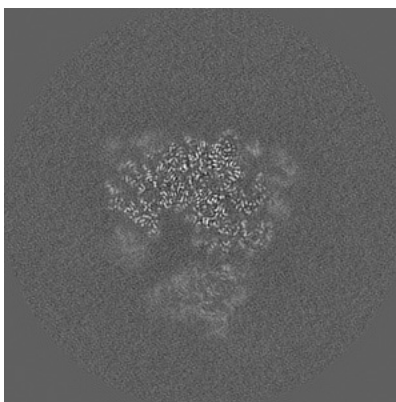
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

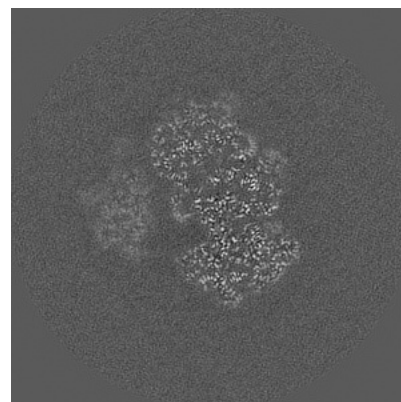
6.2.1 Primary map



X Index: 180



Y Index: 180

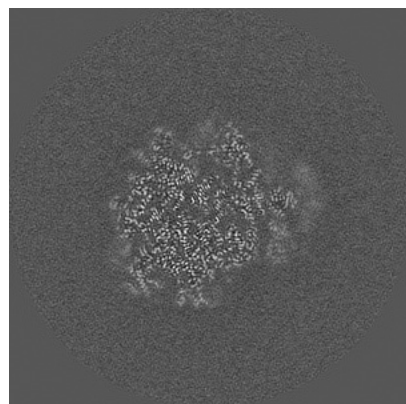


Z Index: 180

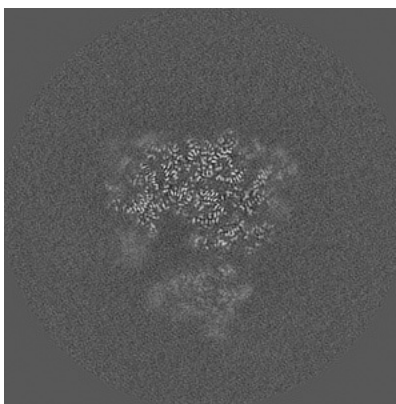
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

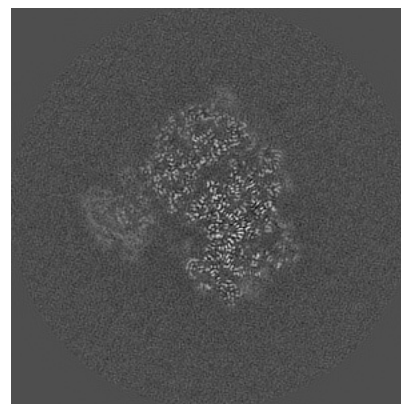
6.3.1 Primary map



X Index: 201



Y Index: 183

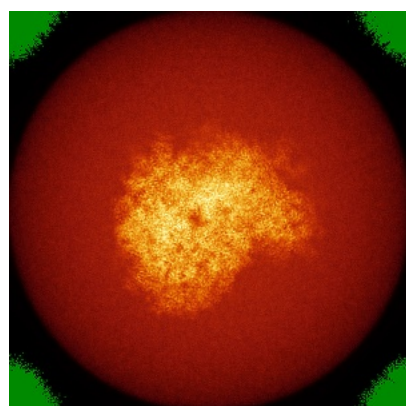


Z Index: 187

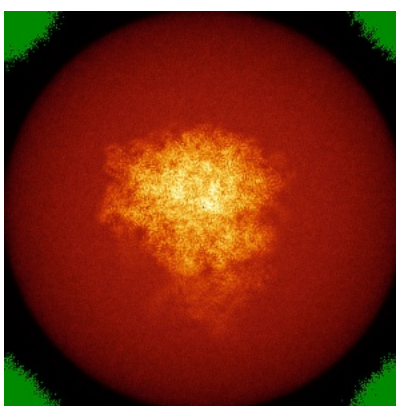
The images above show the largest variance slices of the map in three orthogonal directions.

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

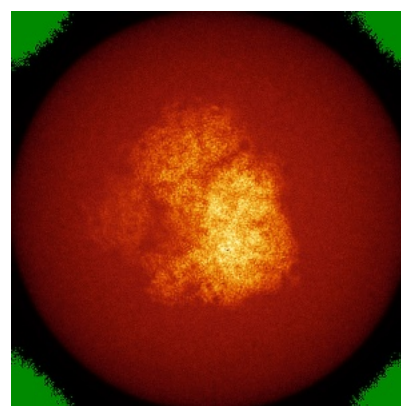
6.4.1 Primary map



X



Y

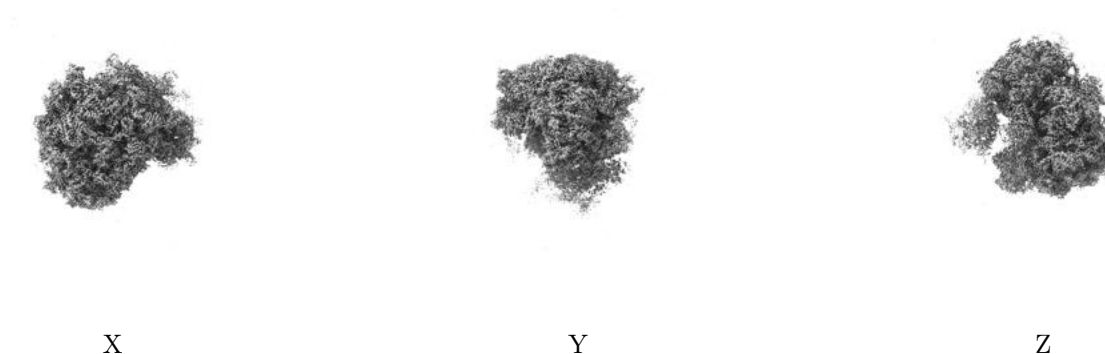


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

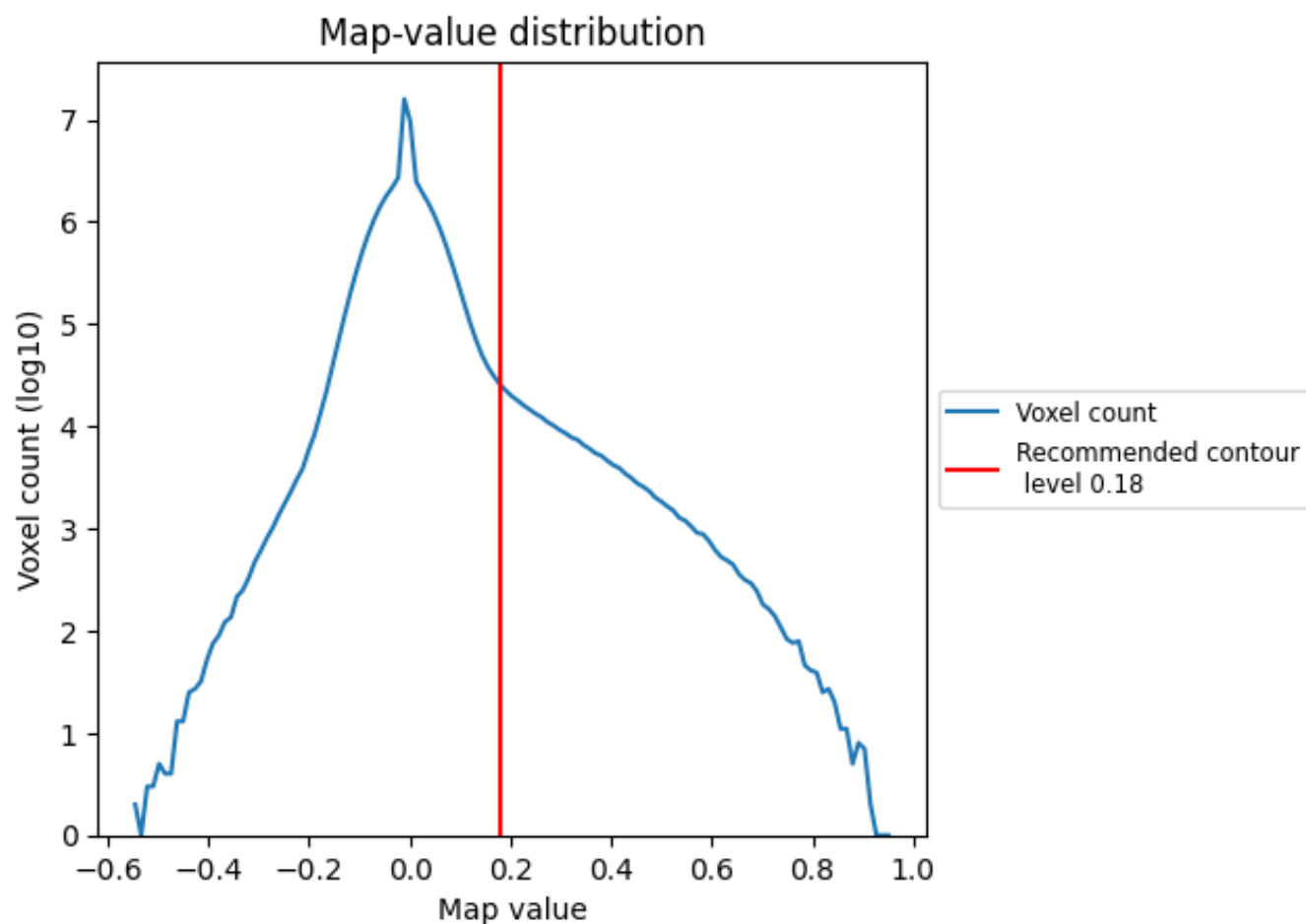
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

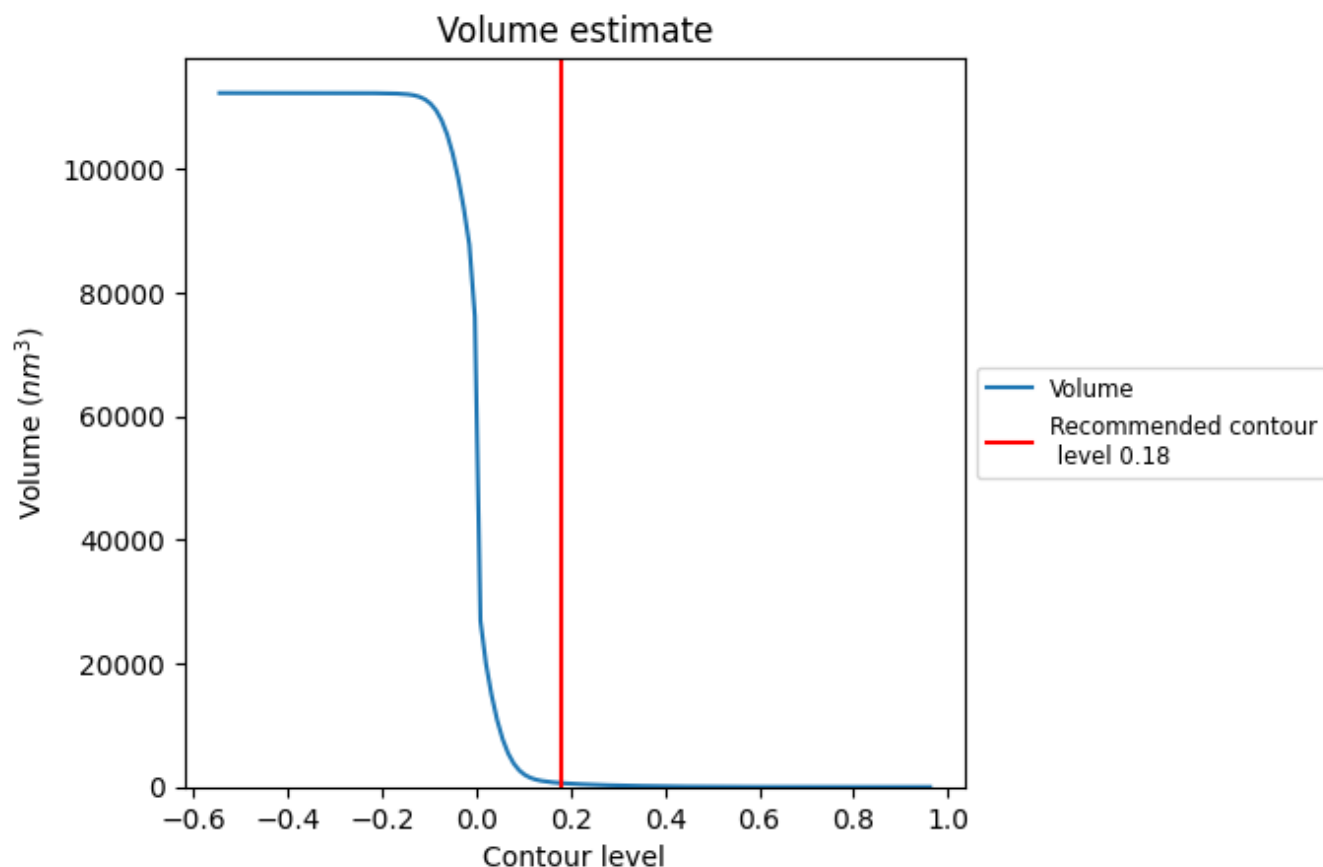
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

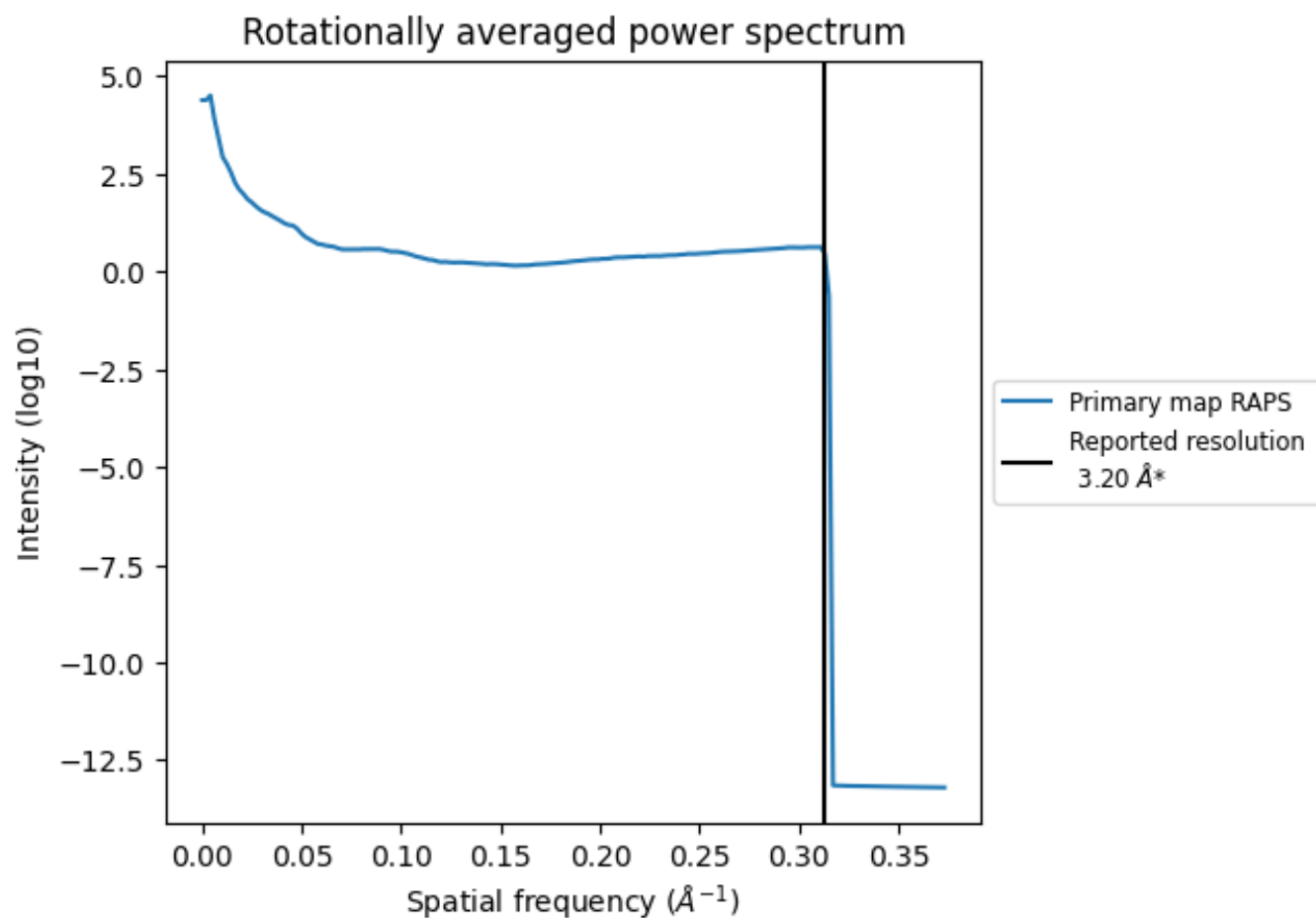
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 628 nm^3 ; this corresponds to an approximate mass of 567 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 0.312 Å⁻¹

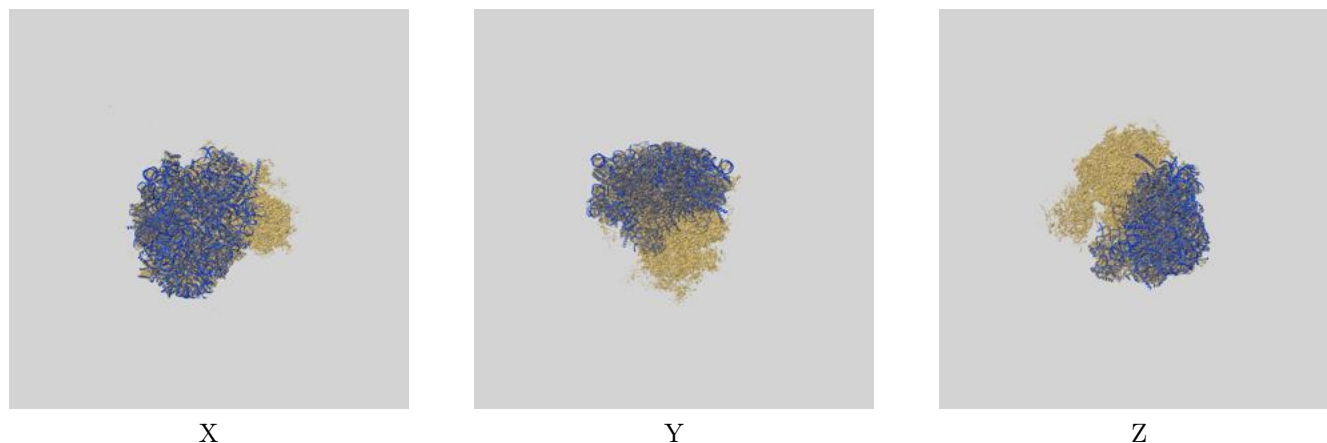
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

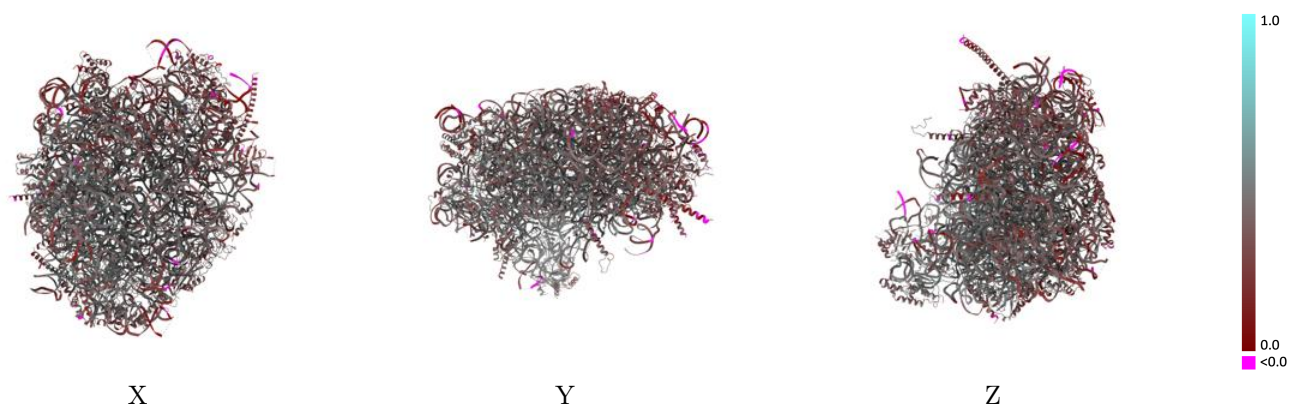
This section contains information regarding the fit between EMDB map EMD-2660 and PDB model 3J79. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



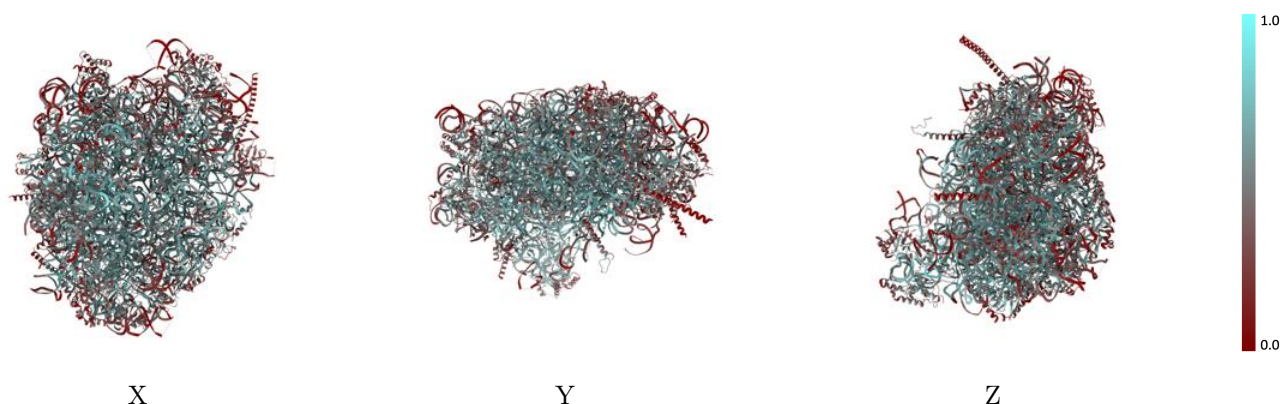
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



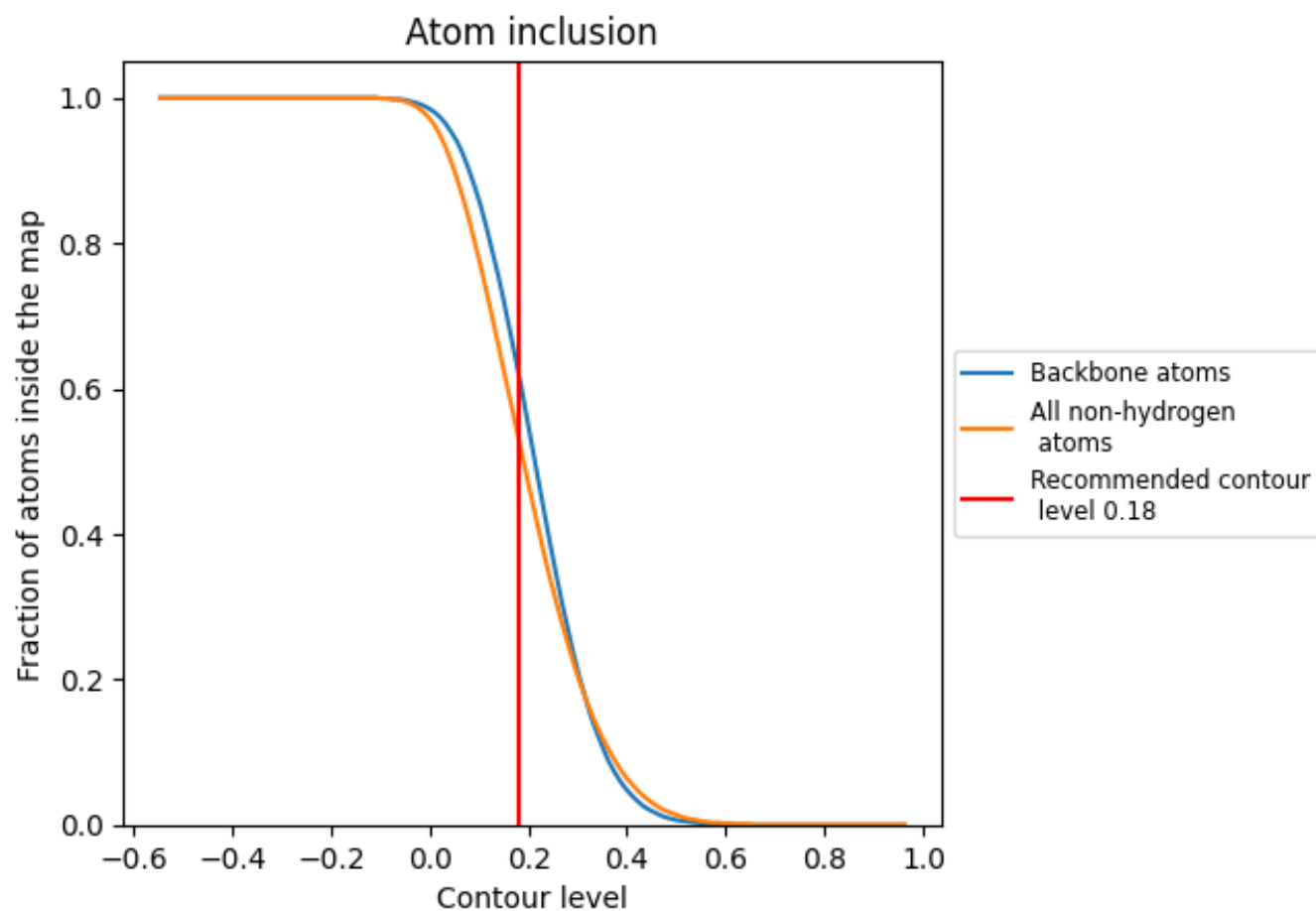
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 53% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5310	 0.4130
0	 0.4280	 0.3590
1	 0.3430	 0.3170
2	 0.4380	 0.4140
3	 0.4240	 0.3430
4	 0.3690	 0.3690
5	 0.5410	 0.4550
6	 0.3500	 0.3010
7	 0.4580	 0.3790
8	 0.5330	 0.4460
9	 0.5650	 0.4670
A	 0.5790	 0.4220
B	 0.6660	 0.4710
C	 0.5840	 0.4100
D	 0.4860	 0.4040
E	 0.4910	 0.4040
F	 0.4730	 0.4010
G	 0.3920	 0.3850
H	 0.4480	 0.4090
I	 0.4170	 0.4080
J	 0.2910	 0.3230
K	 0.5300	 0.4370
L	 0.4750	 0.4030
M	 0.4140	 0.4000
N	 0.4460	 0.4180
O	 0.5780	 0.4660
P	 0.5590	 0.4360
Q	 0.4480	 0.4290
R	 0.4300	 0.4090
S	 0.5580	 0.4590
T	 0.3720	 0.3230
U	 0.5080	 0.4560
V	 0.4810	 0.4410
W	 0.5380	 0.4150
X	 0.2250	 0.2790



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.3430	 0.3370
Z	 0.4150	 0.3610
a	 0.4240	 0.3640
b	 0.4100	 0.3850
c	 0.5340	 0.3980
d	 0.2450	 0.2470
e	 0.4630	 0.3890
f	 0.4870	 0.4140
g	 0.3750	 0.3220
h	 0.4390	 0.3710
i	 0.4780	 0.4550