



Full wwPDB EM Validation Report ⓘ

Oct 20, 2026 – 07:52 pm BST

PDB ID : 9SX5 / pdb_00009sx5
EMDB ID : EMD-55331
Title : Structural characterization of hibernating ribosomes in the Gram-negative pathogen *Enterobacter cloacae* complex
Authors : Vasanthakrishnan, R.K.B.S.; Olivier, D.; Sophie, C.; Yann, L.C.; Sylvie, G.; Sassi, M.; Emmanuel, G.; Reynald, G.
Deposited on : 2025-10-08
Resolution : 2.80 Å (reported)
Based on initial model : 8B0X

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:

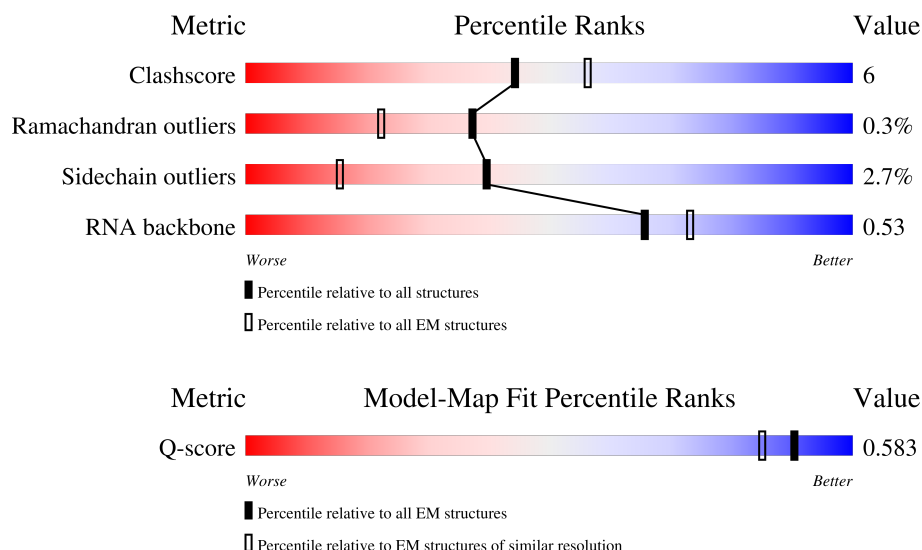
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	0	55	
2	1	46	
3	2	65	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	5	234	
7	A	1541	
8	B	241	
9	C	233	
10	D	206	
11	E	166	
12	F	131	
13	G	156	
14	H	130	
15	I	130	
16	J	103	
17	K	129	
18	L	124	
19	M	118	
20	N	101	
21	O	89	
22	P	82	
23	Q	84	
24	R	75	
25	S	92	
26	T	87	
27	V	77	
28	W	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	X	95	
30	a	2904	
31	b	116	
32	c	273	
33	d	209	
34	e	201	
35	f	179	
36	g	177	
37	h	149	
38	i	142	
39	j	123	
40	k	144	
41	l	136	
42	m	127	
43	n	117	
44	o	115	
45	p	118	
46	q	103	
47	r	110	
48	s	100	
49	t	104	
50	u	94	
51	v	85	
52	w	78	
53	x	63	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	y	59	12% 86% 12%
55	z	57	16% 75% 21%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 146853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	67	Total	C	N	O	S	0	0
			526	325	100	95	6		

- Molecule 6 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	233	Total	C	N	O	S	0	0
			1714	1069	311	328	6		

- Molecule 7 is a RNA chain called 16s rRNA (1539-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1539	Total	C	N	O	P	0	0
			33035	14741	6061	10694	1539		

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	225	Total	C	N	O	S	0	0
			1761	1110	317	326	8		

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	207	Total	C	N	O	S	0	0
			1632	1034	306	289	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	205	Total	C	N	O	S	0	0
			1645	1026	316	299	4		

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 12 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	104	Total	C	N	O	S	0	0
			845	533	152	153	7		

- Molecule 13 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	155	Total	C	N	O	S	0	0
			1228	767	238	219	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	129	Total	C	N	O	S	0	0
			978	618	171	183	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	128	Total	C	N	O	S	0	0
			1028	638	206	181	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	98	Total	C	N	O	S	0	0
			788	493	151	143	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP A0A837F5X1

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	115	Total	C	N	O	S	0	0
			895	554	178	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	100	Total	C	N	O	S	0	0
			796	493	161	139	3		

- Molecule 21 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	88	Total	C	N	O	S	0	0
			709	438	144	126	1		

- Molecule 22 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	82	Total	C	N	O	S	0	0
			640	400	127	112	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	81	Total	C	N	O	S	0	0
			658	416	123	116	3		

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	67	Total	C	N	O	S	0	0
			555	351	106	97	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	86	Total	C	N	O	S	0	0
			668	411	138	116	3		

- Molecule 27 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	V	77	Total	C	N	O	P	S	0	0
			1644	734	297	535	77	1		

- Molecule 28 is a RNA chain called Non Stop mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	W	10	Total	C	N	O	P		0	0
			219	97	41	71	10			

- Molecule 29 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	X	95	Total	C	N	O	S		0	0
			764	481	137	144	2			

- Molecule 30 is a RNA chain called 23S rRNA (2904-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
30	a	2904	Total	C	N	O	P		0	0
			62357	27823	11472	20158	2904			

- Molecule 31 is a RNA chain called 5s rRNA (120-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	b	116	Total	C	N	O	P		0	0
			2481	1105	449	811	116			

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	c	271	Total	C	N	O	S		0	0
			2079	1285	423	364	7			

- Molecule 33 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	d	209	Total	C	N	O	S		0	0
			1568	982	288	295	3			

- Molecule 34 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 35 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	178	Total	C	N	O	S	0	0
			1417	901	251	259	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	176	Total	C	N	O	S	0	0
			1317	833	241	241	2		

- Molecule 37 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	149	Total	C	N	O	S	0	0
			1102	693	197	211	1		

- Molecule 38 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	142	Total	C	N	O	S	0	0
			1130	713	211	201	5		

- Molecule 39 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	123	Total	C	N	O	S	0	0
			947	594	181	166	6		

- Molecule 40 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	144	Total	C	N	O	S	0	0
			1051	651	207	191	2		

- Molecule 41 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	136	Total	C	N	O	S	0	0
			1074	685	204	179	6		

- Molecule 42 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 43 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	116	Total	C	N	O		0	0
			890	550	178	162			

- Molecule 44 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 45 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 46 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	103	Total	C	N	O	S	0	0
			815	515	153	145	2		

- Molecule 47 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	110	Total	C	N	O	S	0	0
			855	530	166	156	3		

- Molecule 48 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	93	Total	C	N	O	S	0	0
			739	467	139	131	2		

- Molecule 49 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	103	Total	C	N	O	S	0	0
			788	498	148	142			

- Molecule 50 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	94	Total	C	N	O	S	0	0
			746	476	135	133	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	78	Total	C	N	O	S	0	0
			592	364	119	108	1		

- Molecule 52 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	77	Total	C	N	O	S	0	0
			626	388	129	107	2		

- Molecule 53 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	62	Total	C	N	O	S	0	0
			499	308	99	91	1		

- Molecule 54 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	58	Total	C	N	O	S	0	0
			453	285	87	79	2		

- Molecule 55 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	55	Total	C	N	O	S	0	0
			435	264	92	78	1		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	95	Total	Mg	0
			95	95	
57	a	252	Total	Mg	0
			252	252	
57	b	5	Total	Mg	0
			5	5	
57	c	2	Total	Mg	0
			2	2	
57	p	2	Total	Mg	0
			2	2	
57	z	1	Total	Mg	0
			1	1	

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	A	45	Total	K	0
			45	45	
58	a	107	Total	K	0
			107	107	
58	b	1	Total	K	0
			1	1	
58	c	5	Total	K	0
			5	5	
58	d	1	Total	K	0
			1	1	
58	e	2	Total	K	0
			2	2	

Continued on next page...

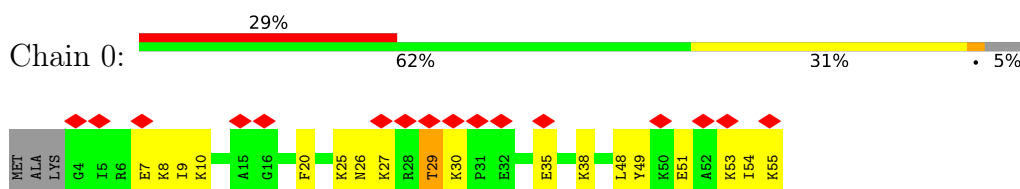
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	f	1	Total	K	0
			1	1	

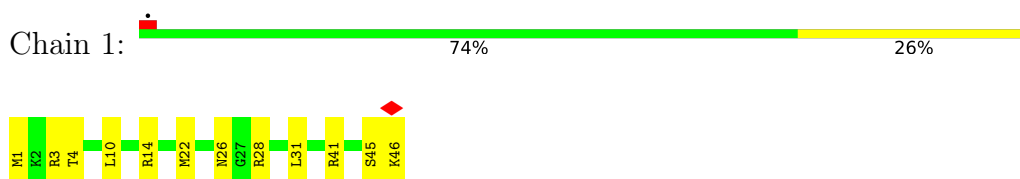
3 Residue-property plots

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.

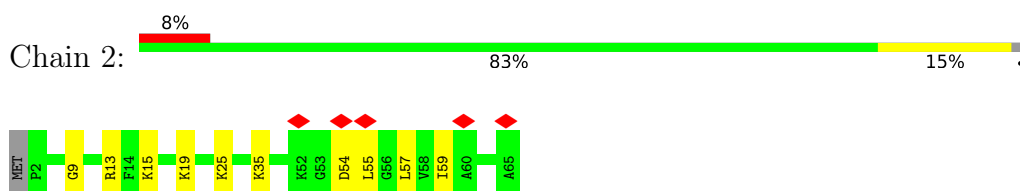
- Molecule 1: Large ribosomal subunit protein bL33



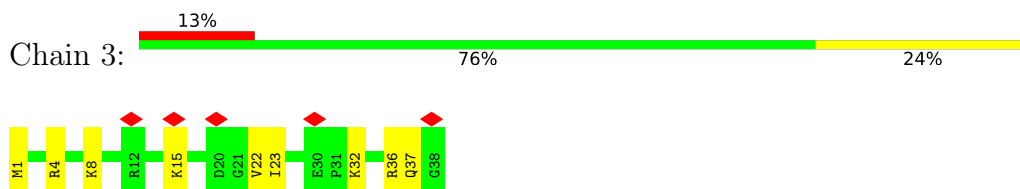
- Molecule 2: Large ribosomal subunit protein bL34



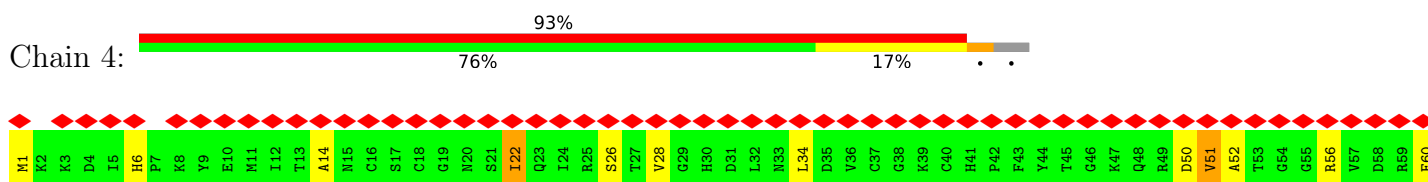
- Molecule 3: Large ribosomal subunit protein bL35

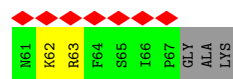


- Molecule 4: Large ribosomal subunit protein bL36

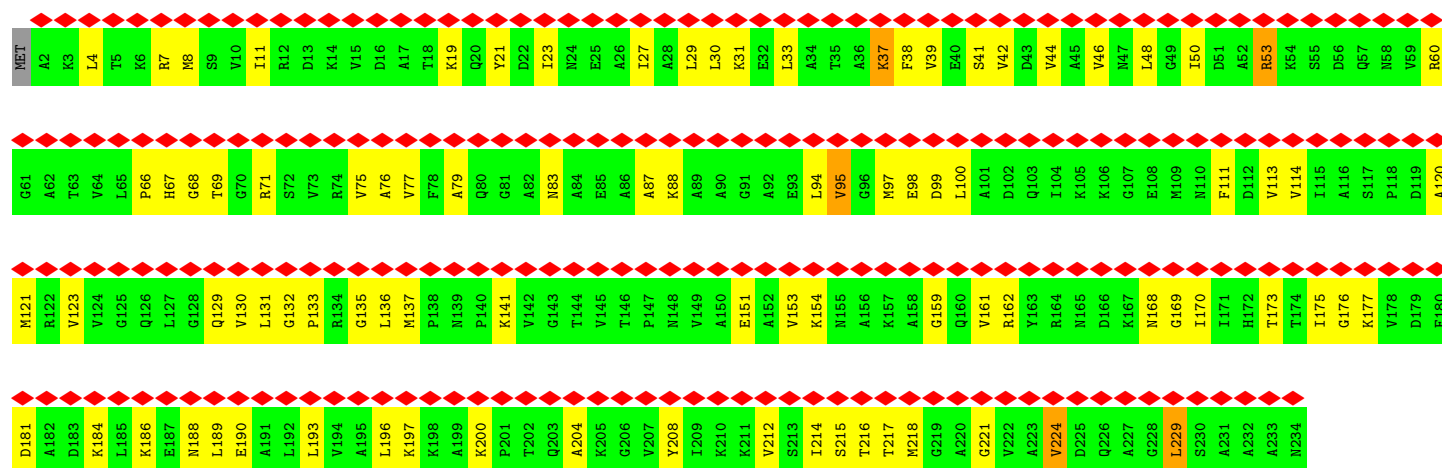


- Molecule 5: Large ribosomal subunit protein bL31

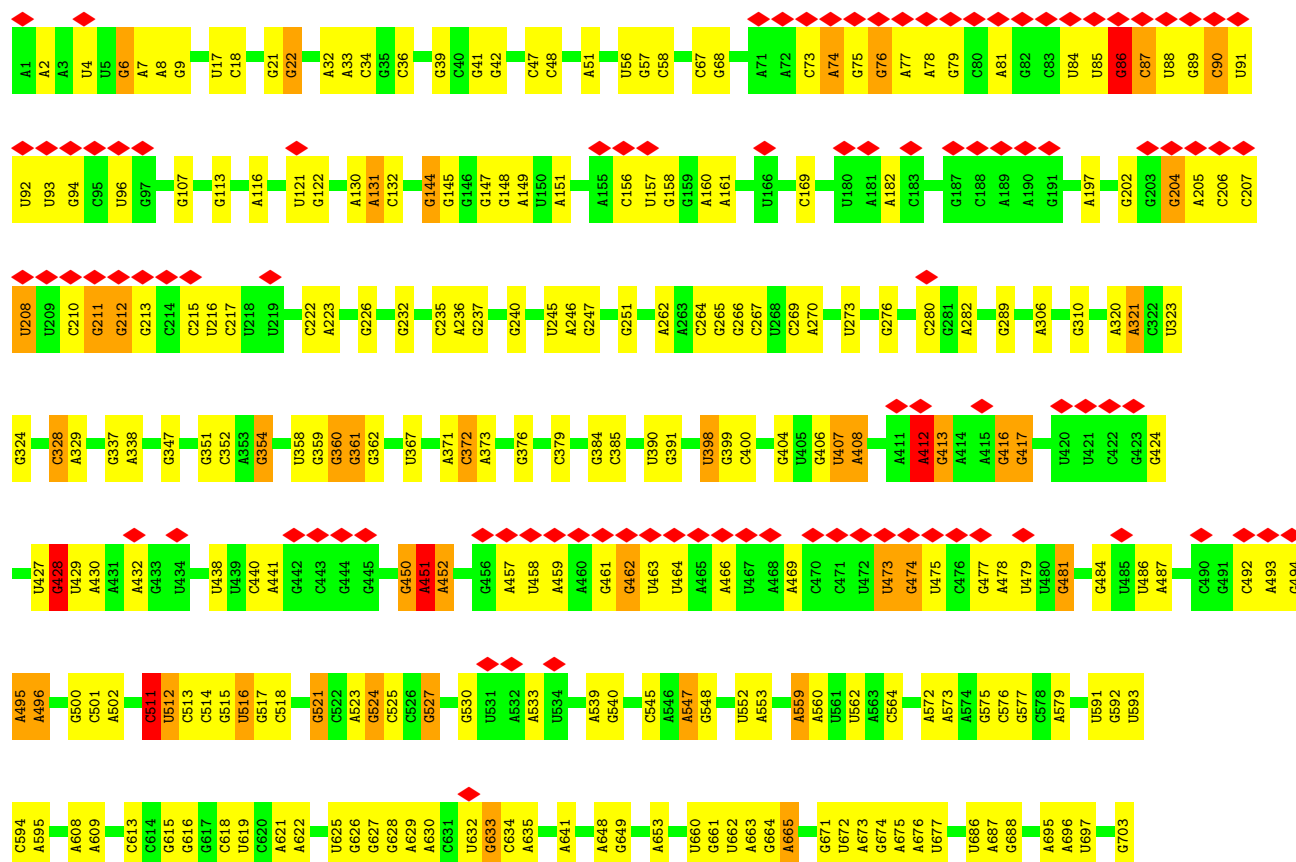


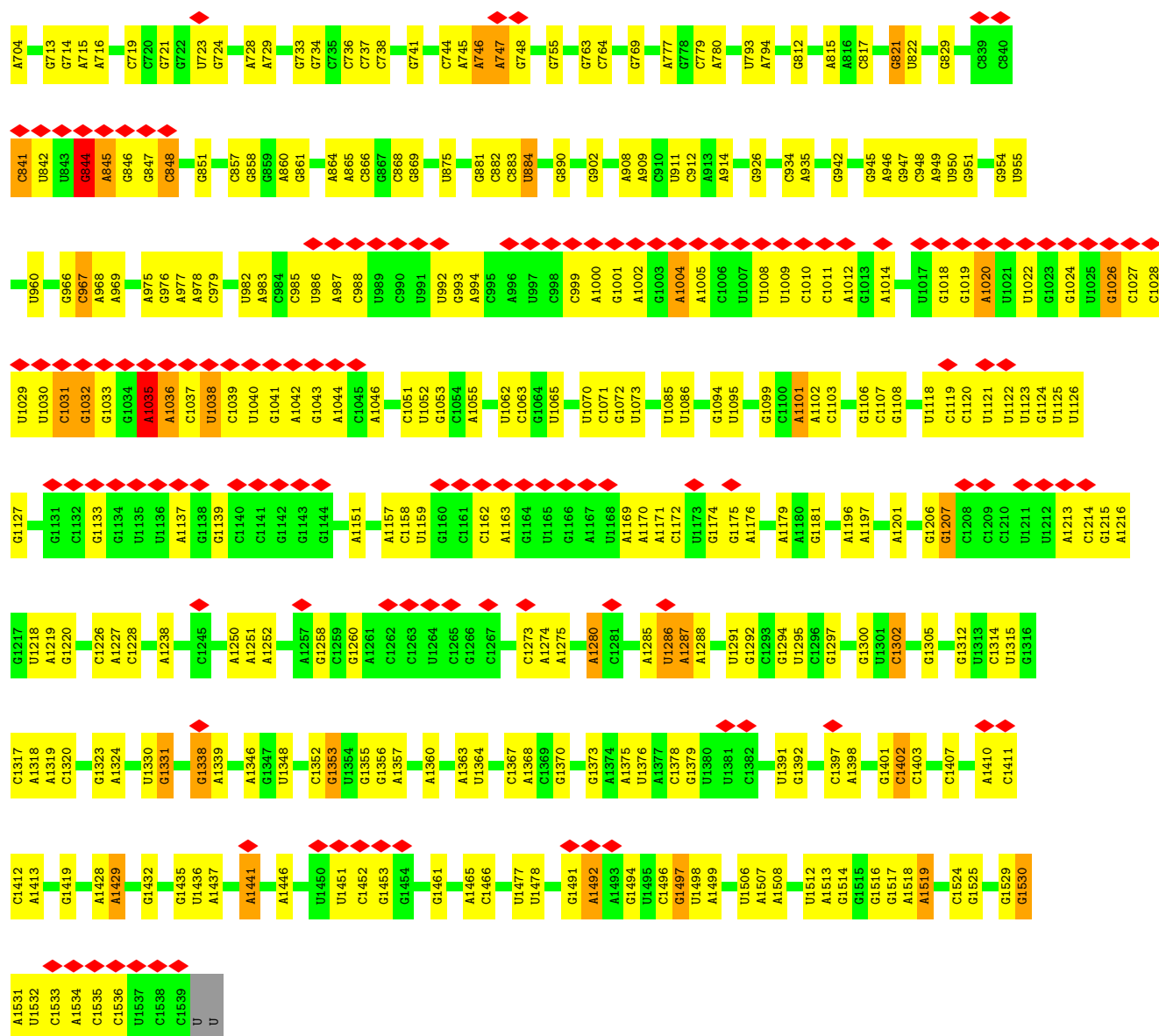


• Molecule 6: Large ribosomal subunit protein uL1

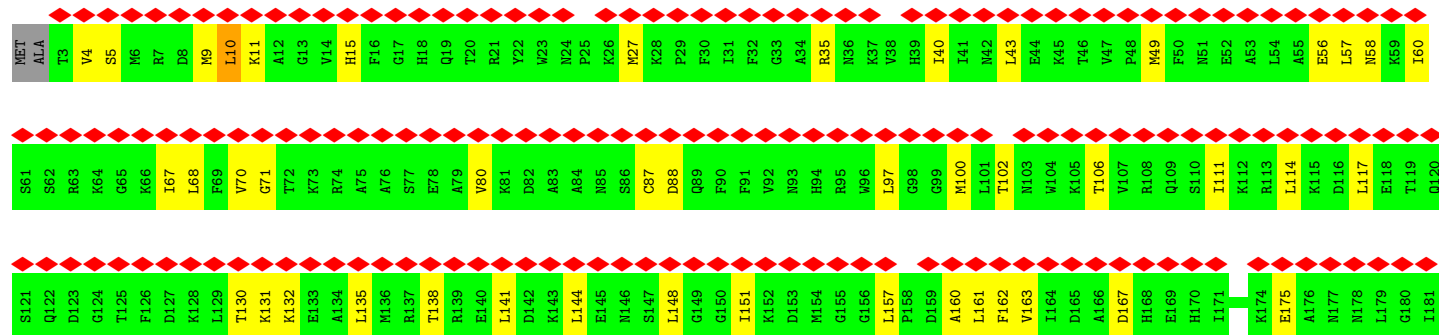
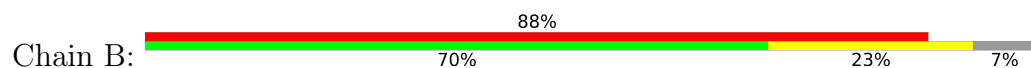


• Molecule 7: 16S rRNA (1539-MER)



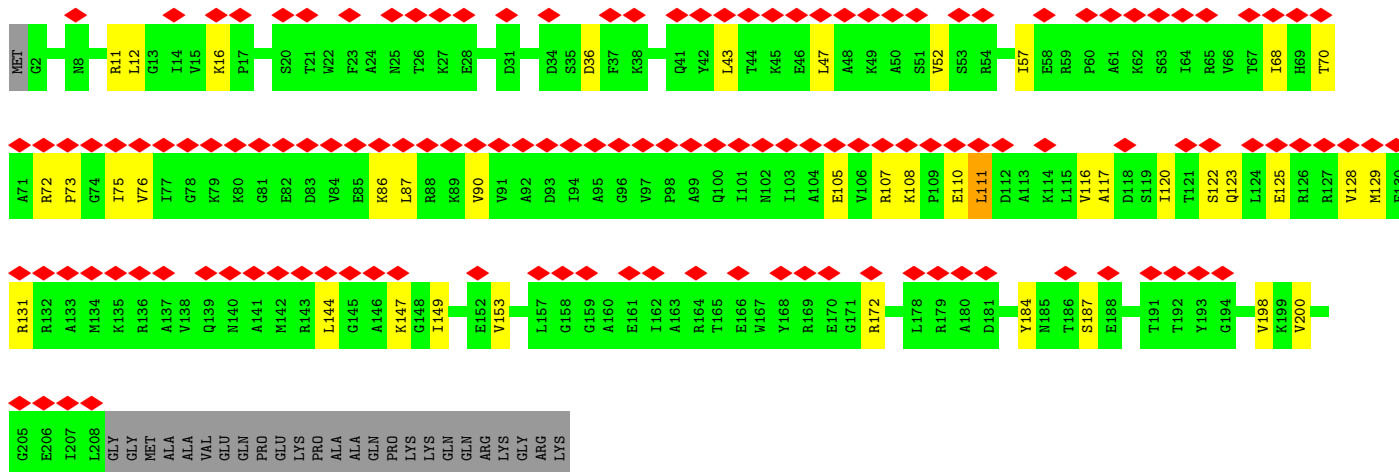
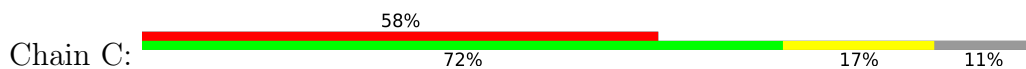


• Molecule 8: Small ribosomal subunit protein uS2

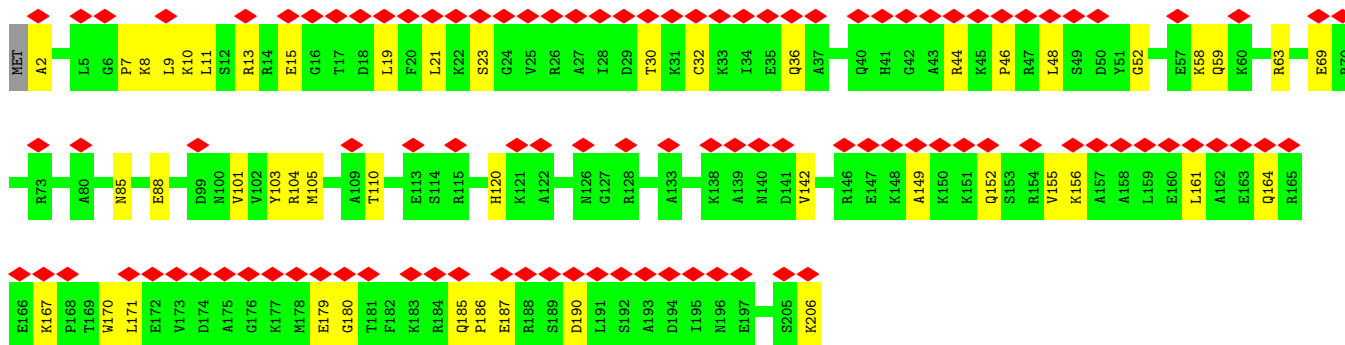
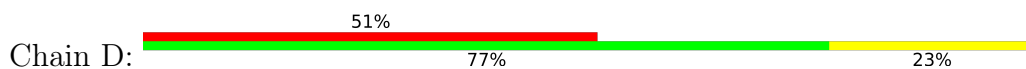




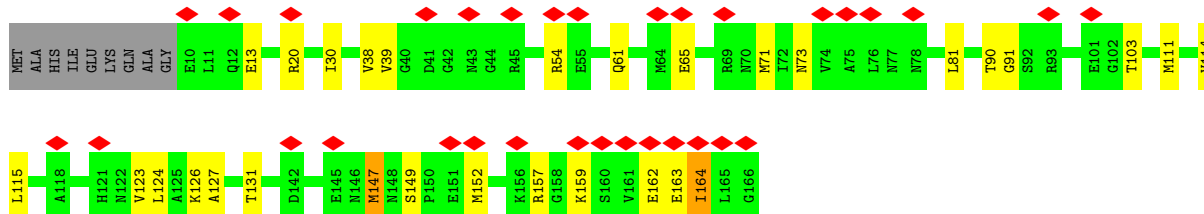
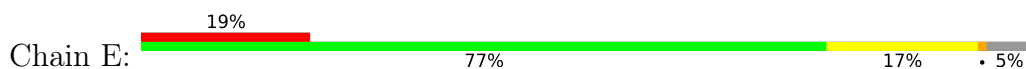
• Molecule 9: Small ribosomal subunit protein uS3



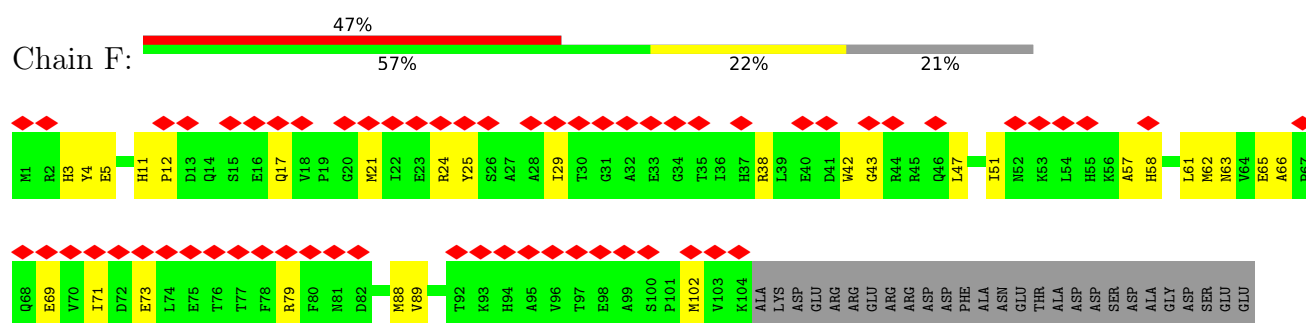
• Molecule 10: Small ribosomal subunit protein uS4



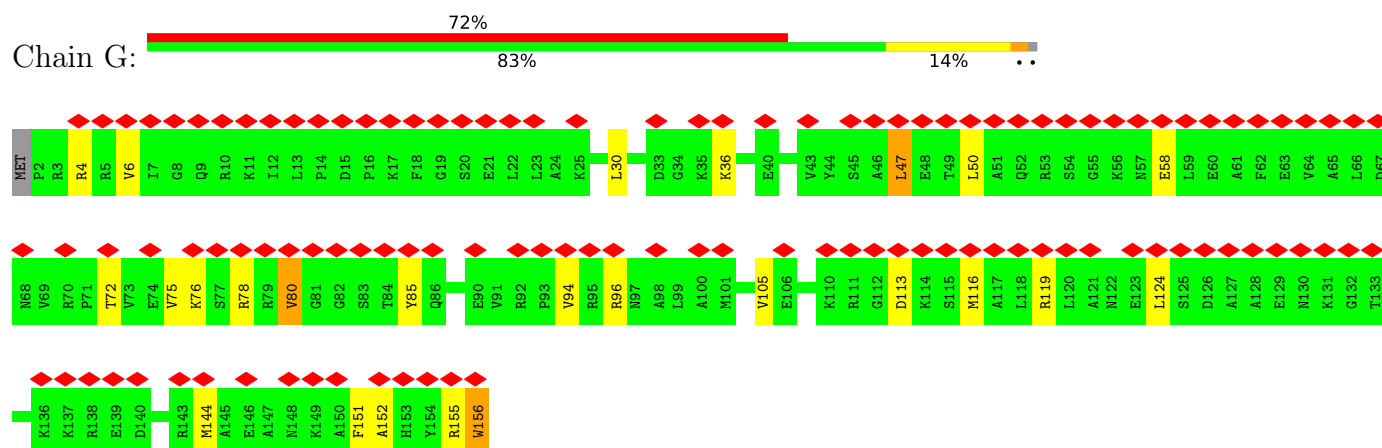
• Molecule 11: Small ribosomal subunit protein uS5



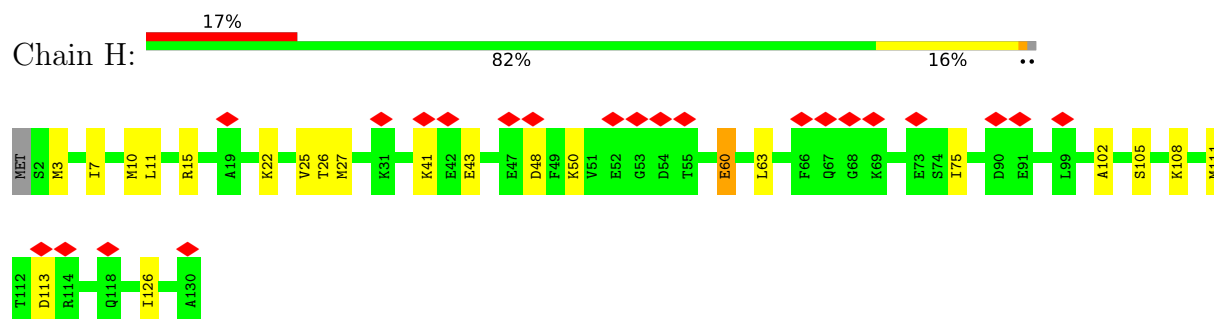
• Molecule 12: Small ribosomal subunit protein bS6



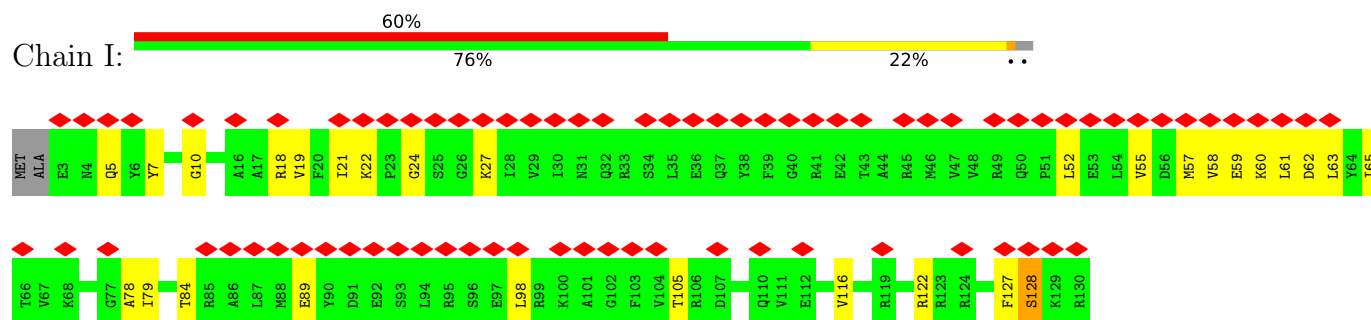
- Molecule 13: Small ribosomal subunit protein uS7



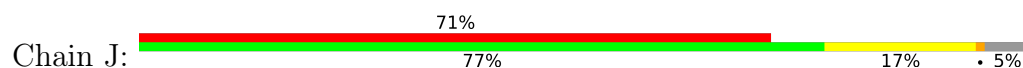
- Molecule 14: Small ribosomal subunit protein uS8

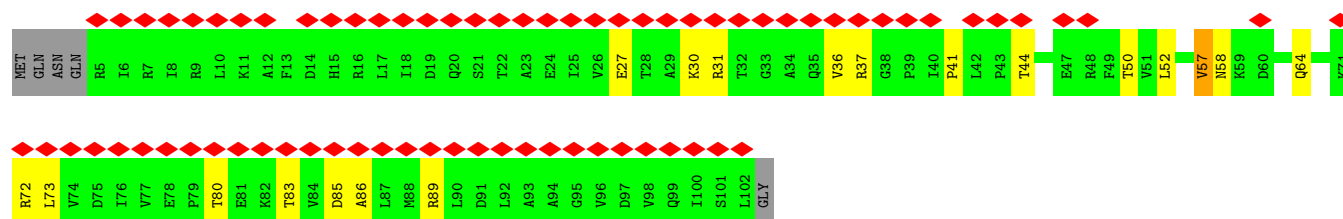


- Molecule 15: Small ribosomal subunit protein uS9

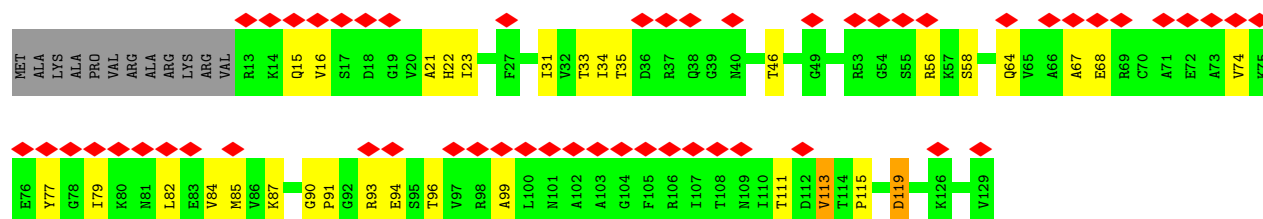
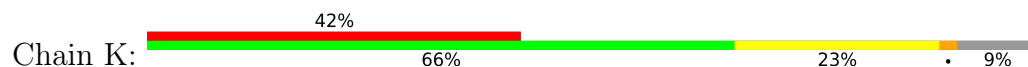


- Molecule 16: Small ribosomal subunit protein uS10

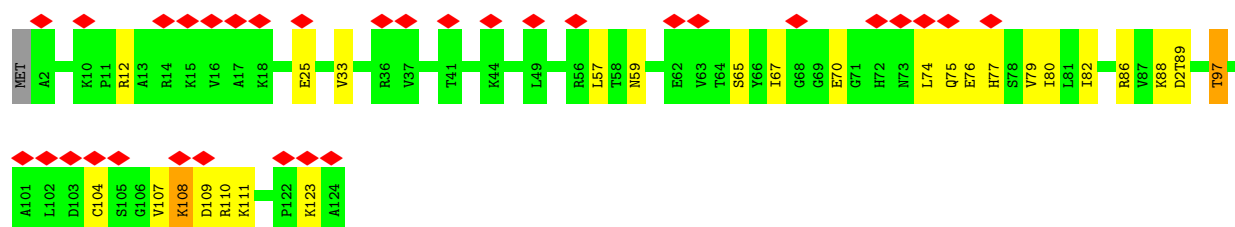
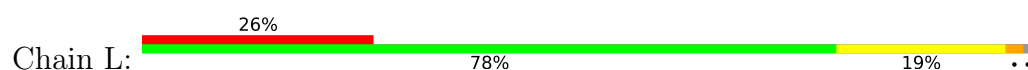




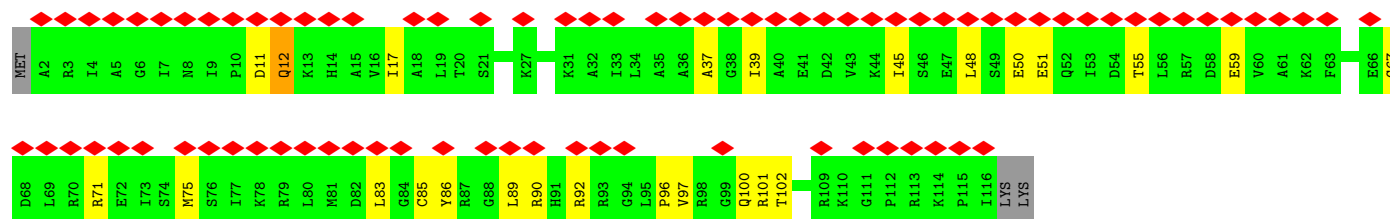
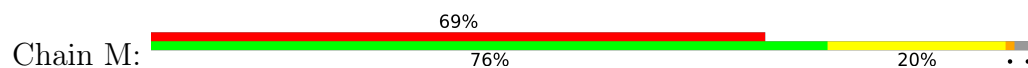
• Molecule 17: Small ribosomal subunit protein uS11



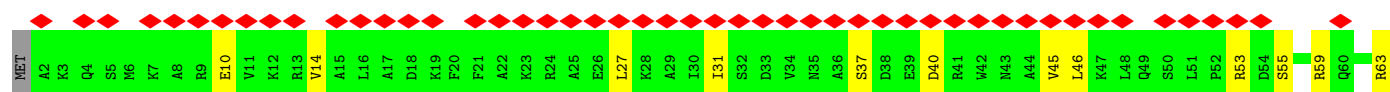
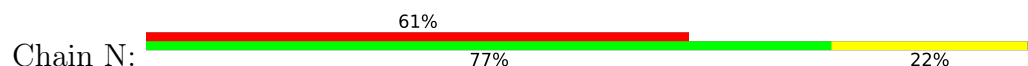
• Molecule 18: Small ribosomal subunit protein uS12

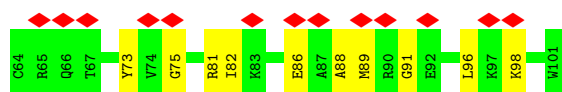


• Molecule 19: Small ribosomal subunit protein uS13

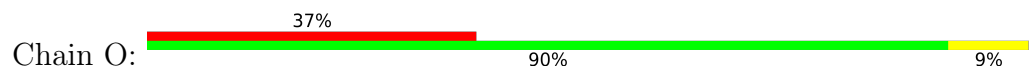


• Molecule 20: Small ribosomal subunit protein uS14

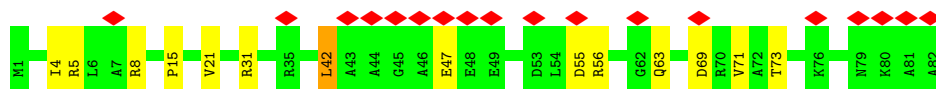
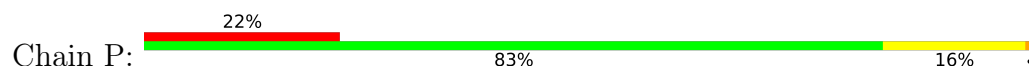




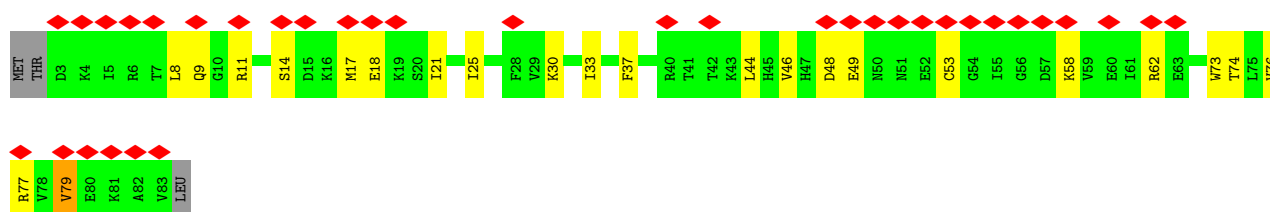
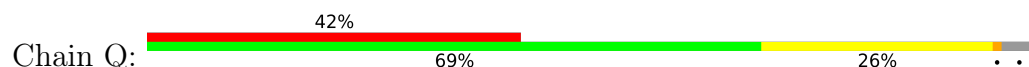
- Molecule 21: Small ribosomal subunit protein uS15



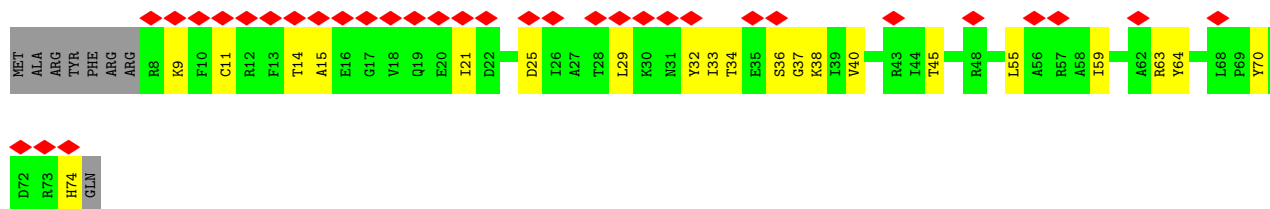
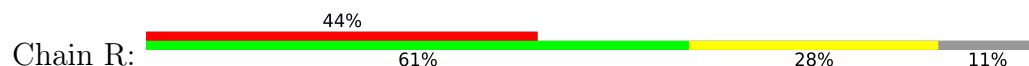
- Molecule 22: Small ribosomal subunit protein bS16



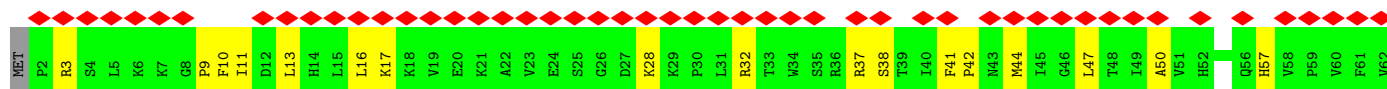
- Molecule 23: Small ribosomal subunit protein uS17

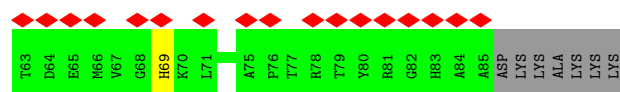


- Molecule 24: Small ribosomal subunit protein bS18

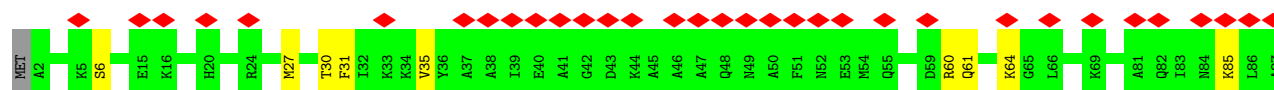
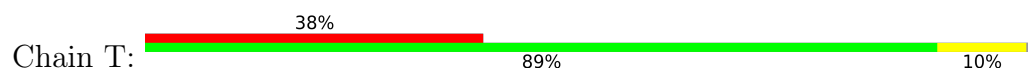


- Molecule 25: Small ribosomal subunit protein uS19





- Molecule 26: Small ribosomal subunit protein bS20



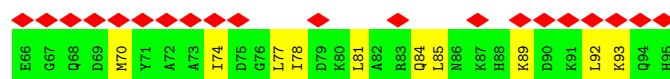
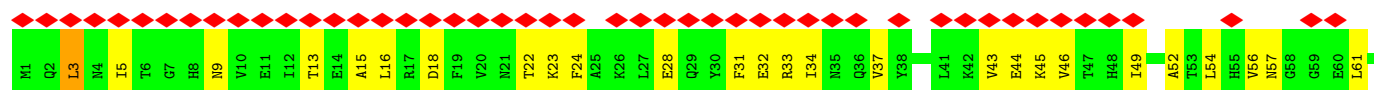
- Molecule 27: tRNA



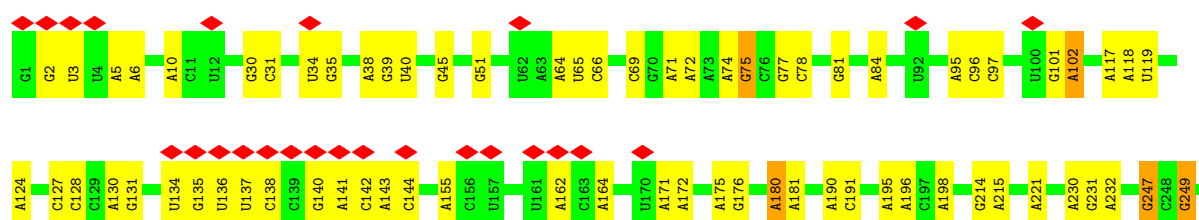
- Molecule 28: Non Stop mRNA



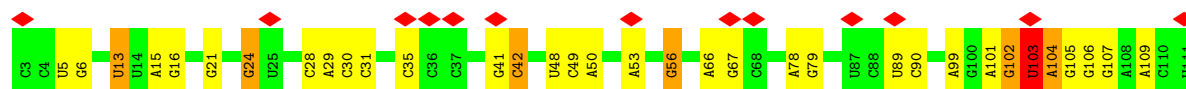
- Molecule 29: Ribosome hibernation promoting factor



- Molecule 30: 23S rRNA (2904-MER)

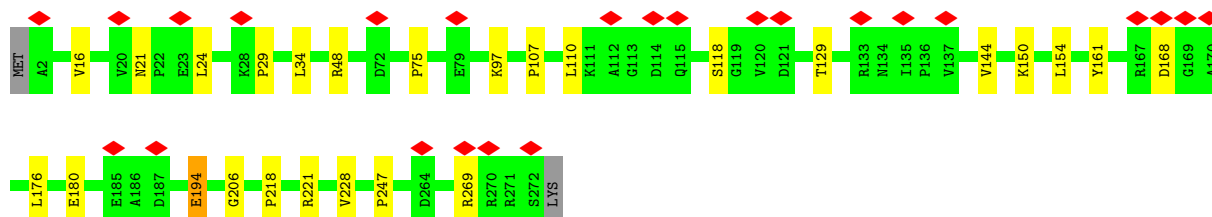




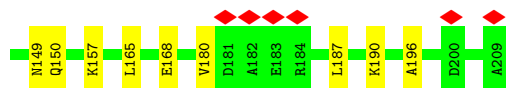
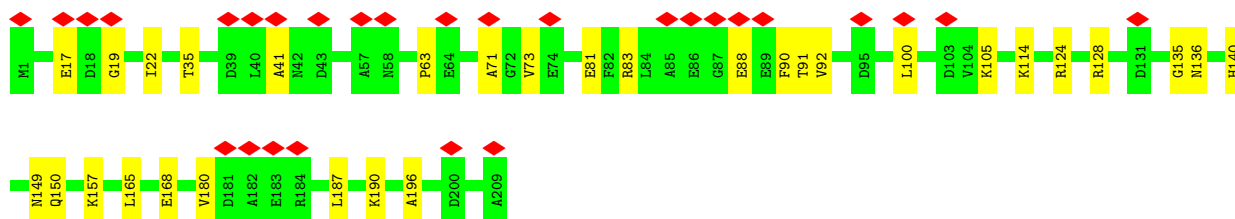
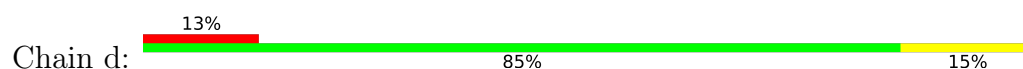




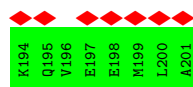
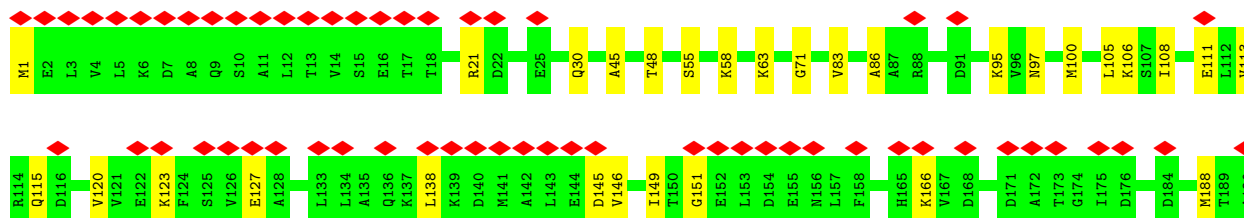
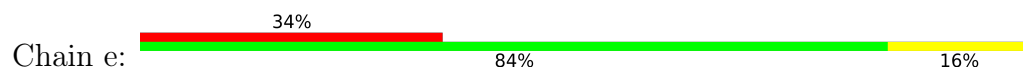
- Molecule 32: Large ribosomal subunit protein uL2



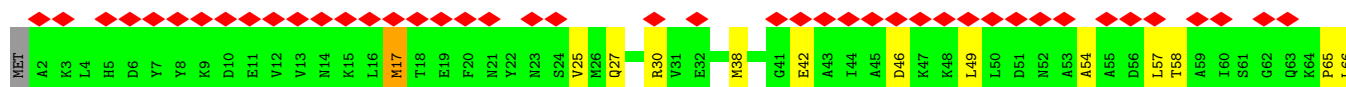
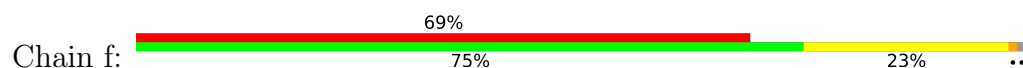
- Molecule 33: Large ribosomal subunit protein uL3

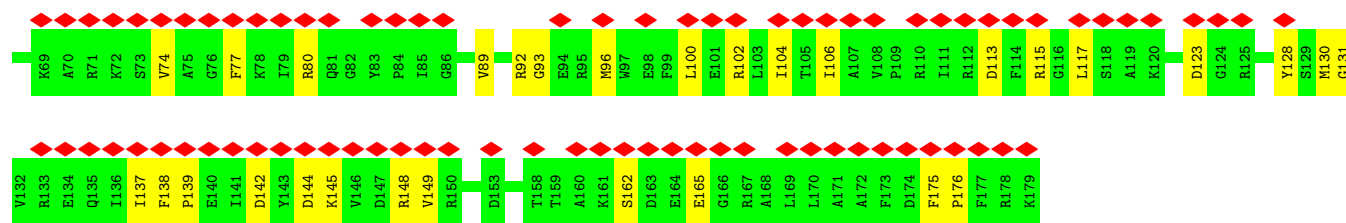


- Molecule 34: Large ribosomal subunit protein uL4

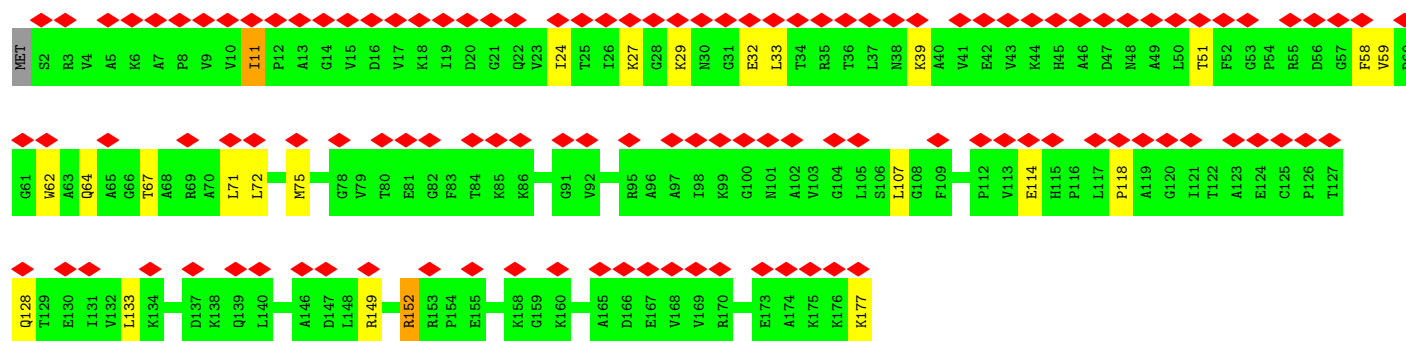
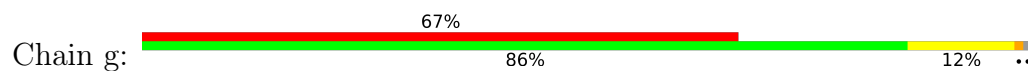


- Molecule 35: Large ribosomal subunit protein uL5

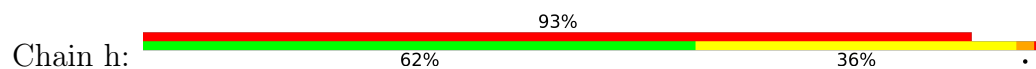




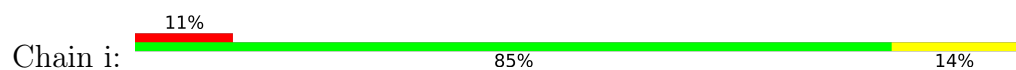
• Molecule 36: Large ribosomal subunit protein uL6



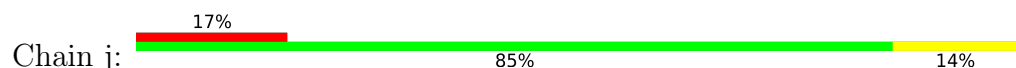
• Molecule 37: Large ribosomal subunit protein bL9

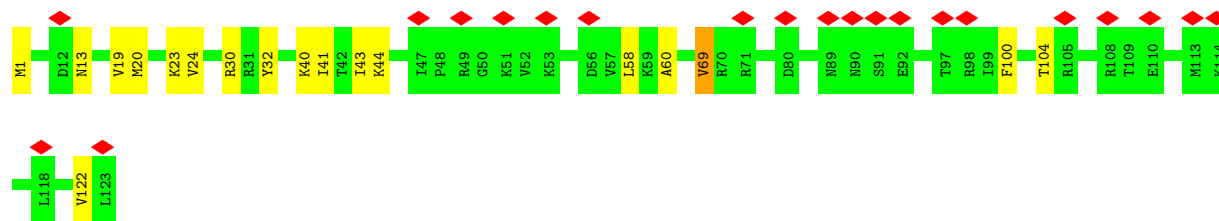


• Molecule 38: Large ribosomal subunit protein uL13

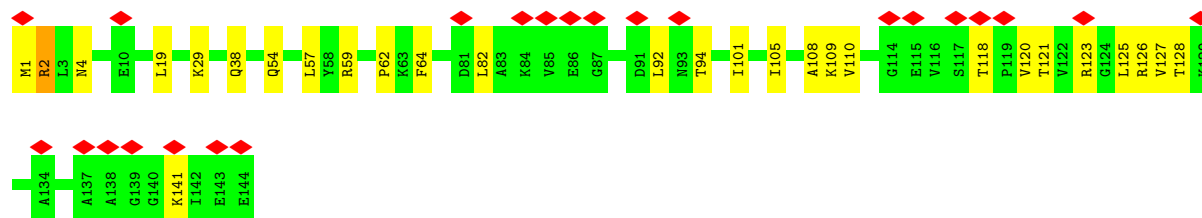
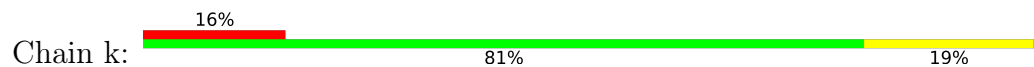


• Molecule 39: Large ribosomal subunit protein uL14

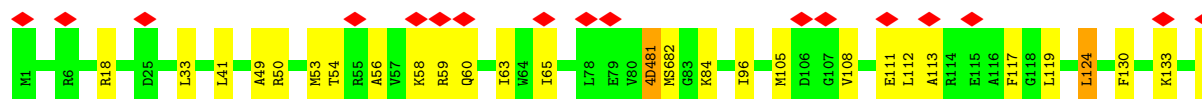
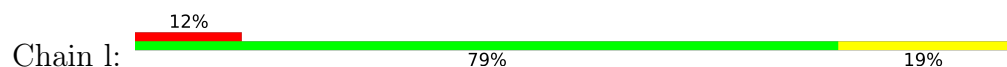




- Molecule 40: Large ribosomal subunit protein uL15



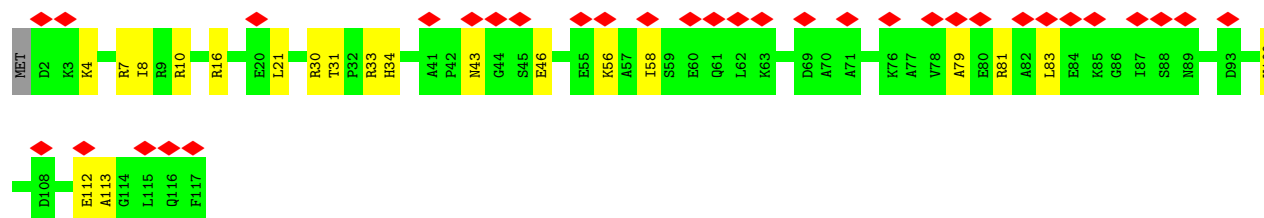
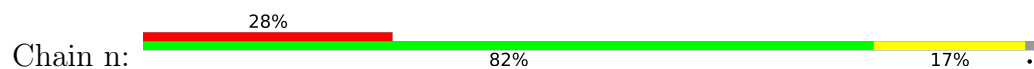
- Molecule 41: Large ribosomal subunit protein uL16



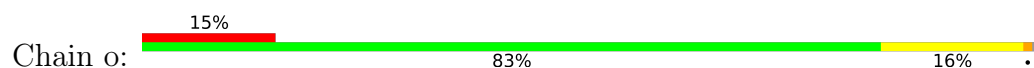
- Molecule 42: Large ribosomal subunit protein bL17

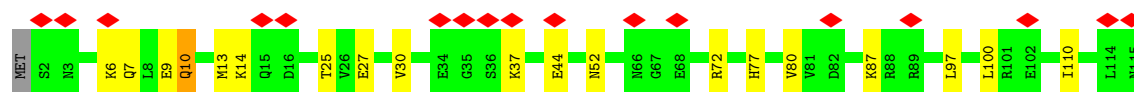


- Molecule 43: Large ribosomal subunit protein uL18

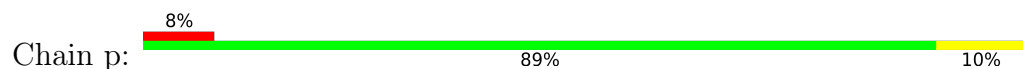


- Molecule 44: Large ribosomal subunit protein bL19

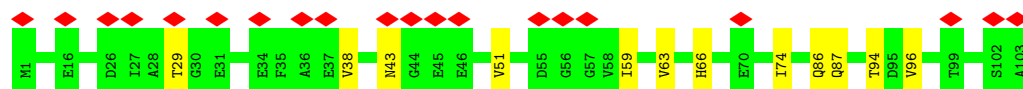
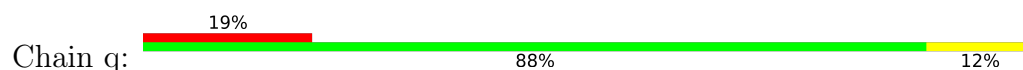




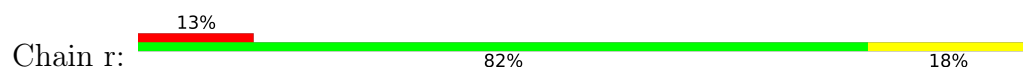
- Molecule 45: Large ribosomal subunit protein bL20



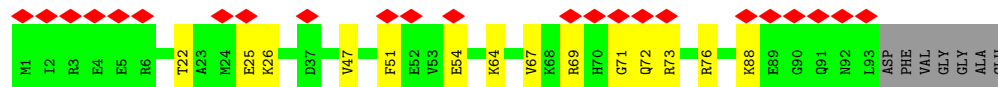
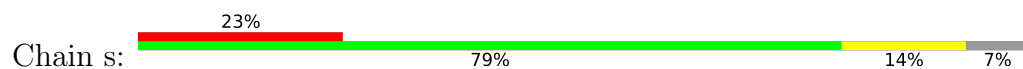
- Molecule 46: Large ribosomal subunit protein bL21



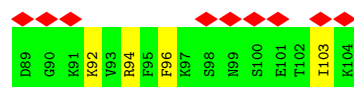
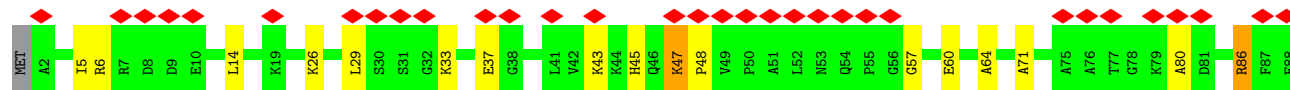
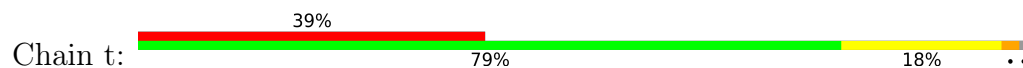
- Molecule 47: Large ribosomal subunit protein uL22



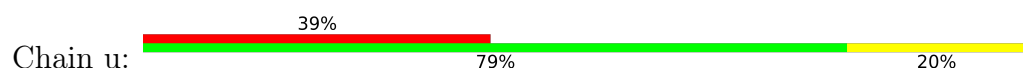
- Molecule 48: Large ribosomal subunit protein uL23

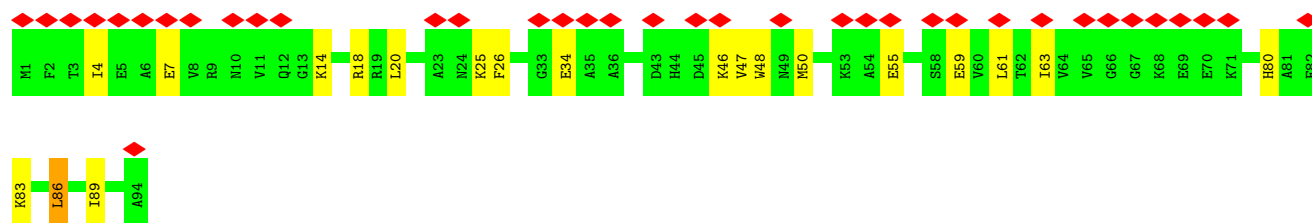


- Molecule 49: Large ribosomal subunit protein uL24

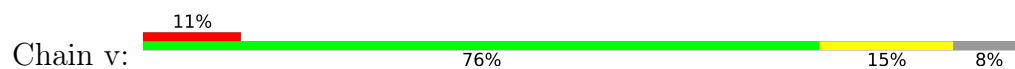


- Molecule 50: Large ribosomal subunit protein bL25

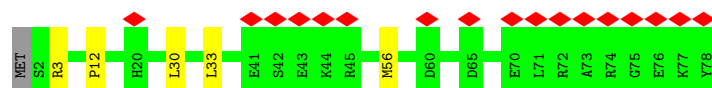
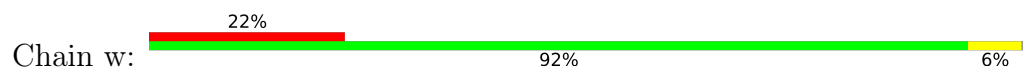




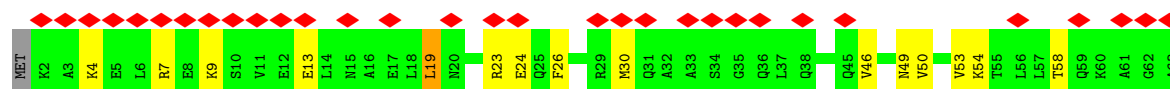
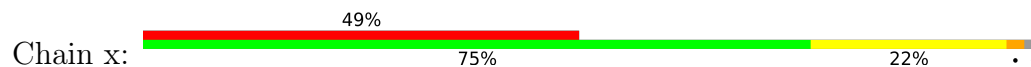
- Molecule 51: Large ribosomal subunit protein bL27



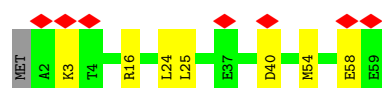
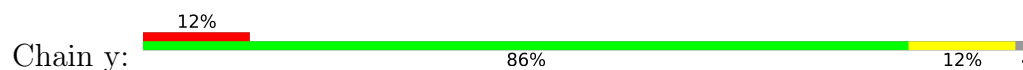
- Molecule 52: Large ribosomal subunit protein bL28



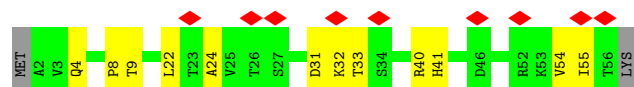
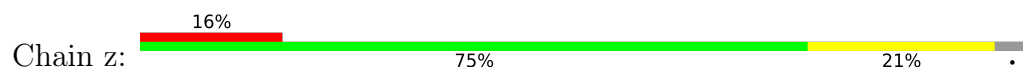
- Molecule 53: Large ribosomal subunit protein uL29



- Molecule 54: Large ribosomal subunit protein uL30



- Molecule 55: Large ribosomal subunit protein bL32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87433	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.484	Depositor
Minimum map value	-1.049	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: D2T, OMC, 5MU, 2MG, K, 4D4, 4SU, ZN, 6MZ, MS6, 3TD, H2U, 5MC, MA6, 1MG, OMU, OMG, PSU, MEQ, G7M, 4OC, MG, 2MA, UR3, IAS

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	0	0.27	0/433	0.34	0/576
2	1	0.30	0/380	0.35	0/498
3	2	0.29	0/513	0.33	0/676
4	3	0.30	0/303	0.34	0/397
5	4	0.18	0/536	0.45	0/718
6	5	0.17	0/1729	0.37	1/2331 (0.0%)
7	A	0.61	0/36710	0.76	11/57263 (0.0%)
8	B	0.18	0/1792	0.36	0/2414
9	C	0.21	0/1659	0.31	0/2236
10	D	0.22	0/1666	0.31	0/2227
11	E	0.27	0/1169	0.39	0/1573
12	F	0.22	0/864	0.39	0/1168
13	G	0.20	0/1246	0.32	0/1673
14	H	0.26	0/988	0.34	0/1325
15	I	0.21	0/1040	0.40	0/1384
16	J	0.21	0/798	0.38	0/1078
17	K	0.23	0/884	0.37	0/1191
18	L	0.26	0/960	0.39	0/1286
19	M	0.22	0/903	0.35	0/1208
20	N	0.19	0/808	0.27	0/1076
21	O	0.23	0/717	0.30	0/955
22	P	0.26	0/650	0.36	0/876
23	Q	0.23	0/667	0.37	0/893
24	R	0.23	0/564	0.41	0/756
25	S	0.19	0/685	0.32	0/922
26	T	0.23	0/674	0.31	0/894
27	V	0.34	1/1724 (0.1%)	0.86	0/2687
28	W	0.34	0/245	0.80	0/381
29	X	0.23	0/775	0.41	0/1041
30	a	0.72	0/69263	0.78	6/108053 (0.0%)
31	b	0.60	0/2773	0.75	1/4323 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.32	0/2117	0.38	0/2845
33	d	0.33	0/1578	0.45	1/2123 (0.0%)
34	e	0.27	0/1571	0.32	0/2113
35	f	0.20	0/1440	0.35	0/1935
36	g	0.26	0/1338	0.46	0/1807
37	h	0.19	0/1113	0.47	1/1504 (0.1%)
38	i	0.33	0/1153	0.41	1/1552 (0.1%)
39	j	0.30	0/956	0.37	0/1281
40	k	0.33	0/1060	0.47	0/1411
41	l	0.28	0/1072	0.31	0/1434
42	m	0.30	0/973	0.39	0/1301
43	n	0.23	0/900	0.35	0/1206
44	o	0.28	0/929	0.33	0/1242
45	p	0.36	0/960	0.43	0/1278
46	q	0.29	0/828	0.40	0/1105
47	r	0.29	0/862	0.37	0/1154
48	s	0.26	0/745	0.34	0/996
49	t	0.31	0/796	0.50	0/1062
50	u	0.25	0/760	0.36	0/1022
51	v	0.30	0/599	0.35	0/795
52	w	0.30	0/636	0.36	0/849
53	x	0.21	0/500	0.32	0/665
54	y	0.27	0/458	0.37	0/613
55	z	0.28	0/441	0.32	0/589
All	All	0.58	1/157903 (0.0%)	0.69	22/235961 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	5	0	1
36	g	0	2
40	k	0	1
41	l	0	1
49	t	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	V	8	4SU	O3'-P	5.03	1.61	1.56

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	412	A	O4'-C1'-N9	7.86	114.49	108.20
30	a	511	G	O4'-C1'-N9	7.73	114.39	108.20
6	5	53	ARG	CG-CD-NE	-6.99	96.62	112.00
30	a	1310	U	C2-N1-C1'	6.95	126.05	117.70
7	A	511	C	N1-C2-O2	6.37	122.72	118.90
7	A	511	C	C2-N1-C1'	6.24	125.67	118.80
7	A	86	G	O4'-C1'-N9	-5.92	103.46	108.20
7	A	1035	A	P-O3'-C3'	5.88	126.76	119.70
30	a	2118	A	O4'-C1'-N9	-5.86	103.51	108.20
31	b	103	U	O4'-C1'-N1	5.81	112.84	108.20
7	A	428	G	P-O3'-C3'	5.80	126.66	119.70
30	a	1298	A	O5'-C5'-C4'	5.61	113.89	109.40
33	d	41	ALA	N-CA-C	-5.59	108.25	114.62
7	A	844	G	C5-C6-O6	-5.53	125.28	128.60
7	A	1158	C	C2-N1-C1'	5.41	124.75	118.80
30	a	2849	G	O4'-C1'-N9	5.36	112.48	108.20
7	A	511	C	N3-C2-O2	-5.24	118.23	121.90
7	A	547	A	P-O3'-C3'	5.24	125.99	119.70
7	A	451	A	O5'-C5'-C4'	5.23	113.58	109.40
37	h	54	LEU	CA-CB-CG	5.07	134.05	116.30
38	i	108	MET	N-CA-C	-5.07	107.15	113.38
30	a	1310	U	N1-C2-O2	5.03	126.32	122.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	53	ARG	Sidechain
36	g	149	ARG	Sidechain
36	g	152	ARG	Sidechain
40	k	2	ARG	Sidechain
41	l	81	4D4	Mainchain
49	t	86	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	426	0	464	10	0
2	1	377	0	418	10	0
3	2	504	0	572	9	0
4	3	302	0	340	8	0
5	4	526	0	522	13	0
6	5	1714	0	1796	74	0
7	A	33035	0	16641	330	0
8	B	1761	0	1780	35	0
9	C	1632	0	1707	23	0
10	D	1645	0	1708	33	0
11	E	1156	0	1199	21	0
12	F	845	0	838	20	0
13	G	1228	0	1276	18	0
14	H	978	0	1035	14	0
15	I	1028	0	1075	21	0
16	J	788	0	830	18	0
17	K	877	0	883	16	0
18	L	957	0	1017	16	0
19	M	895	0	956	22	0
20	N	796	0	830	16	0
21	O	709	0	738	5	0
22	P	640	0	655	11	0
23	Q	658	0	699	14	0
24	R	555	0	578	16	0
25	S	668	0	693	15	0
26	T	668	0	710	5	0
27	V	1644	0	842	29	0
28	W	219	0	108	5	0
29	X	764	0	770	27	0
30	a	62357	0	31372	509	0
31	b	2481	0	1256	24	0
32	c	2079	0	2148	24	0
33	d	1568	0	1619	17	0
34	e	1552	0	1619	19	0
35	f	1417	0	1454	28	0
36	g	1317	0	1376	15	0
37	h	1102	0	1139	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	i	1130	0	1155	12	0
39	j	947	0	1025	13	0
40	k	1051	0	1120	19	0
41	l	1074	0	1137	17	0
42	m	960	0	1000	13	0
43	n	890	0	922	14	0
44	o	917	0	962	9	0
45	p	947	0	1019	9	0
46	q	815	0	837	9	0
47	r	855	0	915	15	0
48	s	739	0	809	6	0
49	t	788	0	843	14	0
50	u	746	0	765	10	0
51	v	592	0	605	7	0
52	w	626	0	652	3	0
53	x	499	0	536	9	0
54	y	453	0	488	3	0
55	z	435	0	447	9	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	95	0	0	0	0
57	a	252	0	0	0	0
57	b	5	0	0	0	0
57	c	2	0	0	0	0
57	p	2	0	0	0	0
57	z	1	0	0	0	0
58	A	45	0	0	0	0
58	a	107	0	0	0	0
58	b	1	0	0	0	0
58	c	5	0	0	0	0
58	d	1	0	0	0	0
58	e	2	0	0	0	0
58	f	1	0	0	0	0
All	All	146853	0	98900	1574	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 6.

All (1574) 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)
30:a:2120:A:N6	30:a:2169:G:H21	1.60	0.98
30:a:2840:G:H4'	42:m:49:GLU:OE1	1.62	0.97
30:a:2120:A:H61	30:a:2169:G:N2	1.66	0.93
37:h:9:VAL:HG12	37:h:10:ALA:H	1.35	0.92
7:A:1535:C:O2	28:W:11:G:N2	2.03	0.90
30:a:2305:G:H22	30:a:2313:U:H3	1.12	0.90
16:J:57:VAL:HG12	16:J:58:ASN:H	1.37	0.89
7:A:511:C:H5	7:A:540:G:H1	1.19	0.88
30:a:2120:A:H61	30:a:2169:G:H21	1.13	0.87
16:J:80:THR:HG22	16:J:83:THR:HG23	1.57	0.86
30:a:289:U:H3	30:a:349:G:H1	1.23	0.86
6:5:131:LEU:HB3	6:5:136:LEU:HB2	1.56	0.86
1:0:53:LYS:HE3	1:0:55:LYS:HE2	1.58	0.86
30:a:2792:G:N2	30:a:2806:C:O2	2.09	0.85
7:A:450:G:H5''	7:A:451:A:H5'	1.59	0.83
30:a:2074:C:H5''	32:c:228:VAL:HG22	1.62	0.81
7:A:413:G:H21	7:A:428:G:H8	1.27	0.80
30:a:2840:G:C4'	42:m:49:GLU:OE1	2.30	0.79
6:5:44:VAL:HG22	6:5:214:ILE:HG22	1.64	0.79
7:A:664:G:H22	7:A:741:G:H1	1.30	0.78
4:3:32:LYS:HE2	30:a:2479:A:H5'	1.65	0.78
30:a:2096:A:H5''	37:h:11:ASN:HD21	1.48	0.77
7:A:1373:G:H5''	13:G:36:LYS:HD2	1.66	0.77
39:j:20:MET:HE3	39:j:44:LYS:HE2	1.67	0.76
19:M:71:ARG:HG3	19:M:75:MET:HE2	1.68	0.75
7:A:844:G:H2'	7:A:845:A:H4'	1.66	0.75
30:a:565:U:H1'	30:a:2031:6MZ:H9C1	1.67	0.75
30:a:1404:G:H1	30:a:1595:G:H22	1.32	0.74
9:C:70:THR:HG21	9:C:76:VAL:HG21	1.68	0.74
43:n:31:THR:HG22	43:n:33:ARG:H	1.52	0.73
6:5:114:VAL:HG21	6:5:136:LEU:HB3	1.69	0.73
36:g:24:ILE:HG12	36:g:72:LEU:HD11	1.71	0.73
30:a:1664:A:H2	39:j:1:MET:HE1	1.54	0.73
36:g:27:LYS:HE2	36:g:32:GLU:HB2	1.71	0.72
6:5:132:GLY:H	6:5:137:MET:HE2	1.55	0.72
32:c:107:PRO:HD2	32:c:110:LEU:HD22	1.72	0.72
37:h:57:LYS:HE3	37:h:57:LYS:HA	1.72	0.72
7:A:673:A:H2'	7:A:674:G:C8	2.23	0.71
7:A:1040:U:H2'	7:A:1041:G:H8	1.54	0.71
35:f:17:MET:HE1	35:f:25:VAL:HG23	1.71	0.71
30:a:2135:A:H2'	30:a:2136:A:C8	2.25	0.71
6:5:67:HIS:CG	6:5:184:LYS:HG2	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:73:PRO:HG3	9:C:105:GLU:HG3	1.72	0.71
7:A:1004:A:C6	7:A:1026:G:H1'	2.27	0.70
15:I:21:ILE:HG12	15:I:61:LEU:HD12	1.73	0.70
7:A:1151:A:H5''	16:J:44:THR:HG23	1.72	0.69
42:m:24:MET:HE2	42:m:44:LEU:HD22	1.73	0.69
37:h:122:LEU:HG	37:h:128:HIS:CD2	2.26	0.69
7:A:1086:U:H3	7:A:1099:G:H22	1.39	0.69
13:G:113:ASP:HB2	13:G:119:ARG:HG2	1.72	0.69
46:q:29:THR:HG22	46:q:66:HIS:HD2	1.56	0.69
22:P:4:ILE:HG12	22:P:21:VAL:HG22	1.74	0.69
30:a:2170:A:H2'	30:a:2171:A:C8	2.27	0.69
3:2:55:LEU:O	3:2:59:ILE:HG13	1.93	0.69
12:F:21:MET:HG3	12:F:24:ARG:HH22	1.58	0.69
30:a:2135:A:H2'	30:a:2136:A:H8	1.56	0.69
30:a:2169:G:H2'	30:a:2170:A:H3'	1.73	0.68
7:A:451:A:H61	7:A:481:G:H5'	1.59	0.68
7:A:967:5MC:H4'	15:I:127:PHE:HZ	1.59	0.68
8:B:58:ASN:OD1	8:B:220:THR:HG22	1.93	0.68
30:a:845:C:H2'	30:a:846:A:H8	1.57	0.68
30:a:2585:U:H2'	30:a:2586:U:H2'	1.75	0.68
7:A:1226:C:H2'	19:M:102:THR:HG22	1.75	0.68
53:x:4:LYS:HZ2	53:x:7:ARG:HH21	1.40	0.68
18:L:33:VAL:HG12	18:L:79:VAL:HG22	1.75	0.67
25:S:3:ARG:HE	25:S:10:PHE:HB2	1.58	0.67
30:a:354:U:H2'	30:a:355:G:H8	1.59	0.67
7:A:946:A:H2'	7:A:947:G:C8	2.30	0.67
7:A:671:G:H4'	12:F:79:ARG:HH22	1.60	0.67
7:A:1348:U:H4'	15:I:122:ARG:HD3	1.77	0.66
6:5:68:GLY:HA2	6:5:159:GLY:HA3	1.77	0.66
20:N:31:ILE:HD12	20:N:45:VAL:HG23	1.77	0.66
23:Q:62:ARG:HG2	23:Q:76:VAL:HG22	1.78	0.66
7:A:1356:G:H2'	7:A:1357:A:C8	2.30	0.66
10:D:149:ALA:HB1	10:D:152:GLN:HE21	1.60	0.66
9:C:108:LYS:HB3	9:C:111:LEU:HB2	1.76	0.66
30:a:1801:A:H2'	30:a:1802:A:C8	2.30	0.66
32:c:144:VAL:HB	32:c:154:LEU:HB2	1.76	0.66
6:5:4:LEU:HD22	6:5:8:MET:HG2	1.77	0.65
1:0:35:GLU:HG2	1:0:48:LEU:HD21	1.78	0.65
29:X:44:GLU:HB2	29:X:49:ILE:HD13	1.78	0.65
34:e:1:MET:HE1	34:e:113:VAL:HG11	1.77	0.65
41:l:41:LEU:HD12	41:l:96:ILE:HG13	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:219:ALA:HA	8:B:222:ARG:HE	1.60	0.65
7:A:458:U:H2'	7:A:459:A:C8	2.31	0.65
15:I:19:VAL:HG22	15:I:65:ILE:HG12	1.79	0.65
11:E:115:LEU:HD13	11:E:123:VAL:HG11	1.77	0.65
34:e:108:ILE:HA	40:k:1:MET:HE1	1.77	0.65
5:4:51:VAL:HG22	5:4:52:ALA:H	1.61	0.65
30:a:482:A:H5''	49:t:47:LYS:HD3	1.79	0.65
20:N:89:MET:HE1	20:N:98:LYS:HD3	1.79	0.65
30:a:1025:A:H2'	30:a:1026:A:C8	2.32	0.65
37:h:6:LEU:HD11	37:h:37:VAL:HG23	1.78	0.64
8:B:56:GLU:O	8:B:60:ILE:HG13	1.97	0.64
30:a:1805:C:O3'	32:c:48:ARG:NH1	2.29	0.64
35:f:42:GLU:HG3	35:f:49:LEU:HD23	1.80	0.64
7:A:337:G:H2'	7:A:338:A:C8	2.33	0.64
30:a:1869:G:H21	30:a:1872:A:H2	1.46	0.64
30:a:2074:C:C5'	32:c:228:VAL:HG22	2.27	0.64
6:5:97:MET:HG3	6:5:120:ALA:HB1	1.80	0.64
30:a:2306:U:H5''	35:f:131:GLY:HA3	1.80	0.64
7:A:407:U:H2'	7:A:408:A:H8	1.61	0.64
30:a:2548:A:H2'	30:a:2549:U:C6	2.33	0.64
6:5:76:ALA:HA	6:5:94:LEU:O	1.99	0.63
25:S:11:ILE:HG13	25:S:38:SER:HB3	1.78	0.63
47:r:95:ARG:HG3	47:r:95:ARG:HH11	1.64	0.63
14:H:26:THR:HG23	14:H:60:GLU:HG2	1.80	0.63
29:X:18:ASP:O	29:X:22:THR:HG23	1.98	0.63
11:E:81:LEU:HG	11:E:147:MET:HE2	1.79	0.63
30:a:737:C:H5'	30:a:1783:A:H3'	1.81	0.63
6:5:39:VAL:HB	6:5:177:LYS:HD2	1.81	0.63
7:A:1124:G:H5''	16:J:37:ARG:HH12	1.64	0.63
6:5:41:SER:HA	6:5:177:LYS:HD3	1.81	0.63
7:A:1040:U:H2'	7:A:1041:G:C8	2.33	0.63
35:f:38:MET:HE2	35:f:57:LEU:HG	1.81	0.63
27:V:21:H2U:H62	27:V:22:A:H4'	1.81	0.62
30:a:2329:A:H2'	30:a:2330:U:C6	2.34	0.62
6:5:30:LEU:HD11	6:5:216:THR:H	1.65	0.62
6:5:69:THR:HA	6:5:176:GLY:HA2	1.81	0.62
30:a:636:U:H2'	30:a:637:C:C6	2.35	0.62
7:A:674:G:H2'	7:A:675:A:H8	1.63	0.62
30:a:876:G:H2'	30:a:877:G:C8	2.35	0.62
45:p:49:ASP:HA	45:p:52:GLN:HB2	1.81	0.62
31:b:103:U:HO2'	31:b:104:A:H8	1.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:97:LEU:HD12	8:B:100:MET:HE3	1.80	0.62
30:a:1429:G:H2'	30:a:1430:A:C8	2.34	0.62
7:A:1071:C:H2'	7:A:1072:G:H8	1.63	0.62
22:P:69:ASP:O	22:P:73:THR:HG23	1.99	0.62
7:A:495:A:H4'	7:A:496:A:H5'	1.82	0.62
50:u:4:ILE:HB	50:u:63:ILE:HD13	1.82	0.61
30:a:2115:A:H3'	30:a:2116:G:H8	1.64	0.61
41:l:54:THR:HG22	41:l:59:ARG:HH11	1.65	0.61
30:a:1795:U:H2'	30:a:1796:G:C8	2.36	0.61
30:a:879:G:H2'	30:a:880:G:H8	1.65	0.61
30:a:1590:A:H2'	30:a:1591:A:H8	1.65	0.61
5:4:60:PHE:CE2	25:S:42:PRO:HD3	2.35	0.61
17:K:56:ARG:HH22	27:V:41:C:H4'	1.65	0.61
19:M:92:ARG:HD3	30:a:885:C:C5	2.34	0.61
30:a:1062:U:H3'	30:a:1063:U:H4'	1.82	0.61
19:M:55:THR:O	19:M:59:GLU:HG2	2.00	0.61
34:e:58:LYS:HG2	34:e:71:GLY:HA2	1.82	0.61
9:C:11:ARG:HG3	9:C:16:LYS:HG2	1.81	0.61
30:a:1466:A:H2'	30:a:1467:A:C8	2.35	0.61
7:A:21:G:H2'	7:A:22:G:C8	2.36	0.61
30:a:2101:G:H2'	30:a:2102:G:C8	2.36	0.61
7:A:714:G:H2'	7:A:715:A:C8	2.36	0.60
8:B:35:ARG:HD3	8:B:40:ILE:HG13	1.81	0.60
30:a:1173:U:H2'	30:a:1174:G:O4'	2.01	0.60
6:5:215:SER:HB3	6:5:221:GLY:HA2	1.81	0.60
7:A:407:U:H2'	7:A:408:A:C8	2.36	0.60
27:V:29:C:H2'	27:V:30:G:H8	1.66	0.60
30:a:1383:C:H2'	30:a:1384:A:C8	2.36	0.60
46:q:29:THR:HG22	46:q:66:HIS:CD2	2.36	0.60
55:z:32:LYS:HG3	55:z:33:THR:HG23	1.82	0.60
6:5:77:VAL:HG21	6:5:87:ALA:HB1	1.83	0.60
7:A:276:G:H5''	23:Q:17:MET:HE2	1.82	0.60
7:A:1535:C:H2'	7:A:1536:C:C6	2.36	0.60
12:F:47:LEU:HD13	12:F:51:ILE:HD12	1.83	0.60
24:R:29:LEU:O	24:R:33:ILE:HG23	2.01	0.60
7:A:1218:U:H2'	7:A:1219:A:C8	2.36	0.60
30:a:1664:A:C2	39:j:1:MET:HE1	2.37	0.60
7:A:147:G:H2'	7:A:148:G:C8	2.37	0.60
47:r:51:LEU:O	47:r:55:ILE:HG13	2.01	0.60
30:a:2184:A:H2'	30:a:2185:A:H8	1.66	0.60
30:a:2274:A:H2'	30:a:2275:A:C8	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:846:G:H2'	7:A:847:G:H8	1.66	0.60
29:X:70:MET:O	29:X:74:ILE:HD12	2.00	0.60
16:J:57:VAL:CG1	16:J:58:ASN:H	2.14	0.60
30:a:1795:U:H2'	30:a:1796:G:H8	1.66	0.60
32:c:176:LEU:HD12	32:c:180:GLU:HB3	1.84	0.60
7:A:73:C:H2'	7:A:74:A:H5'	1.84	0.59
30:a:2184:A:H2'	30:a:2185:A:C8	2.37	0.59
30:a:2205:G:H4'	32:c:150:LYS:HG3	1.84	0.59
7:A:1323:G:H2'	7:A:1324:A:C8	2.37	0.59
30:a:739:A:H2'	30:a:740:A:C8	2.36	0.59
37:h:53:GLU:HA	37:h:57:LYS:HG2	1.82	0.59
30:a:1059:G:H2'	30:a:1060:G:N2	2.17	0.59
37:h:9:VAL:HG12	37:h:10:ALA:N	2.14	0.59
37:h:93:SER:HB3	37:h:123:ARG:CZ	2.32	0.59
21:O:22:SER:HA	21:O:27:VAL:HG11	1.84	0.59
30:a:1793:A:H2'	30:a:1794:C:C6	2.37	0.59
55:z:54:VAL:HG23	55:z:55:ILE:HG12	1.84	0.59
16:J:57:VAL:HG12	16:J:58:ASN:N	2.14	0.59
30:a:413:C:H2'	30:a:414:A:H8	1.66	0.59
16:J:37:ARG:HB3	16:J:37:ARG:NH1	2.17	0.59
20:N:10:GLU:O	20:N:14:VAL:HG23	2.02	0.59
30:a:413:C:H2'	30:a:414:A:C8	2.37	0.59
30:a:1042:C:H4'	30:a:1044:G:H1'	1.84	0.59
30:a:2072:A:H2'	30:a:2073:C:C6	2.37	0.59
36:g:33:LEU:HB3	36:g:75:MET:HE3	1.83	0.59
13:G:50:LEU:HD22	13:G:124:LEU:HB3	1.84	0.59
35:f:104:ILE:HD11	35:f:175:PHE:HA	1.84	0.59
1:O:8:LYS:HB3	1:O:54:ILE:HD12	1.85	0.59
8:B:71:GLY:HA3	8:B:80:VAL:HG11	1.85	0.59
20:N:10:GLU:HG3	20:N:63:ARG:HD2	1.84	0.59
30:a:641:A:H2'	30:a:642:C:O4'	2.03	0.58
30:a:1067:A:H2'	30:a:1094:U:H4'	1.85	0.58
7:A:1441:A:H62	7:A:1461:G:H21	1.49	0.58
7:A:1103:C:H5''	8:B:97:LEU:HD22	1.85	0.58
8:B:70:VAL:HB	8:B:163:VAL:HG22	1.85	0.58
45:p:87:SER:HB2	46:q:51:VAL:HG13	1.84	0.58
30:a:997:A:H2'	30:a:998:A:C8	2.38	0.58
39:j:69:VAL:HG21	39:j:104:THR:HG21	1.84	0.58
13:G:78:ARG:HB2	13:G:156:TRP:HZ3	1.68	0.58
30:a:636:U:H2'	30:a:637:C:H6	1.67	0.58
12:F:25:TYR:O	12:F:29:ILE:HG13	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:42:TRP:CZ2	12:F:61:LEU:HD12	2.38	0.58
16:J:37:ARG:HB3	16:J:37:ARG:HH11	1.69	0.58
33:d:124:ARG:HG3	33:d:165:LEU:HD13	1.86	0.58
7:A:539:A:H2'	7:A:540:G:C8	2.38	0.58
27:V:14:A:H3'	27:V:15:G:H8	1.69	0.58
6:5:60:ARG:HB3	6:5:141:LYS:HD3	1.86	0.58
3:2:54:ASP:HB3	40:k:57:LEU:HD22	1.86	0.58
7:A:427:U:H2'	7:A:428:G:N2	2.19	0.58
7:A:946:A:H2'	7:A:947:G:H8	1.68	0.58
49:t:26:LYS:HD2	49:t:37:GLU:HG3	1.86	0.58
11:E:131:THR:HG22	11:E:131:THR:O	2.04	0.57
30:a:2065:C:H2'	30:a:2066:C:C6	2.39	0.57
42:m:22:ARG:HG3	42:m:70:THR:HA	1.86	0.57
49:t:47:LYS:HG3	49:t:48:PRO:HD2	1.86	0.57
17:K:67:ALA:HB2	17:K:96:THR:HG23	1.84	0.57
51:v:37:ILE:HG21	51:v:80:ILE:HG21	1.86	0.57
7:A:17:U:H2'	7:A:18:C:C6	2.39	0.57
7:A:458:U:H2'	7:A:459:A:H8	1.70	0.57
17:K:22:HIS:HB2	17:K:33:THR:HG22	1.86	0.57
30:a:2292:U:H2'	30:a:2293:U:C6	2.39	0.57
32:c:75:PRO:HG2	32:c:97:LYS:HE2	1.86	0.57
6:5:7:ARG:HH22	6:5:218:MET:HB3	1.68	0.57
6:5:8:MET:HE1	30:a:2176:C:H5''	1.85	0.57
7:A:384:G:H2'	7:A:385:C:C6	2.38	0.57
7:A:73:C:C2'	7:A:74:A:H5'	2.34	0.57
8:B:217:VAL:O	8:B:221:VAL:HG12	2.04	0.57
30:a:885:C:H2'	30:a:886:C:C6	2.38	0.57
30:a:2330:U:H2'	30:a:2331:G:C8	2.39	0.57
9:C:110:GLU:HB2	9:C:144:LEU:HD12	1.87	0.57
10:D:85:ASN:HB3	10:D:88:GLU:HB2	1.86	0.57
23:Q:11:ARG:HH11	23:Q:11:ARG:HB2	1.69	0.57
7:A:207:C:H2'	7:A:208:U:C6	2.39	0.57
7:A:461:G:HO2'	7:A:462:G:H8	1.53	0.57
19:M:90:ARG:HD3	19:M:97:VAL:HA	1.86	0.57
37:h:44:VAL:O	37:h:48:GLU:HB3	2.04	0.57
30:a:1403:U:H2'	30:a:1404:G:C8	2.40	0.57
7:A:131:A:H2'	7:A:132:C:C6	2.40	0.57
7:A:337:G:H2'	7:A:338:A:H8	1.68	0.57
32:c:269:ARG:HB3	32:c:269:ARG:NH1	2.20	0.57
7:A:1356:G:H2'	7:A:1357:A:H8	1.70	0.57
13:G:47:LEU:HB3	13:G:58:GLU:OE1	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1023:G:H2'	30:a:1024:A:H8	1.68	0.56
13:G:116:MET:HA	13:G:119:ARG:HG3	1.86	0.56
7:A:954:G:H2'	7:A:955:U:C6	2.41	0.56
7:A:1018:G:H2'	7:A:1019:G:H8	1.70	0.56
8:B:67:ILE:HG13	8:B:160:ALA:HB3	1.86	0.56
15:I:21:ILE:CG1	15:I:61:LEU:HD12	2.35	0.56
17:K:34:ILE:HB	17:K:74:VAL:HG11	1.87	0.56
30:a:1025:A:N6	30:a:1122:G:H2'	2.20	0.56
30:a:1060:G:H2'	30:a:1061:C:O4'	2.05	0.56
29:X:32:GLU:O	29:X:33:ARG:HD2	2.05	0.56
11:E:90:THR:HG22	11:E:91:GLY:H	1.70	0.56
15:I:65:ILE:HG21	15:I:79:ILE:HG12	1.88	0.56
30:a:1102:U:H2'	30:a:1103:G:C8	2.39	0.56
35:f:54:ALA:O	35:f:58:THR:HG23	2.06	0.56
7:A:514:C:H2'	7:A:515:G:H8	1.70	0.56
7:A:674:G:H2'	7:A:675:A:C8	2.41	0.56
18:L:67:ILE:HD13	18:L:74:LEU:HD12	1.88	0.56
41:l:49:ALA:O	41:l:53:MET:HG2	2.06	0.56
41:l:105:MET:HE1	41:l:113:ALA:HA	1.87	0.56
19:M:96:PRO:HB2	19:M:100:GLN:HB2	1.88	0.56
30:a:2729:U:HO2'	30:a:2730:G:H8	1.52	0.56
2:1:22:MET:HE2	2:1:28:ARG:HG2	1.87	0.56
7:A:269:C:H2'	7:A:270:A:C8	2.40	0.56
30:a:853:G:H2'	30:a:854:G:C8	2.41	0.56
6:5:168:ASN:HB2	6:5:170:ILE:HD12	1.87	0.55
7:A:1291:U:H2'	7:A:1292:G:H8	1.71	0.55
30:a:1415:G:H21	30:a:1580:A:H2	1.54	0.55
30:a:2103:U:H2'	30:a:2104:C:C6	2.41	0.55
30:a:2592:C:H2'	30:a:2593:G:C8	2.42	0.55
9:C:12:LEU:HD11	20:N:91:GLY:HA2	1.88	0.55
6:5:151:GLU:O	6:5:154:LYS:HG2	2.06	0.55
30:a:642:C:H2'	30:a:644:G:C8	2.41	0.55
30:a:829:U:H2'	30:a:830:A:C8	2.41	0.55
7:A:1018:G:H2'	7:A:1019:G:C8	2.42	0.55
29:X:28:GLU:O	29:X:32:GLU:HG3	2.07	0.55
7:A:634:C:H2'	7:A:635:A:C8	2.41	0.55
7:A:1410:A:H2'	7:A:1411:C:C6	2.42	0.55
19:M:71:ARG:HH12	35:f:115:ARG:NH1	2.05	0.55
6:5:133:PRO:HB3	30:a:2170:A:O2'	2.06	0.55
7:A:672:U:H2'	7:A:673:A:C8	2.41	0.55
12:F:42:TRP:HZ2	12:F:61:LEU:HD12	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:152:ALA:HB1	13:G:155:ARG:HH12	1.71	0.55
30:a:642:C:H2'	30:a:644:G:N7	2.22	0.55
11:E:61:GLN:O	11:E:65:GLU:HG2	2.06	0.55
30:a:846:A:H2'	30:a:847:U:C6	2.41	0.55
37:h:87:GLU:HG3	37:h:88:GLY:H	1.71	0.55
6:5:88:LYS:HE3	6:5:95:VAL:HG21	1.87	0.55
10:D:11:LEU:O	10:D:15:GLU:HG2	2.05	0.55
30:a:280:C:H2'	30:a:281:A:C8	2.41	0.55
44:o:6:LYS:O	44:o:10:GLN:NE2	2.39	0.55
7:A:390:U:H2'	7:A:391:G:C8	2.41	0.55
7:A:769:G:H4'	7:A:1513:A:H4'	1.88	0.55
7:A:1273:C:H2'	7:A:1274:A:O4'	2.07	0.55
30:a:778:A:C8	32:c:218:PRO:HG3	2.42	0.55
30:a:1431:A:H2'	30:a:1432:G:C8	2.42	0.55
30:a:878:G:H21	30:a:893:A:H61	1.54	0.55
30:a:2642:G:H5''	38:i:78:THR:HB	1.89	0.55
50:u:80:HIS:CE1	50:u:83:LYS:HD2	2.42	0.55
1:0:9:ILE:HD12	1:0:51:GLU:HG3	1.89	0.54
15:I:55:VAL:HG23	15:I:57:MET:HB3	1.89	0.54
30:a:1466:A:H2'	30:a:1467:A:H8	1.72	0.54
30:a:1570:A:H2'	30:a:1571:A:C8	2.42	0.54
7:A:716:A:N3	17:K:119:IAS:HB2	2.21	0.54
17:K:64:GLN:O	17:K:68:GLU:HG2	2.07	0.54
8:B:102:THR:HG23	8:B:175:GLU:HG2	1.88	0.54
8:B:187:VAL:HG13	8:B:191:SER:HB2	1.89	0.54
25:S:50:ALA:HB1	25:S:57:HIS:HB3	1.89	0.54
30:a:907:A:H2'	30:a:908:A:C8	2.43	0.54
30:a:2015:A:H2'	30:a:2016:A:C8	2.42	0.54
33:d:114:LYS:HE3	33:d:196:ALA:HB2	1.88	0.54
7:A:1120:C:H2'	7:A:1121:U:H6	1.73	0.54
12:F:3:HIS:CE1	12:F:65:GLU:HG3	2.42	0.54
29:X:61:LEU:HD22	29:X:84:GLN:HB3	1.90	0.54
30:a:845:C:H2'	30:a:846:A:C8	2.41	0.54
30:a:2789:C:H2'	30:a:2790:C:C6	2.43	0.54
35:f:74:VAL:HG12	35:f:77:PHE:H	1.73	0.54
6:5:11:ILE:HG12	6:5:33:LEU:HD22	1.88	0.54
6:5:217:THR:O	30:a:2176:C:H1'	2.07	0.54
7:A:745:A:H2'	7:A:746:A:C8	2.42	0.54
30:a:354:U:H2'	30:a:355:G:C8	2.43	0.54
30:a:2087:U:H2'	30:a:2088:G:C8	2.42	0.54
7:A:90:C:H2'	7:A:91:U:C6	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:92:U:H2'	7:A:93:U:O4'	2.08	0.54
7:A:713:G:H2'	7:A:714:G:C8	2.43	0.54
7:A:846:G:H2'	7:A:847:G:C8	2.41	0.54
7:A:1412:C:H2'	7:A:1413:A:C8	2.42	0.54
9:C:72:ARG:HD2	9:C:75:ILE:HG13	1.90	0.54
29:X:31:PHE:HB3	29:X:85:LEU:HD12	1.90	0.54
2:1:22:MET:HE3	2:1:31:LEU:HD12	1.89	0.54
7:A:451:A:N6	7:A:481:G:H5'	2.22	0.54
17:K:31:ILE:HG12	17:K:46:THR:HG23	1.89	0.54
6:5:132:GLY:HA3	6:5:137:MET:HG2	1.90	0.54
30:a:868:U:H2'	30:a:869:U:C6	2.43	0.54
9:C:129:MET:SD	9:C:131:ARG:HB2	2.48	0.54
30:a:72:A:H61	53:x:58:THR:HG21	1.73	0.54
30:a:1855:U:H2'	30:a:1856:G:O4'	2.08	0.54
30:a:2152:U:H2'	30:a:2153:G:H8	1.72	0.54
34:e:97:ASN:HB2	34:e:100:MET:HB2	1.90	0.54
50:u:26:PHE:HZ	50:u:47:VAL:HG11	1.73	0.54
29:X:23:LYS:HG3	29:X:78:ILE:HG12	1.90	0.54
30:a:418:U:H2'	30:a:419:C:C6	2.42	0.53
7:A:1367:C:H5''	15:I:116:VAL:HG22	1.90	0.53
16:J:27:GLU:O	16:J:31:ARG:HG2	2.08	0.53
29:X:61:LEU:HD13	29:X:85:LEU:HD22	1.90	0.53
30:a:1645:G:H5''	30:a:1646:C:H5'	1.91	0.53
30:a:2234:U:H2'	30:a:2235:G:C8	2.43	0.53
40:k:108:ALA:HB3	40:k:125:LEU:HD22	1.90	0.53
6:5:114:VAL:HG23	6:5:162:ARG:HH22	1.72	0.53
8:B:15:HIS:HB3	8:B:43:LEU:HD11	1.89	0.53
8:B:57:LEU:HD13	8:B:217:VAL:HG23	1.90	0.53
12:F:38:ARG:HB3	12:F:63:ASN:HB2	1.91	0.53
30:a:2:G:H2'	30:a:3:U:C6	2.44	0.53
30:a:927:G:H1'	54:y:25:LEU:HD11	1.90	0.53
46:q:63:VAL:HA	46:q:96:VAL:HG12	1.89	0.53
7:A:841:C:H2'	7:A:842:U:C6	2.44	0.53
7:A:1391:U:H2'	7:A:1392:G:C8	2.44	0.53
28:W:11:G:H2'	28:W:12:U:C6	2.43	0.53
7:A:728:A:H2'	7:A:729:A:C8	2.44	0.53
7:A:1226:C:H2'	19:M:102:THR:CG2	2.39	0.53
30:a:1052:G:H2'	30:a:1053:G:O4'	2.08	0.53
30:a:2181:U:H2'	30:a:2182:U:C6	2.44	0.53
24:R:32:TYR:CE1	24:R:45:THR:HG21	2.44	0.53
27:V:29:C:H2'	27:V:30:G:C8	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2244:U:H2'	30:a:2245:U:C6	2.44	0.53
7:A:1106:G:H5''	9:C:172:ARG:HG2	1.90	0.53
17:K:87:LYS:HD3	17:K:115:PRO:HD3	1.90	0.53
18:L:57:LEU:HD21	18:L:82:ILE:HD13	1.91	0.53
30:a:2456:G:H2'	30:a:2457:C:C6	2.43	0.53
30:a:2846:U:H5''	44:o:52:ASN:O	2.08	0.53
7:A:715:A:H2'	7:A:716:A:C8	2.43	0.53
7:A:845:A:H3'	7:A:846:G:H8	1.74	0.53
30:a:2106:U:H2'	30:a:2107:U:C6	2.43	0.53
37:h:54:LEU:CD1	37:h:55:GLU:H	2.21	0.53
49:t:33:LYS:HB3	49:t:64:ALA:HB1	1.91	0.53
6:5:212:VAL:HB	6:5:224:VAL:HG22	1.90	0.53
31:b:66:A:N6	31:b:107:G:H2'	2.24	0.53
9:C:43:LEU:HD13	9:C:68:ILE:HD11	1.90	0.52
10:D:8:LYS:HB3	10:D:21:LEU:HD13	1.90	0.52
12:F:43:GLY:HA2	12:F:58:HIS:CE1	2.44	0.52
30:a:1592:C:H2'	30:a:1593:A:C8	2.43	0.52
14:H:25:VAL:HG13	14:H:63:LEU:HD11	1.90	0.52
30:a:249:G:H4'	40:k:59:ARG:HD2	1.91	0.52
30:a:2092:C:H4'	52:w:56:MET:HE1	1.90	0.52
30:a:2328:A:H2'	30:a:2329:A:C8	2.45	0.52
10:D:19:LEU:HB2	10:D:21:LEU:HG	1.90	0.52
7:A:1175:G:H2'	7:A:1176:A:H8	1.75	0.52
27:V:19:G:H21	27:V:59:A:H5'	1.74	0.52
30:a:2813:G:H2'	30:a:2814:A:C8	2.44	0.52
7:A:501:C:H2'	7:A:502:A:H8	1.75	0.52
31:b:5:U:H2'	31:b:6:G:H8	1.75	0.52
42:m:8:ARG:HD2	42:m:43:GLU:HG2	1.92	0.52
8:B:117:LEU:HD23	8:B:141:LEU:HG	1.91	0.52
9:C:47:LEU:HD21	9:C:87:LEU:HD11	1.92	0.52
30:a:578:C:H2'	30:a:579:A:C8	2.45	0.52
34:e:138:LEU:HD22	34:e:146:VAL:HG11	1.92	0.52
13:G:78:ARG:HD3	13:G:80:VAL:HG23	1.92	0.52
30:a:1079:U:H2'	30:a:1080:U:C2	2.45	0.52
30:a:2105:C:H2'	30:a:2106:U:C6	2.45	0.52
6:5:132:GLY:HA2	6:5:136:LEU:H	1.75	0.52
7:A:204:G:C4	7:A:205:A:C8	2.97	0.52
7:A:328:C:H4'	7:A:329:A:H5'	1.92	0.52
7:A:427:U:H2'	7:A:428:G:H21	1.75	0.52
7:A:1355:G:H2'	7:A:1356:G:H8	1.75	0.52
24:R:33:ILE:HD12	24:R:37:GLY:HA2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:590:U:H2'	30:a:591:U:C6	2.45	0.52
30:a:848:C:H2'	30:a:849:U:C6	2.45	0.52
7:A:1338:G:H2'	7:A:1339:A:C8	2.45	0.52
10:D:152:GLN:HB2	10:D:155:VAL:HG23	1.91	0.52
30:a:482:A:C8	49:t:45:HIS:HD2	2.28	0.52
30:a:1260:U:O2'	55:z:8:PRO:HD2	2.10	0.52
30:a:1391:U:H2'	30:a:1392:A:O4'	2.10	0.52
10:D:101:VAL:O	10:D:105:MET:HG3	2.09	0.52
10:D:185:GLN:HG3	10:D:186:PRO:HD2	1.91	0.52
30:a:1383:C:H2'	30:a:1384:A:H8	1.75	0.52
30:a:1770:C:H2'	30:a:1771:A:C8	2.45	0.52
53:x:9:LYS:HD3	53:x:13:GLU:HG2	1.92	0.52
30:a:5:A:H2'	30:a:6:A:C8	2.44	0.51
30:a:247:G:H5'	30:a:249:G:N7	2.25	0.51
30:a:357:U:H2'	30:a:358:G:C8	2.45	0.51
30:a:493:G:H4'	47:r:6:GLN:HB3	1.90	0.51
30:a:1444:C:H2'	30:a:1445:G:C8	2.45	0.51
37:h:66:ASN:HB3	37:h:135:HIS:HA	1.92	0.51
44:o:100:LEU:HD11	44:o:110:ILE:HD11	1.92	0.51
7:A:390:U:H2'	7:A:391:G:H8	1.75	0.51
7:A:216:U:H2'	7:A:217:C:C6	2.45	0.51
17:K:64:GLN:HG3	17:K:99:ALA:HB2	1.93	0.51
30:a:64:A:H2'	30:a:65:U:C6	2.46	0.51
34:e:188:MET:HB3	34:e:193:VAL:HG23	1.92	0.51
41:l:108:VAL:HB	41:l:112:LEU:HD23	1.92	0.51
7:A:269:C:H2'	7:A:270:A:H8	1.73	0.51
12:F:88:MET:HB2	24:R:64:TYR:HE2	1.75	0.51
30:a:2247:G:H2'	30:a:2248:A:C8	2.46	0.51
37:h:9:VAL:CG1	37:h:10:ALA:H	2.16	0.51
7:A:618:C:H5'	7:A:619:U:H5''	1.92	0.51
30:a:2136:A:H2'	30:a:2137:G:O4'	2.11	0.51
6:5:200:LYS:HE2	6:5:208:TYR:HB2	1.92	0.51
30:a:2490:U:H2'	30:a:2491:G:O4'	2.10	0.51
25:S:44:MET:HA	25:S:47:LEU:HD12	1.93	0.51
30:a:881:C:H2'	30:a:882:C:C6	2.46	0.51
30:a:1350:A:H2'	30:a:1351:A:C8	2.46	0.51
31:b:104:A:H2'	31:b:105:G:O4'	2.10	0.51
40:k:110:VAL:O	40:k:128:THR:HG23	2.11	0.51
7:A:552:U:H2'	7:A:553:A:H8	1.76	0.51
14:H:102:ALA:HB3	14:H:113:ASP:HB3	1.92	0.51
20:N:82:ILE:O	20:N:86:GLU:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:190:A:H2'	30:a:191:C:C6	2.46	0.51
30:a:1057:U:H1'	30:a:1059:G:OP2	2.11	0.51
30:a:1174:G:H2'	30:a:1175:C:C6	2.46	0.51
30:a:1590:A:H2'	30:a:1591:A:C8	2.45	0.51
30:a:2516:C:H2'	30:a:2517:A:H8	1.74	0.51
31:b:48:U:H4'	43:n:100:HIS:CD2	2.46	0.51
34:e:111:GLU:O	34:e:115:GLN:HG2	2.10	0.51
7:A:987:A:H2'	7:A:988:C:C6	2.45	0.51
10:D:152:GLN:O	10:D:156:LYS:HD2	2.11	0.51
14:H:105:SER:HB2	14:H:126:ILE:HD11	1.93	0.51
34:e:145:ASP:HA	34:e:166:LYS:HB3	1.93	0.51
43:n:58:ILE:HD11	43:n:81:ARG:NH2	2.26	0.51
47:r:20:VAL:HG11	47:r:44:ALA:HA	1.93	0.51
48:s:67:VAL:HG12	48:s:76:ARG:HG3	1.92	0.51
7:A:865:A:H2'	7:A:866:C:C6	2.47	0.50
9:C:72:ARG:HB3	9:C:75:ILE:HB	1.93	0.50
11:E:111:MET:HE2	11:E:127:ALA:HB2	1.92	0.50
29:X:45:LYS:HE3	29:X:46:VAL:HG23	1.93	0.50
30:a:1439:U:H2'	30:a:1440:C:C6	2.45	0.50
30:a:1733:G:H2'	30:a:1734:G:H8	1.76	0.50
36:g:71:LEU:O	36:g:75:MET:HG3	2.11	0.50
42:m:32:GLU:HB3	42:m:118:ARG:HG3	1.92	0.50
11:E:90:THR:HG22	11:E:91:GLY:N	2.25	0.50
30:a:2330:U:H2'	30:a:2331:G:H8	1.76	0.50
37:h:79:THR:HG23	37:h:145:ASN:HB3	1.93	0.50
7:A:67:C:H2'	7:A:68:G:C8	2.46	0.50
7:A:501:C:H2'	7:A:502:A:C8	2.47	0.50
10:D:48:LEU:HD22	10:D:52:GLY:HA3	1.91	0.50
14:H:11:LEU:HD22	14:H:75:ILE:HD11	1.92	0.50
24:R:21:ILE:HG21	24:R:55:LEU:HA	1.94	0.50
37:h:53:GLU:O	37:h:54:LEU:HD12	2.11	0.50
5:4:56:ARG:HH21	25:S:69:HIS:CE1	2.29	0.50
30:a:2515:U:H2'	30:a:2516:C:C6	2.47	0.50
7:A:113:G:H1'	7:A:354:G:H5'	1.94	0.50
7:A:746:A:H2'	7:A:747:A:C8	2.46	0.50
32:c:29:PRO:HG2	32:c:34:LEU:HD11	1.92	0.50
41:l:84:LYS:HB3	51:v:8:GLY:HA2	1.93	0.50
25:S:13:LEU:HD11	25:S:17:LYS:HE3	1.92	0.50
27:V:63:C:H2'	27:V:64:G:C8	2.47	0.50
30:a:2075:U:H2'	30:a:2076:U:C6	2.47	0.50
44:o:25:THR:HG22	44:o:44:GLU:OE2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:744:C:H2'	7:A:745:A:C8	2.47	0.50
7:A:1062:U:H2'	7:A:1063:C:C6	2.47	0.50
7:A:1118:U:H2'	7:A:1119:C:H6	1.76	0.50
30:a:1592:C:H2'	30:a:1593:A:H8	1.77	0.50
30:a:2638:U:H2'	30:a:2639:G:O4'	2.12	0.50
32:c:161:TYR:HB3	32:c:194:GLU:HB3	1.92	0.50
49:t:94:ARG:HB2	49:t:103:ILE:HG13	1.93	0.50
18:L:25:GLU:CD	18:L:59:ASN:HD22	2.20	0.50
30:a:190:A:H2'	30:a:191:C:H6	1.77	0.50
30:a:1058:U:H5'	30:a:1059:G:OP2	2.12	0.50
30:a:1095:A:H3'	30:a:1096:G:H8	1.77	0.50
30:a:1391:U:H4'	30:a:1603:A:H4'	1.92	0.50
30:a:2121:G:H2'	30:a:2122:G:H8	1.77	0.50
30:a:2640:A:H2'	30:a:2641:G:O4'	2.12	0.50
35:f:92:ARG:HA	35:f:96:MET:HB2	1.93	0.50
43:n:4:LYS:O	43:n:8:ILE:HG12	2.12	0.50
18:L:107:VAL:O	18:L:108:LYS:HB2	2.10	0.50
29:X:24:PHE:CE1	29:X:78:ILE:HD11	2.46	0.50
30:a:596:A:H2'	30:a:597:G:H8	1.77	0.50
30:a:1138:U:H4'	30:a:1139:A:O4'	2.11	0.50
37:h:114:GLU:HB3	37:h:134:VAL:HG22	1.93	0.50
7:A:524:G:H2'	7:A:525:C:C6	2.47	0.49
7:A:1124:G:H5''	16:J:37:ARG:NH1	2.26	0.49
7:A:1323:G:H2'	7:A:1324:A:H8	1.76	0.49
27:V:51:U:H2'	27:V:52:C:C6	2.47	0.49
30:a:846:A:H2'	30:a:847:U:H6	1.75	0.49
38:i:110:PRO:HD2	38:i:118:MET:HE1	1.94	0.49
47:r:41:LYS:HD2	55:z:22:LEU:HD11	1.94	0.49
7:A:634:C:H2'	7:A:635:A:H8	1.76	0.49
7:A:985:C:H2'	7:A:986:U:C6	2.47	0.49
30:a:1542:U:H2'	30:a:1543:G:O4'	2.11	0.49
30:a:2033:G:C5	33:d:150:MEQ:HE3	2.47	0.49
30:a:2248:A:H2'	30:a:2249:C:H6	1.76	0.49
30:a:2793:A:H2'	30:a:2794:G:O4'	2.11	0.49
37:h:76:GLY:HA2	37:h:142:LEU:HD12	1.95	0.49
47:r:74:ILE:HD12	47:r:105:VAL:HG22	1.94	0.49
7:A:1038:U:H2'	7:A:1039:C:H6	1.78	0.49
7:A:1512:U:H2'	7:A:1513:A:C8	2.47	0.49
30:a:1196:U:H1'	45:p:4:VAL:HG22	1.94	0.49
7:A:763:G:H2'	7:A:764:C:C6	2.48	0.49
17:K:23:ILE:HD13	17:K:84:VAL:HG13	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:45:ARG:HD3	42:m:97:ILE:HD11	1.94	0.49
47:r:23:LEU:HD22	55:z:24:ALA:HB2	1.95	0.49
6:5:181:ASP:H	6:5:184:LYS:HD2	1.77	0.49
7:A:371:A:H2'	7:A:372:C:O4'	2.13	0.49
7:A:672:U:H2'	7:A:673:A:H8	1.75	0.49
7:A:1287:A:H2'	7:A:1288:A:C8	2.47	0.49
7:A:1533:C:H2'	7:A:1534:A:H8	1.77	0.49
30:a:2066:C:H2'	30:a:2067:C:H6	1.78	0.49
30:a:2108:G:H2'	30:a:2109:A:C8	2.47	0.49
1:0:25:LYS:HE2	1:0:27:LYS:NZ	2.28	0.49
6:5:132:GLY:H	6:5:137:MET:CE	2.23	0.49
7:A:235:C:H2'	7:A:236:A:H8	1.76	0.49
7:A:1071:C:H2'	7:A:1072:G:C8	2.45	0.49
7:A:1477:U:H2'	7:A:1478:U:C6	2.48	0.49
30:a:1070:A:C4	30:a:1071:G:C8	3.00	0.49
30:a:1682:G:H2'	30:a:1683:U:C6	2.48	0.49
30:a:2538:U:H2'	30:a:2539:C:C6	2.48	0.49
37:h:129:GLU:HB2	37:h:143:VAL:HG12	1.95	0.49
2:1:4:THR:HG22	30:a:684:C:H1'	1.94	0.49
7:A:539:A:H2'	7:A:540:G:H8	1.77	0.49
30:a:1066:A:C4	30:a:1070:A:C8	3.00	0.49
30:a:1080:U:C2	30:a:1082:A:H5''	2.47	0.49
6:5:67:HIS:CD2	6:5:184:LYS:HA	2.48	0.49
7:A:235:C:H2'	7:A:236:A:C8	2.48	0.49
7:A:416:G:H2'	7:A:417:G:H8	1.77	0.49
7:A:1005:A:H62	7:A:1024:G:H21	1.60	0.49
7:A:1513:A:H2'	7:A:1514:G:C8	2.48	0.49
9:C:86:LYS:O	9:C:90:VAL:HG23	2.12	0.49
11:E:13:GLU:HG2	11:E:39:VAL:HG12	1.94	0.49
15:I:52:LEU:HD11	15:I:63:LEU:HD11	1.95	0.49
27:V:10:G:N2	27:V:27:G:H1'	2.28	0.49
30:a:1430:A:H2'	30:a:1431:A:O4'	2.13	0.49
30:a:1710:G:H4'	30:a:2859:C:O2	2.13	0.49
34:e:83:VAL:HB	34:e:86:ALA:HB2	1.95	0.49
35:f:142:ASP:HB3	35:f:145:LYS:HG3	1.93	0.49
36:g:11:ILE:HD12	36:g:11:ILE:O	2.12	0.49
8:B:88:ASP:HB2	8:B:225:ARG:NH2	2.28	0.49
30:a:363:C:H2'	30:a:364:U:C6	2.47	0.49
30:a:654:U:H2'	30:a:655:U:C6	2.48	0.49
30:a:1402:U:H2'	30:a:1403:U:C6	2.48	0.49
30:a:1933:A:H2'	30:a:1934:G:O4'	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:x:4:LYS:HZ2	53:x:7:ARG:NH2	2.10	0.49
6:5:66:PRO:HD2	6:5:188:ASN:HA	1.94	0.49
29:X:37:VAL:HG22	29:X:54:LEU:HG	1.95	0.49
30:a:629:A:H2'	30:a:630:A:C8	2.48	0.49
30:a:810:U:H2'	30:a:811:C:C6	2.48	0.49
30:a:2117:G:O6	30:a:2163:G:H5'	2.13	0.49
31:b:5:U:H2'	31:b:6:G:C8	2.48	0.49
32:c:118:SER:HB3	32:c:129:THR:HB	1.95	0.49
41:l:41:LEU:HD21	41:l:124:LEU:HG	1.94	0.49
7:A:662:U:H2'	7:A:663:A:C8	2.48	0.48
7:A:979:C:O2	20:N:59:ARG:HD2	2.12	0.48
7:A:1072:G:H2'	7:A:1073:U:C6	2.47	0.48
7:A:1401:G:H2'	7:A:1402:4OC:O4'	2.13	0.48
26:T:27:MET:O	26:T:30:THR:HG22	2.12	0.48
30:a:1508:A:H2'	30:a:1509:A:C8	2.48	0.48
30:a:1884:U:H2'	30:a:1885:G:O4'	2.13	0.48
34:e:149:ILE:HG22	34:e:192:ALA:HB1	1.94	0.48
39:j:24:VAL:HG12	39:j:30:ARG:HD3	1.94	0.48
14:H:22:LYS:O	14:H:63:LEU:HD12	2.13	0.48
27:V:25:U:H2'	27:V:26:C:C6	2.48	0.48
27:V:71:G:H2'	27:V:72:C:C6	2.49	0.48
31:b:48:U:H4'	43:n:100:HIS:HD2	1.78	0.48
7:A:562:U:H1'	18:L:12:ARG:HD2	1.95	0.48
15:I:84:THR:HG23	15:I:98:LEU:HD13	1.95	0.48
30:a:143:A:H2'	30:a:144:C:C6	2.49	0.48
30:a:584:C:C2	40:k:19:LEU:HD12	2.48	0.48
30:a:1770:C:H2'	30:a:1771:A:H8	1.78	0.48
30:a:2157:G:H8	30:a:2157:G:OP2	1.97	0.48
36:g:39:LYS:HE2	36:g:58:PHE:HE1	1.78	0.48
42:m:54:LEU:HD23	42:m:66:ALA:HB2	1.94	0.48
6:5:130:VAL:HG12	6:5:131:LEU:HD23	1.94	0.48
30:a:1056:G:H5''	30:a:1057:U:H5''	1.94	0.48
30:a:2039:G:H2'	30:a:2040:U:O4'	2.12	0.48
43:n:43:ASN:HD21	43:n:46:GLU:HG2	1.77	0.48
6:5:111:PHE:HE1	6:5:136:LEU:HD13	1.79	0.48
7:A:1107:C:C4	7:A:1108:G:C8	3.01	0.48
9:C:153:VAL:HG22	9:C:198:VAL:HG22	1.94	0.48
13:G:30:LEU:HD11	13:G:116:MET:HE2	1.93	0.48
15:I:7:TYR:HE1	15:I:18:ARG:HB3	1.79	0.48
24:R:32:TYR:O	24:R:40:VAL:HG12	2.14	0.48
30:a:1169:C:H2'	30:a:1170:U:O4'	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:11:ILE:HG23	6:5:33:LEU:HD13	1.94	0.48
7:A:1118:U:H2'	7:A:1119:C:C6	2.48	0.48
21:O:10:LYS:O	21:O:14:GLU:HG2	2.14	0.48
24:R:70:TYR:HB2	24:R:74:HIS:CE1	2.49	0.48
30:a:305:U:H2'	30:a:306:G:O4'	2.14	0.48
30:a:579:A:H2'	30:a:580:G:C8	2.49	0.48
30:a:2810:A:H2'	30:a:2811:A:C8	2.48	0.48
33:d:128:ARG:HA	33:d:128:ARG:HD3	1.63	0.48
41:l:136:MET:HE3	41:l:136:MET:HB2	1.71	0.48
6:5:133:PRO:HB2	30:a:2171:A:H5'	1.95	0.48
7:A:523:A:C2	18:L:88:LYS:HB3	2.48	0.48
30:a:700:U:H2'	30:a:701:G:O4'	2.13	0.48
30:a:2592:C:H2'	30:a:2593:G:H8	1.79	0.48
35:f:162:SER:OG	35:f:165:GLU:HG3	2.13	0.48
38:i:11:VAL:HG11	38:i:50:THR:HA	1.96	0.48
44:o:27:GLU:HB2	44:o:87:LYS:HD2	1.95	0.48
6:5:200:LYS:HG3	6:5:208:TYR:CD1	2.48	0.48
22:P:4:ILE:HG22	22:P:71:VAL:HG11	1.96	0.48
24:R:11:CYS:SG	24:R:14:THR:HG22	2.54	0.48
30:a:464:G:H2'	30:a:465:A:C8	2.48	0.48
30:a:577:U:H2'	30:a:578:C:C6	2.49	0.48
30:a:1146:G:H2'	30:a:1147:C:C6	2.48	0.48
7:A:1219:A:H5''	20:N:53:ARG:HH21	1.77	0.48
10:D:11:LEU:HB3	10:D:63:ARG:HD3	1.95	0.48
11:E:39:VAL:HG23	11:E:71:MET:HE2	1.95	0.48
14:H:3:MET:HE3	14:H:3:MET:HA	1.95	0.48
30:a:531:A:H4'	30:a:532:G:C8	2.49	0.48
30:a:1096:G:H2'	30:a:1097:C:O4'	2.14	0.48
30:a:1720:U:H2'	30:a:1721:G:O4'	2.13	0.48
33:d:88:GLU:HG2	33:d:90:PHE:CE1	2.49	0.48
42:m:96:ARG:CZ	42:m:116:VAL:HG12	2.44	0.48
3:2:54:ASP:HA	3:2:57:LEU:HD12	1.96	0.48
4:3:8:LYS:HB2	4:3:8:LYS:HE2	1.48	0.48
7:A:594:C:H2'	7:A:595:A:O4'	2.14	0.48
7:A:908:A:H2'	7:A:909:A:H8	1.79	0.48
11:E:149:SER:OG	11:E:152:MET:HG3	2.13	0.48
30:a:591:U:H2'	30:a:592:C:C6	2.49	0.48
30:a:848:C:H2'	30:a:849:U:H6	1.79	0.48
38:i:13:ARG:HG3	38:i:13:ARG:HH11	1.79	0.48
39:j:122:VAL:O	39:j:122:VAL:HG12	2.14	0.48
2:1:1:MET:HE2	2:1:1:MET:HB3	1.72	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:75:VAL:HG11	6:5:153:VAL:HG22	1.96	0.47
8:B:111:ILE:HG13	8:B:148:LEU:HD22	1.95	0.47
30:a:2021:A:H5'	55:z:9:THR:CG2	2.44	0.47
30:a:2899:U:H2'	30:a:2900:A:C8	2.49	0.47
36:g:24:ILE:HG21	36:g:72:LEU:HD21	1.96	0.47
45:p:76:TYR:CZ	45:p:80:ILE:HG13	2.49	0.47
3:2:19:LYS:HG3	30:a:648:G:H5'	1.95	0.47
7:A:1162:C:H2'	7:A:1163:A:H8	1.80	0.47
29:X:89:LYS:HG3	29:X:93:LYS:HZ2	1.79	0.47
30:a:171:A:H2'	30:a:172:A:C8	2.49	0.47
7:A:206:C:C4	7:A:207:C:C2	3.03	0.47
7:A:1122:U:H2'	7:A:1123:U:C6	2.50	0.47
7:A:1410:A:H2'	7:A:1411:C:H6	1.78	0.47
11:E:20:ARG:HG2	11:E:20:ARG:HH11	1.80	0.47
19:M:67:GLY:HA3	35:f:113:ASP:OD1	2.15	0.47
19:M:92:ARG:HD3	30:a:885:C:C6	2.49	0.47
30:a:711:U:H1'	30:a:714:C:H5	1.79	0.47
37:h:4:ILE:HA	37:h:17:ASP:O	2.13	0.47
3:2:15:LYS:HG2	40:k:64:PHE:HZ	1.80	0.47
7:A:273:U:H1'	23:Q:18:GLU:OE2	2.14	0.47
30:a:289:U:O4	30:a:349:G:O6	2.32	0.47
30:a:1550:U:H2'	30:a:1551:A:C8	2.49	0.47
30:a:1745:A:H2'	30:a:1746:U:C6	2.49	0.47
30:a:1793:A:H2'	30:a:1794:C:H6	1.78	0.47
32:c:269:ARG:HB3	32:c:269:ARG:HH11	1.80	0.47
33:d:157:LYS:HB2	33:d:157:LYS:HE2	1.60	0.47
6:5:131:LEU:HB2	6:5:137:MET:SD	2.53	0.47
7:A:384:G:H2'	7:A:385:C:H6	1.78	0.47
7:A:1031:C:H4'	7:A:1032:G:C6	2.50	0.47
7:A:1535:C:N3	28:W:11:G:N1	2.46	0.47
15:I:27:LYS:HB3	15:I:62:ASP:OD1	2.14	0.47
23:Q:62:ARG:HG2	23:Q:76:VAL:CG2	2.43	0.47
30:a:576:G:H2'	30:a:577:U:C6	2.49	0.47
30:a:822:A:O2'	40:k:54:GLN:HB2	2.15	0.47
30:a:1011:A:H2'	30:a:1012:U:C6	2.49	0.47
30:a:1070:A:C5	30:a:1071:G:C5	3.02	0.47
41:l:105:MET:HE3	41:l:108:VAL:HG21	1.97	0.47
44:o:14:LYS:HE3	44:o:77:HIS:HA	1.95	0.47
6:5:23:ILE:HG23	6:5:186:LYS:HE2	1.95	0.47
7:A:945:G:C2	7:A:946:A:C8	3.02	0.47
7:A:1352:C:H2'	7:A:1353:G:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:31:PHE:O	26:T:35:VAL:HG23	2.14	0.47
30:a:1100:A:H5''	30:a:1101:C:C5	2.50	0.47
30:a:1807:A:H3'	30:a:1808:A:C8	2.49	0.47
30:a:2109:A:H2'	30:a:2110:U:O4'	2.15	0.47
30:a:2558:G:H2'	30:a:2559:C:C6	2.49	0.47
34:e:48:THR:HG22	34:e:86:ALA:HB3	1.95	0.47
35:f:46:ASP:HB2	35:f:49:LEU:HD22	1.97	0.47
6:5:19:LYS:HE2	6:5:21:TYR:HA	1.96	0.47
6:5:75:VAL:HG22	6:5:113:VAL:HB	1.96	0.47
9:C:116:VAL:O	9:C:120:ILE:HG13	2.14	0.47
23:Q:8:LEU:HD13	23:Q:73:TRP:CZ3	2.49	0.47
24:R:70:TYR:HB2	24:R:74:HIS:HE1	1.80	0.47
27:V:28:U:H2'	27:V:29:C:C6	2.49	0.47
29:X:52:ALA:HB2	29:X:77:LEU:HD21	1.97	0.47
30:a:498:U:H5''	49:t:43:LYS:HD2	1.97	0.47
30:a:1025:A:H2'	30:a:1026:A:H8	1.79	0.47
30:a:2568:G:H2'	30:a:2569:U:C6	2.50	0.47
30:a:2699:U:H2'	30:a:2700:C:C6	2.49	0.47
37:h:68:ARG:HH12	37:h:109:LYS:NZ	2.13	0.47
49:t:96:PHE:CZ	49:t:103:ILE:HD13	2.50	0.47
2:1:3:ARG:HA	2:1:3:ARG:HD3	1.73	0.47
22:P:8:ARG:CZ	22:P:15:PRO:HB3	2.45	0.47
29:X:34:ILE:HA	29:X:56:VAL:HG23	1.97	0.47
30:a:586:U:H2'	30:a:587:A:C8	2.49	0.47
30:a:970:A:H5'	30:a:1185:U:H1'	1.96	0.47
30:a:1539:U:H2'	30:a:1540:G:H8	1.80	0.47
30:a:1890:A:H2'	30:a:1891:A:C8	2.50	0.47
7:A:1524:C:H2'	7:A:1525:G:C8	2.50	0.47
10:D:105:MET:HG2	10:D:171:LEU:HD13	1.96	0.47
17:K:23:ILE:HG12	17:K:96:THR:HG21	1.97	0.47
30:a:180:A:H2'	30:a:181:A:C8	2.49	0.47
30:a:1564:C:H2'	30:a:1565:C:C6	2.50	0.47
6:5:27:ILE:O	6:5:31:LYS:HG3	2.14	0.47
7:A:33:A:H2'	7:A:34:C:C6	2.49	0.47
7:A:376:G:H5''	22:P:5:ARG:HB2	1.97	0.47
9:C:184:TYR:HA	9:C:200:VAL:O	2.15	0.47
30:a:578:C:H2'	30:a:579:A:H8	1.79	0.47
30:a:1095:A:H3'	30:a:1096:G:C8	2.49	0.47
30:a:2805:U:H2'	30:a:2806:C:H6	1.80	0.47
36:g:29:LYS:HB2	36:g:29:LYS:HE2	1.76	0.47
7:A:216:U:H2'	7:A:217:C:H6	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:59:GLN:NE2	10:D:63:ARG:HH21	2.13	0.46
30:a:492:G:H2'	30:a:493:G:O4'	2.14	0.46
30:a:605:A:H2'	30:a:606:A:C8	2.51	0.46
30:a:2462:A:H2'	30:a:2463:C:C6	2.50	0.46
30:a:2837:U:H2'	30:a:2838:A:C8	2.50	0.46
9:C:36:ASP:OD1	9:C:57:ILE:HG21	2.15	0.46
9:C:52:VAL:HG22	9:C:70:THR:HG22	1.97	0.46
11:E:38:VAL:HG11	11:E:114:VAL:HG22	1.97	0.46
12:F:47:LEU:HD21	12:F:57:ALA:HB3	1.97	0.46
18:L:108:LYS:HD3	18:L:108:LYS:HA	1.73	0.46
30:a:1051:A:H2'	30:a:1052:G:C8	2.50	0.46
30:a:2282:A:O2'	30:a:2283:G:H5'	2.15	0.46
30:a:2329:A:H2'	30:a:2330:U:H6	1.79	0.46
30:a:2503:G:H5''	30:a:2504:2MA:H5''	1.97	0.46
30:a:2701:A:H2'	30:a:2702:U:C6	2.49	0.46
37:h:70:GLU:HB2	37:h:135:HIS:HB2	1.96	0.46
43:n:7:ARG:HG3	43:n:10:ARG:HH21	1.80	0.46
7:A:205:A:C6	7:A:206:C:C4	3.03	0.46
8:B:162:PHE:HA	8:B:184:PHE:O	2.15	0.46
19:M:86:TYR:CZ	19:M:90:ARG:HD2	2.49	0.46
27:V:26:C:H2'	27:V:27:G:O4'	2.15	0.46
29:X:9:ASN:HD21	29:X:43:VAL:H	1.63	0.46
30:a:39:G:H2'	30:a:40:U:C6	2.50	0.46
30:a:1789:C:H2'	30:a:1790:A:C5	2.51	0.46
30:a:2848:U:H2'	30:a:2849:G:O4'	2.15	0.46
37:h:141:LYS:HD2	37:h:142:LEU:N	2.30	0.46
3:2:35:LYS:HE2	3:2:35:LYS:HB2	1.64	0.46
12:F:4:TYR:CD1	12:F:71:ILE:HG13	2.51	0.46
20:N:73:TYR:CE2	20:N:75:GLY:HA2	2.50	0.46
30:a:2616:U:C2	55:z:4:GLN:HA	2.51	0.46
50:u:55:GLU:HB3	50:u:59:GLU:OE2	2.15	0.46
51:v:37:ILE:HD11	51:v:82:ILE:HD11	1.97	0.46
51:v:41:ARG:HD3	51:v:41:ARG:HA	1.72	0.46
1:0:10:LYS:HG3	1:0:20:PHE:CD1	2.50	0.46
6:5:44:VAL:HB	6:5:173:THR:HG22	1.96	0.46
7:A:78:A:H2'	7:A:79:G:O4'	2.16	0.46
7:A:310:G:H5''	22:P:31:ARG:HB2	1.96	0.46
19:M:37:ALA:HB2	19:M:59:GLU:HG3	1.97	0.46
19:M:71:ARG:NH1	35:f:115:ARG:HD2	2.30	0.46
30:a:781:G:H5'	30:a:782:G:OP1	2.15	0.46
30:a:825:U:H2'	30:a:826:A:C8	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:906:A:H2'	30:a:909:C:C5	2.50	0.46
30:a:1435:U:H2'	30:a:1436:A:H8	1.81	0.46
30:a:1460:C:H2'	30:a:1461:G:C8	2.50	0.46
30:a:1823:G:O3'	32:c:247:PRO:HD3	2.16	0.46
37:h:99:ILE:HD11	37:h:122:LEU:HD22	1.98	0.46
46:q:74:ILE:HB	46:q:87:GLN:HB3	1.98	0.46
48:s:54:GLU:HB3	48:s:88:LYS:HB2	1.97	0.46
5:4:1:MET:HE3	5:4:6:HIS:CD2	2.51	0.46
7:A:676:A:H2'	7:A:677:U:H6	1.81	0.46
7:A:908:A:H2'	7:A:909:A:C8	2.51	0.46
17:K:58:SER:O	17:K:91:PRO:HG2	2.16	0.46
19:M:39:ILE:HG21	19:M:48:LEU:HD11	1.96	0.46
30:a:372:U:H2'	30:a:373:A:H8	1.79	0.46
30:a:1434:C:H2'	30:a:1435:U:C6	2.51	0.46
30:a:1493:A:H2'	30:a:1495:C:C5	2.50	0.46
30:a:2396:C:H2'	30:a:2397:G:O4'	2.15	0.46
30:a:2456:G:H2'	30:a:2457:C:H6	1.78	0.46
30:a:2899:U:H2'	30:a:2900:A:H8	1.81	0.46
34:e:151:GLY:HA3	34:e:191:ASP:OD1	2.16	0.46
43:n:30:ARG:HG2	43:n:30:ARG:HH11	1.81	0.46
5:4:60:PHE:CE1	25:S:9:PRO:HG2	2.51	0.46
7:A:864:A:H4'	11:E:90:THR:HG23	1.97	0.46
33:d:180:VAL:HG22	33:d:187:LEU:HD12	1.96	0.46
2:1:10:LEU:HD11	2:1:14:ARG:HE	1.81	0.46
12:F:11:HIS:ND1	12:F:12:PRO:HD2	2.31	0.46
13:G:30:LEU:HD11	13:G:116:MET:CE	2.46	0.46
30:a:2015:A:H4'	47:r:92:ARG:HH22	1.81	0.46
39:j:19:VAL:HG12	39:j:43:ILE:HG13	1.96	0.46
48:s:22:THR:O	48:s:26:LYS:HB2	2.16	0.46
49:t:14:LEU:HD11	49:t:71:ALA:HB2	1.97	0.46
49:t:92:LYS:HE3	49:t:92:LYS:HB2	1.62	0.46
7:A:75:G:H5'	7:A:76:G:OP2	2.16	0.46
7:A:323:U:H2'	7:A:324:G:O4'	2.16	0.46
7:A:1251:A:H2'	7:A:1252:A:C8	2.50	0.46
11:E:30:ILE:HG23	11:E:54:ARG:NH1	2.31	0.46
15:I:57:MET:O	15:I:57:MET:HG2	2.15	0.46
26:T:60:ARG:O	26:T:64:LYS:HG3	2.16	0.46
30:a:956:A:H2'	30:a:957:A:C8	2.51	0.46
39:j:1:MET:HG2	39:j:32:TYR:CG	2.51	0.46
5:4:60:PHE:HE2	25:S:41:PHE:HA	1.81	0.46
6:5:38:PHE:HE2	30:a:2126:G:H4'	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:193:LEU:HA	6:5:196:LEU:HD12	1.98	0.46
7:A:8:A:C6	10:D:206:LYS:HB3	2.50	0.46
7:A:41:G:H2'	7:A:42:G:H8	1.81	0.46
7:A:875:U:O2'	14:H:15:ARG:HD2	2.16	0.46
12:F:4:TYR:CE1	12:F:71:ILE:HG13	2.51	0.46
30:a:230:A:H2'	30:a:231:G:O4'	2.16	0.46
30:a:2247:G:H2'	30:a:2248:A:H8	1.81	0.46
31:b:66:A:H61	31:b:107:G:H2'	1.80	0.46
37:h:82:SER:HB2	37:h:94:ILE:HD11	1.98	0.46
46:q:43:ASN:OD1	46:q:43:ASN:O	2.34	0.46
6:5:48:LEU:HB2	6:5:169:GLY:O	2.16	0.45
6:5:94:LEU:HD13	6:5:100:LEU:HD21	1.98	0.45
6:5:193:LEU:O	6:5:197:LYS:HG2	2.17	0.45
7:A:500:G:H2'	7:A:501:C:C6	2.51	0.45
13:G:30:LEU:HD13	13:G:105:VAL:HG22	1.98	0.45
14:H:10:MET:HG3	14:H:27:MET:SD	2.56	0.45
25:S:32:ARG:HA	25:S:50:ALA:HB3	1.97	0.45
26:T:85:LYS:HB3	26:T:85:LYS:HE3	1.59	0.45
30:a:280:C:H2'	30:a:281:A:H8	1.81	0.45
30:a:1425:C:C5	30:a:1569:A:H5''	2.51	0.45
30:a:2151:C:H2'	30:a:2152:U:C6	2.51	0.45
38:i:106:LYS:HB2	38:i:106:LYS:HE2	1.61	0.45
50:u:46:LYS:O	50:u:50:MET:HG3	2.16	0.45
4:3:15:LYS:HE3	4:3:15:LYS:HB3	1.77	0.45
7:A:6:G:O2'	7:A:7:A:H8	1.99	0.45
7:A:206:C:H2'	7:A:207:C:O4'	2.16	0.45
7:A:844:G:H2'	7:A:845:A:C4'	2.44	0.45
7:A:864:A:H2'	7:A:865:A:C8	2.51	0.45
7:A:1032:G:H3'	7:A:1032:G:N3	2.31	0.45
7:A:1120:C:H2'	7:A:1121:U:C6	2.50	0.45
16:J:86:ALA:HA	16:J:89:ARG:HG3	1.98	0.45
18:L:111:LYS:HE2	18:L:111:LYS:HB2	1.67	0.45
27:V:63:C:H2'	27:V:64:G:N7	2.31	0.45
30:a:596:A:H2'	30:a:597:G:C8	2.51	0.45
30:a:876:G:H2'	30:a:877:G:H8	1.81	0.45
30:a:1105:U:C4	30:a:1106:C:C4	3.04	0.45
30:a:2573:A:N7	33:d:150:MEQ:HB3	2.31	0.45
35:f:74:VAL:HG11	35:f:77:PHE:CD2	2.50	0.45
6:5:42:VAL:HB	6:5:175:ILE:HG13	1.98	0.45
6:5:97:MET:HE2	6:5:123:VAL:HG13	1.99	0.45
7:A:149:A:H1'	7:A:1446:A:C2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:677:U:H3	7:A:713:G:H22	1.63	0.45
7:A:868:C:H2'	7:A:869:G:O4'	2.16	0.45
10:D:187:GLU:HB2	10:D:190:ASP:OD2	2.16	0.45
18:L:76:GLU:HG3	18:L:77:HIS:N	2.31	0.45
24:R:34:THR:HG23	24:R:36:SER:H	1.81	0.45
29:X:52:ALA:HB3	29:X:81:LEU:HD11	1.97	0.45
30:a:2026:C:H2'	30:a:2027:U:C6	2.51	0.45
43:n:56:LYS:HA	43:n:56:LYS:HD3	1.68	0.45
4:3:23:ILE:HD13	30:a:1029:A:H1'	1.99	0.45
30:a:1508:A:H2'	30:a:1509:A:H8	1.81	0.45
30:a:1597:A:H5''	30:a:1598:A:H5'	1.98	0.45
36:g:107:LEU:HD22	36:g:152:ARG:HB3	1.98	0.45
6:5:71:ARG:HG3	6:5:177:LYS:NZ	2.32	0.45
6:5:193:LEU:HD23	6:5:196:LEU:HD12	1.99	0.45
7:A:56:U:H2'	7:A:57:G:C8	2.51	0.45
7:A:621:A:H2'	7:A:622:A:C8	2.52	0.45
12:F:42:TRP:CZ2	12:F:102:MET:HG3	2.51	0.45
27:V:28:U:H2'	27:V:29:C:H6	1.81	0.45
30:a:906:A:H2'	30:a:909:C:H5	1.81	0.45
30:a:2729:U:O2'	30:a:2730:G:H8	1.99	0.45
7:A:950:U:H2'	7:A:951:G:C8	2.52	0.45
30:a:77:G:H2'	30:a:78:C:C6	2.51	0.45
30:a:631:C:H2'	30:a:632:C:C6	2.52	0.45
30:a:921:A:H2'	30:a:922:A:H8	1.81	0.45
30:a:2123:U:H2'	30:a:2124:G:C8	2.51	0.45
30:a:2701:A:H2'	30:a:2702:U:H6	1.80	0.45
33:d:22:ILE:HG23	33:d:190:LYS:HG3	1.99	0.45
36:g:75:MET:HE2	36:g:75:MET:HB3	1.81	0.45
40:k:121:THR:HA	40:k:141:LYS:O	2.17	0.45
7:A:202:G:H21	7:A:466:A:H61	1.64	0.45
7:A:1118:U:H1'	7:A:1179:A:C5	2.52	0.45
19:M:83:LEU:HD23	19:M:83:LEU:HA	1.78	0.45
19:M:85:CYS:O	19:M:89:LEU:HD13	2.16	0.45
30:a:30:G:H2'	30:a:31:C:C6	2.51	0.45
30:a:1175:C:H2'	30:a:1176:G:C8	2.52	0.45
30:a:1195:U:H2'	30:a:1196:U:C6	2.52	0.45
30:a:2156:U:H3'	30:a:2157:G:C8	2.52	0.45
30:a:2649:G:H2'	30:a:2650:C:C6	2.52	0.45
37:h:41:LYS:NZ	37:h:42:LYS:HD3	2.32	0.45
44:o:30:VAL:HG13	44:o:80:VAL:HG12	1.98	0.45
7:A:559:A:H4'	7:A:560:A:H3'	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:575:G:O2'	7:A:821:G:H5'	2.16	0.45
7:A:779:C:H2'	7:A:780:A:O4'	2.17	0.45
30:a:180:A:H2'	30:a:181:A:H8	1.82	0.45
30:a:1404:G:H1	30:a:1595:G:N2	2.07	0.45
30:a:1441:A:H2'	30:a:1442:G:C8	2.52	0.45
5:4:26:SER:OG	5:4:28:VAL:HG23	2.17	0.45
7:A:987:A:H2'	7:A:988:C:H6	1.81	0.45
7:A:999:C:H2'	7:A:1000:A:C8	2.51	0.45
7:A:999:C:H2'	7:A:1000:A:H8	1.81	0.45
9:C:122:SER:HA	9:C:125:GLU:OE1	2.17	0.45
10:D:105:MET:SD	10:D:180:GLY:HA3	2.57	0.45
30:a:717:U:H2'	30:a:718:A:C8	2.52	0.45
30:a:1672:A:C2	30:a:2583:G:H5'	2.52	0.45
30:a:2151:C:H2'	30:a:2152:U:H6	1.82	0.45
30:a:2183:U:H2'	30:a:2184:A:C8	2.52	0.45
30:a:2409:U:H2'	30:a:2410:G:H8	1.82	0.45
31:b:28:C:P	43:n:31:THR:HG21	2.57	0.45
39:j:43:ILE:HD11	39:j:58:LEU:HD12	1.99	0.45
50:u:26:PHE:HE2	50:u:89:ILE:HG13	1.82	0.45
51:v:53:CYS:SG	51:v:57:HIS:HA	2.57	0.45
7:A:404:G:N7	10:D:2:ALA:HB3	2.32	0.45
7:A:521:G:H4'	18:L:70:GLU:HG3	2.00	0.45
7:A:687:A:C2	7:A:704:A:C5	3.05	0.45
15:I:24:GLY:HA3	15:I:62:ASP:HB2	1.99	0.45
27:V:72:C:H2'	27:V:73:A:C8	2.52	0.45
30:a:353:A:H2'	30:a:354:U:C6	2.51	0.45
30:a:944:A:H2'	30:a:945:C:C6	2.52	0.45
30:a:1103:G:C2	30:a:1104:G:C8	3.05	0.45
30:a:1127:U:C2	30:a:2026:C:H5''	2.51	0.45
30:a:1545:A:H2'	30:a:1546:G:O4'	2.17	0.45
30:a:1641:A:H2'	30:a:1642:G:O4'	2.17	0.45
30:a:2117:G:H2'	30:a:2118:A:C6	2.52	0.45
30:a:2127:A:H4'	30:a:2128:G:O5'	2.17	0.45
30:a:2301:C:H2'	30:a:2302:C:H6	1.82	0.45
30:a:2741:A:H2'	30:a:2742:A:C8	2.52	0.45
30:a:2785:U:H2'	30:a:2786:C:H6	1.82	0.45
37:h:93:SER:HB2	37:h:121:VAL:HG13	1.98	0.45
37:h:110:VAL:HG22	37:h:114:GLU:HG3	1.99	0.45
7:A:948:C:H2'	7:A:949:A:H8	1.83	0.44
13:G:78:ARG:HB2	13:G:156:TRP:CZ3	2.50	0.44
16:J:30:LYS:HB2	16:J:30:LYS:HE2	1.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:96:LEU:HD12	20:N:96:LEU:HA	1.87	0.44
30:a:1089:C:H3'	30:a:1090:G:C8	2.51	0.44
30:a:2292:U:H2'	30:a:2293:U:H6	1.82	0.44
33:d:17:GLU:C	33:d:19:GLY:H	2.24	0.44
37:h:81:ALA:HB2	37:h:147:VAL:HG23	1.98	0.44
40:k:101:ILE:HD12	40:k:105:ILE:HB	1.99	0.44
7:A:215:C:H2'	7:A:216:U:C6	2.52	0.44
7:A:1014:A:C2	7:A:1219:A:H1'	2.52	0.44
7:A:1051:C:H2'	7:A:1052:U:C6	2.52	0.44
7:A:1314:C:H2'	7:A:1315:U:C6	2.52	0.44
19:M:86:TYR:CE2	19:M:90:ARG:HD2	2.52	0.44
22:P:15:PRO:HD2	22:P:42:LEU:HD21	1.99	0.44
30:a:579:A:H2'	30:a:580:G:H8	1.82	0.44
30:a:720:C:H2'	30:a:721:U:O4'	2.17	0.44
30:a:1179:G:H2'	30:a:1180:U:O4'	2.17	0.44
30:a:1444:C:H2'	30:a:1445:G:H8	1.81	0.44
30:a:2144:C:H2'	30:a:2145:G:O4'	2.17	0.44
33:d:71:ALA:HB3	33:d:73:VAL:HG22	1.99	0.44
53:x:54:LYS:O	53:x:58:THR:HG22	2.17	0.44
7:A:358:U:H2'	7:A:359:G:H8	1.83	0.44
7:A:428:G:H5'	7:A:430:A:O4'	2.17	0.44
7:A:1101:A:H4'	7:A:1102:A:O5'	2.16	0.44
8:B:43:LEU:HD12	8:B:43:LEU:H	1.81	0.44
10:D:167:LYS:HB2	10:D:167:LYS:HE2	1.79	0.44
30:a:65:U:H2'	30:a:66:C:H6	1.82	0.44
30:a:921:A:H2'	30:a:922:A:C8	2.51	0.44
30:a:1016:U:H2'	30:a:1017:A:C8	2.52	0.44
30:a:2133:U:O2'	30:a:2134:G:H5'	2.17	0.44
36:g:64:GLN:O	36:g:67:THR:HG22	2.16	0.44
38:i:34:ARG:HG3	38:i:39:LYS:HB2	1.99	0.44
40:k:1:MET:O	40:k:1:MET:HG2	2.18	0.44
47:r:11:ARG:HH11	47:r:82:MET:HE1	1.82	0.44
5:4:1:MET:HE3	5:4:1:MET:HB3	1.71	0.44
7:A:2:A:H1'	7:A:613:C:O2'	2.17	0.44
7:A:842:U:H2'	7:A:844:G:C6	2.53	0.44
13:G:152:ALA:O	13:G:155:ARG:HG2	2.17	0.44
15:I:127:PHE:HD2	15:I:127:PHE:O	2.00	0.44
23:Q:11:ARG:NH2	23:Q:58:LYS:HB2	2.32	0.44
30:a:555:U:H2'	30:a:556:G:C8	2.52	0.44
30:a:931:U:H2'	30:a:932:C:C6	2.52	0.44
30:a:2104:C:H2'	30:a:2105:C:C6	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2220:U:H2'	30:a:2221:U:O4'	2.17	0.44
30:a:2283:G:H4'	30:a:2390:G:O2'	2.18	0.44
30:a:2506:G:O2'	30:a:2507:U:H5''	2.18	0.44
37:h:66:ASN:N	37:h:66:ASN:HD22	2.16	0.44
6:5:30:LEU:HG	6:5:216:THR:HG23	1.98	0.44
7:A:1507:A:H2'	7:A:1508:A:C8	2.52	0.44
13:G:85:TYR:HB3	13:G:151:PHE:CD2	2.53	0.44
14:H:7:ILE:O	14:H:11:LEU:HG	2.17	0.44
30:a:1289:G:H2'	30:a:1290:C:C6	2.52	0.44
30:a:1852:A:H2'	30:a:1853:A:C8	2.53	0.44
30:a:2082:U:H2'	30:a:2083:A:H8	1.82	0.44
30:a:2108:G:H2'	30:a:2109:A:H8	1.82	0.44
37:h:23:ALA:O	37:h:27:ARG:HB3	2.18	0.44
38:i:35:ARG:HB2	38:i:54:ILE:HD11	1.98	0.44
49:t:71:ALA:HB3	49:t:80:ALA:HB1	1.98	0.44
1:0:7:GLU:HG3	1:0:27:LYS:HE2	2.00	0.44
2:1:45:SER:C	2:1:46:LYS:HG2	2.42	0.44
7:A:860:A:H2'	7:A:861:G:O4'	2.17	0.44
7:A:1038:U:H2'	7:A:1039:C:C6	2.52	0.44
7:A:1491:G:H5''	7:A:1492:A:OP2	2.17	0.44
8:B:27:MET:HE2	8:B:27:MET:HB2	1.66	0.44
12:F:88:MET:HE2	24:R:64:TYR:HD2	1.81	0.44
16:J:27:GLU:HG2	16:J:31:ARG:HD3	1.99	0.44
21:O:3:LEU:HD23	21:O:3:LEU:HA	1.83	0.44
30:a:1772:A:N7	30:a:1828:A:H1'	2.33	0.44
31:b:102:G:H2'	31:b:102:G:N3	2.32	0.44
31:b:112:G:H2'	31:b:113:C:C6	2.53	0.44
37:h:68:ARG:O	37:h:72:ILE:HG13	2.17	0.44
6:5:189:LEU:HD23	6:5:229:LEU:HD21	1.99	0.44
7:A:107:G:H1	26:T:6:SER:HB2	1.83	0.44
7:A:821:G:H2'	7:A:822:U:C6	2.52	0.44
7:A:1533:C:H42	28:W:13:A:N6	2.15	0.44
8:B:135:LEU:O	8:B:138:THR:HG22	2.18	0.44
18:L:65:SER:OG	18:L:97:THR:HG22	2.18	0.44
23:Q:30:LYS:HB2	23:Q:37:PHE:CE2	2.53	0.44
27:V:8:4SU:H6	27:V:8:4SU:O5'	2.17	0.44
30:a:196:A:H62	30:a:2431:A:H2'	1.83	0.44
30:a:564:U:H2'	30:a:565:U:O4'	2.18	0.44
30:a:1709:U:H2'	30:a:1710:G:H8	1.83	0.44
30:a:1873:C:H2'	30:a:1874:G:C8	2.52	0.44
30:a:2248:A:H2'	30:a:2249:C:C6	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2591:A:H2'	30:a:2592:C:H6	1.82	0.44
32:c:21:ASN:HB3	32:c:24:LEU:HG	2.00	0.44
7:A:212:G:H2'	7:A:213:G:C8	2.53	0.44
7:A:1286:U:H2'	7:A:1287:A:H5'	1.98	0.44
10:D:44:ARG:HG3	10:D:46:PRO:HD3	1.99	0.44
11:E:20:ARG:HG2	11:E:20:ARG:NH1	2.33	0.44
23:Q:11:ARG:HH12	23:Q:58:LYS:HD3	1.83	0.44
30:a:585:U:H2'	30:a:586:U:C6	2.53	0.44
30:a:830:A:H2'	30:a:831:G:C8	2.52	0.44
30:a:2107:U:H2'	30:a:2108:G:H8	1.82	0.44
30:a:2132:U:H4'	30:a:2133:U:H2'	2.00	0.44
30:a:2821:A:N3	30:a:2821:A:H2'	2.32	0.44
38:i:13:ARG:HG3	38:i:13:ARG:NH1	2.33	0.44
51:v:47:ALA:HB2	51:v:59:LEU:CD2	2.47	0.44
5:4:63:ARG:HG3	5:4:63:ARG:HH11	1.82	0.44
7:A:77:A:H2'	7:A:78:A:C8	2.52	0.44
7:A:361:G:H2'	7:A:362:G:O4'	2.18	0.44
7:A:512:U:H2'	7:A:513:C:C6	2.53	0.44
7:A:552:U:H2'	7:A:553:A:C8	2.53	0.44
7:A:978:A:C2	7:A:1319:A:C4	3.06	0.44
7:A:994:A:C5	7:A:1216:A:H4'	2.53	0.44
7:A:1041:G:C2	7:A:1042:A:C5	3.06	0.44
7:A:1127:G:H5'	7:A:1280:A:O2'	2.17	0.44
30:a:287:U:H2'	30:a:288:G:H8	1.83	0.44
30:a:1479:G:H2'	30:a:1480:A:H8	1.83	0.44
30:a:2013:G:OP1	47:r:98:LYS:HG2	2.17	0.44
30:a:2120:A:N6	30:a:2169:G:N2	2.34	0.44
30:a:2390:G:H5''	30:a:2391:U:O4'	2.18	0.44
32:c:34:LEU:HD23	32:c:34:LEU:HA	1.90	0.44
40:k:82:LEU:HD13	40:k:120:VAL:HG21	2.00	0.44
43:n:79:ALA:HB3	43:n:113:ALA:HB3	2.00	0.44
54:y:3:LYS:O	54:y:40:ASP:HB2	2.17	0.44
5:4:14:ALA:HB3	5:4:22:ILE:HG13	2.00	0.43
7:A:360:G:H2'	7:A:361:G:C8	2.53	0.43
1:0:29:THR:HG23	1:0:30:LYS:HG2	1.99	0.43
6:5:79:ALA:HB1	6:5:83:ASN:HB3	2.00	0.43
6:5:121:MET:HE3	6:5:121:MET:HB3	1.84	0.43
7:A:591:U:H2'	7:A:592:G:H8	1.83	0.43
7:A:1496:C:H2'	7:A:1497:G:O4'	2.18	0.43
8:B:11:LYS:HA	8:B:11:LYS:HD3	1.58	0.43
10:D:58:LYS:HE3	10:D:58:LYS:HB3	1.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:593:U:H2'	30:a:594:G:H8	1.83	0.43
30:a:1057:U:C1'	30:a:1059:G:H5'	2.48	0.43
30:a:1409:U:H2'	30:a:1410:A:C8	2.54	0.43
30:a:1534:U:H2'	30:a:1536:C:C6	2.53	0.43
30:a:1614:A:C6	47:r:87:PRO:HB3	2.53	0.43
30:a:1668:A:H4'	30:a:1669:A:O5'	2.18	0.43
30:a:2681:U:O2'	30:a:2682:C:H5'	2.18	0.43
48:s:71:GLY:O	48:s:72:GLN:HG3	2.18	0.43
54:y:24:LEU:HD11	54:y:54:MET:HE1	1.99	0.43
7:A:513:C:H2'	7:A:514:C:H6	1.82	0.43
7:A:1055:A:C6	7:A:1206:G:C5	3.06	0.43
7:A:1121:U:H2'	7:A:1122:U:H6	1.83	0.43
7:A:1220:G:P	20:N:53:ARG:HH22	2.41	0.43
9:C:68:ILE:HG22	9:C:70:THR:HG23	1.99	0.43
14:H:43:GLU:OE2	14:H:43:GLU:HA	2.17	0.43
27:V:30:G:H2'	27:V:31:G:H8	1.82	0.43
30:a:1065:G:H21	30:a:1093:A:H5'	1.83	0.43
30:a:2040:U:H2'	30:a:2041:G:C8	2.53	0.43
30:a:2121:G:H2'	30:a:2122:G:C8	2.53	0.43
6:5:129:GLN:O	30:a:2170:A:H4'	2.19	0.43
6:5:186:LYS:O	6:5:190:GLU:HG3	2.18	0.43
7:A:211:G:C4	7:A:212:G:H1'	2.53	0.43
7:A:593:U:H2'	7:A:594:C:C6	2.53	0.43
7:A:616:G:O2'	22:P:47:GLU:HG3	2.19	0.43
7:A:881:G:H2'	7:A:882:C:O4'	2.19	0.43
7:A:1171:A:H2'	7:A:1172:C:C6	2.54	0.43
16:J:52:LEU:HB2	20:N:81:ARG:HD2	2.00	0.43
29:X:81:LEU:O	29:X:85:LEU:HD23	2.19	0.43
30:a:714:C:H3'	30:a:715:A:H8	1.83	0.43
30:a:829:U:H2'	30:a:830:A:H8	1.82	0.43
30:a:1274:G:O2'	42:m:24:MET:HG2	2.18	0.43
30:a:1279:U:H2'	30:a:1280:G:O4'	2.18	0.43
30:a:2082:U:H2'	30:a:2083:A:C8	2.52	0.43
30:a:2100:U:H2'	30:a:2101:G:H8	1.84	0.43
30:a:2163:G:H2'	30:a:2164:C:O4'	2.18	0.43
31:b:13:U:O2'	31:b:15:A:H2'	2.17	0.43
47:r:21:ALA:HB1	47:r:74:ILE:HG12	2.01	0.43
7:A:857:C:H2'	7:A:858:G:O4'	2.18	0.43
7:A:1027:C:H2'	7:A:1028:C:C6	2.52	0.43
7:A:1532:U:H2'	7:A:1533:C:C6	2.54	0.43
8:B:131:LYS:HE3	8:B:131:LYS:HB3	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2804:C:H2'	30:a:2805:U:C6	2.54	0.43
35:f:149:VAL:HG12	35:f:149:VAL:O	2.19	0.43
44:o:72:ARG:HE	44:o:72:ARG:HB3	1.70	0.43
50:u:20:LEU:HD22	50:u:25:LYS:HB2	2.00	0.43
7:A:399:G:H2'	7:A:400:C:C6	2.53	0.43
7:A:745:A:H2'	7:A:746:A:H8	1.81	0.43
23:Q:21:ILE:HG13	23:Q:46:VAL:HB	2.00	0.43
27:V:77:A:N6	30:a:2422:G:H2'	2.34	0.43
30:a:836:U:H2'	30:a:837:C:C6	2.54	0.43
30:a:2444:C:OP1	34:e:63:LYS:HD3	2.18	0.43
30:a:2688:U:H2'	30:a:2689:G:O4'	2.18	0.43
41:l:56:ALA:HB2	41:l:119:LEU:HD12	2.00	0.43
48:s:47:VAL:HG13	48:s:51:PHE:HD2	1.82	0.43
8:B:114:LEU:HB2	8:B:144:LEU:HB3	2.00	0.43
30:a:38:A:H2'	30:a:39:G:O4'	2.19	0.43
30:a:860:A:H2'	30:a:861:G:C8	2.53	0.43
30:a:884:U:H4'	30:a:886:C:H41	1.82	0.43
30:a:1100:A:H5''	30:a:1101:C:H5	1.84	0.43
30:a:2066:C:H2'	30:a:2067:C:C6	2.53	0.43
36:g:128:GLN:OE1	36:g:128:GLN:HA	2.19	0.43
38:i:73:MET:SD	38:i:88:THR:HG22	2.58	0.43
40:k:141:LYS:HE2	40:k:141:LYS:HB3	1.56	0.43
6:5:38:PHE:CE2	30:a:2126:G:H4'	2.54	0.43
7:A:205:A:C5	7:A:206:C:C5	3.06	0.43
7:A:737:C:H2'	7:A:738:C:H6	1.84	0.43
7:A:1162:C:H2'	7:A:1163:A:C8	2.54	0.43
7:A:1428:A:H2'	7:A:1429:A:O4'	2.19	0.43
10:D:59:GLN:HE21	10:D:63:ARG:HH21	1.66	0.43
16:J:41:PRO:HA	16:J:72:ARG:HD3	2.00	0.43
30:a:363:C:H2'	30:a:364:U:H6	1.83	0.43
31:b:42:C:C6	35:f:66:LEU:HB2	2.54	0.43
32:c:16:VAL:HG22	32:c:206:GLY:HA3	2.00	0.43
37:h:42:LYS:HA	37:h:42:LYS:HD2	1.67	0.43
55:z:54:VAL:O	55:z:55:ILE:HD13	2.18	0.43
5:4:60:PHE:C	5:4:60:PHE:CD1	2.95	0.43
6:5:50:ILE:HG22	6:5:204:ALA:HB2	2.01	0.43
7:A:1035:A:H1'	7:A:1036:A:OP1	2.18	0.43
11:E:126:LYS:HA	11:E:126:LYS:HD2	1.90	0.43
16:J:85:ASP:HB3	16:J:89:ARG:NH1	2.34	0.43
30:a:656:G:H4'	34:e:95:LYS:HD3	2.01	0.43
31:b:49:C:H2'	31:b:50:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:35:ARG:HD2	38:i:140:LEU:HD21	2.00	0.43
6:5:37:LYS:H	6:5:37:LYS:HD2	1.84	0.43
7:A:56:U:H2'	7:A:57:G:H8	1.84	0.43
7:A:461:G:O2'	7:A:462:G:H8	2.02	0.43
7:A:495:A:N6	10:D:120:HIS:HE1	2.17	0.43
7:A:545:C:H5'	10:D:69:GLU:CB	2.49	0.43
7:A:950:U:H2'	7:A:951:G:H8	1.84	0.43
7:A:1000:A:H2'	7:A:1001:G:C8	2.54	0.43
7:A:1375:A:H2'	7:A:1376:U:O4'	2.18	0.43
10:D:13:ARG:HB3	10:D:36:GLN:O	2.19	0.43
15:I:5:GLN:HG3	15:I:22:LYS:CG	2.49	0.43
15:I:60:LYS:O	15:I:61:LEU:HD22	2.19	0.43
20:N:88:ALA:HB2	20:N:96:LEU:HD23	2.01	0.43
30:a:2126:G:H21	30:a:2174:A:H62	1.67	0.43
30:a:2128:G:C6	30:a:2163:G:C2	3.07	0.43
30:a:2301:C:H2'	30:a:2302:C:C6	2.54	0.43
30:a:2409:U:H2'	30:a:2410:G:C8	2.54	0.43
46:q:51:VAL:O	46:q:51:VAL:HG12	2.19	0.43
7:A:451:A:H1'	7:A:452:A:C2	2.54	0.42
7:A:719:C:O2'	24:R:38:LYS:HB3	2.19	0.42
30:a:482:A:O2'	49:t:57:GLY:HA2	2.18	0.42
30:a:1364:A:N7	30:a:1365:G:H1'	2.34	0.42
30:a:2788:C:H1'	33:d:63:PRO:HG3	2.00	0.42
31:b:48:U:H2'	31:b:49:C:C6	2.54	0.42
31:b:49:C:H2'	31:b:50:A:H8	1.84	0.42
34:e:123:LYS:HB3	34:e:123:LYS:HE3	1.66	0.42
36:g:11:ILE:H	36:g:11:ILE:HG13	1.68	0.42
50:u:48:TRP:HE3	50:u:86:LEU:HD12	1.83	0.42
7:A:160:A:H2'	7:A:161:A:O4'	2.19	0.42
7:A:493:A:H2'	7:A:494:G:C8	2.54	0.42
7:A:845:A:P	24:R:15:ALA:HA	2.59	0.42
7:A:979:C:H41	7:A:1360:A:H62	1.67	0.42
19:M:51:GLU:O	19:M:55:THR:HG22	2.19	0.42
30:a:84:A:C2	30:a:102:A:C5	3.07	0.42
30:a:196:A:N6	30:a:2431:A:H2'	2.34	0.42
30:a:403:A:H1'	30:a:404:U:OP2	2.19	0.42
30:a:840:G:H2'	30:a:841:A:C8	2.54	0.42
30:a:1076:C:H2'	30:a:1077:A:C8	2.54	0.42
30:a:1431:A:H2'	30:a:1432:G:H8	1.82	0.42
30:a:2272:G:OP1	51:v:18:ALA:HB1	2.19	0.42
30:a:2650:C:H2'	30:a:2651:U:H6	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:29:A:H2'	31:b:30:C:C6	2.54	0.42
36:g:39:LYS:HE2	36:g:58:PHE:CE1	2.54	0.42
43:n:16:ARG:HE	43:n:16:ARG:HB3	1.49	0.42
7:A:156:C:H2'	7:A:157:U:O4'	2.19	0.42
7:A:232:G:H1'	7:A:262:A:N1	2.33	0.42
7:A:513:C:H2'	7:A:514:C:C6	2.55	0.42
7:A:1005:A:H4'	7:A:1037:C:O2'	2.18	0.42
7:A:1219:A:H2'	7:A:1220:G:C8	2.55	0.42
9:C:117:ALA:HB1	9:C:187:SER:OG	2.20	0.42
27:V:21:H2U:H1'	27:V:22:A:H5'	2.01	0.42
30:a:2413:A:H2'	30:a:2414:G:O4'	2.18	0.42
30:a:2637:U:H4'	33:d:81:GLU:OE1	2.19	0.42
35:f:93:GLY:H	35:f:96:MET:HE3	1.85	0.42
44:o:9:GLU:O	44:o:13:MET:HG3	2.20	0.42
50:u:14:LYS:O	50:u:18:ARG:HG3	2.19	0.42
55:z:40:ARG:HG2	55:z:41:HIS:ND1	2.33	0.42
7:A:246:A:C2	7:A:282:A:C5	3.07	0.42
7:A:660:U:H2'	7:A:661:G:O4'	2.20	0.42
7:A:736:C:H2'	7:A:737:C:C6	2.54	0.42
7:A:950:U:OP2	19:M:101:ARG:HD2	2.19	0.42
8:B:10:LEU:HD12	8:B:10:LEU:HA	1.89	0.42
16:J:50:THR:HG23	16:J:64:GLN:HG2	2.01	0.42
17:K:16:VAL:HG23	17:K:77:TYR:HB3	2.01	0.42
30:a:38:A:H5'	34:e:45:ALA:HB3	2.01	0.42
30:a:1180:U:H2'	30:a:1181:U:C6	2.54	0.42
30:a:2305:G:N2	30:a:2313:U:H3	1.96	0.42
30:a:2374:G:H2'	30:a:2375:C:C6	2.54	0.42
30:a:2691:U:O2'	30:a:2873:A:H1'	2.19	0.42
6:5:94:LEU:HD23	6:5:94:LEU:HA	1.91	0.42
7:A:57:G:H2'	7:A:58:C:C6	2.54	0.42
7:A:1319:A:C8	7:A:1323:G:C6	3.07	0.42
20:N:37:SER:HB3	20:N:40:ASP:OD2	2.19	0.42
27:V:9:G:H21	27:V:46:G:H3'	1.85	0.42
27:V:20:G:N2	27:V:58:A:H1'	2.33	0.42
30:a:555:U:H2'	30:a:556:G:H8	1.85	0.42
30:a:1589:U:H2'	30:a:1590:A:H8	1.84	0.42
37:h:5:LEU:HD21	37:h:12:LEU:HD23	2.01	0.42
47:r:95:ARG:HG3	47:r:95:ARG:NH1	2.32	0.42
49:t:47:LYS:HB2	49:t:47:LYS:HE3	1.66	0.42
6:5:114:VAL:HG11	6:5:131:LEU:HD13	2.02	0.42
6:5:154:LYS:HB2	6:5:154:LYS:HE2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:412:A:O2'	7:A:413:G:H4'	2.18	0.42
7:A:695:A:H2'	7:A:696:A:C8	2.54	0.42
8:B:68:LEU:HD21	8:B:151:ILE:HG22	2.02	0.42
29:X:56:VAL:HG22	29:X:57:ASN:H	1.84	0.42
30:a:30:G:H2'	30:a:31:C:H6	1.85	0.42
30:a:142:C:H2'	30:a:143:A:C8	2.54	0.42
30:a:825:U:H4'	30:a:828:G:N1	2.35	0.42
30:a:2176:C:H2'	30:a:2177:A:H8	1.85	0.42
30:a:2252:OMG:HM23	30:a:2252:OMG:H1'	1.75	0.42
30:a:2651:U:H2'	30:a:2652:C:H6	1.83	0.42
31:b:78:A:H2'	31:b:79:G:O4'	2.20	0.42
35:f:106:ILE:HG21	35:f:139:PRO:HG3	2.02	0.42
41:l:58:LYS:HE3	41:l:58:LYS:HB3	1.88	0.42
6:5:79:ALA:O	6:5:97:MET:HB2	2.19	0.42
6:5:161:VAL:HG11	6:5:173:THR:OG1	2.20	0.42
7:A:264:C:H2'	7:A:265:G:O4'	2.20	0.42
7:A:1004:A:C5	7:A:1026:G:H1'	2.55	0.42
8:B:49:MET:HE2	8:B:199:VAL:O	2.18	0.42
12:F:102:MET:HE3	12:F:102:MET:HB3	1.75	0.42
15:I:10:GLY:HA3	15:I:78:ALA:O	2.20	0.42
30:a:2:G:H2'	30:a:3:U:H6	1.84	0.42
30:a:5:A:H2'	30:a:6:A:H8	1.84	0.42
30:a:1785:A:H1'	30:a:1939:A:N6	2.35	0.42
30:a:2234:U:H2'	30:a:2235:G:H8	1.83	0.42
30:a:2681:U:OP1	33:d:114:LYS:HG3	2.20	0.42
40:k:123:ARG:HG2	40:k:123:ARG:HH11	1.84	0.42
45:p:15:LYS:HB3	45:p:15:LYS:HE3	1.64	0.42
46:q:94:THR:HG22	46:q:96:VAL:HG13	2.01	0.42
52:w:12:PRO:HB3	52:w:30:LEU:HD23	2.00	0.42
6:5:60:ARG:HD3	6:5:141:LYS:HD3	2.02	0.42
7:A:845:A:H2'	7:A:846:G:O4'	2.20	0.42
10:D:7:PRO:HB2	10:D:10:LYS:HB2	2.02	0.42
14:H:50:LYS:HE3	14:H:50:LYS:HB3	1.78	0.42
19:M:12:GLN:CD	19:M:12:GLN:H	2.28	0.42
30:a:478:A:N3	30:a:480:G:H5''	2.34	0.42
30:a:2108:G:H1	30:a:2183:U:H3	1.68	0.42
30:a:2757:U:H1'	30:a:2758:A:H5''	2.01	0.42
38:i:4:PHE:CD2	45:p:100:VAL:HG11	2.55	0.42
53:x:19:LEU:O	53:x:23:ARG:HG3	2.20	0.42
2:1:26:ASN:CG	30:a:679:G:H5'	2.45	0.42
4:3:1:MET:HE3	30:a:2743:G:H5''	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:7:A:H2'	11:E:124:LEU:HD22	2.02	0.42
7:A:986:U:H2'	7:A:987:A:O4'	2.19	0.42
19:M:11:ASP:HA	19:M:45:ILE:HB	2.01	0.42
27:V:25:U:H2'	27:V:26:C:H6	1.85	0.42
30:a:1102:U:H2'	30:a:1103:G:H8	1.82	0.42
30:a:2548:A:H2'	30:a:2549:U:H6	1.84	0.42
35:f:117:LEU:HD12	35:f:176:PRO:HG2	2.01	0.42
42:m:72:ASP:HB3	42:m:75:ILE:HB	2.02	0.42
2:1:26:ASN:ND2	30:a:679:G:H5'	2.35	0.42
3:2:35:LYS:HD3	30:a:2391:U:P	2.60	0.42
7:A:148:G:H2'	7:A:149:A:O4'	2.20	0.42
7:A:398:U:H2'	7:A:399:G:C8	2.55	0.42
7:A:744:C:H2'	7:A:745:A:H8	1.85	0.42
7:A:1206:G:C4	7:A:1207:2MG:C8	3.08	0.42
7:A:1436:U:H2'	7:A:1437:A:C8	2.55	0.42
14:H:111:MET:HE2	14:H:111:MET:HB3	1.73	0.42
29:X:45:LYS:HG2	29:X:46:VAL:HG23	2.02	0.42
30:a:175:A:O2'	30:a:176:G:H5'	2.19	0.42
30:a:1492:A:H2'	30:a:1493:A:C8	2.55	0.42
30:a:2178:C:H2'	30:a:2179:C:O4'	2.20	0.42
30:a:2190:U:H2'	30:a:2191:G:O4'	2.19	0.42
30:a:2515:U:H2'	30:a:2516:C:H6	1.83	0.42
6:5:48:LEU:HA	6:5:208:TYR:O	2.19	0.41
7:A:222:C:H2'	7:A:223:A:H8	1.85	0.41
7:A:473:U:H3'	7:A:474:G:H8	1.84	0.41
7:A:1011:C:H2'	7:A:1012:A:C8	2.54	0.41
7:A:1072:G:N2	8:B:106:THR:HG21	2.35	0.41
7:A:1218:U:H2'	7:A:1219:A:H8	1.83	0.41
7:A:1330:U:H2'	7:A:1331:G:O4'	2.20	0.41
18:L:80:ILE:HG22	18:L:104:CYS:HB2	2.02	0.41
24:R:55:LEU:HG	24:R:59:ILE:HD12	2.02	0.41
27:V:37:U:H2'	27:V:38:A:O4'	2.20	0.41
30:a:595:U:H2'	30:a:596:A:H8	1.84	0.41
30:a:816:A:H5''	30:a:970:A:N1	2.35	0.41
30:a:888:G:H2'	30:a:889:G:C8	2.55	0.41
30:a:981:A:N3	30:a:981:A:H2'	2.35	0.41
30:a:1176:G:H2'	30:a:1177:U:C6	2.55	0.41
30:a:1439:U:H2'	30:a:1440:C:H6	1.85	0.41
30:a:1826:U:OP2	32:c:221:ARG:HD2	2.20	0.41
31:b:30:C:H2'	31:b:31:C:H5'	2.02	0.41
31:b:112:G:H2'	31:b:113:C:H6	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:h:47:PHE:CE1	37:h:56:ALA:HB2	2.55	0.41
4:3:1:MET:HE2	4:3:1:MET:HB2	1.87	0.41
5:4:56:ARG:HD2	5:4:56:ARG:HA	1.85	0.41
7:A:205:A:C4	7:A:206:C:C5	3.08	0.41
7:A:211:G:C5	7:A:212:G:H1'	2.54	0.41
7:A:376:G:H5''	22:P:5:ARG:HD2	2.01	0.41
7:A:967:5MC:H4'	15:I:127:PHE:CZ	2.47	0.41
8:B:87:CYS:HB2	8:B:221:VAL:HG13	2.01	0.41
10:D:11:LEU:HD13	10:D:63:ARG:HG2	2.02	0.41
18:L:86:ARG:NH1	18:L:88:LYS:HD2	2.35	0.41
29:X:33:ARG:HB3	29:X:57:ASN:HB2	2.02	0.41
30:a:589:A:H2'	30:a:590:U:C6	2.55	0.41
35:f:57:LEU:HD23	35:f:57:LEU:HA	1.75	0.41
40:k:110:VAL:HB	40:k:127:VAL:HG13	2.01	0.41
41:l:50:ARG:HD3	41:l:65:ILE:HD11	2.02	0.41
1:0:38:LYS:HB2	1:0:49:TYR:CD1	2.55	0.41
2:1:45:SER:HB3	2:1:46:LYS:NZ	2.35	0.41
7:A:1121:U:H2'	7:A:1122:U:C6	2.55	0.41
7:A:1169:A:H2'	7:A:1170:A:C8	2.54	0.41
7:A:1402:4OC:H2'	7:A:1403:C:O4'	2.20	0.41
7:A:1446:A:H8	7:A:1446:A:OP1	2.03	0.41
17:K:21:ALA:HB2	17:K:82:LEU:HD13	2.03	0.41
18:L:108:LYS:HB3	18:L:109:ASP:H	1.54	0.41
25:S:11:ILE:HG21	25:S:16:LEU:HG	2.01	0.41
30:a:1039:G:H2'	30:a:1040:C:C6	2.55	0.41
30:a:1743:A:H3'	30:a:1744:A:H8	1.85	0.41
33:d:136:ASN:HB3	33:d:140:HIS:CE1	2.56	0.41
38:i:110:PRO:O	38:i:115:GLY:HA3	2.20	0.41
50:u:48:TRP:CE3	50:u:86:LEU:HD12	2.55	0.41
7:A:883:C:O2'	7:A:884:U:H5'	2.20	0.41
7:A:1465:A:H2'	7:A:1466:C:C6	2.55	0.41
8:B:130:THR:C	8:B:132:LYS:H	2.29	0.41
9:C:123:GLN:HB3	9:C:128:VAL:HB	2.02	0.41
27:V:15:G:N2	27:V:49:C:O2	2.45	0.41
30:a:1221:U:H2'	30:a:1222:G:C8	2.55	0.41
30:a:1441:A:H2'	30:a:1442:G:H8	1.85	0.41
30:a:1511:G:H2'	30:a:1512:C:C6	2.55	0.41
30:a:2074:C:C5'	32:c:228:VAL:CG2	2.96	0.41
31:b:106:G:H2'	31:b:107:G:O4'	2.20	0.41
40:k:92:LEU:HD23	40:k:92:LEU:HA	1.76	0.41
6:5:98:GLU:HG2	6:5:99:ASP:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:41:G:H2'	7:A:42:G:C8	2.55	0.41
7:A:608:A:H2'	7:A:609:A:O4'	2.20	0.41
7:A:1120:C:C2	7:A:1121:U:C5	3.09	0.41
7:A:1319:A:C8	7:A:1323:G:C5	3.09	0.41
10:D:104:ARG:HD2	10:D:170:TRP:CZ2	2.55	0.41
11:E:159:LYS:HB2	11:E:164:ILE:HD13	2.01	0.41
23:Q:44:LEU:HD22	23:Q:73:TRP:CD1	2.56	0.41
25:S:3:ARG:NE	25:S:10:PHE:HB2	2.32	0.41
29:X:3:LEU:HD12	29:X:5:ILE:HG13	2.01	0.41
30:a:595:U:H2'	30:a:596:A:C8	2.54	0.41
30:a:1806:G:P	32:c:48:ARG:NH1	2.94	0.41
35:f:137:ILE:HG13	35:f:138:PHE:N	2.34	0.41
41:l:133:LYS:HB3	41:l:133:LYS:HE3	1.87	0.41
47:r:13:SER:O	47:r:17:VAL:HG23	2.20	0.41
48:s:69:ARG:HA	48:s:73:ARG:O	2.21	0.41
5:4:62:LYS:HE3	5:4:62:LYS:HB3	1.89	0.41
7:A:1435:G:H2'	7:A:1436:U:C6	2.56	0.41
8:B:15:HIS:CB	8:B:43:LEU:HD11	2.51	0.41
12:F:66:ALA:HB3	12:F:71:ILE:HD11	2.02	0.41
13:G:76:LYS:HE2	13:G:156:TRP:CE2	2.56	0.41
22:P:55:ASP:OD2	22:P:55:ASP:C	2.63	0.41
30:a:1100:A:N3	30:a:1100:A:H2'	2.35	0.41
30:a:1680:U:H2'	30:a:1681:G:O4'	2.20	0.41
30:a:2120:A:N7	30:a:2171:A:C6	2.87	0.41
30:a:2334:A:H5'	30:a:2336:A:H1'	2.03	0.41
30:a:2468:C:H2'	30:a:2469:A:O4'	2.20	0.41
30:a:2785:U:H2'	30:a:2786:C:C6	2.56	0.41
30:a:2820:G:H2'	30:a:2822:A:N7	2.35	0.41
34:e:21:ARG:HD3	34:e:106:LYS:HB3	2.02	0.41
36:g:62:TRP:CE3	36:g:62:TRP:HA	2.55	0.41
39:j:23:LYS:HB3	39:j:40:LYS:HB3	2.01	0.41
7:A:86:G:C8	7:A:87:C:C4	3.08	0.41
7:A:91:U:H2'	7:A:92:U:C6	2.55	0.41
7:A:144:G:H2'	7:A:145:G:C8	2.56	0.41
7:A:632:U:H5''	7:A:633:G:C8	2.55	0.41
7:A:911:U:H2'	7:A:912:C:C6	2.55	0.41
7:A:1001:G:H2'	7:A:1002:A:H8	1.85	0.41
7:A:1125:U:O2'	7:A:1126:U:H2'	2.21	0.41
7:A:1294:G:H2'	7:A:1295:U:C6	2.55	0.41
8:B:5:SER:O	8:B:9:MET:HG3	2.21	0.41
13:G:72:THR:HA	13:G:96:ARG:HE	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:127:PHE:O	15:I:128:SER:HB3	2.19	0.41
17:K:85:MET:HB3	17:K:113:VAL:HG21	2.03	0.41
17:K:90:GLY:O	17:K:93:ARG:HG2	2.20	0.41
20:N:46:LEU:HD22	25:S:13:LEU:HD13	2.03	0.41
24:R:63:ARG:HD3	24:R:70:TYR:CD1	2.56	0.41
27:V:65:G:C6	27:V:66:C:C4	3.09	0.41
30:a:474:C:H4'	30:a:509:C:H5'	2.01	0.41
30:a:637:C:H2'	30:a:638:U:C6	2.56	0.41
30:a:859:G:H2'	30:a:860:A:O4'	2.21	0.41
30:a:1061:C:H5'	30:a:1063:U:C4	2.56	0.41
30:a:2231:G:H2'	30:a:2232:U:C6	2.56	0.41
30:a:2675:G:H4'	39:j:30:ARG:HG3	2.02	0.41
31:b:101:A:N3	31:b:102:G:H1'	2.36	0.41
35:f:102:ARG:O	35:f:106:ILE:HB	2.19	0.41
42:m:71:ARG:HA	42:m:71:ARG:HD2	1.86	0.41
53:x:49:ASN:O	53:x:53:VAL:HG23	2.20	0.41
1:O:26:ASN:HB3	1:O:29:THR:HG22	2.01	0.41
7:A:215:C:H2'	7:A:216:U:H6	1.85	0.41
7:A:763:G:H2'	7:A:764:C:H6	1.86	0.41
13:G:4:ARG:O	13:G:6:VAL:HG23	2.21	0.41
14:H:41:LYS:HD2	14:H:48:ASP:HA	2.03	0.41
20:N:27:LEU:O	20:N:31:ILE:HG12	2.19	0.41
25:S:16:LEU:HD23	25:S:16:LEU:HA	1.86	0.41
27:V:35:C:C5	29:X:92:LEU:HG	2.55	0.41
30:a:95:A:H2'	30:a:96:C:O4'	2.20	0.41
30:a:1057:U:H1'	30:a:1059:G:H5'	2.03	0.41
30:a:1174:G:H2'	30:a:1175:C:H6	1.84	0.41
30:a:2020:A:H4'	45:p:34:VAL:HG21	2.03	0.41
30:a:2470:A:H2'	30:a:2471:G:O4'	2.21	0.41
30:a:2638:U:H5''	33:d:83:ARG:NH1	2.36	0.41
35:f:80:ARG:H	35:f:80:ARG:HG2	1.74	0.41
39:j:41:ILE:HD13	39:j:60:ALA:HB2	2.03	0.41
53:x:26:PHE:HE1	53:x:30:MET:HE2	1.85	0.41
3:2:9:GLY:O	3:2:13:ARG:HD3	2.21	0.41
4:3:22:VAL:HG21	4:3:36:ARG:NH2	2.36	0.41
6:5:111:PHE:CD1	6:5:114:VAL:HG22	2.56	0.41
7:A:76:G:N3	7:A:76:G:H2'	2.36	0.41
7:A:157:U:O2'	7:A:158:G:H5'	2.21	0.41
7:A:440:C:H2'	7:A:441:A:H8	1.84	0.41
7:A:696:A:H2'	7:A:697:U:H6	1.85	0.41
7:A:745:A:O2'	7:A:746:A:H5'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1011:C:H2'	7:A:1012:A:H8	1.86	0.41
7:A:1302:C:C5	19:M:17:ILE:HG13	2.56	0.41
7:A:1530:G:H2'	7:A:1531:A:C8	2.56	0.41
8:B:167:ASP:OD1	8:B:167:ASP:C	2.64	0.41
10:D:8:LYS:HB3	10:D:21:LEU:HB3	2.02	0.41
11:E:152:MET:HG3	11:E:152:MET:H	1.66	0.41
11:E:157:ARG:NE	11:E:164:ILE:HD11	2.36	0.41
11:E:162:GLU:HG2	11:E:163:GLU:N	2.35	0.41
21:O:8:LYS:HG2	21:O:31:LEU:HD22	2.03	0.41
30:a:96:C:H2'	30:a:97:C:C6	2.55	0.41
30:a:277:A:N3	30:a:277:A:H3'	2.36	0.41
30:a:894:C:H2'	30:a:895:C:C6	2.56	0.41
30:a:1033:G:C6	30:a:1117:G:C6	3.09	0.41
30:a:1427:G:H2'	30:a:1428:A:O4'	2.21	0.41
30:a:1806:G:OP1	32:c:48:ARG:NH1	2.46	0.41
30:a:1988:A:H2'	30:a:1989:G:H8	1.86	0.41
30:a:2106:U:H2'	30:a:2107:U:H6	1.84	0.41
30:a:2378:A:H2'	30:a:2379:A:C8	2.55	0.41
35:f:128:TYR:CE2	35:f:130:MET:HB3	2.55	0.41
41:l:117:PHE:HD2	41:l:130:PHE:CD1	2.39	0.41
43:n:33:ARG:HG2	43:n:34:HIS:CD2	2.55	0.41
46:q:38:VAL:HG22	46:q:59:ILE:HG13	2.02	0.41
52:w:3:ARG:O	52:w:12:PRO:HD3	2.21	0.41
53:x:46:VAL:O	53:x:50:VAL:HG23	2.21	0.41
3:2:25:LYS:HB3	40:k:62:PRO:HG2	2.03	0.41
6:5:71:ARG:HG3	6:5:177:LYS:HZ3	1.84	0.41
7:A:492:C:H2'	7:A:493:A:C8	2.56	0.41
7:A:665:A:H1'	7:A:733:G:H5'	2.04	0.41
10:D:9:LEU:HD13	10:D:32:CYS:HB3	2.03	0.41
21:O:14:GLU:HG2	21:O:14:GLU:H	1.79	0.41
27:V:57:C:H2'	27:V:58:A:O4'	2.21	0.41
30:a:740:A:OP1	33:d:135:GLY:HA2	2.21	0.41
30:a:781:G:C6	32:c:228:VAL:HG21	2.56	0.41
30:a:945:C:H1'	30:a:981:A:C8	2.56	0.41
30:a:1709:U:H2'	30:a:1710:G:C8	2.55	0.41
30:a:1774:U:O4	30:a:1788:A:H2	2.04	0.41
30:a:2365:C:H2'	30:a:2366:G:O4'	2.21	0.41
35:f:57:LEU:HD13	35:f:89:VAL:HG23	2.03	0.41
41:l:33:LEU:HD13	41:l:117:PHE:HB3	2.02	0.41
45:p:31:VAL:HG12	45:p:34:VAL:H	1.86	0.41
6:5:132:GLY:C	6:5:135:GLY:H	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:236:A:H2'	7:A:237:G:C8	2.56	0.40
7:A:847:G:H2'	7:A:848:C:C6	2.56	0.40
7:A:1010:C:H2'	7:A:1011:C:C6	2.56	0.40
7:A:1019:G:H2'	7:A:1020:A:O4'	2.21	0.40
16:J:73:LEU:HD12	16:J:73:LEU:HA	1.81	0.40
18:L:75:GLN:O	18:L:76:GLU:HB3	2.20	0.40
23:Q:77:ARG:NH2	23:Q:79:VAL:HG12	2.35	0.40
30:a:1076:C:C5	30:a:1085:A:C4	3.08	0.40
30:a:1082:A:H1'	30:a:1102:U:H1'	2.02	0.40
30:a:1196:U:H2'	30:a:1197:C:C6	2.56	0.40
30:a:2347:A:H3'	30:a:2348:C:H5''	2.02	0.40
30:a:2805:U:H2'	30:a:2806:C:C6	2.56	0.40
31:b:24:G:N7	31:b:56:G:H2'	2.36	0.40
34:e:127:GLU:HA	34:e:127:GLU:OE1	2.21	0.40
39:j:13:ASN:HB3	39:j:100:PHE:CZ	2.55	0.40
41:l:18:ARG:HE	41:l:18:ARG:HB3	1.77	0.40
47:r:55:ILE:HG13	47:r:55:ILE:H	1.69	0.40
49:t:6:ARG:HE	49:t:6:ARG:HB3	1.79	0.40
7:A:77:A:H2'	7:A:78:A:H8	1.86	0.40
7:A:593:U:H2'	7:A:594:C:H6	1.86	0.40
7:A:1355:G:H2'	7:A:1356:G:C8	2.54	0.40
12:F:5:GLU:HG3	12:F:63:ASN:ND2	2.37	0.40
24:R:25:ASP:O	24:R:29:LEU:HG	2.21	0.40
29:X:13:THR:HG22	29:X:15:ALA:H	1.85	0.40
30:a:96:C:H2'	30:a:97:C:H6	1.86	0.40
30:a:127:C:H2'	30:a:128:C:H6	1.86	0.40
30:a:467:G:H5''	34:e:55:SER:HB3	2.03	0.40
30:a:2199:A:C4	37:h:29:PHE:HB2	2.57	0.40
30:a:2481:C:H2'	30:a:2482:G:O4'	2.20	0.40
30:a:2650:C:H2'	30:a:2651:U:C6	2.55	0.40
31:b:28:C:OP1	43:n:31:THR:HG21	2.21	0.40
7:A:625:U:H2'	7:A:626:G:H8	1.86	0.40
7:A:648:A:H2'	7:A:649:G:O4'	2.22	0.40
8:B:157:LEU:HD23	8:B:157:LEU:HA	1.86	0.40
9:C:147:LYS:HD3	9:C:147:LYS:HA	1.82	0.40
13:G:47:LEU:HD12	13:G:58:GLU:HB3	2.03	0.40
27:V:20:G:H4'	27:V:21:H2U:OP2	2.22	0.40
29:X:23:LYS:HE2	29:X:23:LYS:HB2	1.90	0.40
30:a:69:C:H4'	30:a:75:G:N7	2.37	0.40
30:a:130:A:H2'	30:a:131:G:C8	2.56	0.40
30:a:753:A:H2'	30:a:754:G:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1414:C:H2'	30:a:1415:G:O4'	2.20	0.40
30:a:1424:A:H4'	30:a:1425:C:O4'	2.21	0.40
30:a:1505:A:N3	30:a:1505:A:H2'	2.36	0.40
30:a:1781:U:H1'	30:a:2610:U:H5''	2.03	0.40
30:a:2462:A:H2'	30:a:2463:C:H6	1.87	0.40
37:h:73:ASN:O	37:h:142:LEU:HD13	2.22	0.40
40:k:109:LYS:HA	40:k:126:ARG:O	2.22	0.40
7:A:131:A:H2'	7:A:132:C:H6	1.85	0.40
7:A:320:A:H2'	7:A:321:A:O4'	2.20	0.40
7:A:440:C:C2	7:A:441:A:C8	3.10	0.40
7:A:486:U:H2'	7:A:487:A:H8	1.86	0.40
7:A:982:U:H4'	7:A:983:A:O4'	2.21	0.40
7:A:1157:A:C2	7:A:1181:G:C4	3.10	0.40
7:A:1250:A:H2'	7:A:1251:A:C8	2.56	0.40
7:A:1318:A:O2'	25:S:37:ARG:HD3	2.21	0.40
7:A:1534:A:H2'	7:A:1535:C:H6	1.86	0.40
8:B:161:LEU:HD23	8:B:183:VAL:HG13	2.02	0.40
10:D:21:LEU:HD23	10:D:21:LEU:HA	1.89	0.40
10:D:103:TYR:CE1	10:D:110:THR:HA	2.56	0.40
29:X:45:LYS:HE2	29:X:45:LYS:HB3	1.92	0.40
30:a:498:U:H2'	30:a:499:G:O4'	2.21	0.40
30:a:739:A:H2'	30:a:740:A:H8	1.84	0.40
30:a:976:A:H2'	30:a:979:C:H42	1.86	0.40
30:a:1324:A:H2'	30:a:1325:A:O4'	2.22	0.40
30:a:1550:U:H2'	30:a:1551:A:H8	1.84	0.40
30:a:1653:G:H3'	42:m:2:ARG:HG2	2.02	0.40
30:a:1683:U:H2'	30:a:1684:G:C8	2.56	0.40
30:a:1789:C:H2'	30:a:1790:A:C8	2.56	0.40
30:a:1811:U:H2'	30:a:1812:G:H8	1.86	0.40
30:a:2516:C:H2'	30:a:2517:A:C8	2.55	0.40
35:f:58:THR:HG22	35:f:65:PRO:HD3	2.04	0.40
41:l:63:ILE:HG12	41:l:105:MET:CG	2.52	0.40
4:3:4:ARG:O	4:3:37:GLN:HA	2.22	0.40
7:A:629:A:H2'	7:A:630:A:O4'	2.21	0.40
7:A:1513:A:H2'	7:A:1514:G:H8	1.86	0.40
7:A:1533:C:H42	28:W:13:A:H61	1.69	0.40
10:D:23:SER:HB2	10:D:161:LEU:HD13	2.03	0.40
10:D:142:VAL:HG13	10:D:179:GLU:OE1	2.21	0.40
12:F:17:GLN:N	12:F:17:GLN:OE1	2.55	0.40
15:I:22:LYS:O	15:I:61:LEU:HD13	2.20	0.40
22:P:56:ARG:HD2	22:P:56:ARG:HA	1.67	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:8:LEU:HD23	23:Q:25:ILE:HG12	2.04	0.40
23:Q:21:ILE:HD13	23:Q:53:CYS:SG	2.62	0.40
29:X:74:ILE:O	29:X:78:ILE:HD13	2.22	0.40
30:a:593:U:H2'	30:a:594:G:C8	2.56	0.40
30:a:802:G:H5''	40:k:38:GLN:HG3	2.04	0.40
30:a:1042:C:C4'	30:a:1044:G:H1'	2.51	0.40
30:a:1418:G:C2	30:a:1419:G:C8	3.09	0.40
30:a:1462:G:H2'	30:a:1463:U:O4'	2.22	0.40
30:a:1805:C:O2'	32:c:48:ARG:HD2	2.20	0.40
30:a:2472:A:H2'	30:a:2473:G:O4'	2.21	0.40
35:f:100:LEU:HD12	35:f:100:LEU:HA	1.89	0.40
37:h:57:LYS:HA	37:h:57:LYS:CE	2.45	0.40
37:h:80:ILE:O	37:h:146:VAL:HA	2.21	0.40
37:h:90:LEU:HD12	37:h:90:LEU:HA	1.96	0.40
45:p:95:LEU:HA	45:p:95:LEU:HD23	1.88	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	
1	0	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
3	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	65/70 (93%)	59 (91%)	4 (6%)	2 (3%)	3	12
6	5	231/234 (99%)	215 (93%)	16 (7%)	0	100	100
8	B	223/241 (92%)	202 (91%)	21 (9%)	0	100	100
9	C	205/233 (88%)	197 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	D	203/206 (98%)	195 (96%)	8 (4%)	0	100	100
11	E	155/166 (93%)	145 (94%)	10 (6%)	0	100	100
12	F	102/131 (78%)	101 (99%)	1 (1%)	0	100	100
13	G	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
14	H	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
15	I	126/130 (97%)	116 (92%)	9 (7%)	1 (1%)	16	44
16	J	96/103 (93%)	87 (91%)	8 (8%)	1 (1%)	12	38
17	K	113/129 (88%)	106 (94%)	6 (5%)	1 (1%)	14	41
18	L	120/124 (97%)	108 (90%)	10 (8%)	2 (2%)	7	25
19	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
20	N	98/101 (97%)	98 (100%)	0	0	100	100
21	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
22	P	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
23	Q	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
24	R	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
25	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
26	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
29	X	93/95 (98%)	86 (92%)	7 (8%)	0	100	100
32	c	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
33	d	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	24	55
34	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
35	f	176/179 (98%)	167 (95%)	8 (4%)	1 (1%)	21	51
36	g	174/177 (98%)	157 (90%)	15 (9%)	2 (1%)	11	36
37	h	147/149 (99%)	126 (86%)	18 (12%)	3 (2%)	6	21
38	i	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
39	j	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
40	k	142/144 (99%)	133 (94%)	8 (6%)	1 (1%)	18	47
41	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
42	m	118/127 (93%)	109 (92%)	9 (8%)	0	100	100
43	n	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
44	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
46	q	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
47	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
48	s	91/100 (91%)	83 (91%)	8 (9%)	0	100	100
49	t	101/104 (97%)	86 (85%)	14 (14%)	1 (1%)	12	38
50	u	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
51	v	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
52	w	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
53	x	60/63 (95%)	60 (100%)	0	0	100	100
54	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
55	z	53/57 (93%)	52 (98%)	1 (2%)	0	100	100
All	All	5869/6143 (96%)	5558 (95%)	295 (5%)	16 (0%)	37	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	4	22	ILE
5	4	51	VAL
16	J	57	VAL
18	L	108	LYS
18	L	123	LYS
33	d	149	ASN
35	f	123	ASP
37	h	9	VAL
37	h	112	LYS
40	k	4	ASN
15	I	128	SER
17	K	79	ILE
36	g	51	THR
37	h	54	LEU
36	g	118	PRO
49	t	29	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/49 (96%)	46 (98%)	1 (2%)	47	79
2	1	38/38 (100%)	37 (97%)	1 (3%)	40	75
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	59/60 (98%)	57 (97%)	2 (3%)	32	68
6	5	177/178 (99%)	171 (97%)	6 (3%)	32	68
8	B	189/201 (94%)	187 (99%)	2 (1%)	65	87
9	C	171/190 (90%)	168 (98%)	3 (2%)	51	82
10	D	172/173 (99%)	170 (99%)	2 (1%)	63	87
11	E	119/125 (95%)	115 (97%)	4 (3%)	32	68
12	F	91/113 (80%)	87 (96%)	4 (4%)	25	59
13	G	127/128 (99%)	121 (95%)	6 (5%)	23	57
14	H	104/105 (99%)	102 (98%)	2 (2%)	50	81
15	I	106/107 (99%)	102 (96%)	4 (4%)	29	64
16	J	87/91 (96%)	86 (99%)	1 (1%)	65	87
17	K	89/98 (91%)	84 (94%)	5 (6%)	19	50
18	L	102/103 (99%)	100 (98%)	2 (2%)	48	80
19	M	94/97 (97%)	92 (98%)	2 (2%)	47	79
20	N	82/83 (99%)	81 (99%)	1 (1%)	63	87
21	O	75/76 (99%)	74 (99%)	1 (1%)	61	86
22	P	63/63 (100%)	61 (97%)	2 (3%)	34	70
23	Q	75/78 (96%)	68 (91%)	7 (9%)	8	27
24	R	58/65 (89%)	57 (98%)	1 (2%)	53	83
25	S	72/79 (91%)	71 (99%)	1 (1%)	59	85
26	T	65/66 (98%)	64 (98%)	1 (2%)	57	84
29	X	82/82 (100%)	80 (98%)	2 (2%)	43	77
32	c	215/217 (99%)	213 (99%)	2 (1%)	70	89
33	d	163/163 (100%)	157 (96%)	6 (4%)	30	65
34	e	165/165 (100%)	162 (98%)	3 (2%)	51	82
35	f	150/151 (99%)	145 (97%)	5 (3%)	33	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	g	135/136 (99%)	130 (96%)	5 (4%)	30	65
37	h	112/112 (100%)	108 (96%)	4 (4%)	31	66
38	i	116/116 (100%)	111 (96%)	5 (4%)	26	60
39	j	104/104 (100%)	103 (99%)	1 (1%)	68	88
40	k	103/103 (100%)	99 (96%)	4 (4%)	28	64
41	l	107/107 (100%)	104 (97%)	3 (3%)	38	73
42	m	100/103 (97%)	99 (99%)	1 (1%)	68	88
43	n	87/88 (99%)	84 (97%)	3 (3%)	32	68
44	o	99/100 (99%)	95 (96%)	4 (4%)	28	63
45	p	89/90 (99%)	88 (99%)	1 (1%)	65	87
46	q	84/84 (100%)	83 (99%)	1 (1%)	63	87
47	r	92/92 (100%)	90 (98%)	2 (2%)	45	78
48	s	80/84 (95%)	78 (98%)	2 (2%)	42	76
49	t	84/85 (99%)	80 (95%)	4 (5%)	23	56
50	u	77/77 (100%)	73 (95%)	4 (5%)	21	53
51	v	60/64 (94%)	57 (95%)	3 (5%)	22	54
52	w	68/69 (99%)	67 (98%)	1 (2%)	57	84
53	x	53/54 (98%)	51 (96%)	2 (4%)	29	64
54	y	48/49 (98%)	46 (96%)	2 (4%)	26	61
55	z	47/49 (96%)	46 (98%)	1 (2%)	47	79
All	All	4867/4996 (97%)	4735 (97%)	132 (3%)	40	74

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	29	THR
2	1	41	ARG
5	4	34	LEU
5	4	50	ASP
6	5	29	LEU
6	5	37	LYS
6	5	46	VAL
6	5	95	VAL
6	5	224	VAL
6	5	229	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	B	4	VAL
8	B	10	LEU
9	C	107	ARG
9	C	111	LEU
9	C	149	ILE
10	D	30	THR
10	D	164	GLN
11	E	73	ASN
11	E	103	THR
11	E	147	MET
11	E	164	ILE
12	F	62	MET
12	F	69	GLU
12	F	73	GLU
12	F	89	VAL
13	G	47	LEU
13	G	75	VAL
13	G	80	VAL
13	G	94	VAL
13	G	144	MET
13	G	156	TRP
14	H	60	GLU
14	H	108	LYS
15	I	58	VAL
15	I	59	GLU
15	I	89	GLU
15	I	105	THR
16	J	36	VAL
17	K	15	GLN
17	K	35	THR
17	K	94	GLU
17	K	111	THR
17	K	113	VAL
18	L	97	THR
18	L	110	ARG
19	M	12	GLN
19	M	50	GLU
20	N	55	SER
21	O	40	GLN
22	P	42	LEU
22	P	63	GLN
23	Q	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	Q	14	SER
23	Q	33	ILE
23	Q	48	ASP
23	Q	49	GLU
23	Q	74	THR
23	Q	79	VAL
24	R	9	LYS
25	S	28	LYS
26	T	61	GLN
29	X	3	LEU
29	X	16	LEU
32	c	168	ASP
32	c	194	GLU
33	d	35	THR
33	d	91	THR
33	d	92	VAL
33	d	100	LEU
33	d	105	LYS
33	d	168	GLU
34	e	30	GLN
34	e	105	LEU
34	e	120	VAL
35	f	17	MET
35	f	27	GLN
35	f	30	ARG
35	f	144	ASP
35	f	148	ARG
36	g	11	ILE
36	g	59	VAL
36	g	114	GLU
36	g	133	LEU
36	g	177	LYS
37	h	15	LEU
37	h	80	ILE
37	h	124	THR
37	h	134	VAL
38	i	5	THR
38	i	10	THR
38	i	64	VAL
38	i	106	LYS
38	i	138	GLN
39	j	69	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	k	2	ARG
40	k	29	LYS
40	k	94	THR
40	k	118	THR
41	l	60	GLN
41	l	111	GLU
41	l	124	LEU
42	m	98	LEU
43	n	21	LEU
43	n	83	LEU
43	n	112	GLU
44	o	7	GLN
44	o	10	GLN
44	o	37	LYS
44	o	97	LEU
45	p	6	ARG
46	q	86	GLN
47	r	1	MET
47	r	4	LEU
48	s	25	GLU
48	s	64	LYS
49	t	5	ILE
49	t	47	LYS
49	t	60	GLU
49	t	86	ARG
50	u	7	GLU
50	u	34	GLU
50	u	61	LEU
50	u	86	LEU
51	v	39	ARG
51	v	43	THR
51	v	85	GLU
52	w	33	LEU
53	x	19	LEU
53	x	24	GLU
54	y	16	ARG
54	y	58	GLU
55	z	31	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	26	ASN
3	2	28	ASN
8	B	39	HIS
9	C	3	GLN
9	C	123	GLN
9	C	185	ASN
10	D	40	GLN
10	D	59	GLN
10	D	196	ASN
10	D	198	HIS
11	E	61	GLN
14	H	21	ASN
15	I	5	GLN
16	J	15	HIS
17	K	15	GLN
21	O	46	HIS
21	O	62	GLN
22	P	63	GLN
26	T	3	ASN
29	X	2	GLN
29	X	29	GLN
29	X	86	ASN
32	c	25	HIS
32	c	53	HIS
33	d	42	ASN
34	e	90	GLN
34	e	92	HIS
36	g	48	ASN
36	g	88	GLN
37	h	11	ASN
37	h	66	ASN
39	j	3	GLN
40	k	4	ASN
43	n	43	ASN
43	n	98	GLN
44	o	10	GLN
44	o	66	ASN
45	p	72	ASN
47	r	9	HIS
48	s	91	GLN
52	w	20	HIS
52	w	36	HIS
53	x	15	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	y	9	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	V	76/77 (98%)	32 (42%)	1 (1%)
28	W	9/15 (60%)	3 (33%)	0
30	a	2902/2904 (99%)	433 (14%)	0
31	b	115/116 (99%)	17 (14%)	0
7	A	1538/1541 (99%)	233 (15%)	9 (0%)
All	All	4640/4653 (99%)	718 (15%)	10 (0%)

All (718) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	4	U
7	A	6	G
7	A	9	G
7	A	22	G
7	A	32	A
7	A	36	C
7	A	39	G
7	A	47	C
7	A	48	C
7	A	51	A
7	A	74	A
7	A	76	G
7	A	81	A
7	A	84	U
7	A	85	U
7	A	86	G
7	A	87	C
7	A	88	U
7	A	89	G
7	A	90	C
7	A	94	G
7	A	96	U
7	A	116	A
7	A	121	U
7	A	122	G
7	A	130	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	131	A
7	A	144	G
7	A	151	A
7	A	169	C
7	A	182	A
7	A	197	A
7	A	204	G
7	A	208	U
7	A	210	C
7	A	211	G
7	A	212	G
7	A	226	G
7	A	240	G
7	A	245	U
7	A	247	G
7	A	251	G
7	A	266	G
7	A	267	C
7	A	280	C
7	A	289	G
7	A	306	A
7	A	321	A
7	A	328	C
7	A	347	G
7	A	351	G
7	A	352	C
7	A	354	G
7	A	361	G
7	A	367	U
7	A	372	C
7	A	373	A
7	A	379	C
7	A	398	U
7	A	406	G
7	A	407	U
7	A	408	A
7	A	412	A
7	A	413	G
7	A	416	G
7	A	417	G
7	A	424	G
7	A	428	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	429	U
7	A	432	A
7	A	438	U
7	A	450	G
7	A	451	A
7	A	452	A
7	A	457	A
7	A	462	G
7	A	463	U
7	A	464	U
7	A	469	A
7	A	473	U
7	A	474	G
7	A	475	U
7	A	477	G
7	A	478	A
7	A	479	U
7	A	481	G
7	A	484	G
7	A	495	A
7	A	496	A
7	A	511	C
7	A	512	U
7	A	517	G
7	A	518	C
7	A	521	G
7	A	524	G
7	A	527	G7M
7	A	530	G
7	A	533	A
7	A	547	A
7	A	548	G
7	A	559	A
7	A	564	C
7	A	572	A
7	A	573	A
7	A	576	C
7	A	577	G
7	A	579	A
7	A	615	G
7	A	627	G
7	A	628	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	633	G
7	A	641	A
7	A	653	A
7	A	665	A
7	A	686	U
7	A	688	G
7	A	703	G
7	A	721	G
7	A	723	U
7	A	724	G
7	A	734	G
7	A	746	A
7	A	747	A
7	A	748	G
7	A	755	G
7	A	777	A
7	A	793	U
7	A	794	A
7	A	812	G
7	A	815	A
7	A	817	C
7	A	821	G
7	A	829	G
7	A	841	C
7	A	844	G
7	A	845	A
7	A	848	C
7	A	851	G
7	A	884	U
7	A	890	G
7	A	902	G
7	A	914	A
7	A	926	G
7	A	934	C
7	A	935	A
7	A	942	G
7	A	960	U
7	A	968	A
7	A	969	A
7	A	975	A
7	A	976	G
7	A	977	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	992	U
7	A	993	G
7	A	1004	A
7	A	1008	U
7	A	1009	U
7	A	1020	A
7	A	1022	U
7	A	1026	G
7	A	1029	U
7	A	1030	U
7	A	1031	C
7	A	1032	G
7	A	1033	G
7	A	1036	A
7	A	1038	U
7	A	1043	G
7	A	1044	A
7	A	1046	A
7	A	1053	G
7	A	1065	U
7	A	1070	U
7	A	1085	U
7	A	1094	G
7	A	1095	U
7	A	1101	A
7	A	1133	G
7	A	1137	A
7	A	1139	G
7	A	1159	U
7	A	1174	G
7	A	1196	A
7	A	1197	A
7	A	1201	A
7	A	1213	A
7	A	1214	C
7	A	1215	G
7	A	1227	A
7	A	1228	C
7	A	1238	A
7	A	1258	G
7	A	1260	G
7	A	1275	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	1280	A
7	A	1285	A
7	A	1286	U
7	A	1287	A
7	A	1297	G
7	A	1300	G
7	A	1302	C
7	A	1305	G
7	A	1312	G
7	A	1317	C
7	A	1320	C
7	A	1331	G
7	A	1338	G
7	A	1346	A
7	A	1353	G
7	A	1363	A
7	A	1364	U
7	A	1368	A
7	A	1370	G
7	A	1378	C
7	A	1379	G
7	A	1397	C
7	A	1398	A
7	A	1419	G
7	A	1429	A
7	A	1432	G
7	A	1441	A
7	A	1451	U
7	A	1452	C
7	A	1453	G
7	A	1492	A
7	A	1494	G
7	A	1497	G
7	A	1499	A
7	A	1506	U
7	A	1517	G
7	A	1519	MA6
7	A	1529	G
7	A	1530	G
27	V	4	G
27	V	7	G
27	V	9	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	V	11	A
27	V	12	G
27	V	16	C
27	V	18	U
27	V	19	G
27	V	20	G
27	V	21	H2U
27	V	22	A
27	V	23	G
27	V	32	G
27	V	33	OMC
27	V	42	C
27	V	45	A
27	V	47	A
27	V	48	U
27	V	50	G
27	V	52	C
27	V	53	G
27	V	54	G
27	V	56	PSU
27	V	59	A
27	V	63	C
27	V	68	C
27	V	70	C
27	V	71	G
27	V	72	C
27	V	75	C
27	V	76	C
27	V	77	A
28	W	7	U
28	W	10	G
28	W	11	G
30	a	10	A
30	a	34	U
30	a	35	G
30	a	45	G
30	a	51	G
30	a	71	A
30	a	74	A
30	a	75	G
30	a	81	G
30	a	101	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	102	A
30	a	117	A
30	a	118	A
30	a	119	U
30	a	124	A
30	a	134	U
30	a	135	G
30	a	136	U
30	a	137	U
30	a	138	C
30	a	140	G
30	a	141	A
30	a	155	A
30	a	162	A
30	a	164	A
30	a	180	A
30	a	195	A
30	a	198	A
30	a	214	G
30	a	215	A
30	a	221	A
30	a	232	A
30	a	247	G
30	a	249	G
30	a	266	C
30	a	275	U
30	a	276	G
30	a	277	A
30	a	278	A
30	a	284	U
30	a	286	G
30	a	289	U
30	a	290	G
30	a	301	G
30	a	310	A
30	a	328	G
30	a	329	A
30	a	330	U
30	a	332	G
30	a	344	A
30	a	345	A
30	a	361	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	385	G
30	a	395	G
30	a	401	A
30	a	404	U
30	a	410	G
30	a	434	C
30	a	458	U
30	a	474	C
30	a	480	G
30	a	490	G
30	a	494	G
30	a	503	A
30	a	504	A
30	a	508	C
30	a	509	C
30	a	529	G
30	a	530	C
30	a	531	A
30	a	544	U
30	a	545	C
30	a	546	G
30	a	547	G
30	a	560	A
30	a	568	U
30	a	570	U
30	a	572	A
30	a	574	G
30	a	600	A
30	a	612	U
30	a	624	A
30	a	634	A
30	a	642	C
30	a	644	G
30	a	651	A
30	a	652	A
30	a	682	A
30	a	683	U
30	a	708	G
30	a	714	C
30	a	723	G
30	a	727	A
30	a	735	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	737	C
30	a	744	5MU
30	a	761	A
30	a	772	G
30	a	773	G
30	a	774	G
30	a	779	A
30	a	781	G
30	a	782	G
30	a	786	A
30	a	789	A
30	a	802	G
30	a	809	C
30	a	824	U
30	a	825	U
30	a	842	A
30	a	843	C
30	a	844	U
30	a	856	G
30	a	866	G
30	a	874	U
30	a	876	G
30	a	881	C
30	a	882	C
30	a	883	A
30	a	885	C
30	a	887	C
30	a	888	G
30	a	892	U
30	a	893	A
30	a	894	C
30	a	904	G
30	a	907	A
30	a	943	C
30	a	956	A
30	a	958	C
30	a	971	G
30	a	980	A
30	a	986	G
30	a	993	A
30	a	1007	A
30	a	1009	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1010	C
30	a	1023	G
30	a	1030	U
30	a	1043	A
30	a	1044	G
30	a	1051	A
30	a	1056	G
30	a	1057	U
30	a	1058	U
30	a	1059	G
30	a	1060	G
30	a	1061	C
30	a	1063	U
30	a	1065	G
30	a	1066	A
30	a	1067	A
30	a	1068	G
30	a	1069	C
30	a	1073	C
30	a	1075	U
30	a	1076	C
30	a	1078	U
30	a	1080	U
30	a	1081	A
30	a	1084	G
30	a	1085	A
30	a	1086	A
30	a	1087	A
30	a	1088	G
30	a	1091	U
30	a	1092	A
30	a	1095	A
30	a	1098	U
30	a	1100	A
30	a	1103	G
30	a	1104	G
30	a	1107	G
30	a	1108	A
30	a	1109	G
30	a	1119	G
30	a	1125	G
30	a	1127	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1129	U
30	a	1130	A
30	a	1132	C
30	a	1139	A
30	a	1168	G
30	a	1173	U
30	a	1174	G
30	a	1209	G
30	a	1233	G
30	a	1247	G
30	a	1250	A
30	a	1253	G
30	a	1268	G
30	a	1269	A
30	a	1270	U
30	a	1284	A
30	a	1297	G
30	a	1298	A
30	a	1299	A
30	a	1349	U
30	a	1362	A
30	a	1375	A
30	a	1376	U
30	a	1380	A
30	a	1389	A
30	a	1400	A
30	a	1404	G
30	a	1413	G
30	a	1424	A
30	a	1425	C
30	a	1449	G
30	a	1450	A
30	a	1479	G
30	a	1482	G
30	a	1483	U
30	a	1490	U
30	a	1494	U
30	a	1500	A
30	a	1506	U
30	a	1507	U
30	a	1515	A
30	a	1529	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1535	A
30	a	1536	C
30	a	1537	G
30	a	1554	U
30	a	1566	A
30	a	1569	A
30	a	1577	C
30	a	1580	A
30	a	1583	A
30	a	1584	U
30	a	1585	C
30	a	1586	A
30	a	1607	C
30	a	1608	A
30	a	1622	G
30	a	1626	A
30	a	1634	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1653	G
30	a	1654	A
30	a	1674	G
30	a	1715	G
30	a	1728	C
30	a	1730	G
30	a	1731	C
30	a	1732	G
30	a	1734	G
30	a	1737	G
30	a	1755	G
30	a	1758	A
30	a	1763	C
30	a	1772	A
30	a	1787	C
30	a	1799	C
30	a	1800	A
30	a	1806	G
30	a	1807	A
30	a	1815	C
30	a	1828	A
30	a	1847	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1857	A
30	a	1868	G
30	a	1869	G
30	a	1870	C
30	a	1871	A
30	a	1873	C
30	a	1885	G
30	a	1907	G
30	a	1914	A
30	a	1930	G
30	a	1931	G
30	a	1937	A
30	a	1938	A
30	a	1956	U
30	a	1965	G
30	a	1968	C
30	a	1971	A
30	a	1972	U
30	a	1973	G
30	a	1992	U
30	a	1993	G
30	a	1994	U
30	a	2017	U
30	a	2021	A
30	a	2024	C
30	a	2031	6MZ
30	a	2032	A
30	a	2034	A
30	a	2036	G
30	a	2044	C
30	a	2056	C
30	a	2057	G
30	a	2061	A
30	a	2062	G
30	a	2070	G7M
30	a	2094	G
30	a	2104	C
30	a	2105	C
30	a	2111	G
30	a	2113	G
30	a	2115	A
30	a	2116	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2117	G
30	a	2119	U
30	a	2120	A
30	a	2127	A
30	a	2130	C
30	a	2131	U
30	a	2132	U
30	a	2133	U
30	a	2134	G
30	a	2135	A
30	a	2142	G
30	a	2146	C
30	a	2147	C
30	a	2148	A
30	a	2155	G
30	a	2157	G
30	a	2158	G
30	a	2160	G
30	a	2162	C
30	a	2165	C
30	a	2166	C
30	a	2167	U
30	a	2168	U
30	a	2170	A
30	a	2172	A
30	a	2173	U
30	a	2174	A
30	a	2175	C
30	a	2177	A
30	a	2179	C
30	a	2183	U
30	a	2188	G
30	a	2189	C
30	a	2192	G
30	a	2194	G
30	a	2199	A
30	a	2205	G
30	a	2212	G
30	a	2214	U
30	a	2226	A
30	a	2239	G
30	a	2240	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2280	G
30	a	2284	C
30	a	2288	A
30	a	2289	A
30	a	2306	U
30	a	2309	G
30	a	2312	A
30	a	2322	U
30	a	2323	A
30	a	2326	G
30	a	2334	A
30	a	2335	U
30	a	2336	A
30	a	2346	G
30	a	2348	C
30	a	2351	C
30	a	2362	G
30	a	2384	G
30	a	2386	C
30	a	2397	G
30	a	2403	U
30	a	2404	C
30	a	2407	A
30	a	2426	A
30	a	2430	G
30	a	2431	A
30	a	2436	A
30	a	2442	U
30	a	2449	A
30	a	2476	C
30	a	2477	A
30	a	2479	A
30	a	2492	U
30	a	2495	G
30	a	2499	OMC
30	a	2503	G
30	a	2506	G
30	a	2507	U
30	a	2519	A
30	a	2521	C
30	a	2526	G
30	a	2530	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2548	A
30	a	2567	A
30	a	2568	G
30	a	2574	C
30	a	2603	A
30	a	2610	U
30	a	2614	U
30	a	2616	U
30	a	2630	U
30	a	2631	G
30	a	2647	C
30	a	2655	A
30	a	2664	G
30	a	2690	U
30	a	2691	U
30	a	2715	G
30	a	2717	C
30	a	2721	U
30	a	2727	A
30	a	2733	G
30	a	2734	A
30	a	2745	G
30	a	2749	A
30	a	2758	A
30	a	2766	A
30	a	2779	A
30	a	2781	G
30	a	2794	G
30	a	2796	C
30	a	2797	C
30	a	2798	U
30	a	2799	U
30	a	2801	A
30	a	2819	U
30	a	2821	A
30	a	2822	A
30	a	2834	U
30	a	2837	U
30	a	2850	U
30	a	2874	A
30	a	2880	A
30	a	2881	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2884	A
30	a	2885	U
30	a	2892	U
31	b	13	U
31	b	16	G
31	b	21	G
31	b	24	G
31	b	35	C
31	b	41	G
31	b	42	C
31	b	53	A
31	b	56	G
31	b	67	G
31	b	89	U
31	b	90	C
31	b	99	A
31	b	102	G
31	b	103	U
31	b	104	A
31	b	109	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	360	G
7	A	406	G
7	A	407	U
7	A	416	G
7	A	428	G
7	A	516	PSU
7	A	547	A
7	A	1035	A
7	A	1506	U
27	V	20	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

45 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	H2U	V	21	27	18,21,22	4.31	5 (27%)	21,30,33	5.02	6 (28%)
30	PSU	a	2505	58,30	18,21,22	2.14	7 (38%)	22,30,33	1.88	3 (13%)
7	2MG	A	1207	58,7	23,26,27	2.58	6 (26%)	32,38,41	2.03	10 (31%)
30	OMG	a	2252	58,30	23,26,27	2.36	6 (26%)	33,38,41	1.84	9 (27%)
30	OMU	a	2553	57,58,30	19,22,23	2.64	7 (36%)	26,31,34	1.79	6 (23%)
7	4OC	A	1402	7	20,23,24	2.24	3 (15%)	26,32,35	1.03	2 (7%)
30	PSU	a	1918	30	18,21,22	2.04	7 (38%)	22,30,33	1.82	4 (18%)
7	5MC	A	967	7	18,22,23	1.93	6 (33%)	26,32,35	1.34	2 (7%)
30	2MG	a	1834	30	23,26,27	2.57	7 (30%)	32,38,41	2.17	10 (31%)
30	6MZ	a	1618	30	22,25,26	2.41	3 (13%)	30,36,39	2.27	10 (33%)
30	2MA	a	2504	57,58,30	22,25,26	1.33	2 (9%)	33,37,40	2.03	7 (21%)
30	OMC	a	2499	57,30	19,22,23	1.81	5 (26%)	26,31,34	1.14	2 (7%)
41	4D4	l	81	41	9,11,12	0.79	0	8,13,15	1.69	2 (25%)
7	MA6	A	1518	7	23,26,27	1.25	3 (13%)	34,38,41	2.22	9 (26%)
7	5MC	A	1407	7	18,22,23	1.98	6 (33%)	26,32,35	1.32	2 (7%)
41	MS6	l	82	41	5,7,8	0.57	0	2,7,9	1.52	1 (50%)
27	PSU	V	56	27	18,21,22	1.88	6 (33%)	22,30,33	1.77	3 (13%)
7	UR3	A	1498	7	19,22,23	2.54	6 (31%)	26,32,35	1.37	2 (7%)
7	PSU	A	516	57,7	18,21,22	2.01	7 (38%)	22,30,33	1.91	4 (18%)
30	PSU	a	1912	30	18,21,22	2.06	7 (38%)	22,30,33	1.87	4 (18%)
30	PSU	a	743	57,30	18,21,22	2.10	9 (50%)	22,30,33	1.86	3 (13%)
30	6MZ	a	2031	30	22,25,26	2.39	4 (18%)	30,36,39	2.54	10 (33%)
7	G7M	A	527	58,7	23,26,27	2.17	5 (21%)	35,39,42	1.90	7 (20%)
30	5MC	a	1963	58,30	18,22,23	1.95	6 (33%)	26,32,35	1.37	2 (7%)
30	PSU	a	2581	58,30	18,21,22	2.22	9 (50%)	22,30,33	1.88	5 (22%)
7	MA6	A	1519	7	23,26,27	1.26	3 (13%)	34,38,41	2.29	9 (26%)
30	G7M	a	2070	58,30	23,26,27	2.22	5 (21%)	35,39,42	1.84	7 (20%)
30	2MG	a	2446	30	23,26,27	2.59	7 (30%)	32,38,41	2.13	12 (37%)
30	1MG	a	742	30	22,26,27	2.53	6 (27%)	33,39,42	2.06	6 (18%)
30	5MU	a	1940	58,30	19,22,23	2.59	7 (36%)	28,32,35	3.83	10 (35%)
30	PSU	a	2458	30	18,21,22	2.22	8 (44%)	22,30,33	1.88	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	D2T	L	89	18	7,9,10	1.18	0	6,11,13	1.58	1 (16%)
27	4SU	V	8	27	18,21,22	3.74	8 (44%)	26,30,33	2.17	5 (19%)
7	2MG	A	966	7	23,26,27	2.57	5 (21%)	32,38,41	2.07	9 (28%)
30	H2U	a	2450	30	18,21,22	4.10	5 (27%)	21,30,33	5.15	7 (33%)
30	PSU	a	952	30	18,21,22	2.12	8 (44%)	22,30,33	1.86	4 (18%)
33	MEQ	d	150	33	8,9,10	0.96	0	5,10,12	0.54	0
30	5MU	a	744	30	19,22,23	2.51	7 (36%)	28,32,35	3.77	11 (39%)
30	3TD	a	1916	-	18,22,23	2.75	7 (38%)	22,32,35	1.71	3 (13%)
17	IAS	K	119	17	6,7,8	1.72	1 (16%)	6,8,10	2.38	1 (16%)
30	PSU	a	2606	30	18,21,22	2.12	7 (38%)	22,30,33	1.81	3 (13%)
27	5MU	V	55	27	19,22,23	2.41	7 (36%)	28,32,35	3.57	10 (35%)
7	2MG	A	1516	7	23,26,27	2.58	6 (26%)	32,38,41	2.11	10 (31%)
30	PSU	a	2605	30	18,21,22	2.07	7 (38%)	22,30,33	1.83	3 (13%)
27	OMC	V	33	27	19,22,23	1.77	4 (21%)	26,31,34	0.97	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	H2U	V	21	27	-	5/7/38/39	0/2/2/2
30	PSU	a	2505	58,30	-	2/7/25/26	0/2/2/2
7	2MG	A	1207	58,7	-	2/9/27/28	0/3/3/3
30	OMG	a	2252	58,30	-	1/9/27/28	0/3/3/3
30	OMU	a	2553	57,58,30	-	0/9/27/28	0/2/2/2
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
30	PSU	a	1918	30	-	0/7/25/26	0/2/2/2
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
30	2MG	a	1834	30	-	0/9/27/28	0/3/3/3
30	6MZ	a	1618	30	-	0/9/27/28	0/3/3/3
30	2MA	a	2504	57,58,30	-	2/7/25/26	0/3/3/3
30	OMC	a	2499	57,30	-	1/9/27/28	0/2/2/2
41	4D4	l	81	41	-	3/11/12/14	-
7	MA6	A	1518	7	-	0/11/29/30	0/3/3/3
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
41	MS6	l	82	41	-	3/4/6/8	-
27	PSU	V	56	27	-	3/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	UR3	A	1498	7	-	0/7/25/26	0/2/2/2
7	PSU	A	516	57,7	-	0/7/25/26	0/2/2/2
30	PSU	a	1912	30	-	0/7/25/26	0/2/2/2
30	PSU	a	743	57,30	-	1/7/25/26	0/2/2/2
30	6MZ	a	2031	30	-	2/9/27/28	0/3/3/3
7	G7M	A	527	58,7	-	3/7/25/26	0/3/3/3
30	5MC	a	1963	58,30	-	0/7/25/26	0/2/2/2
30	PSU	a	2581	58,30	-	0/7/25/26	0/2/2/2
7	MA6	A	1519	7	-	5/11/29/30	0/3/3/3
30	G7M	a	2070	58,30	-	1/7/25/26	0/3/3/3
30	2MG	a	2446	30	-	1/9/27/28	0/3/3/3
30	1MG	a	742	30	-	0/7/25/26	0/3/3/3
30	5MU	a	1940	58,30	-	0/7/25/26	0/2/2/2
30	PSU	a	2458	30	-	0/7/25/26	0/2/2/2
18	D2T	L	89	18	-	2/7/12/14	-
27	4SU	V	8	27	-	0/7/25/26	0/2/2/2
7	2MG	A	966	7	-	0/9/27/28	0/3/3/3
30	H2U	a	2450	30	-	0/7/38/39	0/2/2/2
30	PSU	a	952	30	-	0/7/25/26	0/2/2/2
33	MEQ	d	150	33	-	2/8/9/11	-
30	5MU	a	744	30	-	0/7/25/26	0/2/2/2
30	3TD	a	1916	-	-	2/7/25/26	0/2/2/2
17	IAS	K	119	17	-	1/7/7/8	-
30	PSU	a	2606	30	-	0/7/25/26	0/2/2/2
27	5MU	V	55	27	-	0/7/25/26	0/2/2/2
7	2MG	A	1516	7	-	0/9/27/28	0/3/3/3
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
27	OMC	V	33	27	-	2/9/27/28	0/2/2/2

All (240) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	V	21	H2U	O4-C4	10.29	1.44	1.23
30	a	1618	6MZ	C6-N6	9.97	1.45	1.34
30	a	2450	H2U	O4-C4	9.88	1.43	1.23
30	a	2031	6MZ	C6-N6	9.54	1.44	1.34
7	A	1207	2MG	O6-C6	9.13	1.40	1.23
7	A	966	2MG	O6-C6	9.00	1.40	1.23
7	A	1516	2MG	O6-C6	8.97	1.40	1.23
30	a	1834	2MG	O6-C6	8.89	1.40	1.23
30	a	2446	2MG	O6-C6	8.81	1.40	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1498	UR3	O4-C4	8.55	1.42	1.23
27	V	21	H2U	C2-N1	8.51	1.47	1.35
27	V	21	H2U	O2-C2	8.41	1.38	1.23
30	a	2252	OMG	O6-C6	8.41	1.39	1.23
30	a	2450	H2U	C2-N1	8.15	1.47	1.35
30	a	1916	3TD	O4-C4	8.14	1.40	1.23
30	a	2450	H2U	O2-C2	8.14	1.37	1.23
30	a	742	1MG	O6-C6	8.01	1.40	1.23
30	a	2553	OMU	O4-C4	7.96	1.40	1.24
7	A	527	G7M	O6-C6	7.86	1.38	1.23
27	V	8	4SU	C4-N3	7.79	1.46	1.37
30	a	2070	G7M	O6-C6	7.79	1.38	1.23
27	V	21	H2U	C2-N3	7.22	1.50	1.38
27	V	8	4SU	C2-N3	7.18	1.50	1.38
27	V	8	4SU	C4-S4	-6.83	1.55	1.68
30	a	2450	H2U	C2-N3	6.69	1.49	1.38
7	A	1402	4OC	O2-C2	6.54	1.35	1.23
30	a	1940	5MU	C2-N1	-6.49	1.28	1.38
30	a	744	5MU	C2-N1	-5.96	1.28	1.38
7	A	1516	2MG	C2-N2	5.94	1.46	1.33
7	A	966	2MG	C2-N2	5.88	1.46	1.33
30	a	742	1MG	C2-N2	5.86	1.44	1.34
7	A	1207	2MG	C2-N2	5.78	1.46	1.33
27	V	55	5MU	C2-N1	-5.70	1.29	1.38
30	a	1834	2MG	C2-N2	5.67	1.46	1.33
30	a	2446	2MG	C2-N2	5.53	1.45	1.33
27	V	21	H2U	C4-N3	5.49	1.46	1.37
7	A	1402	4OC	C4-N4	5.43	1.47	1.35
27	V	8	4SU	C6-C5	5.08	1.46	1.35
30	a	2450	H2U	C4-N3	4.97	1.46	1.37
27	V	33	OMC	C4-N4	4.92	1.45	1.33
30	a	1940	5MU	C2-N3	-4.91	1.29	1.38
30	a	744	5MU	C2-N3	-4.84	1.29	1.38
30	a	744	5MU	C6-N1	-4.68	1.30	1.38
27	V	55	5MU	C2-N3	-4.67	1.29	1.38
30	a	1940	5MU	C6-N1	-4.65	1.30	1.38
30	a	2499	OMC	C4-N4	4.61	1.44	1.33
27	V	8	4SU	C2-N1	4.43	1.45	1.38
30	a	2504	2MA	C6-N6	4.30	1.44	1.34
30	a	2553	OMU	C2-N1	-4.20	1.31	1.38
7	A	967	5MC	C4-N4	4.19	1.45	1.34
27	V	8	4SU	C5-C4	4.17	1.47	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	V	55	5MU	C6-N1	-4.15	1.31	1.38
30	a	2581	PSU	C2-N1	-4.14	1.31	1.36
30	a	2458	PSU	C4-N3	-4.12	1.31	1.38
30	a	1963	5MC	C2-N1	-4.10	1.31	1.40
30	a	1916	3TD	C2-N1	-4.09	1.31	1.37
30	a	2499	OMC	C2-N1	-4.08	1.31	1.40
27	V	8	4SU	C6-N1	4.08	1.47	1.38
30	a	2505	PSU	C2-N1	-4.07	1.31	1.36
7	A	1407	5MC	C4-N4	4.07	1.44	1.34
30	a	742	1MG	C6-N1	-4.06	1.31	1.40
30	a	2252	OMG	C6-N1	-4.06	1.31	1.38
30	a	2458	PSU	C2-N1	-4.04	1.31	1.36
30	a	2581	PSU	C4-N3	-4.04	1.31	1.38
30	a	2606	PSU	C2-N1	-4.00	1.31	1.36
30	a	743	PSU	C2-N1	-3.99	1.31	1.36
7	A	967	5MC	C2-N1	-3.99	1.31	1.40
30	a	2605	PSU	C4-N3	-3.98	1.31	1.38
27	V	33	OMC	C2-N1	-3.98	1.31	1.40
30	a	2252	OMG	C2-N2	3.95	1.43	1.34
30	a	952	PSU	C4-N3	-3.94	1.31	1.38
7	A	1407	5MC	C2-N1	-3.94	1.31	1.40
30	a	2606	PSU	C4-N3	-3.92	1.31	1.38
30	a	1963	5MC	C4-N4	3.91	1.44	1.34
30	a	2505	PSU	C4-N3	-3.91	1.31	1.38
30	a	2458	PSU	C2-N3	-3.89	1.30	1.37
30	a	1916	3TD	C4-N3	-3.88	1.32	1.40
30	a	2070	G7M	C5-N7	-3.84	1.34	1.39
30	a	2553	OMU	C4-N3	-3.83	1.31	1.38
30	a	1918	PSU	C4-N3	-3.83	1.31	1.38
30	a	2505	PSU	C2-N3	-3.79	1.31	1.37
27	V	56	PSU	C6-C5	3.77	1.39	1.35
30	a	952	PSU	C2-N1	-3.77	1.31	1.36
30	a	1912	PSU	C2-N1	-3.74	1.31	1.36
7	A	1402	4OC	C2-N1	-3.73	1.31	1.40
30	a	2553	OMU	C2-N3	-3.73	1.31	1.38
30	a	2605	PSU	C2-N3	-3.73	1.31	1.37
7	A	1498	UR3	C4-N3	-3.71	1.32	1.40
7	A	516	PSU	C2-N1	-3.70	1.31	1.36
30	a	743	PSU	C4-N3	-3.70	1.32	1.38
30	a	2606	PSU	C2-N3	-3.68	1.31	1.37
7	A	516	PSU	C4-N3	-3.64	1.32	1.38
30	a	952	PSU	C2-N3	-3.61	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	1912	PSU	C4-N3	-3.61	1.32	1.38
30	a	2581	PSU	C2-N3	-3.60	1.31	1.37
30	a	2070	G7M	C6-N1	-3.56	1.32	1.38
27	V	8	4SU	O2-C2	-3.52	1.16	1.23
30	a	1963	5MC	C6-N1	-3.51	1.32	1.38
30	a	744	5MU	C4-N3	-3.51	1.32	1.38
27	V	55	5MU	C6-C5	3.51	1.40	1.34
17	K	119	IAS	OD1-CG	3.50	1.39	1.19
30	a	2605	PSU	C2-N1	-3.48	1.32	1.36
30	a	1918	PSU	C2-N1	-3.48	1.32	1.36
7	A	516	PSU	C2-N3	-3.43	1.31	1.37
7	A	527	G7M	C6-N1	-3.42	1.32	1.38
30	a	1912	PSU	C2-N3	-3.42	1.31	1.37
30	a	1940	5MU	C4-N3	-3.40	1.32	1.38
27	V	56	PSU	C4-N3	-3.40	1.32	1.38
30	a	743	PSU	C2-N3	-3.39	1.31	1.37
7	A	527	G7M	C5-N7	-3.39	1.35	1.39
30	a	2446	2MG	C6-N1	-3.38	1.32	1.38
7	A	1518	MA6	C8-N9	-3.38	1.31	1.37
30	a	2031	6MZ	C8-N9	-3.38	1.31	1.37
30	a	1918	PSU	C2-N3	-3.37	1.31	1.37
7	A	1518	MA6	C6-N6	3.34	1.46	1.36
30	a	1618	6MZ	C8-N9	-3.34	1.31	1.37
27	V	55	5MU	C4-N3	-3.33	1.32	1.38
7	A	1519	MA6	C6-N6	3.32	1.46	1.36
7	A	1519	MA6	C8-N9	-3.29	1.31	1.37
7	A	1407	5MC	C6-N1	-3.29	1.32	1.38
7	A	1498	UR3	C2-N3	-3.28	1.32	1.39
7	A	967	5MC	C6-N1	-3.28	1.32	1.38
30	a	1940	5MU	C6-C5	3.26	1.40	1.34
30	a	1916	3TD	C6-C5	3.15	1.39	1.35
27	V	56	PSU	C2-N1	-3.15	1.32	1.36
30	a	744	5MU	C6-C5	3.14	1.39	1.34
7	A	527	G7M	C2-N2	3.14	1.41	1.34
30	a	1918	PSU	C6-C5	3.13	1.39	1.35
30	a	1912	PSU	C6-C5	3.12	1.39	1.35
7	A	1407	5MC	O2-C2	-3.09	1.18	1.23
30	a	1916	3TD	C2-N3	-3.06	1.31	1.38
30	a	1834	2MG	C5-N7	-3.06	1.33	1.39
30	a	1834	2MG	C6-N1	-3.05	1.33	1.38
7	A	1516	2MG	C6-N1	-3.05	1.33	1.38
7	A	1498	UR3	C2-N1	-3.03	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	966	2MG	C6-N1	-3.01	1.33	1.38
30	a	1963	5MC	O2-C2	-3.01	1.18	1.23
7	A	966	2MG	C5-N7	-2.89	1.33	1.39
30	a	952	PSU	C6-C5	2.88	1.38	1.35
7	A	516	PSU	C6-C5	2.85	1.38	1.35
30	a	2070	G7M	C2-N2	2.85	1.41	1.34
7	A	1207	2MG	C6-N1	-2.85	1.33	1.38
7	A	967	5MC	O2-C2	-2.84	1.18	1.23
30	a	2581	PSU	C6-N1	-2.84	1.31	1.36
7	A	1207	2MG	C5-N7	-2.83	1.33	1.39
30	a	2458	PSU	O4-C4	-2.83	1.18	1.23
7	A	1516	2MG	C5-N7	-2.83	1.33	1.39
30	a	2446	2MG	C5-N7	-2.82	1.33	1.39
30	a	952	PSU	O4-C4	-2.82	1.18	1.23
30	a	2605	PSU	O4-C4	-2.80	1.18	1.23
30	a	1918	PSU	O4-C4	-2.78	1.18	1.23
30	a	2252	OMG	C8-N9	-2.78	1.31	1.37
30	a	2458	PSU	C6-C5	2.75	1.38	1.35
30	a	2505	PSU	C6-N1	-2.74	1.31	1.36
27	V	56	PSU	C2-N3	-2.73	1.32	1.37
30	a	2581	PSU	O4-C4	-2.73	1.18	1.23
30	a	2606	PSU	O4-C4	-2.73	1.18	1.23
30	a	2605	PSU	C6-C5	2.73	1.38	1.35
30	a	743	PSU	C6-C5	2.69	1.38	1.35
30	a	2031	6MZ	C5-N7	-2.69	1.33	1.39
30	a	743	PSU	C6-N1	-2.69	1.31	1.36
30	a	2458	PSU	C6-N1	-2.69	1.31	1.36
30	a	2553	OMU	O2-C2	-2.69	1.18	1.23
30	a	1940	5MU	O4-C4	-2.68	1.18	1.23
30	a	744	5MU	O4-C4	-2.68	1.18	1.23
30	a	743	PSU	O4-C4	-2.68	1.18	1.23
30	a	2606	PSU	C6-N1	-2.68	1.31	1.36
30	a	742	1MG	C8-N9	-2.67	1.31	1.37
30	a	1940	5MU	O2-C2	-2.67	1.18	1.23
30	a	742	1MG	C5-N7	-2.66	1.33	1.39
30	a	1912	PSU	O4-C4	-2.66	1.18	1.23
7	A	516	PSU	O4-C4	-2.65	1.18	1.23
30	a	2606	PSU	C6-C5	2.64	1.38	1.35
30	a	2070	G7M	C2-N1	-2.62	1.31	1.37
30	a	2581	PSU	C6-C5	2.59	1.38	1.35
30	a	1618	6MZ	C5-N7	-2.59	1.34	1.39
30	a	2505	PSU	O4-C4	-2.59	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2505	PSU	C6-C5	2.58	1.38	1.35
30	a	2581	PSU	O4'-C1'	-2.57	1.40	1.43
27	V	55	5MU	O4-C4	-2.55	1.18	1.23
30	a	2581	PSU	O2-C2	-2.54	1.18	1.23
7	A	967	5MC	C6-C5	2.53	1.38	1.34
7	A	1407	5MC	C6-C5	2.53	1.38	1.34
30	a	2252	OMG	C5-N7	-2.51	1.34	1.39
30	a	2458	PSU	O2-C2	-2.51	1.18	1.23
7	A	527	G7M	C2-N1	-2.49	1.31	1.37
30	a	744	5MU	O2-C2	-2.46	1.18	1.23
30	a	2605	PSU	C6-N1	-2.46	1.32	1.36
30	a	2446	2MG	C4-N9	-2.45	1.31	1.38
30	a	2252	OMG	C2-N1	-2.45	1.31	1.37
30	a	952	PSU	O2-C2	-2.45	1.18	1.23
30	a	1916	3TD	C6-N1	-2.45	1.32	1.36
30	a	1912	PSU	O2-C2	-2.44	1.18	1.23
30	a	2553	OMU	C6-N1	-2.44	1.32	1.38
30	a	2505	PSU	O2-C2	-2.44	1.18	1.23
30	a	1916	3TD	O2-C2	-2.42	1.18	1.23
30	a	1918	PSU	C6-N1	-2.41	1.32	1.36
30	a	2606	PSU	O2-C2	-2.40	1.18	1.23
30	a	1912	PSU	C6-N1	-2.40	1.32	1.36
30	a	952	PSU	C6-N1	-2.40	1.32	1.36
7	A	1407	5MC	C2-N3	-2.39	1.31	1.36
7	A	1519	MA6	C5-N7	-2.38	1.34	1.39
7	A	516	PSU	C6-N1	-2.37	1.32	1.36
27	V	56	PSU	O4-C4	-2.37	1.19	1.23
30	a	2605	PSU	O2-C2	-2.34	1.18	1.23
7	A	516	PSU	O2-C2	-2.33	1.18	1.23
30	a	2499	OMC	C5-C4	-2.31	1.37	1.42
7	A	1498	UR3	C6-N1	-2.29	1.32	1.38
30	a	2553	OMU	C5-C4	-2.27	1.38	1.43
27	V	55	5MU	O2-C2	-2.26	1.18	1.23
30	a	743	PSU	O2-C2	-2.25	1.18	1.23
7	A	1518	MA6	C5-N7	-2.23	1.34	1.39
30	a	1963	5MC	C2-N3	-2.21	1.31	1.36
30	a	2446	2MG	CM2-N2	-2.21	1.41	1.45
7	A	1498	UR3	O2-C2	2.21	1.26	1.22
7	A	1516	2MG	C4-N9	-2.21	1.32	1.38
30	a	1918	PSU	O2-C2	-2.21	1.18	1.23
7	A	966	2MG	C4-N9	-2.20	1.32	1.38
7	A	1207	2MG	C4-N9	-2.19	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	V	33	OMC	C6-C5	2.17	1.40	1.35
30	a	1834	2MG	CM2-N2	-2.17	1.41	1.45
30	a	1834	2MG	C8-N9	-2.17	1.32	1.37
30	a	2504	2MA	C5-N7	-2.17	1.34	1.39
30	a	2499	OMC	C2-N3	-2.16	1.31	1.36
30	a	2581	PSU	C4-C5	-2.14	1.38	1.44
30	a	1834	2MG	C4-N9	-2.13	1.32	1.38
30	a	2458	PSU	C4-C5	-2.13	1.38	1.44
30	a	1963	5MC	C6-C5	2.13	1.38	1.34
7	A	1516	2MG	CM2-N2	-2.12	1.41	1.45
30	a	2031	6MZ	C6-N1	-2.11	1.31	1.35
30	a	742	1MG	C5-C6	-2.11	1.40	1.45
30	a	2446	2MG	C8-N9	-2.10	1.32	1.37
30	a	743	PSU	O4'-C1'	-2.08	1.40	1.43
7	A	967	5MC	C2-N3	-2.08	1.32	1.36
27	V	33	OMC	C5-C4	-2.06	1.38	1.42
27	V	56	PSU	C6-N1	-2.03	1.32	1.36
30	a	743	PSU	C4-C5	-2.02	1.38	1.44
7	A	1207	2MG	C8-N9	-2.00	1.33	1.37
30	a	952	PSU	C4-C5	-2.00	1.38	1.44
30	a	2499	OMC	C6-C5	2.00	1.39	1.35

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2450	H2U	C4-N3-C2	-15.27	113.13	125.79
27	V	21	H2U	O2-C2-N1	-13.83	105.75	123.11
27	V	21	H2U	C4-N3-C2	-13.45	114.64	125.79
30	a	2450	H2U	O2-C2-N1	-11.02	109.28	123.11
30	a	1940	5MU	C4-N3-C2	-8.60	116.21	127.35
30	a	1940	5MU	C5M-C5-C4	8.49	128.11	118.77
30	a	744	5MU	C5M-C5-C4	8.46	128.08	118.77
30	a	1940	5MU	N3-C2-N1	8.37	126.00	114.89
30	a	744	5MU	C4-N3-C2	-8.29	116.61	127.35
30	a	744	5MU	N3-C2-N1	8.18	125.75	114.89
30	a	2450	H2U	O4-C4-N3	-8.15	107.36	120.28
27	V	55	5MU	C4-N3-C2	-7.99	117.00	127.35
27	V	55	5MU	N3-C2-N1	7.97	125.47	114.89
27	V	55	5MU	C5M-C5-C4	7.80	127.35	118.77
27	V	8	4SU	C4-N3-C2	-7.65	119.91	127.34
30	a	1940	5MU	C5-C6-N1	-7.64	115.48	123.34
30	a	2031	6MZ	C9-N6-C6	-7.49	116.42	122.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1834	2MG	C2-N3-C4	7.40	121.21	112.04
30	a	744	5MU	C5-C6-N1	-7.39	115.74	123.34
7	A	1516	2MG	C2-N3-C4	7.25	121.03	112.04
30	a	2504	2MA	C5-C4-N3	-7.22	119.06	127.19
30	a	2446	2MG	C2-N3-C4	7.22	121.00	112.04
27	V	21	H2U	O4-C4-N3	-7.13	108.97	120.28
30	a	742	1MG	C5-C4-N3	-7.09	116.95	128.46
27	V	55	5MU	C5-C6-N1	-7.04	116.09	123.34
7	A	966	2MG	C2-N3-C4	7.00	120.72	112.04
27	V	21	H2U	O2-C2-N3	-6.97	108.51	121.50
7	A	1207	2MG	C2-N3-C4	6.94	120.65	112.04
30	a	744	5MU	C5M-C5-C6	-6.93	113.60	122.85
30	a	1940	5MU	C5M-C5-C6	-6.75	113.83	122.85
30	a	2450	H2U	O4-C4-C5	-6.64	107.99	122.17
30	a	1916	3TD	N1-C2-N3	6.61	121.35	116.14
30	a	2450	H2U	N3-C2-N1	-6.53	109.75	116.65
30	a	2450	H2U	O2-C2-N3	-6.32	109.72	121.50
27	V	21	H2U	O4-C4-C5	-6.29	108.73	122.17
27	V	55	5MU	C5M-C5-C6	-6.16	114.62	122.85
30	a	1940	5MU	C5-C4-N3	6.03	120.46	115.31
27	V	55	5MU	C5-C4-N3	5.92	120.36	115.31
7	A	1519	MA6	C5-C4-N3	-5.82	119.15	126.75
30	a	2505	PSU	N1-C2-N3	5.77	121.67	115.13
7	A	1518	MA6	C5-C4-N3	-5.77	119.22	126.75
30	a	2458	PSU	N1-C2-N3	5.74	121.63	115.13
30	a	744	5MU	C5-C4-N3	5.72	120.20	115.31
30	a	1912	PSU	N1-C2-N3	5.72	121.61	115.13
30	a	743	PSU	N1-C2-N3	5.67	121.55	115.13
30	a	2581	PSU	N1-C2-N3	5.63	121.51	115.13
30	a	1618	6MZ	C5-C4-N3	-5.60	119.44	126.75
30	a	2553	OMU	N3-C2-N1	5.59	122.32	114.89
30	a	952	PSU	N1-C2-N3	5.57	121.45	115.13
7	A	516	PSU	N1-C2-N3	5.51	121.37	115.13
30	a	1918	PSU	N1-C2-N3	5.48	121.34	115.13
30	a	2605	PSU	N1-C2-N3	5.47	121.33	115.13
30	a	1834	2MG	C5-C4-N3	-5.42	119.66	128.46
30	a	2504	2MA	N3-C4-N9	5.40	134.49	126.99
27	V	56	PSU	N1-C2-N3	5.40	121.25	115.13
27	V	8	4SU	C5-C4-N3	5.37	119.67	114.69
7	A	527	G7M	C2-N3-C4	5.36	121.85	112.30
30	a	2606	PSU	N1-C2-N3	5.31	121.15	115.13
7	A	967	5MC	C5-C6-N1	-5.25	117.94	123.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	119	IAS	OD1-CG-CB	-5.23	110.17	125.43
30	a	1963	5MC	C5-C6-N1	-5.22	117.97	123.34
30	a	742	1MG	C2-N3-C4	5.17	123.59	111.98
30	a	742	1MG	N9-C4-N3	5.16	136.30	125.94
7	A	1407	5MC	C5-C6-N1	-5.15	118.04	123.34
30	a	2070	G7M	C2-N3-C4	5.12	121.42	112.30
30	a	2252	OMG	C5-C4-N3	-5.11	120.17	128.46
7	A	966	2MG	C5-C4-N3	-5.10	120.19	128.46
7	A	1519	MA6	N1-C2-N3	-5.07	120.67	128.60
30	a	2031	6MZ	C5-C4-N3	-5.04	120.17	126.75
7	A	1516	2MG	C5-C4-N3	-4.99	120.36	128.46
7	A	1498	UR3	C4-N3-C2	-4.89	119.96	124.56
30	a	2031	6MZ	N1-C2-N3	-4.88	120.97	128.60
7	A	1207	2MG	C5-C4-N3	-4.86	120.58	128.46
30	a	2446	2MG	C5-C4-N3	-4.85	120.60	128.46
7	A	1518	MA6	N1-C2-N3	-4.83	121.05	128.60
30	a	1618	6MZ	N1-C2-N3	-4.74	121.19	128.60
7	A	527	G7M	C5-C4-N3	-4.62	119.28	128.15
7	A	1519	MA6	N3-C4-N9	4.56	134.60	127.08
30	a	2252	OMG	C2-N3-C4	4.49	120.29	112.30
30	a	2553	OMU	C4-N3-C2	-4.43	120.73	126.58
7	A	527	G7M	C5-C6-N1	4.34	120.85	111.79
30	a	1940	5MU	O2-C2-N1	-4.29	117.08	122.79
30	a	2070	G7M	C5-C4-N3	-4.28	119.95	128.15
7	A	1519	MA6	C2-N3-C4	4.25	121.80	111.75
7	A	1518	MA6	N3-C4-N9	4.20	134.00	127.08
30	a	2070	G7M	C5-C6-N1	4.16	120.47	111.79
7	A	1518	MA6	C2-N1-C6	4.15	121.54	111.75
7	A	1518	MA6	C2-N3-C4	4.13	121.51	111.75
7	A	1519	MA6	C2-N1-C6	4.09	121.42	111.75
30	a	1618	6MZ	C2-N3-C4	3.97	121.12	111.75
30	a	2031	6MZ	C2-N3-C4	3.94	121.06	111.75
27	V	8	4SU	N3-C2-N1	3.86	120.02	114.89
30	a	1940	5MU	O4-C4-N3	-3.83	112.77	120.12
30	a	1618	6MZ	N3-C4-N9	3.82	133.38	127.08
30	a	744	5MU	O4-C4-N3	-3.81	112.81	120.12
30	a	2031	6MZ	C6-C5-N7	3.79	136.49	132.39
30	a	743	PSU	C4-N3-C2	-3.79	120.88	126.34
30	a	1618	6MZ	C9-N6-C6	-3.78	119.61	122.87
30	a	2606	PSU	C4-N3-C2	-3.74	120.94	126.34
30	a	2070	G7M	C6-C5-N7	3.71	136.74	132.25
30	a	2505	PSU	C4-N3-C2	-3.71	120.99	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1912	PSU	C4-N3-C2	-3.71	121.00	126.34
7	A	527	G7M	C6-C5-N7	3.70	136.72	132.25
27	V	55	5MU	O4-C4-N3	-3.70	113.03	120.12
30	a	2605	PSU	C4-N3-C2	-3.69	121.02	126.34
30	a	952	PSU	C4-N3-C2	-3.68	121.04	126.34
30	a	2458	PSU	C4-N3-C2	-3.67	121.05	126.34
7	A	1519	MA6	N9-C8-N7	-3.67	108.89	113.91
30	a	1834	2MG	N9-C4-N3	3.65	133.27	125.94
7	A	516	PSU	C4-N3-C2	-3.65	121.08	126.34
30	a	743	PSU	O2-C2-N1	-3.63	118.79	122.79
7	A	1518	MA6	N9-C8-N7	-3.60	108.98	113.91
7	A	1518	MA6	C5-N7-C8	3.57	108.58	103.51
7	A	527	G7M	N9-C4-N3	3.57	133.11	125.94
30	a	1918	PSU	C4-N3-C2	-3.55	121.22	126.34
30	a	2252	OMG	N9-C4-N3	3.51	132.99	125.94
30	a	2581	PSU	C4-N3-C2	-3.45	121.37	126.34
7	A	1519	MA6	C5-N7-C8	3.44	108.39	103.51
7	A	527	G7M	O6-C6-C5	-3.39	120.40	128.06
7	A	966	2MG	N9-C4-N3	3.39	132.74	125.94
30	a	2499	OMC	O2-C2-N3	-3.39	116.82	122.33
30	a	2070	G7M	O6-C6-C5	-3.38	120.43	128.06
7	A	1518	MA6	C4-C5-N7	-3.35	106.54	110.62
27	V	56	PSU	C4-N3-C2	-3.33	121.54	126.34
7	A	1519	MA6	C4-N9-C8	3.31	109.32	105.73
30	a	2505	PSU	O2-C2-N1	-3.31	119.14	122.79
30	a	1618	6MZ	C5-N7-C8	3.31	108.21	103.51
30	a	2070	G7M	N9-C4-N3	3.26	132.48	125.94
41	l	81	4D4	NE-CZ-NH2	3.25	126.41	120.70
30	a	2031	6MZ	C5-N7-C8	3.24	108.11	103.51
30	a	2581	PSU	O2-C2-N1	-3.24	119.22	122.79
30	a	744	5MU	O2-C2-N1	-3.24	118.48	122.79
30	a	2031	6MZ	C4-C5-N7	-3.23	106.68	110.62
30	a	2446	2MG	C6-C5-N7	3.22	136.23	130.25
7	A	1516	2MG	N9-C4-N3	3.21	132.38	125.94
30	a	1618	6MZ	C4-C5-N7	-3.20	106.72	110.62
27	V	21	H2U	N3-C2-N1	-3.19	113.28	116.65
30	a	2031	6MZ	N9-C8-N7	-3.19	109.56	113.91
30	a	2031	6MZ	N3-C4-N9	3.15	132.28	127.08
27	V	56	PSU	O2-C2-N1	-3.13	119.34	122.79
7	A	1518	MA6	C4-N9-C8	3.13	109.12	105.73
30	a	2252	OMG	C6-C5-N7	3.13	136.06	130.25
30	a	1912	PSU	O2-C2-N1	-3.12	119.36	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	V	55	5MU	O2-C2-N1	-3.12	118.64	122.79
7	A	1207	2MG	N9-C4-N3	3.09	132.14	125.94
30	a	744	5MU	O2-C2-N3	-3.08	115.77	121.50
27	V	8	4SU	C5-C4-S4	-3.06	120.53	124.47
7	A	516	PSU	O2-C2-N1	-3.06	119.42	122.79
7	A	1516	2MG	C6-C5-N7	3.05	135.92	130.25
30	a	2446	2MG	N9-C4-N3	3.03	132.02	125.94
27	V	55	5MU	O2-C2-N3	-3.02	115.88	121.50
7	A	1207	2MG	C6-C5-N7	2.99	135.80	130.25
30	a	952	PSU	O2-C2-N1	-2.98	119.51	122.79
30	a	2605	PSU	O2-C2-N1	-2.97	119.52	122.79
30	a	2504	2MA	N9-C8-N7	-2.96	109.86	113.91
30	a	1918	PSU	O2-C2-N1	-2.94	119.56	122.79
30	a	2458	PSU	O2-C2-N1	-2.93	119.56	122.79
30	a	1618	6MZ	N9-C8-N7	-2.92	109.92	113.91
30	a	744	5MU	C1'-N1-C6	-2.90	116.30	121.12
30	a	1618	6MZ	C6-C5-N7	2.90	135.53	132.39
7	A	1519	MA6	C4-C5-N7	-2.85	107.14	110.62
30	a	2504	2MA	C5-N7-C8	2.85	107.55	103.51
18	L	89	D2T	OD1-CG-CB	-2.80	116.57	122.44
30	a	2606	PSU	O2-C2-N1	-2.79	119.72	122.79
7	A	966	2MG	C6-C5-N7	2.73	135.33	130.25
30	a	2553	OMU	O2-C2-N1	-2.72	119.17	122.79
7	A	527	G7M	C2-N1-C6	-2.72	120.15	125.10
30	a	2446	2MG	CM2-N2-C2	-2.71	117.87	123.86
27	V	33	OMC	O2-C2-N3	-2.67	117.98	122.33
30	a	1834	2MG	C2-N1-C6	-2.63	121.45	124.48
30	a	2553	OMU	C5-C4-N3	2.59	118.72	114.84
30	a	2070	G7M	C2-N1-C6	-2.58	120.39	125.10
30	a	1834	2MG	C6-C5-N7	2.56	135.02	130.25
30	a	2446	2MG	C4-C5-N7	-2.56	106.67	110.72
30	a	1834	2MG	CM2-N2-C2	-2.54	118.25	123.86
7	A	966	2MG	CM2-N2-C2	-2.53	118.27	123.86
30	a	742	1MG	C5-C6-N1	2.53	119.79	114.91
30	a	2252	OMG	C4-C5-N7	-2.52	106.73	110.72
30	a	2252	OMG	C8-N7-C5	2.52	108.81	104.24
30	a	2553	OMU	O4-C4-C5	-2.50	120.77	125.16
7	A	1207	2MG	C4-C5-N7	-2.50	106.77	110.72
7	A	1402	4OC	O2-C2-N3	-2.49	118.28	122.33
30	a	1834	2MG	O6-C6-C5	-2.49	120.00	126.60
7	A	1516	2MG	C4-C5-N7	-2.48	106.79	110.72
30	a	2581	PSU	O4'-C1'-C2'	2.48	108.64	105.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1940	5MU	C6-N1-C2	2.46	123.79	121.30
30	a	1940	5MU	O2-C2-N3	-2.46	116.92	121.50
7	A	967	5MC	C5-C4-N3	-2.45	119.03	121.67
30	a	2252	OMG	N9-C8-N7	-2.43	108.82	113.39
30	a	2252	OMG	C5-C6-N1	2.42	119.33	113.19
7	A	966	2MG	O6-C6-C5	-2.41	120.21	126.60
7	A	966	2MG	C2-N1-C6	-2.41	121.71	124.48
30	a	2504	2MA	C4-N9-C8	2.40	108.33	105.73
30	a	2499	OMC	N1-C2-N3	2.40	123.17	118.81
27	V	8	4SU	O2-C2-N1	-2.33	119.68	122.79
30	a	1834	2MG	C4-C5-N7	-2.33	107.03	110.72
30	a	2504	2MA	C4-C5-N7	-2.32	107.80	110.62
7	A	1516	2MG	N1-C2-N3	-2.31	120.38	123.95
41	l	81	4D4	NH1-CZ-NE	-2.31	113.86	119.19
7	A	1516	2MG	O6-C6-C5	-2.30	120.49	126.60
7	A	516	PSU	O3'-C3'-C2'	2.28	119.21	111.82
7	A	966	2MG	C4-C5-N7	-2.28	107.11	110.72
30	a	2504	2MA	N3-C2-N1	-2.28	121.53	125.72
30	a	2446	2MG	O6-C6-C5	-2.28	120.56	126.60
30	a	1916	3TD	C4-N3-C2	-2.25	122.16	124.61
30	a	2446	2MG	N1-C2-N3	-2.25	120.47	123.95
30	a	2450	H2U	C5-C4-N3	-2.25	114.12	116.65
7	A	1516	2MG	C5-C6-N1	2.24	118.87	113.19
7	A	1407	5MC	C5-C4-N3	-2.23	119.27	121.67
30	a	2446	2MG	C5-C6-N1	2.23	118.85	113.19
7	A	1498	UR3	C5-C6-N1	-2.23	118.08	121.81
7	A	1207	2MG	O6-C6-C5	-2.22	120.71	126.60
30	a	2446	2MG	N9-C8-N7	-2.21	109.23	113.39
30	a	1834	2MG	C5-C6-N1	2.21	118.79	113.19
30	a	2446	2MG	C8-N7-C5	2.20	108.22	104.24
7	A	966	2MG	C5-C6-N1	2.19	118.76	113.19
30	a	2031	6MZ	C4-N9-C8	2.19	108.10	105.73
7	A	1207	2MG	C2-N1-C6	-2.18	121.97	124.48
30	a	2446	2MG	C2-N1-C6	-2.17	121.98	124.48
7	A	1207	2MG	CM2-N2-C2	-2.17	119.08	123.86
30	a	742	1MG	C4-C5-N7	-2.16	107.30	110.72
30	a	2581	PSU	C6-N1-C2	-2.14	120.49	122.68
7	A	1516	2MG	C8-N7-C5	2.14	108.11	104.24
30	a	2458	PSU	C6-N1-C2	-2.13	120.51	122.68
27	V	55	5MU	C1'-N1-C6	-2.12	117.59	121.12
30	a	1963	5MC	C5-C4-N3	-2.12	119.39	121.67
30	a	742	1MG	C6-C5-N7	2.09	134.08	129.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1402	4OC	C5-C4-N3	-2.09	119.23	122.59
7	A	1516	2MG	C2-N1-C6	-2.09	122.08	124.48
7	A	1207	2MG	C8-N7-C5	2.09	108.02	104.24
27	V	33	OMC	N1-C2-N3	2.09	122.61	118.81
30	a	1912	PSU	C6-N1-C2	-2.08	120.55	122.68
7	A	1207	2MG	C5-C6-N1	2.08	118.46	113.19
41	l	82	MS6	CE-SD-CG	2.07	107.51	100.40
30	a	1618	6MZ	C4-N9-C8	2.07	107.97	105.73
30	a	1916	3TD	O4'-C1'-C2'	2.07	108.06	105.14
30	a	1834	2MG	C8-N7-C5	2.06	107.96	104.24
30	a	744	5MU	C6-N1-C2	2.05	123.38	121.30
30	a	1918	PSU	C6-N1-C2	-2.04	120.59	122.68
30	a	952	PSU	C6-N1-C2	-2.04	120.60	122.68
30	a	2252	OMG	O6-C6-C5	-2.02	121.25	126.60
30	a	2553	OMU	C5-C6-N1	-2.01	118.44	121.81

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1207	2MG	N1-C2-N2-CM2
7	A	1207	2MG	N3-C2-N2-CM2
7	A	1519	MA6	C5-C6-N6-C10
27	V	21	H2U	O4'-C4'-C5'-O5'
27	V	21	H2U	C3'-C4'-C5'-O5'
27	V	21	H2U	O4'-C1'-N1-C6
27	V	56	PSU	C3'-C4'-C5'-O5'
27	V	56	PSU	O4'-C4'-C5'-O5'
41	l	82	MS6	CA-CB-CG-SD
17	K	119	IAS	N-CA-CB-CG
30	a	2252	OMG	C1'-C2'-O2'-CM2
7	A	1519	MA6	O4'-C4'-C5'-O5'
30	a	1916	3TD	C3'-C4'-C5'-O5'
30	a	2031	6MZ	O4'-C4'-C5'-O5'
30	a	2031	6MZ	C3'-C4'-C5'-O5'
30	a	1916	3TD	O4'-C4'-C5'-O5'
30	a	2505	PSU	O4'-C4'-C5'-O5'
41	l	82	MS6	CB-CG-SD-CE
7	A	1519	MA6	C3'-C4'-C5'-O5'
7	A	527	G7M	C3'-C4'-C5'-O5'
27	V	33	OMC	O4'-C4'-C5'-O5'
30	a	2505	PSU	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	V	33	OMC	C3'-C4'-C5'-O5'
7	A	1519	MA6	C5-C6-N6-C9
41	l	81	4D4	OB-CB-CG-CD
30	a	2446	2MG	C3'-C4'-C5'-O5'
18	L	89	D2T	CG-CB-SB-CB1
41	l	82	MS6	N-CA-CB-CG
33	d	150	MEQ	N-CA-CB-CG
27	V	56	PSU	C4'-C5'-O5'-P
7	A	527	G7M	O4'-C4'-C5'-O5'
7	A	527	G7M	C4'-C5'-O5'-P
41	l	81	4D4	NE-CD-CG-CB
41	l	81	4D4	CA-CB-CG-CD
18	L	89	D2T	SB-CB-CG-OD2
7	A	1519	MA6	N1-C6-N6-C10
30	a	2504	2MA	C4'-C5'-O5'-P
27	V	21	H2U	C2'-C1'-N1-C2
30	a	743	PSU	O4'-C1'-C5-C6
30	a	2499	OMC	O4'-C4'-C5'-O5'
30	a	2504	2MA	O4'-C4'-C5'-O5'
27	V	21	H2U	O4'-C1'-N1-C2
33	d	150	MEQ	OE1-CD-CG-CB
30	a	2070	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	V	21	H2U	3	0
7	A	1207	2MG	1	0
30	a	2252	OMG	1	0
7	A	1402	4OC	2	0
7	A	967	5MC	2	0
30	a	2504	2MA	1	0
30	a	2031	6MZ	1	0
27	V	8	4SU	1	0
33	d	150	MEQ	2	0
17	K	119	IAS	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 521 ligands modelled in this entry, 521 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	a	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1915:C	O3'	1916:3TD	P	4.59
1	a	1916:3TD	O3'	1917:A	P	3.37

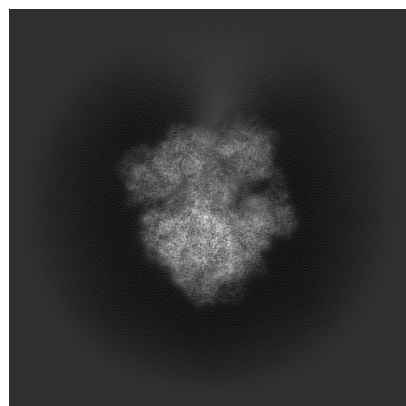
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55331. These allow visual inspection of the internal detail of the map and identification of artifacts.

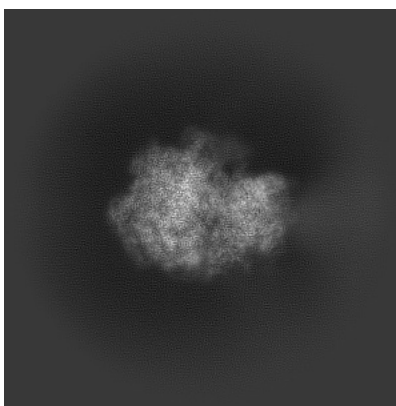
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

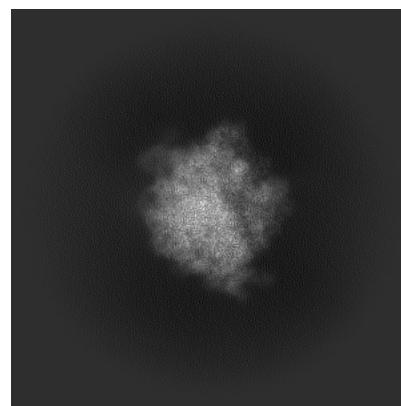
6.1.1 Primary map



X

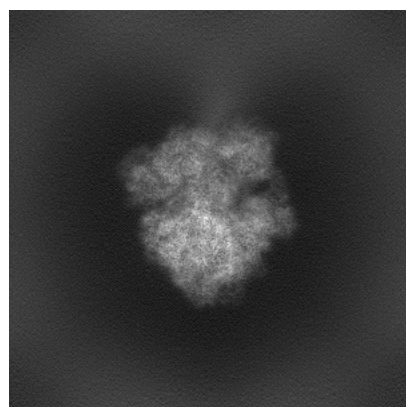


Y

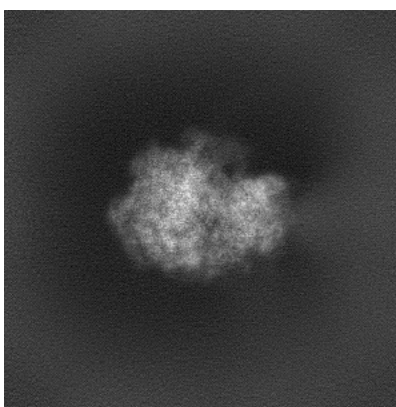


Z

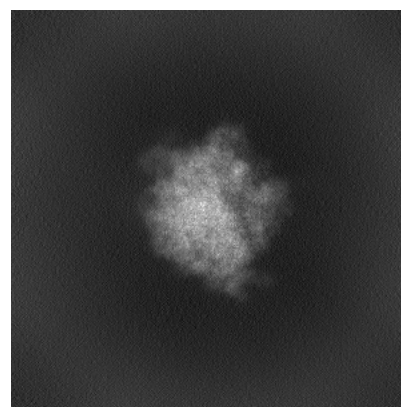
6.1.2 Raw map



X



Y

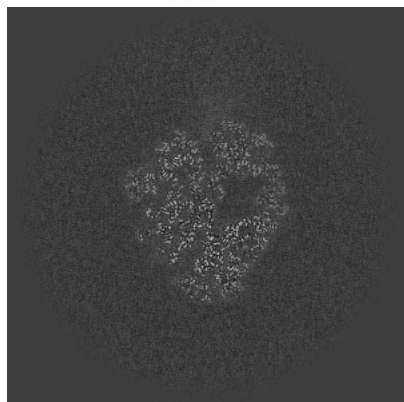


Z

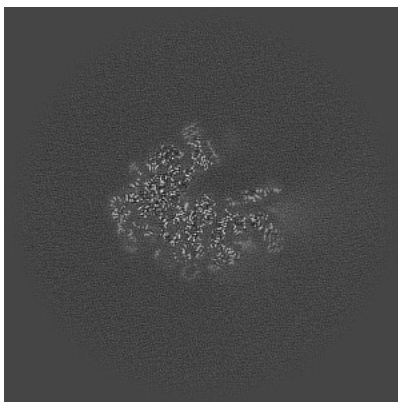
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

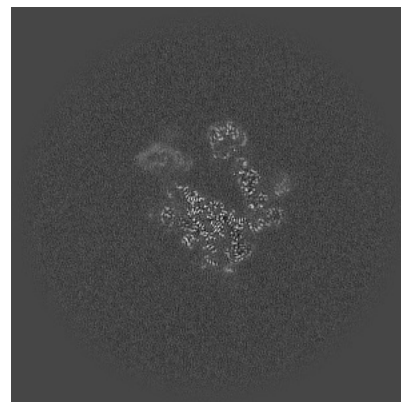
6.2.1 Primary map



X Index: 256

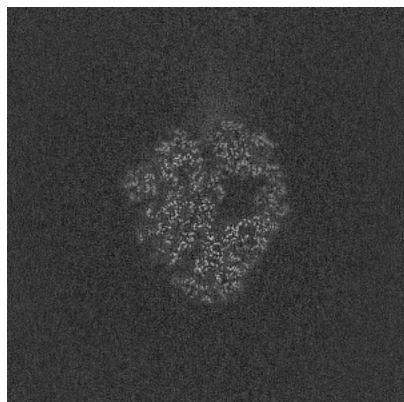


Y Index: 256

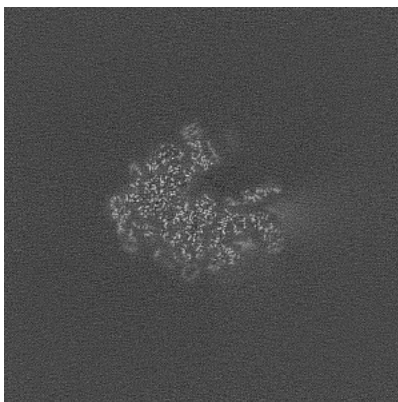


Z Index: 256

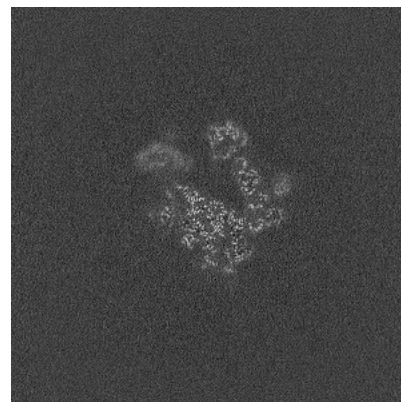
6.2.2 Raw map



X Index: 256



Y Index: 256

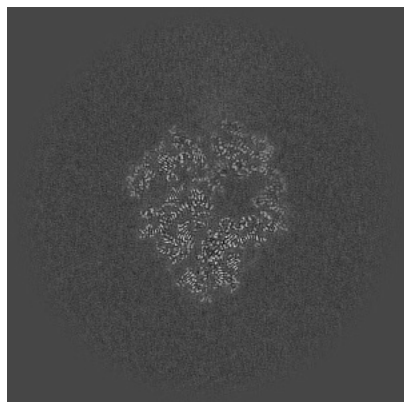


Z Index: 256

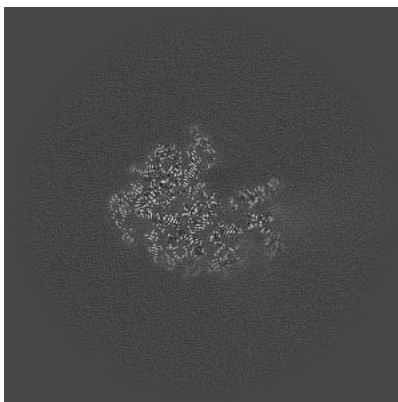
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

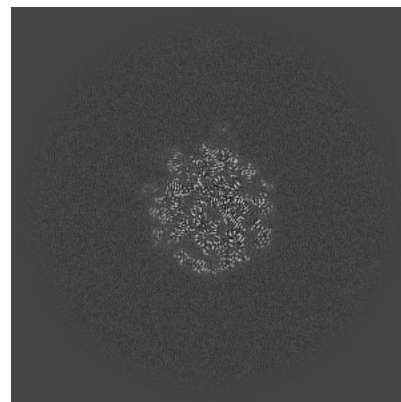
6.3.1 Primary map



X Index: 261

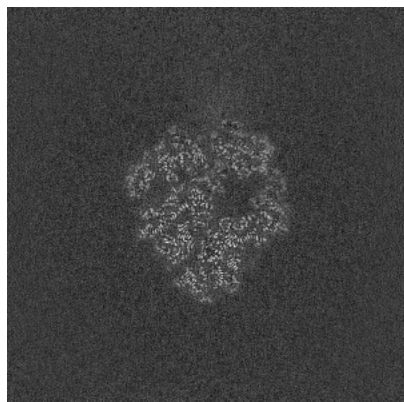


Y Index: 250

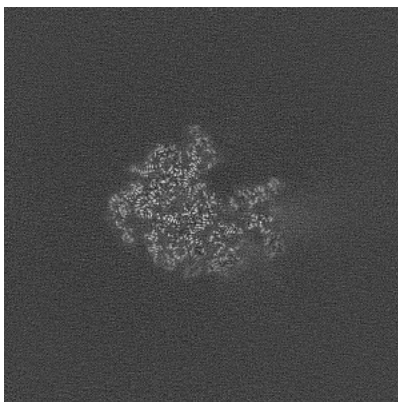


Z Index: 216

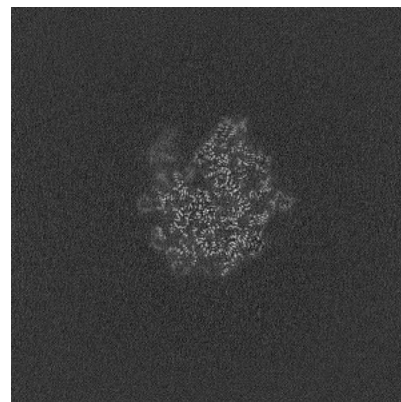
6.3.2 Raw map



X Index: 261



Y Index: 250

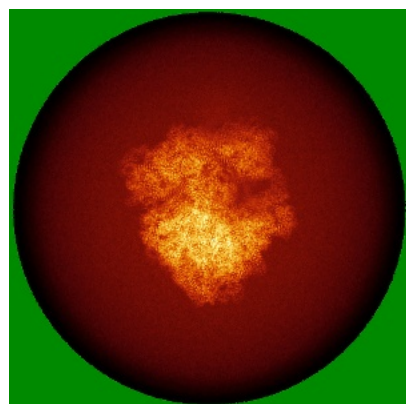


Z Index: 234

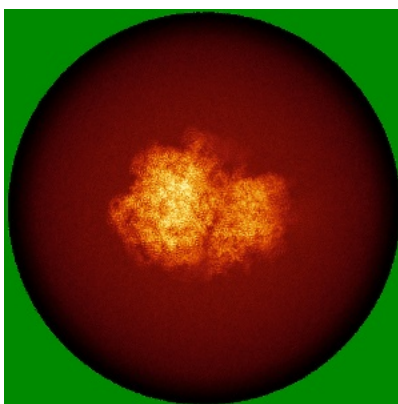
The images above show the largest variance slices of the map in three orthogonal directions.

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

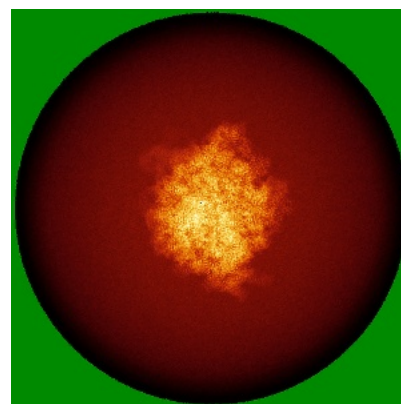
6.4.1 Primary map



X

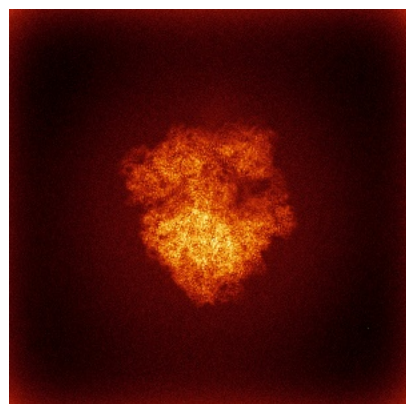


Y

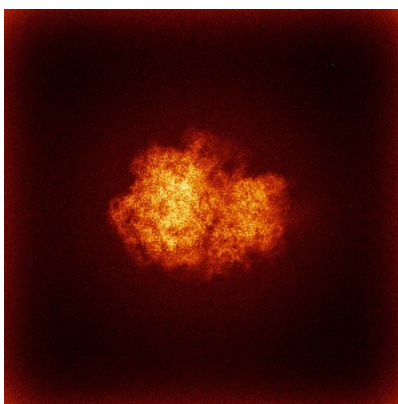


Z

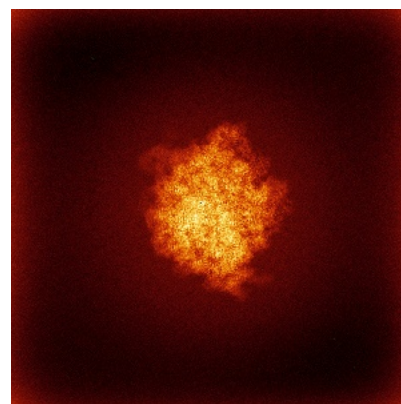
6.4.2 Raw map



X



Y

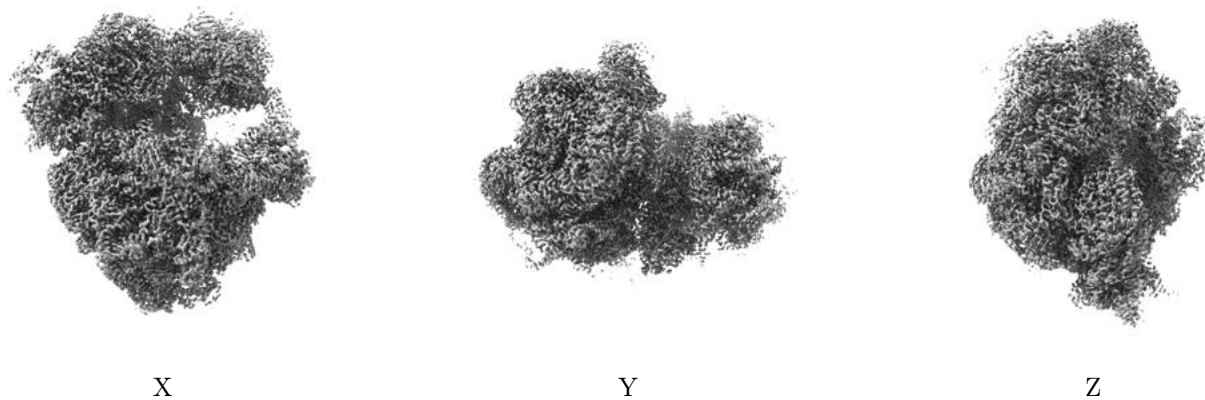


Z

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

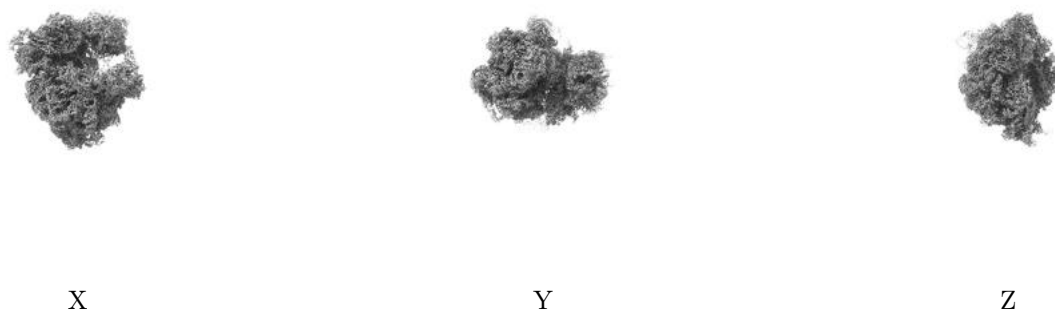
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

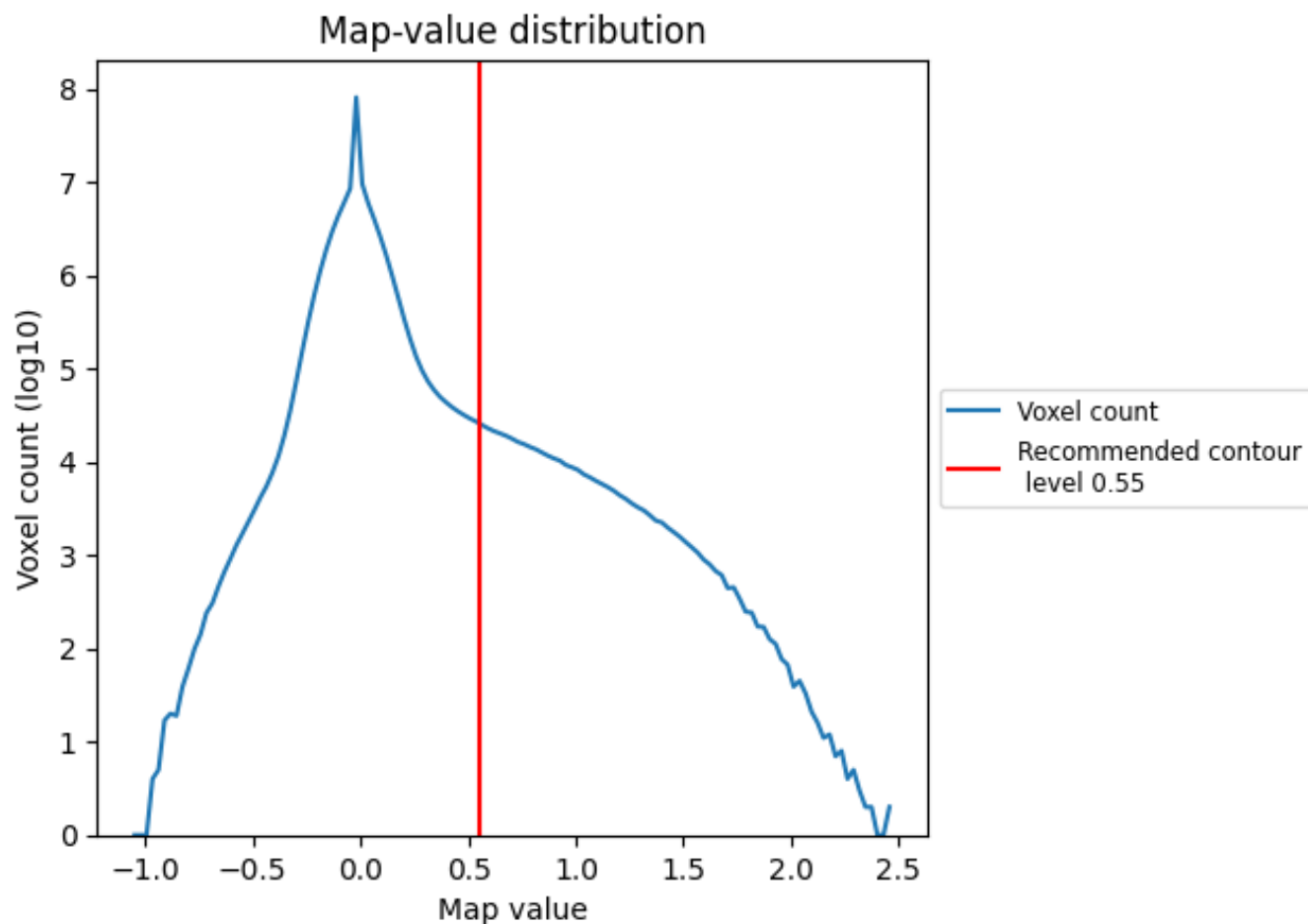
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

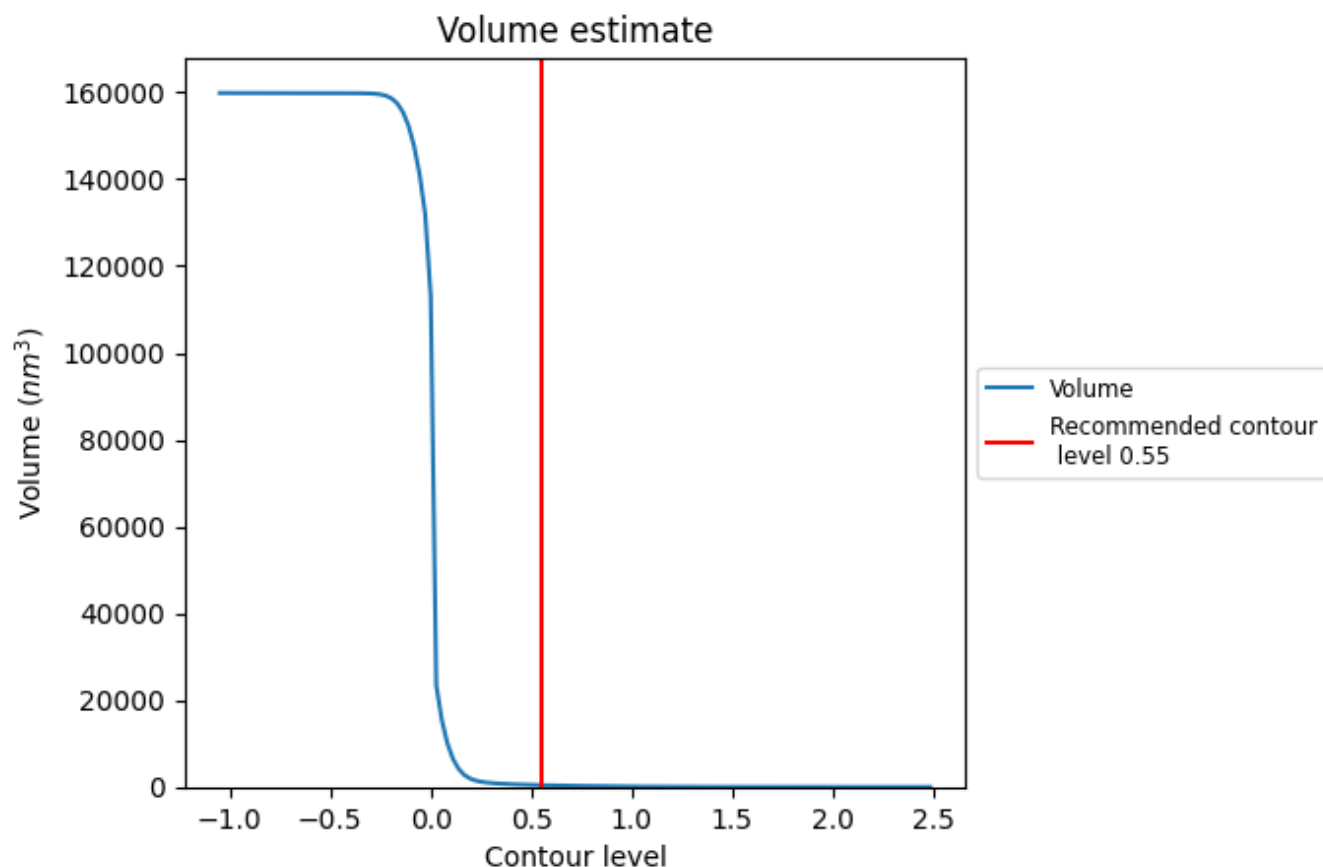
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

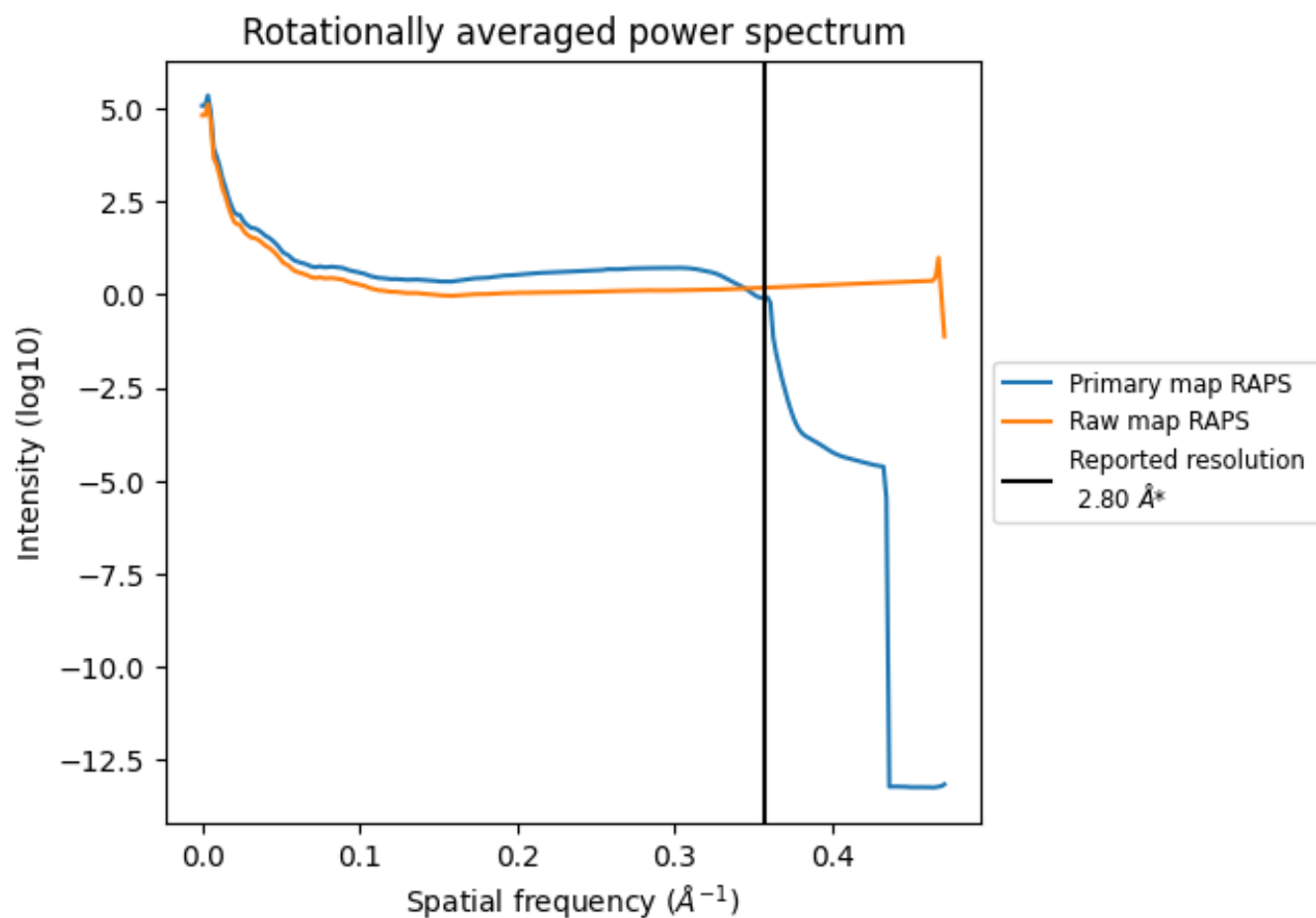
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm^3 ; this corresponds to an approximate mass of 375 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 ⓘ

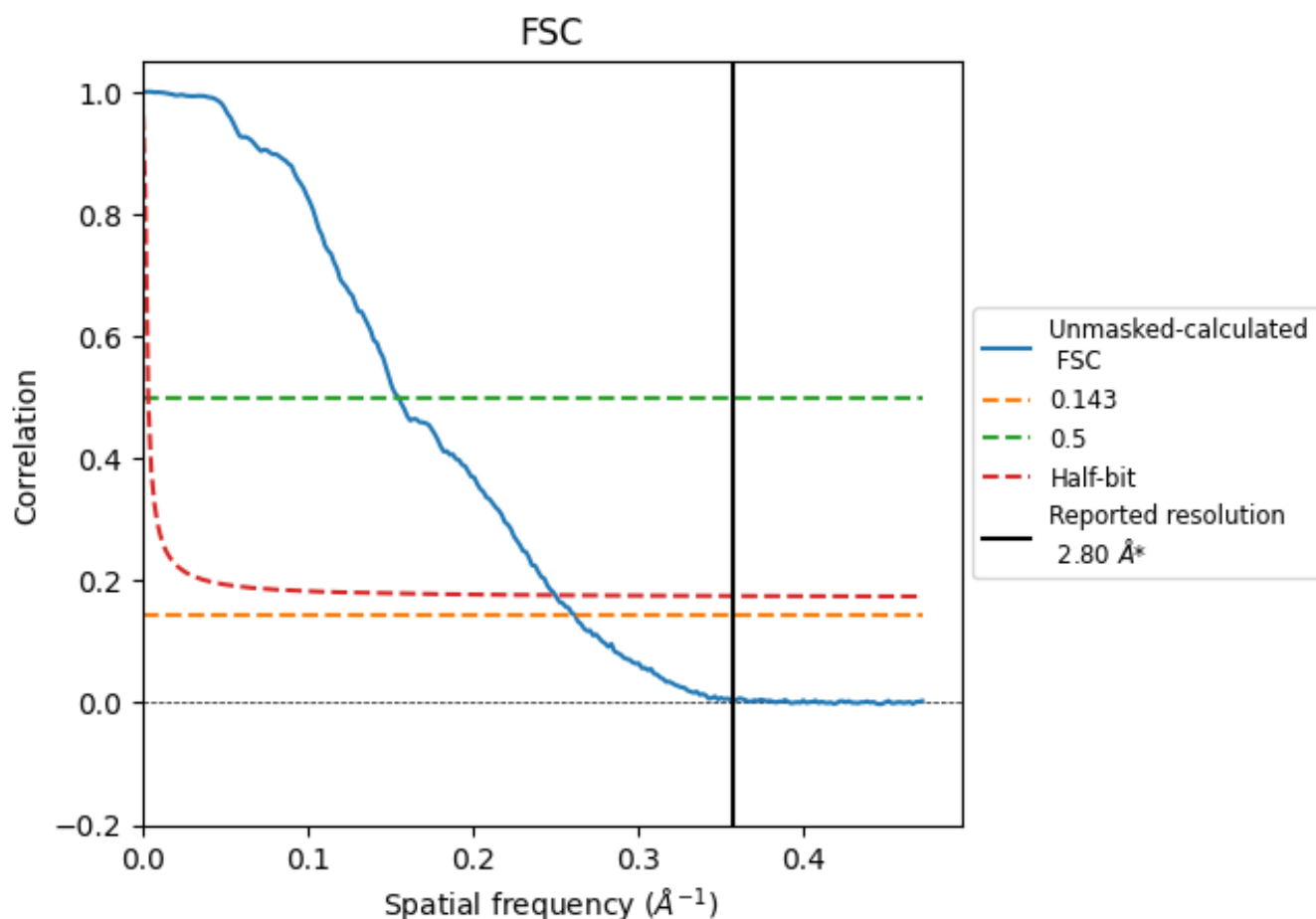


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

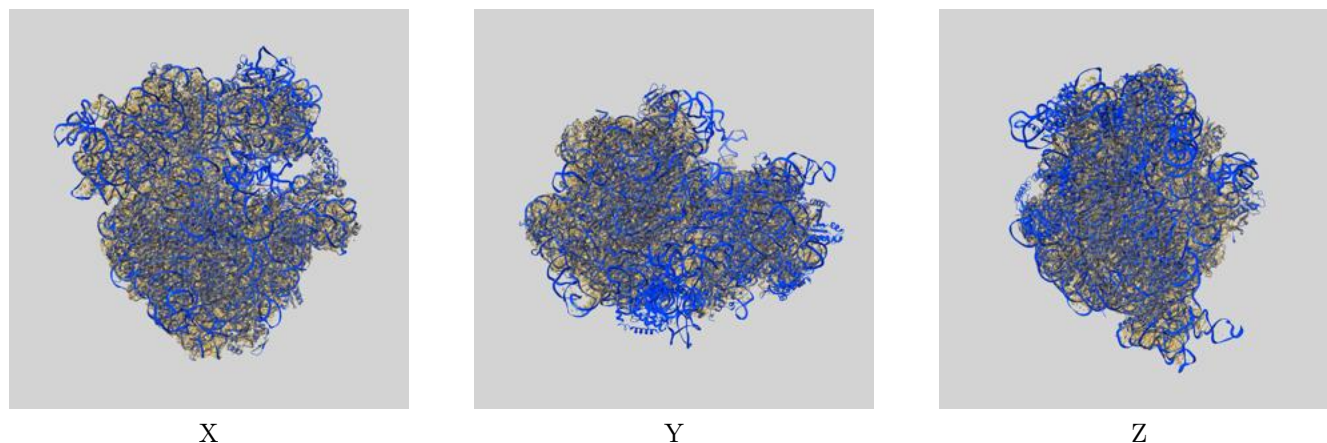
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	6.46	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

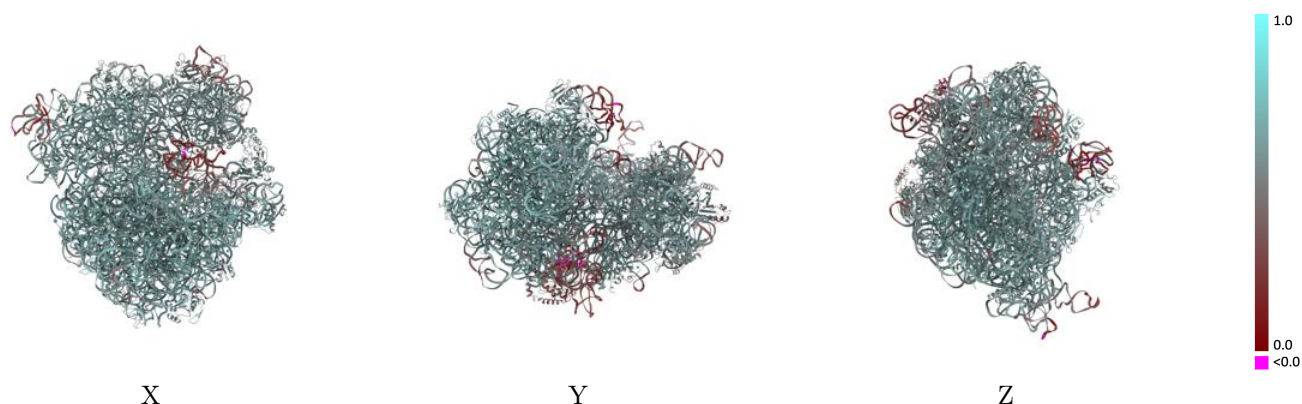
This section contains information regarding the fit between EMDB map EMD-55331 and PDB model 9SX5. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



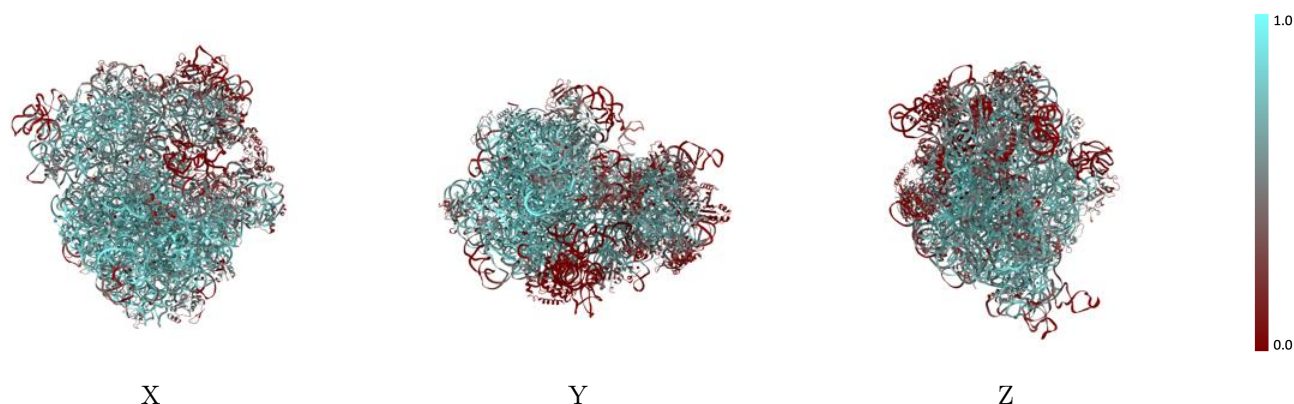
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



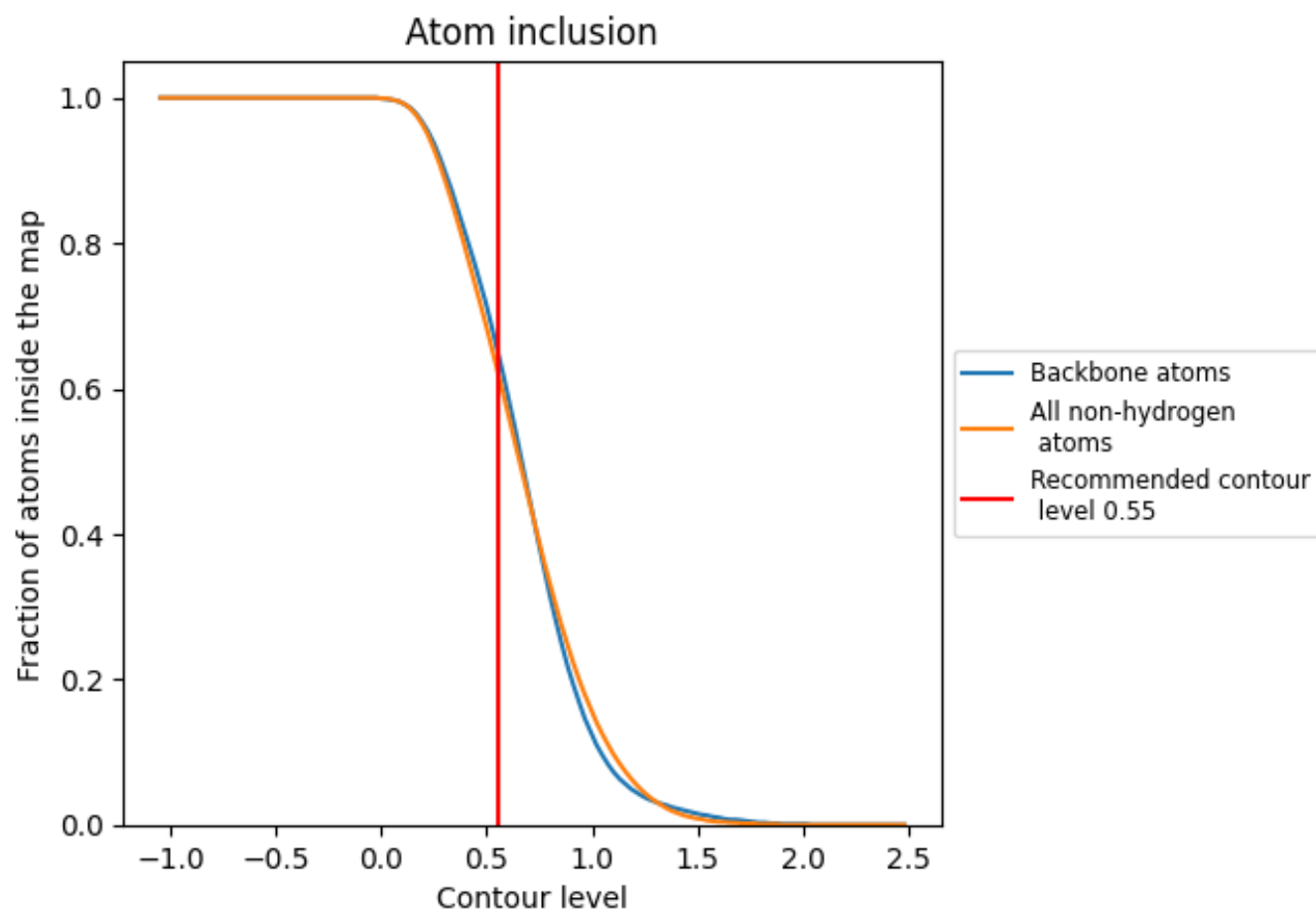
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 63% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6260	 0.5830
0	 0.5310	 0.6100
1	 0.7770	 0.6430
2	 0.7370	 0.6350
3	 0.6380	 0.6200
4	 0.0890	 0.5130
5	 0.0010	 0.3050
A	 0.6610	 0.5780
B	 0.1270	 0.5240
C	 0.3470	 0.5670
D	 0.4010	 0.5790
E	 0.5560	 0.6090
F	 0.3600	 0.5650
G	 0.2790	 0.5480
H	 0.5650	 0.6100
I	 0.3530	 0.5650
J	 0.2320	 0.5270
K	 0.4230	 0.5820
L	 0.5330	 0.5970
M	 0.2880	 0.5640
N	 0.3530	 0.5660
O	 0.5080	 0.5990
P	 0.5700	 0.5970
Q	 0.4520	 0.5880
R	 0.4130	 0.5480
S	 0.2640	 0.5450
T	 0.4920	 0.5850
V	 0.0130	 0.3660
W	 0.0550	 0.4100
X	 0.2890	 0.5680
a	 0.7440	 0.5950
b	 0.6730	 0.5890
c	 0.7050	 0.6350
d	 0.6650	 0.6260
e	 0.5520	 0.6100



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.2900	 0.5630
g	 0.2960	 0.5580
h	 0.0630	 0.4430
i	 0.6710	 0.6230
j	 0.6260	 0.6290
k	 0.6330	 0.6200
l	 0.6050	 0.6200
m	 0.7390	 0.6280
n	 0.5300	 0.5980
o	 0.6240	 0.6250
p	 0.7330	 0.6340
q	 0.5940	 0.6190
r	 0.6460	 0.6230
s	 0.5440	 0.6100
t	 0.4360	 0.5810
u	 0.5020	 0.6030
v	 0.6710	 0.6290
w	 0.6280	 0.6140
x	 0.4190	 0.5670
y	 0.6480	 0.6140
z	 0.6650	 0.6280