



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:31 PM UTC

PDB ID : 7O5B / pdb_00007o5b
EMDB ID : EMD-12734
Title : Cryo-EM structure of a Bacillus subtilis MifM-stalled ribosome-nascent chain complex with (p)ppGpp-SRP bound
Authors : Kratzat, H.; Czech, L.; Berninghausen, O.; Bange, G.; Beckmann, R.
Deposited on : 2021-04-08
Resolution : 3.33 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

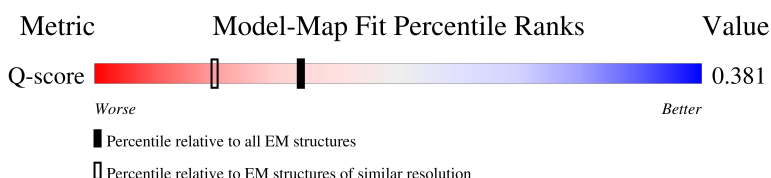
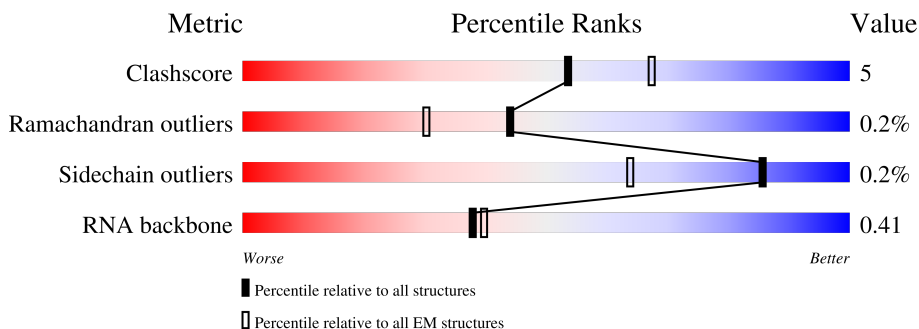
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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	14484 (2.83 - 3.83)

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	U	77	8% 70% 22% 8%
2	V	8	38% 62% 25% 12%
3	W	266	44% 37% 50% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	g	447	
5	h	96	
6	p	166	
7	q	141	
8	X	2887	
9	Y	112	
10	Z	277	
11	a	208	
12	b	207	
13	c	179	
14	d	179	
15	e	145	
16	f	122	
17	i	146	
18	j	144	
19	k	120	
20	l	120	
21	m	115	
22	n	119	
23	o	102	
24	r	113	
25	s	95	
26	t	103	
27	u	94	
28	v	62	

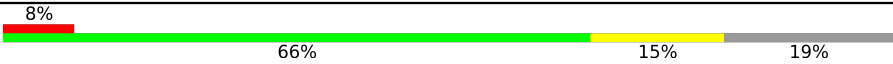
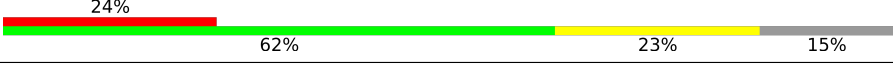
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	w	66	
30	x	59	
31	0	59	
32	1	49	
33	2	44	
34	3	66	
35	4	37	
36	6	66	
37	A	1533	
38	B	246	
39	C	218	
40	D	200	
41	E	166	
42	F	95	
43	G	156	
44	H	132	
45	I	130	
46	J	102	
47	K	131	
48	L	138	
49	M	121	
50	N	61	
51	O	89	
52	P	90	
53	Q	87	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	R	79	
55	S	92	
56	T	88	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 150422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	77	Total	C	N	O	P	0	0
			1643	731	290	545	77		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	8	Total	C	N	O	P	0	0
			177	79	38	52	8		

- Molecule 3 is a RNA chain called SRP RNA (266-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	266	Total	C	N	O	P	0	0
			5685	2535	1018	1866	266		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	?	-	U	deletion	GB 1837880844

- Molecule 4 is a protein called Signal recognition particle protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	g	403	Total	C	N	O	0	0
			1911	1097	410	404		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	-2	HIS	-	expression tag	UNP P37105
g	-1	MET	-	expression tag	UNP P37105
g	0	GLY	-	expression tag	UNP P37105

- Molecule 5 is a protein called MifM-stalling construct.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	h	43	Total	C	N	O	0	0
			189	114	43	32		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	p	123	Total	C	N	O	S	0	0
			955	602	163	189	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	154	THR	ALA	conflict	UNP P42923

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	133	Total	C	N	O	S	0	0
			981	617	173	185	6		

- Molecule 8 is a RNA chain called 23S rRNA (2887-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	2887	Total	C	N	O	P	0	0
			61997	27661	11460	19992	2884		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	243	G	A	conflict	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	G	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961
X	?	-	C	deletion	GB 1491848961
X	?	-	G	deletion	GB 1491848961
X	?	-	G	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	?	-	C	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	C	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	C	deletion	GB 1491848961
X	?	-	C	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	640	U	C	conflict	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	C	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961
X	?	-	G	deletion	GB 1491848961
X	?	-	U	deletion	GB 1491848961
X	?	-	A	deletion	GB 1491848961
X	?	-	G	deletion	GB 1491848961

- Molecule 9 is a RNA chain called 5S rRNA (112-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 10 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 12 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

- Molecule 13 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	176	Total	C	N	O	S	0	0
			1386	882	241	256	7		

- Molecule 14 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	120	Total	C	N	O	S	0	0
			912	564	176	171	1		

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	115	Total	C	N	O	S	0	0
			944	600	185	158	1		

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	o	101	Total	C	N	O	0	0
			786	501	139	146		

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	r	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	s	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	t	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	82	Total	C	N	O	S	0	0
			630	390	123	117			

- Molecule 28 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	x	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 31 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	0	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 32 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 34 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 35 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 36 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	6	63	Total	C	N	O	S	0	0
			499	312	91	91	5		

- Molecule 37 is a RNA chain called 16S rRNA (1533-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	A	1533	Total	C	N	O	P	0	0
			32891	14667	6034	10657	1533		

- Molecule 38 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B	218	Total	C	N	O	S	0	0
			1757	1119	309	323	6		

- Molecule 39 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	C	206	Total	C	N	O	S	0	0
			1619	1011	304	301	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	213	THR	ASN	conflict	UNP P21465

- Molecule 40 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	D	195	Total	C	N	O	S	0	0
			1568	991	291	284	2		

- Molecule 41 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	E	164	Total	C	N	O	S	0	0
			1218	767	225	224	2		

- Molecule 42 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	F	92	Total	C	N	O	S	0	0
			755	476	132	146	1		

- Molecule 43 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	G	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

- Molecule 44 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	H	131	Total	C	N	O	S	0	0
			1036	655	191	187	3		

- Molecule 45 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	I	125	Total	C	N	O	S	0	0
			966	599	191	175	1		

- Molecule 46 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	J	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

- Molecule 47 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	K	114	Total	C	N	O	S	0	0
			838	516	164	156	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	7	GLN	SER	conflict	UNP P04969

- Molecule 48 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L	136	Total	C	N	O	S	0	0
			1052	653	211	186	2		

- Molecule 49 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	M	108	Total	C	N	O	S	0	0
			868	534	176	158			

- Molecule 50 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	N	60	Total	C	N	O	S	0	0
			497	317	98	77	5		

- Molecule 51 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	O	85	Total	C	N	O	S	0	0
			710	436	144	129	1		

- Molecule 52 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	P	88	Total	C	N	O	S	0	0
			695	441	128	124	2		

- Molecule 53 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Q	84	Total	C	N	O	S	0	0
			691	435	128	126	2		

- Molecule 54 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	R	64	Total	C	N	O	S	0	0
			518	332	96	88	2		

- Molecule 55 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S	78	Total	C	N	O	S	0	0
			633	409	112	110	2		

- Molecule 56 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	T	83	Total	C	N	O	S	0	0
			637	390	130	116	1		

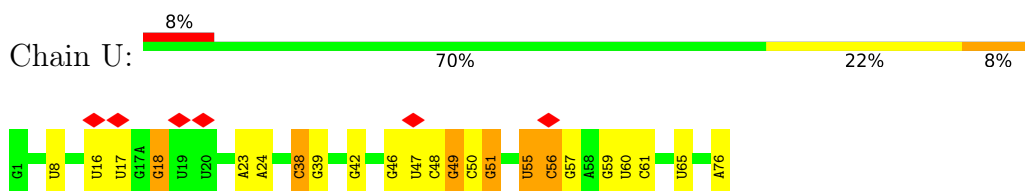
- Molecule 57 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).



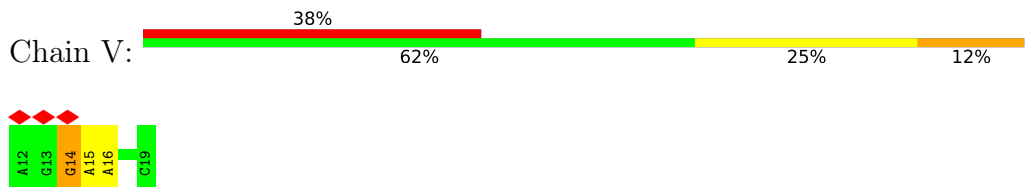
3 Residue-property plots [i](#)

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.

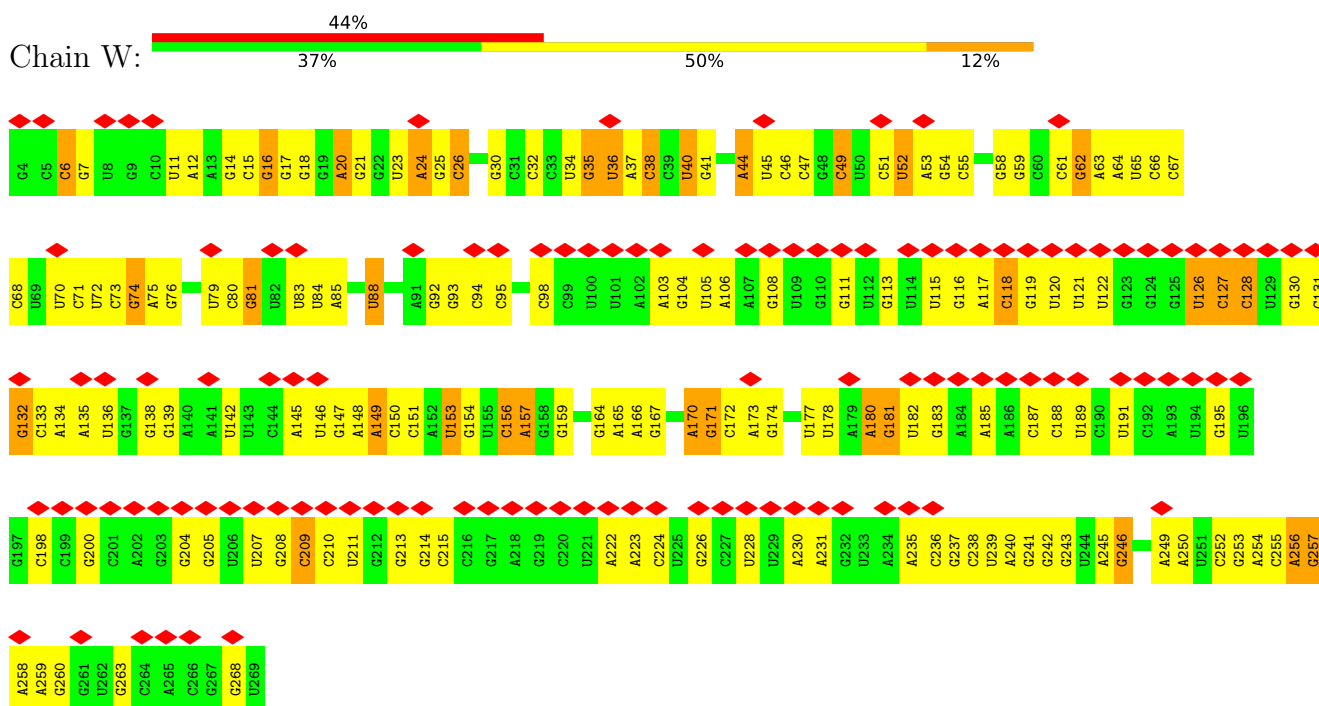
- Molecule 1: tRNA



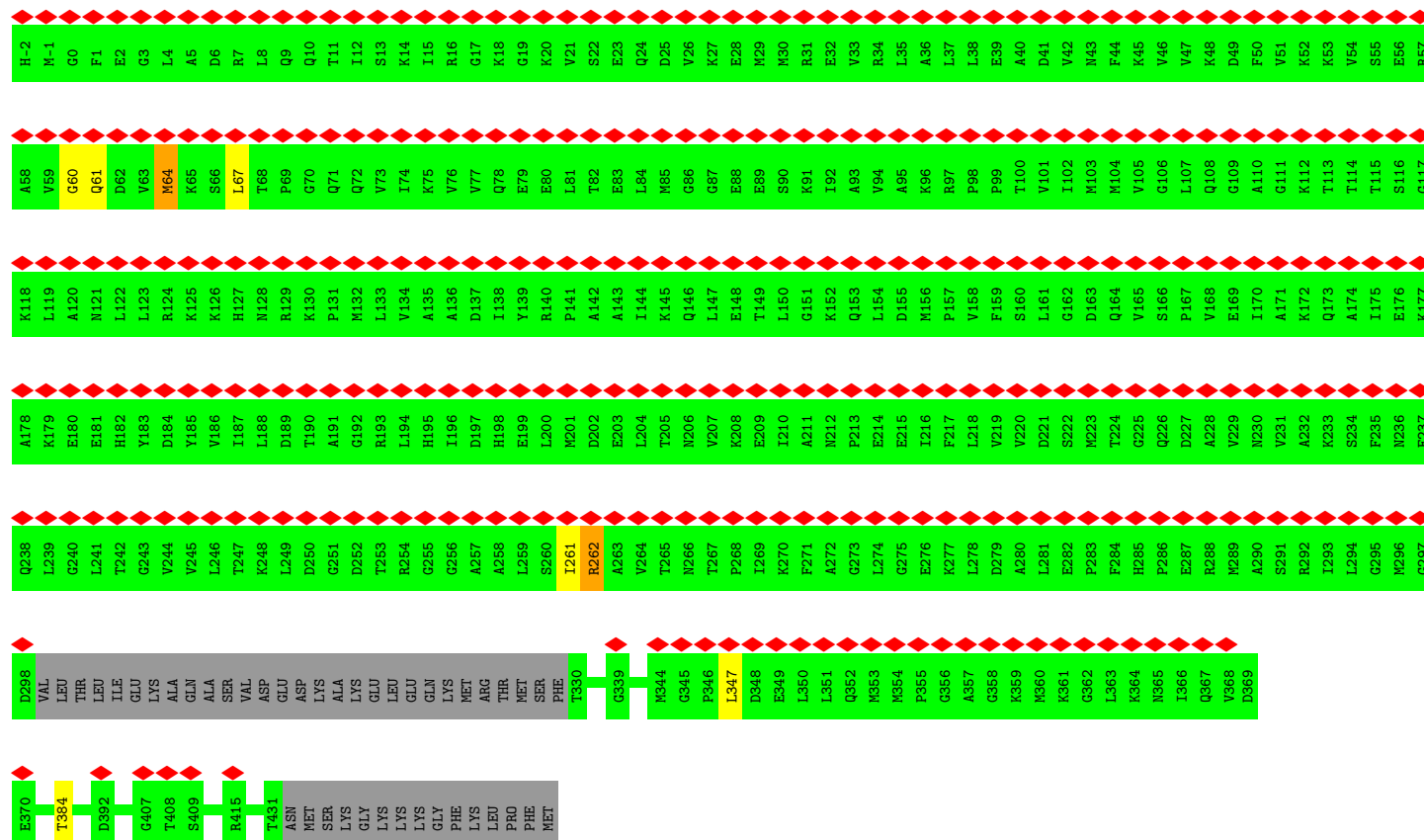
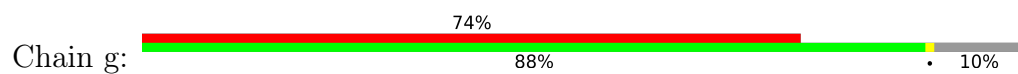
- Molecule 2: mRNA



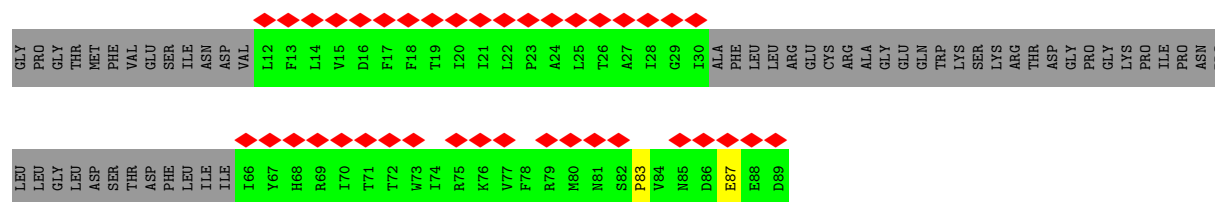
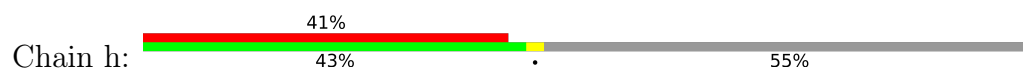
- Molecule 3: SRP RNA (266-MER)



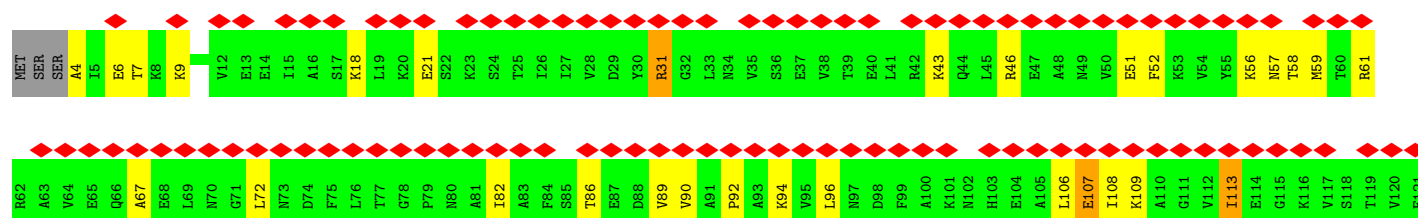
- Molecule 4: Signal recognition particle protein

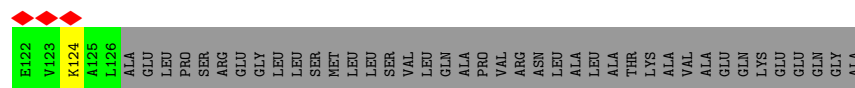


• Molecule 5: MifM-stalling construct

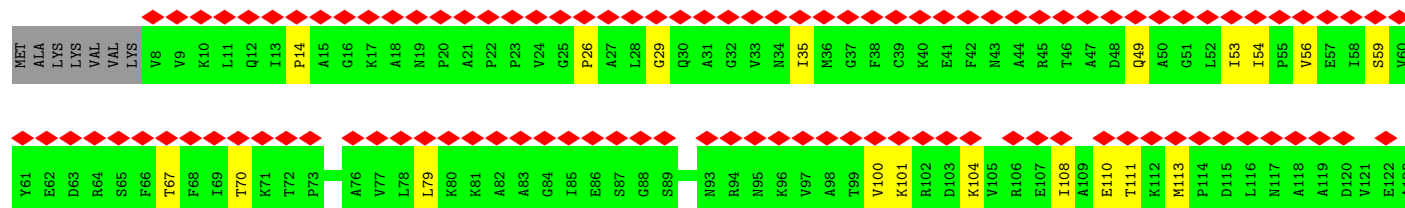
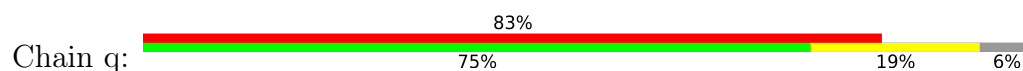


• Molecule 6: 50S ribosomal protein L10

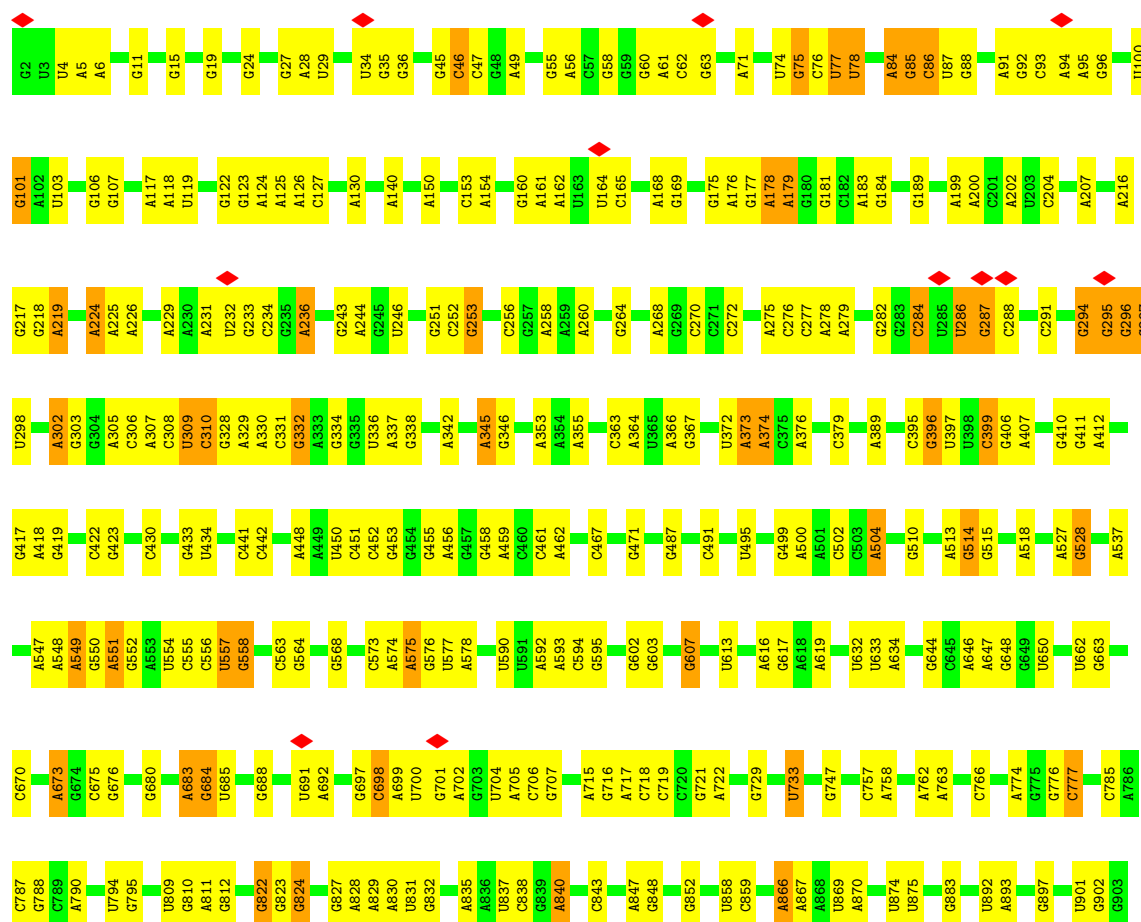




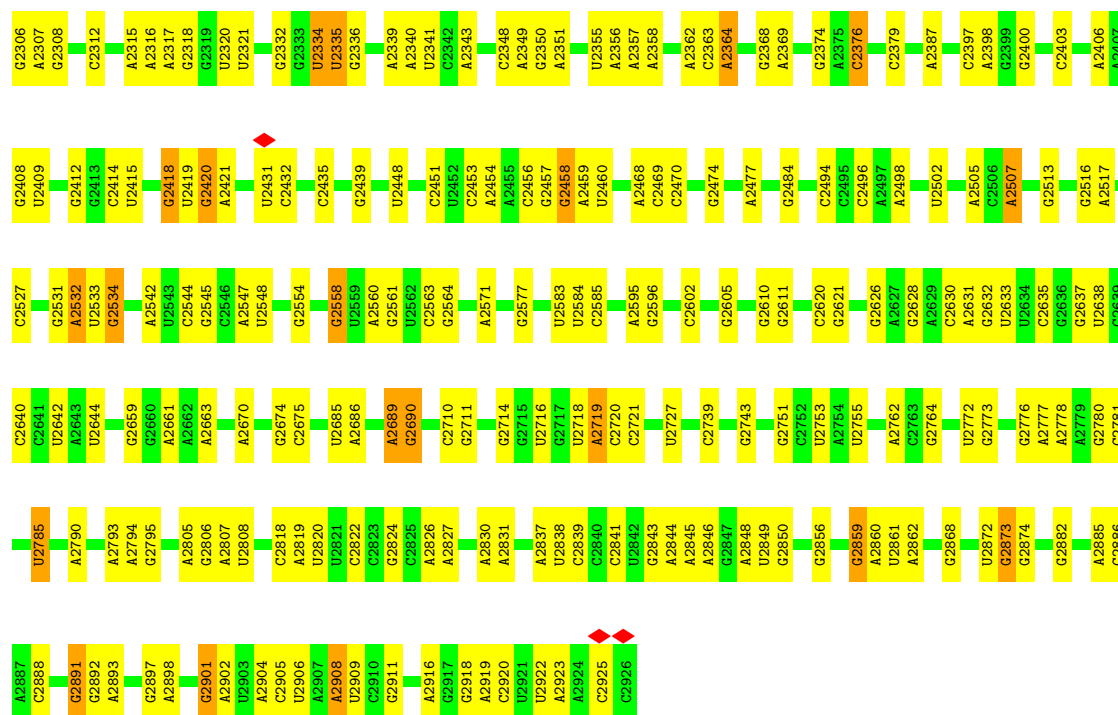
- Molecule 7: 50S ribosomal protein L11



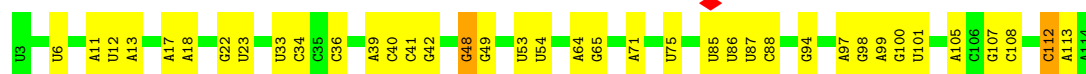
- Molecule 8: 23S rRNA (2887-MER)



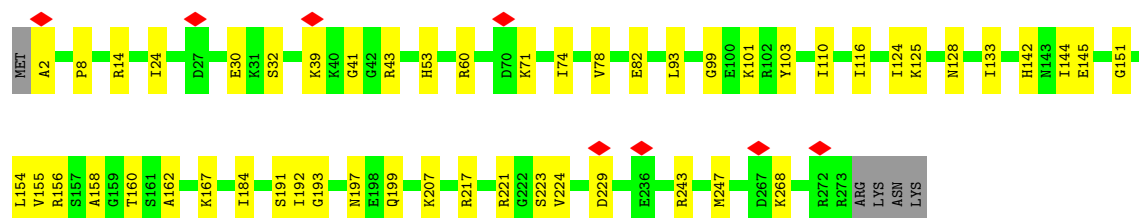
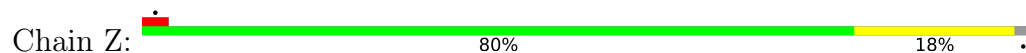




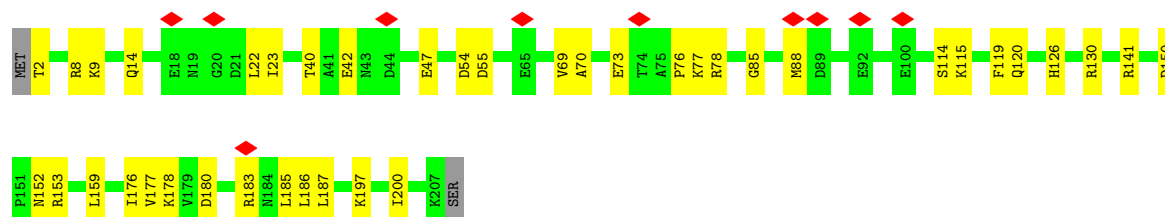
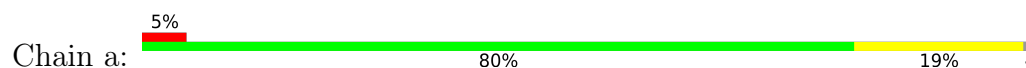
• Molecule 9: 5S rRNA (112-MER)



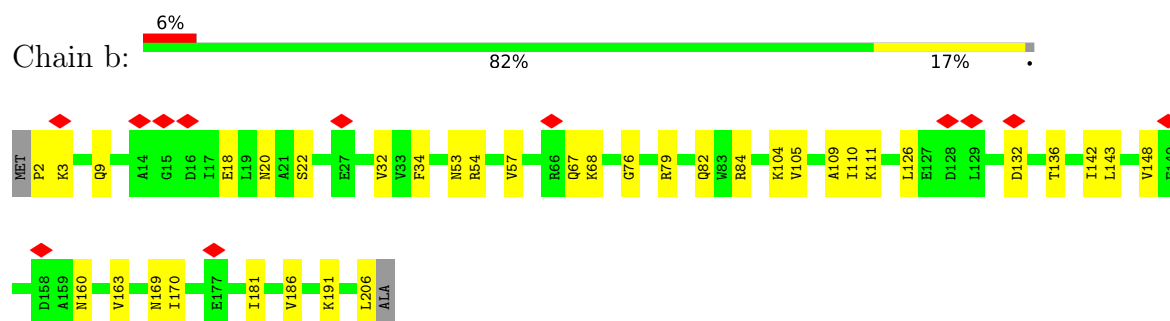
• Molecule 10: 50S ribosomal protein L2



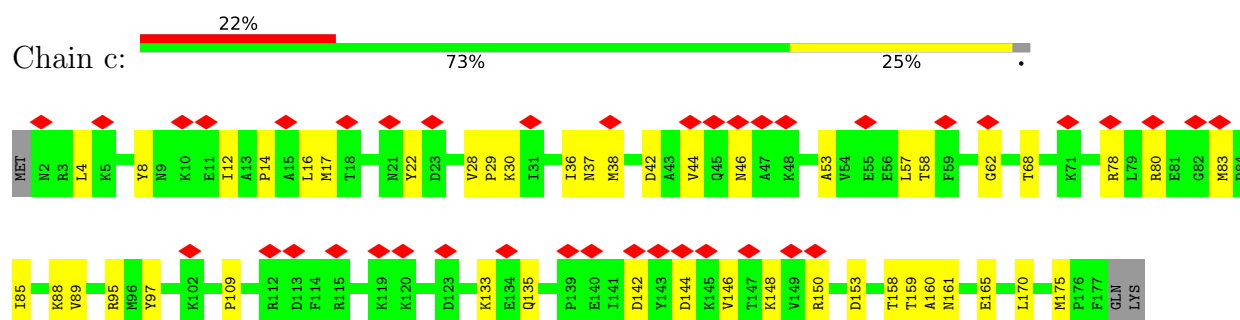
• Molecule 11: 50S ribosomal protein L3



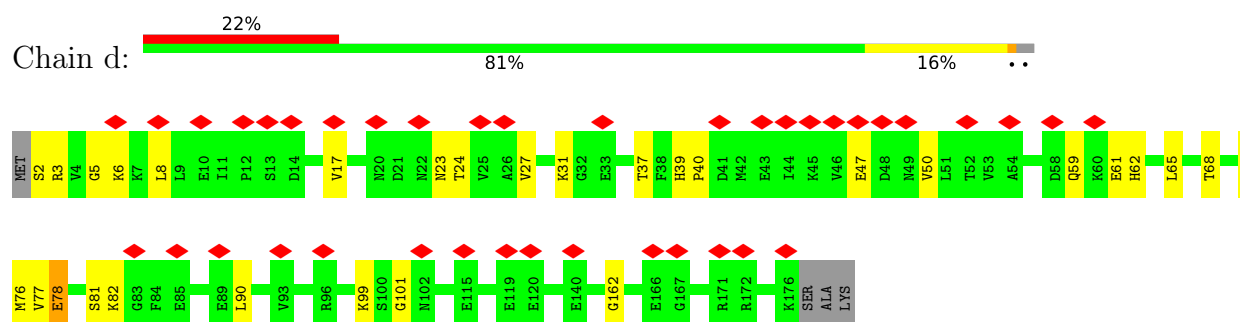
- Molecule 12: 50S ribosomal protein L4



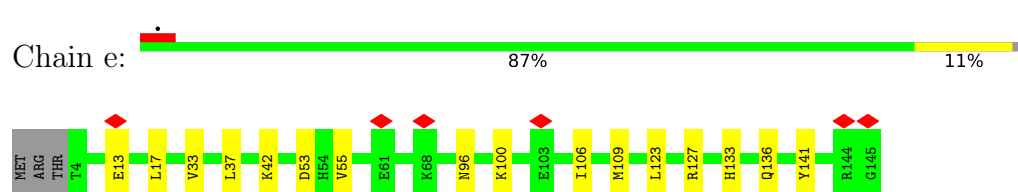
- Molecule 13: 50S ribosomal protein L5



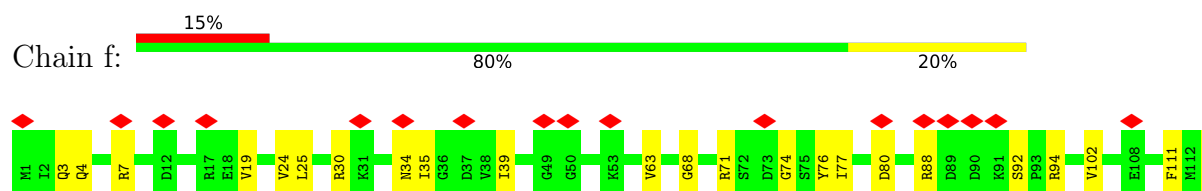
- Molecule 14: 50S ribosomal protein L6

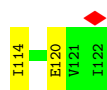


- Molecule 15: 50S ribosomal protein L13

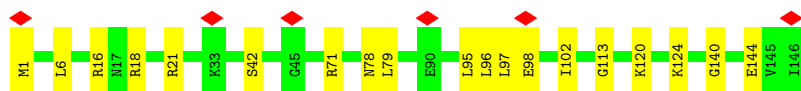
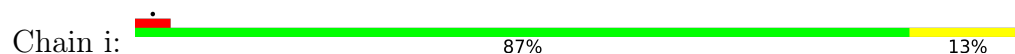


- Molecule 16: 50S ribosomal protein L14

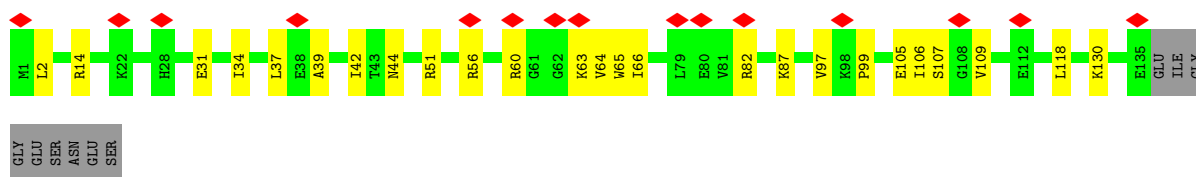
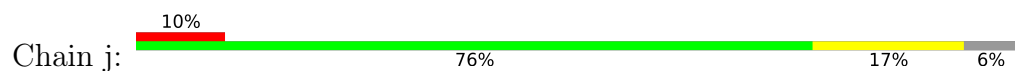




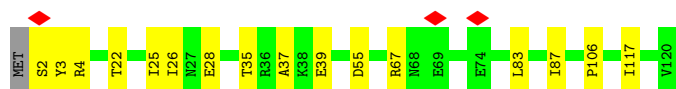
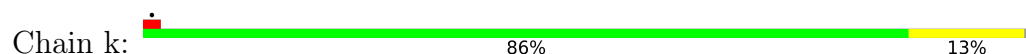
- Molecule 17: 50S ribosomal protein L15



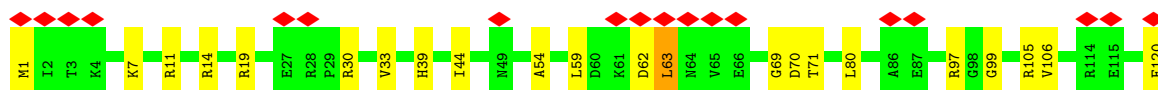
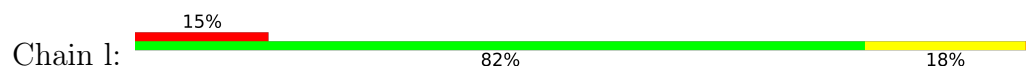
- Molecule 18: 50S ribosomal protein L16



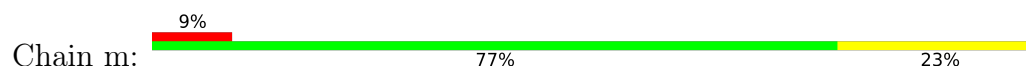
- Molecule 19: 50S ribosomal protein L17



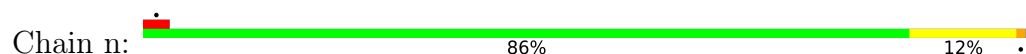
- Molecule 20: 50S ribosomal protein L18

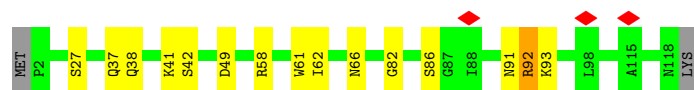


- Molecule 21: 50S ribosomal protein L19

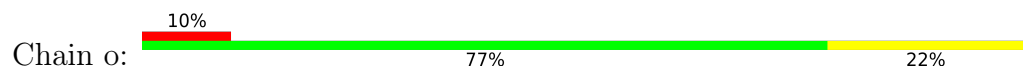


- Molecule 22: 50S ribosomal protein L20

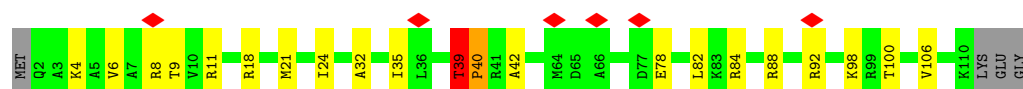
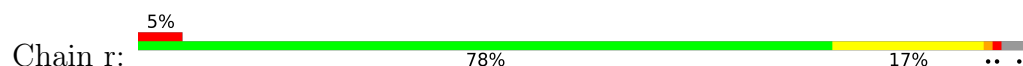




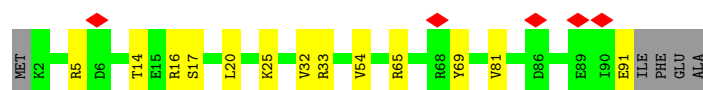
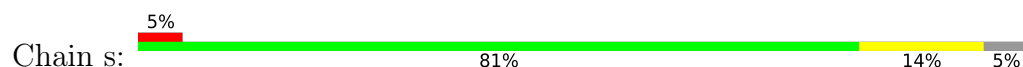
- Molecule 23: 50S ribosomal protein L21



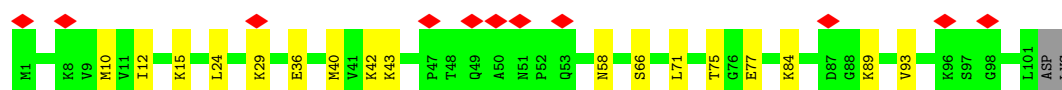
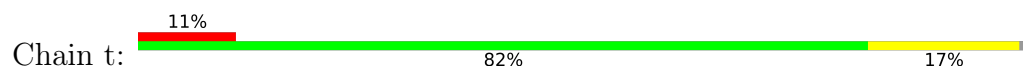
- Molecule 24: 50S ribosomal protein L22



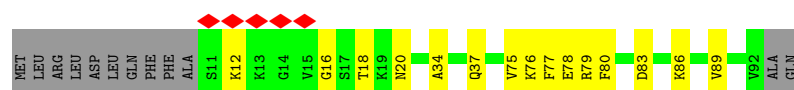
- Molecule 25: 50S ribosomal protein L23



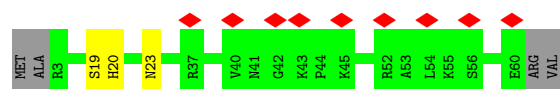
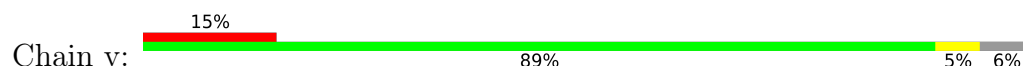
- Molecule 26: 50S ribosomal protein L24



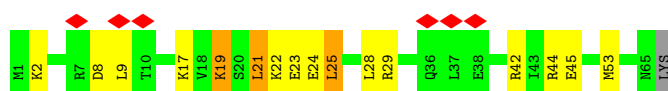
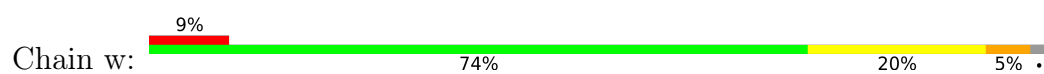
- Molecule 27: 50S ribosomal protein L27



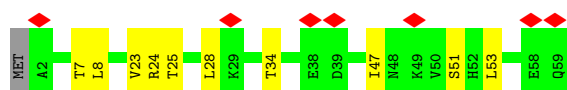
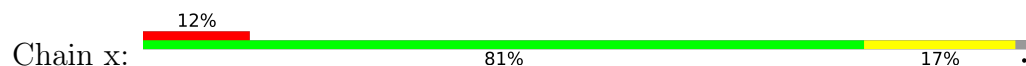
- Molecule 28: 50S ribosomal protein L28



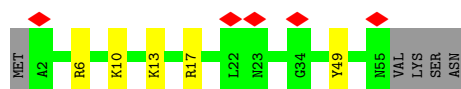
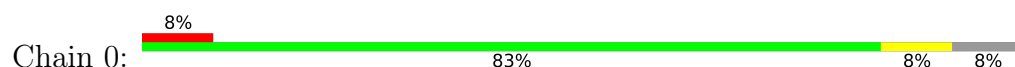
- Molecule 29: 50S ribosomal protein L29



- Molecule 30: 50S ribosomal protein L30



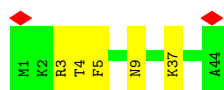
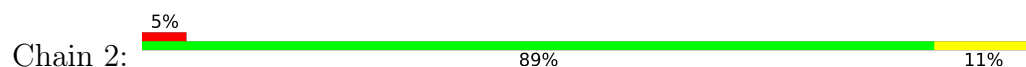
- Molecule 31: 50S ribosomal protein L32



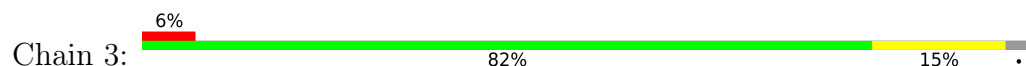
- Molecule 32: 50S ribosomal protein L33 1



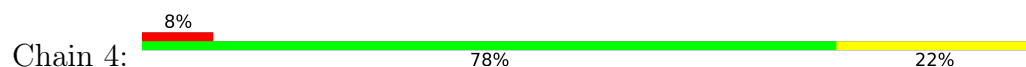
- Molecule 33: 50S ribosomal protein L34

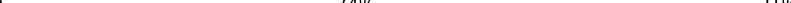


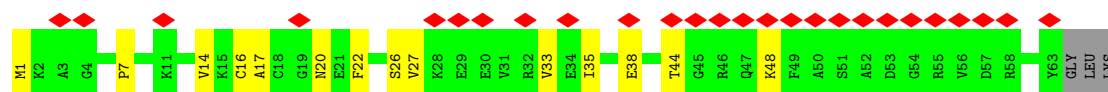
- Molecule 34: 50S ribosomal protein L35

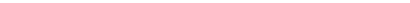


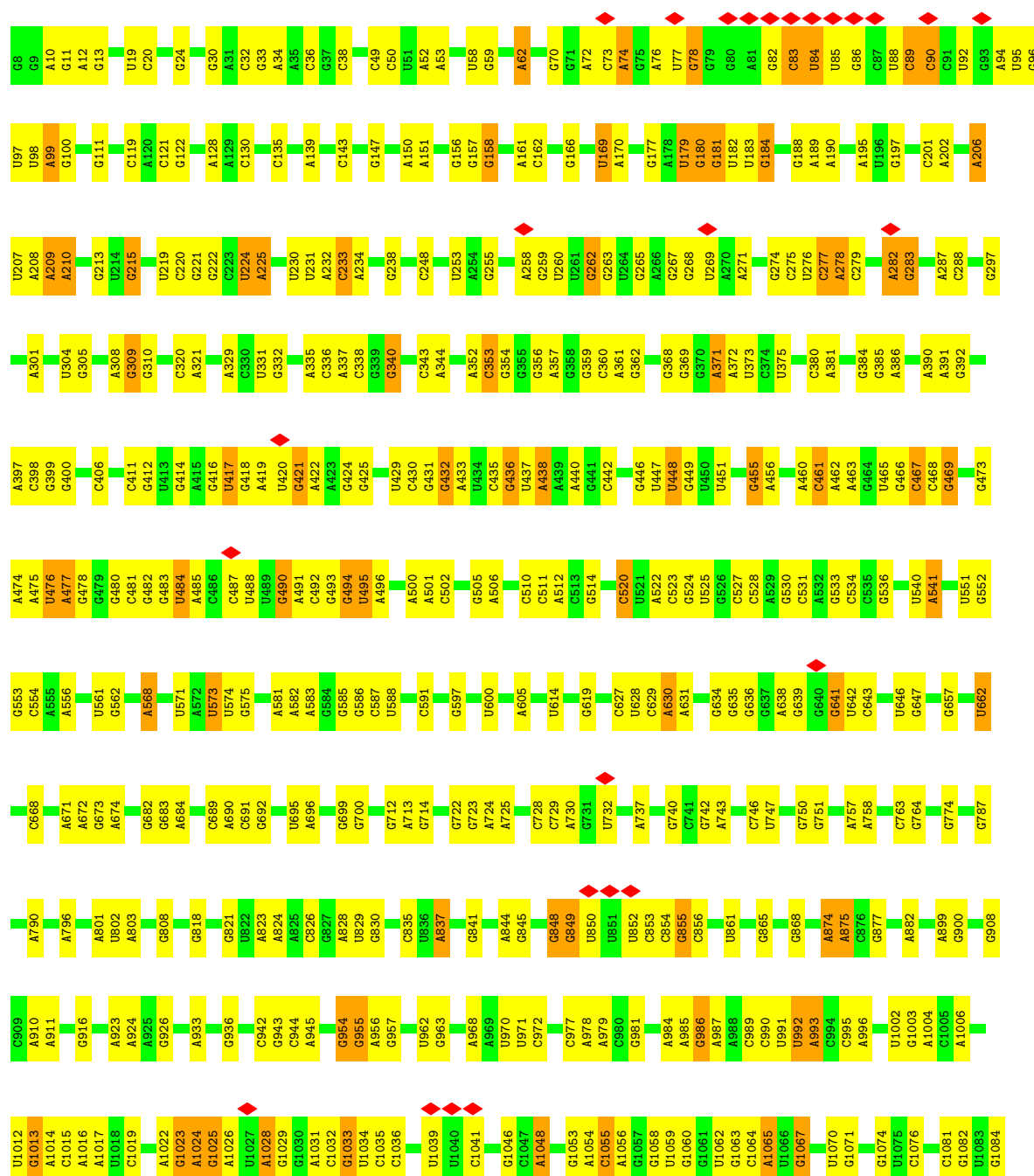
- Molecule 35: 50S ribosomal protein L36

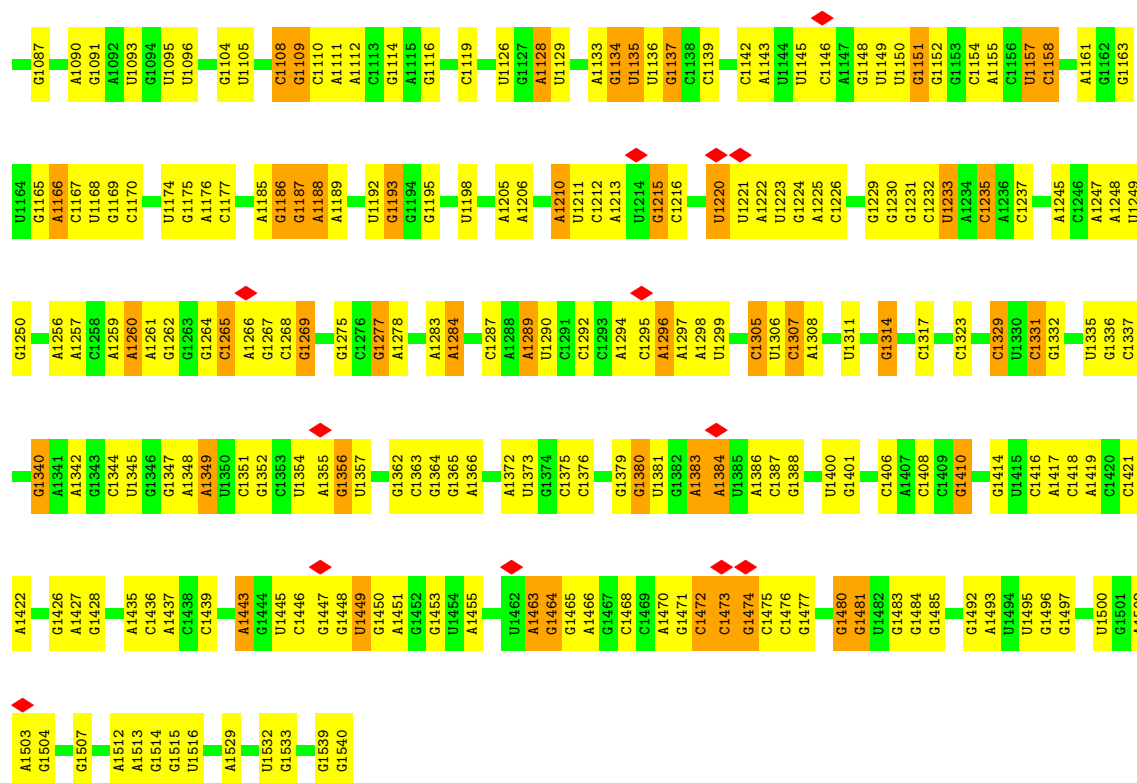


- Chain 6: 

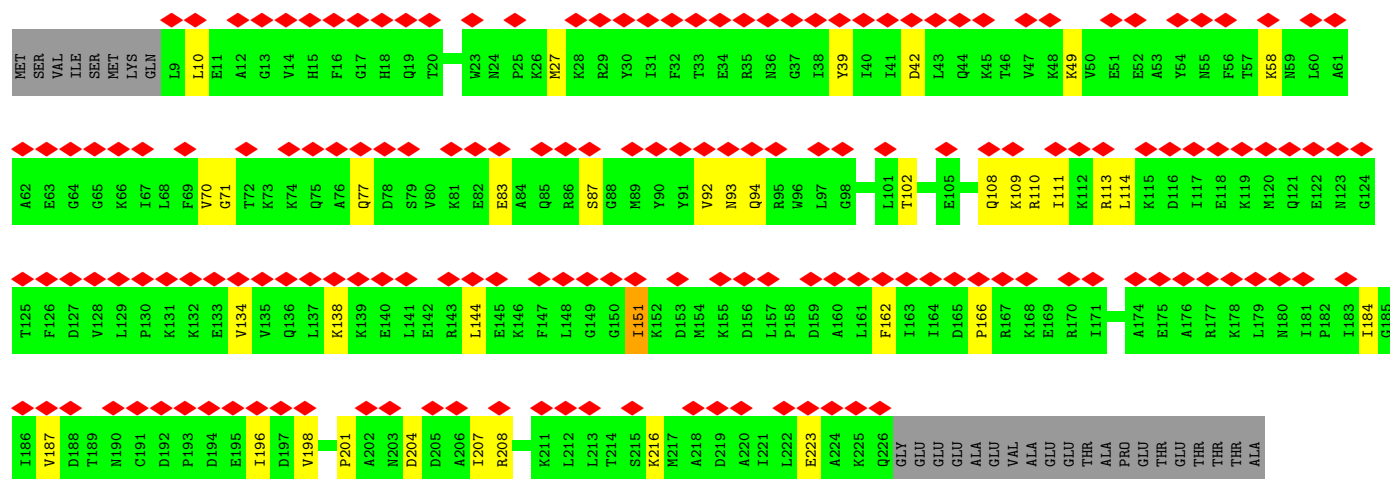
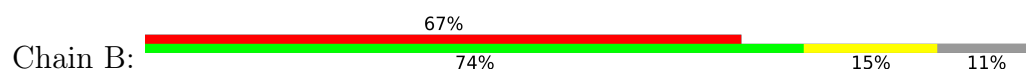


- Chain A:  56% 36% 8%

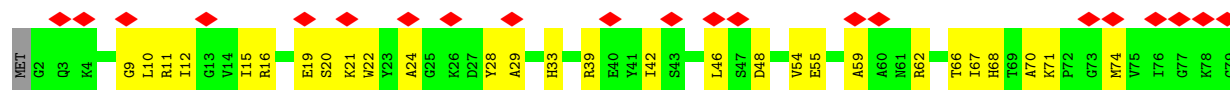


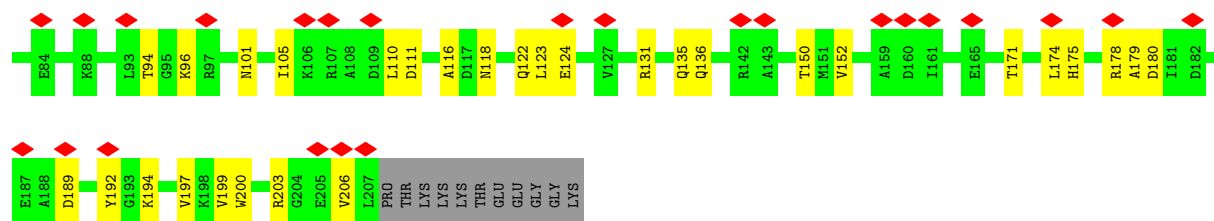


• Molecule 38: 30S ribosomal protein S2

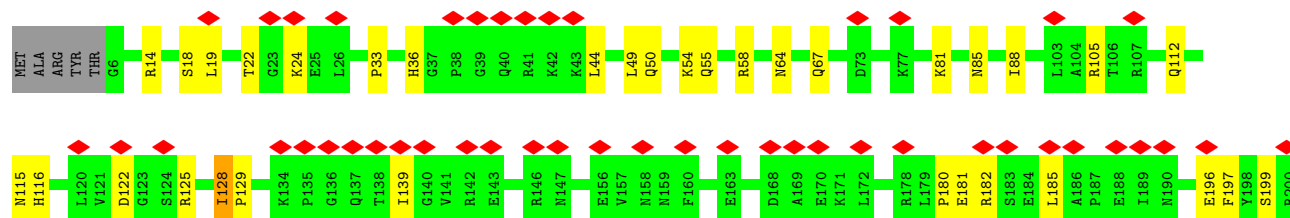
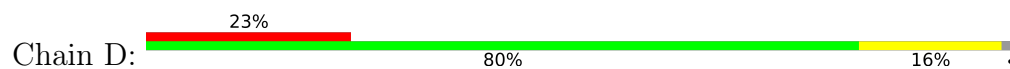


• Molecule 39: 30S ribosomal protein S3

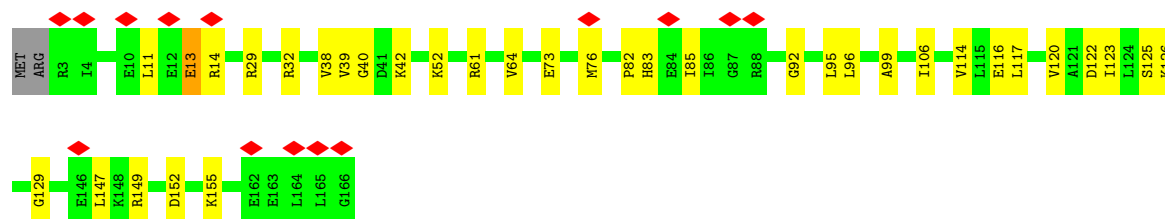
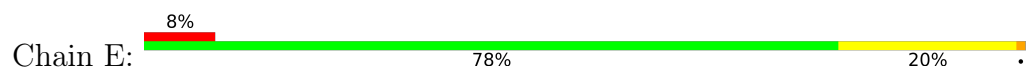




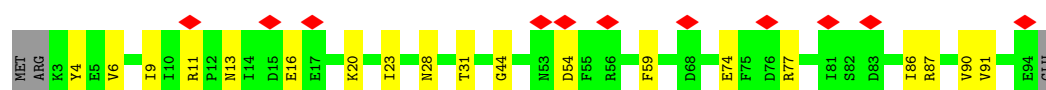
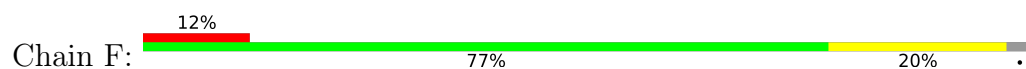
- Molecule 40: 30S ribosomal protein S4



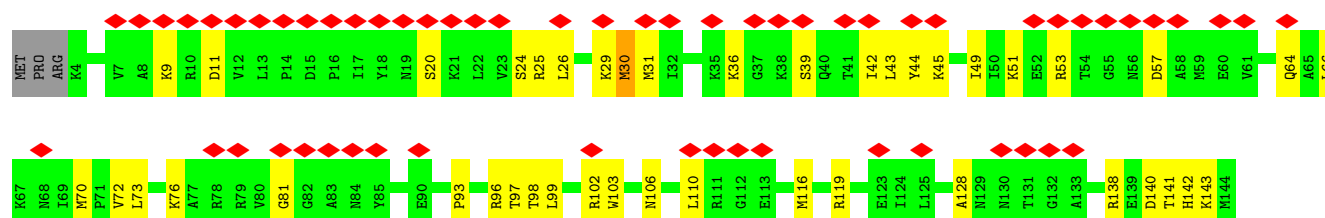
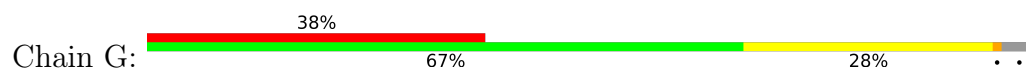
- Molecule 41: 30S ribosomal protein S5

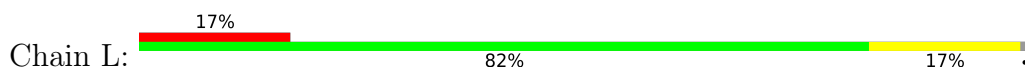


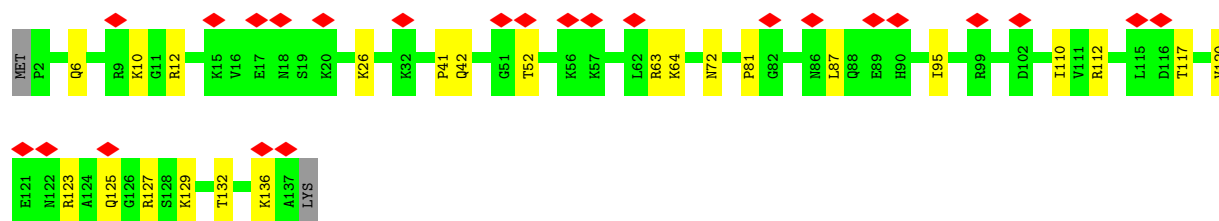
- Molecule 42: 30S ribosomal protein S6



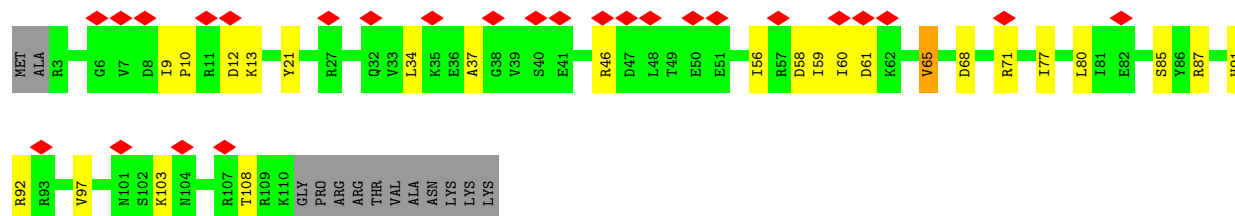
- Molecule 43: 30S ribosomal protein S7



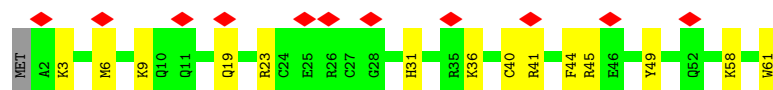
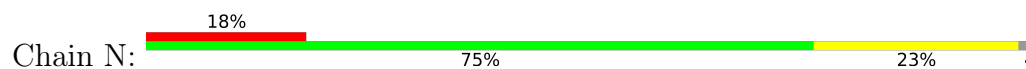




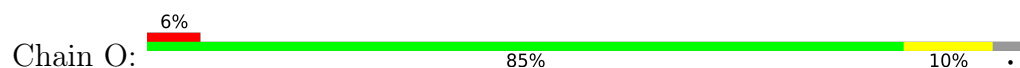
- Molecule 49: 30S ribosomal protein S13



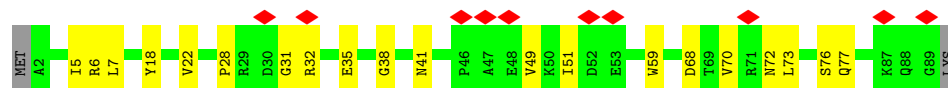
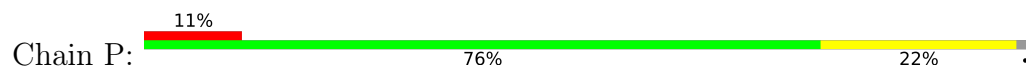
- Molecule 50: 30S ribosomal protein S14



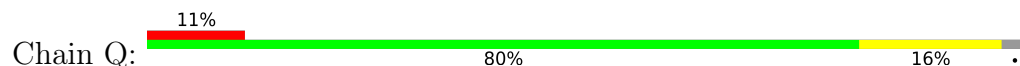
- Molecule 51: 30S ribosomal protein S15



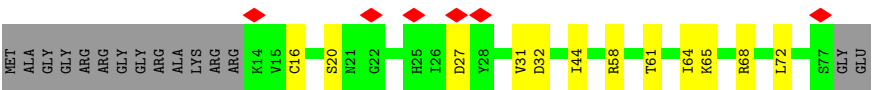
- Molecule 52: 30S ribosomal protein S16



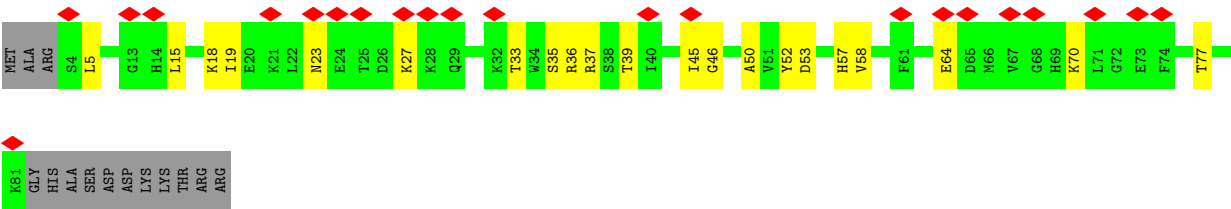
- Molecule 53: 30S ribosomal protein S17



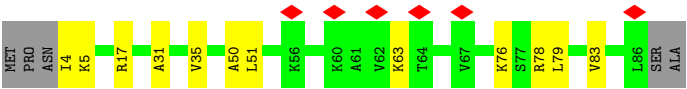
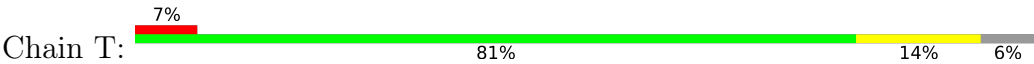
- Molecule 54: 30S ribosomal protein S18



• Molecule 55: 30S ribosomal protein S19



• Molecule 56: 30S ribosomal protein S20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21229	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.675	Depositor
Minimum map value	-0.494	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	0.479	Depositor
Map size ($\text{\AA}$)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.059, 1.059, 1.059	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G4P

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	U	0.19	0/1834	0.34	0/2858
2	V	0.21	0/199	0.36	0/309
3	W	0.14	0/6357	0.32	0/9911
4	g	0.30	0/1909	0.65	2/2593 (0.1%)
5	h	0.27	0/187	0.86	0/236
6	p	0.25	0/963	0.73	5/1298 (0.4%)
7	q	0.21	0/995	0.52	0/1346
8	X	0.37	0/69443	0.43	1/108331 (0.0%)
9	Y	0.23	0/2675	0.40	1/4170 (0.0%)
10	Z	0.42	0/2120	0.60	0/2845
11	a	0.42	0/1591	0.70	0/2132
12	b	0.37	0/1580	0.63	1/2132 (0.0%)
13	c	0.29	0/1405	0.76	1/1887 (0.1%)
14	d	0.25	0/1360	0.68	3/1832 (0.2%)
15	e	0.32	0/1146	0.62	1/1542 (0.1%)
16	f	0.38	0/927	0.67	0/1245
17	i	0.34	0/1093	0.57	0/1457
18	j	0.33	0/1099	0.63	0/1468
19	k	0.41	0/960	0.68	1/1284 (0.1%)
20	l	0.28	0/921	0.73	1/1236 (0.1%)
21	m	0.33	0/957	0.59	0/1279
22	n	0.38	0/952	0.66	2/1266 (0.2%)
23	o	0.38	0/797	0.74	0/1070
24	r	0.40	0/851	0.71	1/1146 (0.1%)
25	s	0.38	0/731	0.62	0/974
26	t	0.35	0/772	0.72	0/1032
27	u	0.36	0/638	0.88	4/847 (0.5%)
28	v	0.36	0/448	0.74	0/596
29	w	0.60	2/531 (0.4%)	0.75	0/707
30	x	0.34	0/457	0.77	0/613
31	0	0.36	0/433	0.73	0/574
32	1	0.28	0/406	0.63	0/540

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	2	0.45	0/370	0.60	0/483
34	3	0.33	0/519	0.58	0/680
35	4	0.30	0/299	0.68	0/393
36	6	0.20	0/509	0.51	0/678
37	A	0.28	0/36826	0.40	2/57450 (0.0%)
38	B	0.25	0/1782	0.68	1/2392 (0.0%)
39	C	0.29	0/1641	0.72	3/2208 (0.1%)
40	D	0.27	0/1598	0.69	0/2147
41	E	0.33	0/1230	0.74	1/1655 (0.1%)
42	F	0.31	0/766	0.71	0/1031
43	G	0.29	0/1196	0.79	2/1604 (0.1%)
44	H	0.33	0/1048	0.73	0/1407
45	I	0.27	0/979	0.74	0/1315
46	J	0.29	0/773	0.71	0/1044
47	K	0.27	0/852	0.66	0/1153
48	L	0.31	0/1069	0.60	0/1435
49	M	0.29	0/873	0.79	0/1166
50	N	0.35	0/507	0.91	3/672 (0.4%)
51	O	0.35	0/718	0.71	0/960
52	P	0.31	0/708	0.73	0/950
53	Q	0.28	0/699	0.62	0/933
54	R	0.29	0/526	0.56	0/705
55	S	0.21	0/649	0.61	0/872
56	T	0.30	0/639	0.69	0/852
All	All	0.33	2/163513 (0.0%)	0.50	36/244941 (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
11	a	0	1
13	c	0	1
21	m	0	1
24	r	0	1
27	u	0	1
40	D	0	1
43	G	0	1
47	K	0	2
49	M	0	1
54	R	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	w	29	ARG	C-O	-8.55	1.14	1.24
29	w	29	ARG	CA-C	-5.66	1.45	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	u	77	PHE	CA-C-N	-9.38	111.27	122.44
27	u	77	PHE	C-N-CA	-9.38	111.27	122.44
14	d	78	GLU	N-CA-CB	6.87	121.59	110.40
6	p	89	VAL	CA-C-N	6.78	134.17	121.97
6	p	89	VAL	C-N-CA	6.78	134.17	121.97
41	E	13	GLU	CA-CB-CG	6.66	127.41	114.10
38	B	151	ILE	CG1-CB-CG2	-6.06	92.51	110.70
27	u	78	GLU	CA-CB-CG	5.91	125.91	114.10
13	c	83	MET	CA-CB-CG	5.81	125.72	114.10
4	g	262	ARG	CB-CA-C	-5.80	101.52	110.81
24	r	39	THR	C-N-CD	-5.66	101.78	125.00
27	u	78	GLU	N-CA-C	5.63	119.58	111.02
6	p	107	GLU	CA-C-N	5.59	132.03	121.97
6	p	107	GLU	C-N-CA	5.59	132.03	121.97
6	p	31	ARG	CA-CB-CG	5.56	125.22	114.10
4	g	64	MET	CB-CA-C	-5.54	101.94	110.81
19	k	28	GLU	CA-CB-CG	5.51	125.13	114.10
50	N	31	HIS	CA-C-N	5.48	132.00	121.54
50	N	31	HIS	C-N-CA	5.48	132.00	121.54
37	A	1013	G	N9-C1'-C2'	5.34	120.01	112.00
43	G	29	LYS	CA-C-N	5.32	129.92	122.36
43	G	29	LYS	C-N-CA	5.32	129.92	122.36
39	C	124	GLU	N-CA-CB	5.28	119.29	110.41
20	l	63	LEU	CA-CB-CG	5.21	134.55	116.30
50	N	36	LYS	CA-CB-CG	5.21	124.52	114.10
15	e	100	LYS	CB-CG-CD	5.17	123.20	111.30
9	Y	48	G	P-O3'-C3'	5.17	127.95	120.20
39	C	123	LEU	CA-C-N	-5.15	111.53	121.58
39	C	123	LEU	C-N-CA	-5.15	111.53	121.58
14	d	77	VAL	CA-C-N	-5.11	112.19	121.14
14	d	77	VAL	C-N-CA	-5.11	112.19	121.14
22	n	91	ASN	CA-C-N	5.08	131.25	121.54
22	n	91	ASN	C-N-CA	5.08	131.25	121.54
12	b	3	LYS	CB-CG-CD	5.06	122.95	111.30
37	A	1013	G	O4'-C1'-N9	5.06	116.09	108.50
8	X	396	G	P-O3'-C3'	5.01	127.72	120.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	D	128	ILE	Peptide
43	G	30	MET	Peptide
47	K	120	HIS	Peptide
47	K	84	LEU	Peptide
49	M	65	VAL	Peptide
54	R	27	ASP	Peptide
11	a	120	GLN	Peptide
13	c	53	ALA	Peptide
21	m	106	LYS	Peptide
24	r	39	THR	Peptide
27	u	79	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	1643	0	831	8	0
2	V	177	0	89	2	0
3	W	5685	0	2865	55	0
4	g	1911	0	845	6	0
5	h	189	0	79	0	0
6	p	955	0	990	17	0
7	q	981	0	1020	18	0
8	X	61997	0	31209	348	0
9	Y	2392	0	1213	4	0
10	Z	2083	0	2168	38	0
11	a	1569	0	1637	26	0
12	b	1561	0	1647	25	0
13	c	1386	0	1446	29	0
14	d	1342	0	1388	22	0
15	e	1123	0	1162	10	0
16	f	920	0	977	17	0
17	i	1081	0	1132	17	0
18	j	1076	0	1145	16	0
19	k	953	0	983	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	l	912	0	947	15	0
21	m	944	0	1020	19	0
22	n	940	0	1005	12	0
23	o	786	0	826	13	0
24	r	842	0	899	14	0
25	s	725	0	770	16	0
26	t	762	0	821	13	0
27	u	630	0	644	9	0
28	v	444	0	487	2	0
29	w	530	0	568	18	0
30	x	455	0	491	6	0
31	0	426	0	445	5	0
32	1	401	0	413	10	0
33	2	367	0	410	5	0
34	3	512	0	564	8	0
35	4	296	0	342	7	0
36	6	499	0	491	9	0
37	A	32891	0	16559	278	0
38	B	1757	0	1830	22	0
39	C	1619	0	1658	35	0
40	D	1568	0	1604	25	0
41	E	1218	0	1300	22	0
42	F	755	0	746	11	0
43	G	1181	0	1235	26	0
44	H	1036	0	1095	17	0
45	I	966	0	1005	32	0
46	J	761	0	795	14	0
47	K	838	0	854	15	0
48	L	1052	0	1112	18	0
49	M	868	0	925	16	0
50	N	497	0	531	11	0
51	O	710	0	735	5	0
52	P	695	0	721	13	0
53	Q	691	0	728	11	0
54	R	518	0	555	8	0
55	S	633	0	649	14	0
56	T	637	0	696	13	0
57	g	36	0	11	0	0
All	All	150422	0	99313	1233	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 5.

All (1233) 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)
25:s:5:ARG:NH2	29:w:23:GLU:HG3	1.65	1.11
8:X:47:C:C2	8:X:181:G:N2	2.27	1.00
37:A:1126:U:H3	37:A:1193:G:H1	1.02	0.98
25:s:5:ARG:CZ	29:w:23:GLU:HG3	1.93	0.98
37:A:1129:U:H3	37:A:1163:G:H1	0.96	0.96
8:X:1528:U:H3	8:X:1557:G:H1	1.10	0.93
37:A:774:G:H1	37:A:821:G:HO2'	1.16	0.92
37:A:455:G:H21	37:A:496:A:H62	1.20	0.90
8:X:616:A:H61	8:X:2058:G:H21	1.00	0.90
37:A:955:G:H1	37:A:1245:A:H61	1.20	0.89
37:A:215:G:H1	37:A:224:U:H3	0.88	0.87
1:U:49:G:H1	1:U:65:U:H3	0.87	0.86
37:A:1269:G:H21	37:A:1284:A:H62	1.22	0.85
37:A:954:G:H21	37:A:1348:A:N6	1.74	0.84
8:X:616:A:N6	8:X:2058:G:H21	1.75	0.84
8:X:616:A:H61	8:X:2058:G:N2	1.76	0.84
3:W:126:U:H3	3:W:209:C:H42	1.24	0.83
29:w:25:LEU:HD12	29:w:25:LEU:O	1.78	0.83
25:s:5:ARG:HH22	29:w:23:GLU:HG3	1.44	0.82
13:c:142:ASP:O	13:c:146:VAL:HB	1.80	0.81
37:A:455:G:H21	37:A:496:A:N6	1.79	0.80
37:A:1062:U:H3	37:A:1215:G:H1	1.30	0.79
16:f:68:GLY:HA3	16:f:77:ILE:O	1.83	0.78
8:X:721:G:H5''	12:b:76:GLY:H	1.48	0.76
37:A:455:G:N2	37:A:496:A:H62	1.85	0.75
37:A:673:G:H22	37:A:750:G:H1	1.34	0.75
3:W:126:U:H3	3:W:209:C:N4	1.84	0.75
29:w:19:LYS:NZ	29:w:19:LYS:HB3	2.02	0.75
8:X:2135:G:N2	8:X:2212:C:C2	2.56	0.74
12:b:2:PRO:O	12:b:18:GLU:HA	1.89	0.73
16:f:71:ARG:HH21	16:f:77:ILE:HD11	1.55	0.72
37:A:954:G:N2	37:A:1348:A:N6	2.36	0.72
3:W:58:G:C6	3:W:59:G:O6	2.43	0.72
3:W:15:C:N4	3:W:38:C:N4	2.37	0.72
8:X:87:U:H5'	8:X:88:G:H5'	1.71	0.72
8:X:47:C:C2	8:X:181:G:C2	2.78	0.71
37:A:986:G:N2	37:A:1372:A:N7	2.38	0.71
37:A:467:C:H42	37:A:484:U:H3	1.39	0.70
37:A:954:G:N2	37:A:1348:A:C6	2.60	0.69
8:X:1290:G:N7	17:i:18:ARG:NH2	2.41	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:s:5:ARG:NH1	29:w:23:GLU:HG3	2.08	0.68
19:k:83:LEU:O	19:k:87:ILE:HB	1.94	0.68
37:A:158:G:H21	37:A:161:A:H62	1.40	0.68
37:A:1269:G:N2	37:A:1284:A:H62	1.90	0.68
11:a:22:LEU:HD12	16:f:74:GLY:HA3	1.75	0.68
37:A:700:G:N7	47:K:30:ASN:ND2	2.42	0.67
37:A:1116:G:H5''	39:C:171:THR:HG22	1.75	0.67
29:w:25:LEU:HD12	29:w:25:LEU:C	2.19	0.67
55:S:36:ARG:HH22	55:S:53:ASP:HA	1.59	0.67
37:A:1269:G:H21	37:A:1284:A:N6	1.93	0.66
2:V:14:G:N7	2:V:16:A:N6	2.43	0.66
54:R:16:CYS:O	54:R:20:SER:HB3	1.96	0.66
37:A:1449:U:O2	37:A:1471:G:N2	2.29	0.66
4:g:67:LEU:CB	25:s:91:GLU:HG2	2.26	0.66
45:I:71:GLY:O	45:I:75:GLN:HB2	1.95	0.66
8:X:1136:U:C4	8:X:1148:C:C4	2.84	0.66
37:A:1143:A:N1	37:A:1151:G:C6	2.63	0.65
3:W:138:G:H1	3:W:191:U:H3	0.78	0.65
45:I:34:GLU:O	45:I:38:HIS:HB3	1.97	0.65
8:X:1886:G:H8	8:X:1914:A:H62	1.45	0.65
3:W:157:A:N7	3:W:170:A:N6	2.44	0.65
29:w:17:LYS:O	29:w:21:LEU:HB2	1.95	0.65
39:C:19:GLU:HG3	39:C:39:ARG:HH12	1.62	0.65
45:I:55:THR:HG23	45:I:57:THR:H	1.61	0.65
8:X:1310:C:H5''	8:X:1311:G:H5'	1.78	0.65
51:O:12:ILE:O	51:O:16:LYS:HB2	1.97	0.64
37:A:467:C:N4	37:A:484:U:H3	1.95	0.64
37:A:955:G:H1	37:A:1245:A:N6	1.92	0.64
8:X:161:A:N6	8:X:168:A:N7	2.45	0.64
37:A:531:C:H41	48:L:63:ARG:HH22	1.45	0.64
36:6:16:CYS:HA	36:6:33:VAL:HB	1.80	0.64
43:G:106:ASN:O	43:G:110:LEU:HB2	1.97	0.64
8:X:47:C:O2	8:X:181:G:N2	2.31	0.63
8:X:673:A:N7	17:i:78:ASN:ND2	2.45	0.63
8:X:1808:U:OP2	8:X:1813:A:N6	2.31	0.63
16:f:76:TYR:HB2	21:m:73:THR:HB	1.79	0.63
37:A:70:G:H1	37:A:99:A:H61	1.46	0.63
16:f:7:ARG:HA	16:f:19:VAL:O	1.97	0.63
48:L:87:LEU:HD11	48:L:117:THR:HG22	1.80	0.63
49:M:60:ILE:HG23	49:M:65:VAL:HG21	1.80	0.63
6:p:58:THR:HG21	6:p:82:ILE:H	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:16:G:N1	3:W:34:U:N3	2.47	0.63
37:A:1365:G:H2'	37:A:1366:A:H8	1.63	0.62
19:k:106:PRO:HG2	24:r:40:PRO:HG2	1.80	0.62
8:X:2859:G:H21	8:X:2908:A:H62	1.46	0.62
21:m:27:ARG:HB2	21:m:42:ILE:HD11	1.81	0.62
22:n:92:ARG:NH2	23:o:11:GLN:O	2.31	0.62
23:o:62:VAL:HG12	23:o:95:VAL:HG22	1.81	0.62
37:A:436:G:N3	37:A:438:A:N6	2.48	0.62
8:X:353:A:N7	8:X:374:A:N6	2.47	0.62
37:A:332:G:H5'	56:T:17:ARG:HH12	1.64	0.62
11:a:176:ILE:HD12	11:a:186:LEU:HD22	1.82	0.62
8:X:364:A:N3	12:b:169:ASN:ND2	2.47	0.62
8:X:972:U:H2'	8:X:973:G:H8	1.65	0.62
37:A:1004:A:N6	37:A:1225:A:O2'	2.33	0.62
52:P:7:LEU:HD12	52:P:18:TYR:HB3	1.81	0.62
3:W:106:A:N1	3:W:224:C:N4	2.48	0.62
8:X:921:G:H1	8:X:950:U:H3	1.47	0.62
36:6:16:CYS:SG	36:6:17:ALA:N	2.73	0.61
8:X:256:C:OP2	34:3:5:LYS:NZ	2.34	0.61
37:A:954:G:N2	37:A:1347:G:N7	2.49	0.61
39:C:66:THR:HG22	39:C:101:ASN:HB2	1.83	0.61
8:X:2841:C:O2	8:X:2908:A:O2'	2.20	0.60
55:S:15:LEU:HA	55:S:18:LYS:HB2	1.83	0.60
3:W:121:U:H5'	3:W:122:U:H5'	1.81	0.60
8:X:1856:U:OP2	10:Z:221:ARG:NH1	2.33	0.60
18:j:39:ALA:HB2	18:j:99:PRO:HD3	1.82	0.60
40:D:122:ASP:H	40:D:139:ILE:HG21	1.65	0.60
45:I:19:VAL:HG12	45:I:65:VAL:HG22	1.83	0.60
53:Q:70:SER:O	53:Q:74:ARG:NH2	2.34	0.60
8:X:1290:G:OP2	17:i:21:ARG:NH1	2.34	0.60
8:X:2039:G:H5''	24:r:42:ALA:HB2	1.83	0.60
22:n:82:GLY:O	22:n:86:SER:HB3	2.01	0.60
37:A:908:G:N2	37:A:911:A:OP2	2.35	0.60
8:X:77:U:H3'	29:w:2:LYS:HD2	1.83	0.60
3:W:156:C:H5''	3:W:171:G:H8	1.67	0.60
8:X:1820:A:N6	8:X:1857:G:O2'	2.30	0.60
10:Z:142:HIS:ND1	10:Z:193:GLY:O	2.34	0.60
56:T:35:VAL:HG22	56:T:50:ALA:HB1	1.84	0.60
6:p:56:LYS:NZ	8:X:1131:A:N1	2.49	0.60
25:s:54:VAL:HG22	25:s:81:VAL:HG12	1.84	0.60
53:Q:26:VAL:HG12	53:Q:45:LYS:HB3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:B:162:PHE:HA	38:B:184:ILE:O	2.02	0.59
37:A:1376:C:H5'	46:J:62:ARG:HH21	1.67	0.59
39:C:94:THR:HG23	39:C:96:LYS:H	1.67	0.59
45:I:15:SER:HB2	45:I:70:GLY:HA3	1.83	0.59
8:X:2785:U:OP2	35:4:19:ARG:NH2	2.35	0.59
13:c:68:THR:OG1	13:c:85:ILE:O	2.19	0.59
49:M:80:LEU:HD21	49:M:87:ARG:HG2	1.84	0.59
8:X:1783:C:OP1	21:m:94:ARG:NH1	2.35	0.59
37:A:627:C:N4	37:A:630:A:OP2	2.34	0.59
46:J:53:ARG:O	50:N:45:ARG:NH1	2.36	0.59
37:A:1473:C:OP2	37:A:1475:C:N4	2.36	0.59
45:I:114:LYS:HA	45:I:121:ALA:HB2	1.85	0.59
8:X:78:U:H3	8:X:107:G:H1	1.50	0.58
37:A:1226:C:OP1	50:N:9:LYS:NZ	2.36	0.58
37:A:1406:C:OP2	41:E:29:ARG:NH2	2.35	0.58
13:c:8:TYR:HA	13:c:12:ILE:HD13	1.84	0.58
37:A:1260:A:N6	37:A:1363:C:O2'	2.36	0.58
11:a:55:ASP:OD1	11:a:77:LYS:NZ	2.36	0.58
37:A:468:C:N4	37:A:469:G:O6	2.36	0.58
14:d:23:ASN:ND2	14:d:39:HIS:O	2.36	0.58
47:K:61:THR:HG22	47:K:63:PHE:H	1.68	0.58
8:X:835:A:OP1	8:X:838:C:N4	2.36	0.58
8:X:2776:G:OP1	14:d:75:ASN:ND2	2.36	0.58
9:Y:98:G:N2	9:Y:99:A:N7	2.51	0.58
8:X:1846:G:OP2	10:Z:156:ARG:NH2	2.36	0.58
8:X:1087:U:H3	8:X:1160:G:H1	1.52	0.58
23:o:65:GLN:HG2	23:o:93:THR:HG22	1.86	0.58
45:I:52:LEU:HD12	45:I:58:ALA:HA	1.86	0.58
3:W:15:C:C4	3:W:38:C:N4	2.72	0.58
8:X:86:C:H4'	8:X:103:U:H1'	1.86	0.58
8:X:2035:C:O2'	8:X:2848:A:N3	2.37	0.58
37:A:1016:A:N6	37:A:1033:G:O2'	2.36	0.57
38:B:58:LYS:NZ	38:B:223:GLU:OE2	2.37	0.57
37:A:1259:A:O2'	37:A:1296:A:N6	2.37	0.57
3:W:127:C:O2	3:W:128:C:N4	2.37	0.57
8:X:1465:A:H62	8:X:1626:U:H3	1.50	0.57
10:Z:144:ILE:HB	10:Z:154:LEU:HB2	1.87	0.57
21:m:39:ARG:NH2	37:A:354:G:OP1	2.37	0.57
39:C:118:ASN:O	39:C:122:GLN:NE2	2.36	0.57
8:X:1513:U:HO2'	8:X:1594:G:HO2'	1.49	0.57
23:o:76:TYR:HA	23:o:82:VAL:O	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:I:46:GLU:HA	45:I:49:LYS:HG2	1.85	0.57
8:X:904:A:H61	8:X:967:G:H1	1.53	0.57
8:X:2785:U:H5'	35:4:19:ARG:HG3	1.87	0.57
14:d:8:LEU:HD11	14:d:50:VAL:HG13	1.86	0.57
19:k:2:SER:OG	19:k:3:TYR:N	2.36	0.57
32:1:30:VAL:HG22	32:1:47:GLU:HB2	1.85	0.57
8:X:2710:C:OP1	11:a:115:LYS:NZ	2.37	0.57
23:o:48:VAL:HB	23:o:51:PRO:HB3	1.87	0.57
3:W:146:U:O2	3:W:181:G:N2	2.38	0.57
19:k:22:THR:HG21	19:k:67:ARG:HB2	1.86	0.57
25:s:5:ARG:NH1	29:w:23:GLU:CG	2.68	0.57
8:X:827:G:N1	10:Z:229:ASP:OD2	2.37	0.57
8:X:897:G:H1'	30:x:25:THR:HG21	1.87	0.57
14:d:17:VAL:HG12	14:d:27:VAL:HG22	1.87	0.57
37:A:73:C:OP2	37:A:74:A:N6	2.37	0.57
44:H:80:ILE:HG22	44:H:87:VAL:HG11	1.87	0.57
8:X:607:G:N3	22:n:37:GLN:NE2	2.53	0.56
10:Z:24:ILE:HG23	10:Z:82:GLU:HA	1.87	0.56
16:f:80:ASP:OD2	21:m:104:ARG:NH2	2.38	0.56
37:A:1186:G:O6	37:A:1187:G:N2	2.38	0.56
8:X:557:U:H4'	8:X:1275:G:H4'	1.87	0.56
12:b:111:LYS:HE3	12:b:206:LEU:HD22	1.88	0.56
40:D:182:ARG:NH1	40:D:182:ARG:O	2.38	0.56
3:W:58:G:O6	3:W:59:G:O6	2.23	0.56
3:W:149:A:H2	4:g:384:THR:H	1.53	0.56
8:X:2376:C:OP1	32:1:34:LYS:NZ	2.38	0.56
10:Z:133:ILE:HD12	10:Z:167:LYS:HD2	1.87	0.56
37:A:89:C:O2	37:A:90:C:N4	2.38	0.56
37:A:1229:G:OP1	55:S:37:ARG:NH2	2.38	0.56
44:H:68:GLN:NE2	44:H:69:ASN:OD1	2.38	0.56
47:K:71:THR:HA	47:K:74:LYS:HG2	1.87	0.56
7:q:49:GLN:HB2	7:q:54:ILE:HD11	1.87	0.56
9:Y:6:U:OP1	20:l:11:ARG:NH2	2.38	0.56
39:C:110:LEU:HD13	39:C:203:ARG:HD3	1.88	0.56
52:P:41:ASN:H	52:P:49:VAL:HG11	1.70	0.56
8:X:2922:U:H2'	8:X:2923:A:H8	1.70	0.56
17:i:79:LEU:HD13	17:i:113:GLY:HA2	1.87	0.56
19:k:37:ALA:HB1	19:k:117:ILE:HD11	1.88	0.56
46:J:59:LYS:O	46:J:62:ARG:NH1	2.38	0.56
44:H:11:LEU:HD22	44:H:77:LEU:HD23	1.87	0.56
52:P:35:GLU:OE2	52:P:59:TRP:NE1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:72:U:OP1	3:W:257:G:N2	2.38	0.56
23:o:39:LEU:HD12	23:o:47:LYS:HE3	1.87	0.56
37:A:36:C:H1'	48:L:42:GLN:HE22	1.71	0.56
37:A:1443:A:H62	37:A:1477:G:H21	1.53	0.56
46:J:27:GLU:HB3	46:J:31:ARG:HH21	1.71	0.56
8:X:2105:U:OP2	8:X:2267:G:N2	2.38	0.56
12:b:181:ILE:HG23	12:b:186:VAL:HG21	1.87	0.56
37:A:835:C:O2	44:H:16:ASN:ND2	2.39	0.56
37:A:1134:G:N2	37:A:1135:U:O4	2.39	0.56
20:l:63:LEU:HD21	20:l:80:LEU:HD11	1.88	0.56
50:N:40:CYS:O	50:N:44:PHE:HB3	2.06	0.56
8:X:345:A:H1'	26:t:12:ILE:HG23	1.89	0.55
8:X:822:G:OP1	8:X:824:G:O2'	2.22	0.55
37:A:1427:A:N6	37:A:1492:G:O2'	2.39	0.55
12:b:110:ILE:HD11	12:b:181:ILE:HG22	1.88	0.55
36:6:20:ASN:ND2	36:6:38:GLU:OE2	2.39	0.55
37:A:1356:G:N2	37:A:1383:A:OP1	2.38	0.55
8:X:1093:G:N2	8:X:1157:A:OP2	2.38	0.55
44:H:25:LEU:O	44:H:61:ARG:HA	2.06	0.55
8:X:1102:G:H22	8:X:1148:C:H5	1.55	0.55
11:a:14:GLN:HE21	11:a:22:LEU:HD13	1.72	0.55
36:6:44:THR:O	36:6:48:LYS:NZ	2.40	0.55
37:A:421:G:N2	37:A:436:G:O2'	2.38	0.55
8:X:518:A:OP1	12:b:84:ARG:NH2	2.40	0.55
8:X:1131:A:OP1	8:X:1150:C:O2'	2.25	0.55
8:X:1828:G:N2	10:Z:154:LEU:O	2.39	0.55
13:c:14:PRO:HA	13:c:17:MET:HG3	1.89	0.55
6:p:57:ASN:HB3	6:p:59:MET:HE1	1.88	0.55
6:p:61:ARG:NH2	8:X:1091:U:O2'	2.39	0.55
37:A:573:U:OP2	48:L:12:ARG:NH2	2.35	0.55
55:S:45:ILE:HD12	55:S:64:GLU:HA	1.87	0.55
3:W:16:G:O6	3:W:34:U:C4	2.60	0.55
8:X:1191:C:H2'	8:X:1192:G:H8	1.72	0.55
37:A:1087:G:N2	37:A:1090:A:OP2	2.37	0.55
1:U:18:G:H1	1:U:55:U:H3	1.55	0.55
11:a:8:ARG:NH1	11:a:197:LYS:O	2.40	0.55
37:A:183:U:H1'	56:T:76:LYS:HD2	1.89	0.55
3:W:131:C:N4	3:W:132:G:O6	2.39	0.54
8:X:920:G:O3'	18:j:63:LYS:NZ	2.40	0.54
45:I:20:ARG:HG3	45:I:64:LEU:HB2	1.89	0.54
8:X:2577:G:O2'	16:f:4:GLN:OE1	2.25	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:1848:A:H5'	10:Z:160:THR:HG21	1.88	0.54
8:X:2104:U:OP1	10:Z:243:ARG:NH1	2.40	0.54
11:a:23:ILE:HG21	11:a:177:VAL:HG21	1.87	0.54
11:a:47:GLU:HB3	11:a:88:MET:HE2	1.89	0.54
18:j:60:ARG:HH22	18:j:109:VAL:HA	1.73	0.54
20:l:69:GLY:O	20:l:105:ARG:NH1	2.37	0.54
8:X:47:C:N3	8:X:181:G:N1	2.55	0.54
8:X:353:A:N3	8:X:373:A:O2'	2.40	0.54
8:X:2129:G:O6	8:X:2218:U:O2	2.25	0.54
37:A:340:G:OP2	56:T:4:ILE:N	2.40	0.54
41:E:73:GLU:OE2	41:E:149:ARG:NH2	2.41	0.54
48:L:6:GLN:O	48:L:10:LYS:HB2	2.08	0.54
8:X:515:G:OP2	33:2:37:LYS:NZ	2.38	0.54
8:X:2144:G:N2	8:X:2148:A:OP1	2.41	0.54
27:u:34:ALA:HB3	27:u:37:GLN:HB2	1.88	0.54
37:A:728:C:O2	54:R:44:ILE:N	2.37	0.54
2:V:14:G:N2	43:G:81:GLY:O	2.41	0.54
8:X:2296:A:H5''	8:X:2297:A:H5''	1.89	0.54
21:m:83:LYS:NZ	21:m:85:GLU:OE2	2.40	0.54
37:A:1297:A:H2'	37:A:1298:A:H8	1.71	0.54
40:D:50:GLN:HB3	40:D:197:PHE:HB2	1.90	0.54
43:G:64:GLN:NE2	43:G:128:ALA:O	2.39	0.54
45:I:27:ARG:NH1	45:I:28:ILE:O	2.40	0.54
8:X:1033:C:O2'	8:X:1046:A:N3	2.37	0.54
14:d:23:ASN:HD22	14:d:40:PRO:HA	1.72	0.54
18:j:106:ILE:HG13	18:j:118:LEU:HD21	1.89	0.54
24:r:82:LEU:HB2	24:r:98:LYS:HB2	1.89	0.54
44:H:5:ASP:OD2	44:H:79:ARG:NH1	2.40	0.54
52:P:6:ARG:NH2	52:P:28:PRO:O	2.40	0.54
52:P:28:PRO:HG2	52:P:31:GLY:HA3	1.89	0.54
3:W:49:C:O2'	3:W:53:A:N6	2.41	0.54
12:b:57:VAL:HG12	12:b:79:ARG:HH11	1.73	0.54
13:c:38:MET:HE3	13:c:57:LEU:HD21	1.89	0.54
24:r:4:LYS:HG2	24:r:106:VAL:HG22	1.90	0.54
37:A:38:C:O2'	48:L:127:ARG:NH2	2.40	0.54
37:A:683:G:H2'	37:A:684:A:H8	1.71	0.54
45:I:50:GLN:OE1	45:I:80:ARG:NH2	2.41	0.54
8:X:1542:A:O2'	8:X:1544:C:N4	2.35	0.54
8:X:1941:A:N6	37:A:1416:C:O2'	2.40	0.54
37:A:10:A:N7	40:D:199:SER:OG	2.41	0.54
16:f:25:LEU:O	16:f:30:ARG:NH2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:989:C:O2	50:N:19:GLN:NE2	2.40	0.54
3:W:156:C:H3'	3:W:171:G:H1'	1.90	0.53
37:A:523:C:H2'	37:A:524:G:H8	1.74	0.53
39:C:15:ILE:HD11	39:C:206:VAL:HG11	1.89	0.53
43:G:140:ASP:HA	43:G:143:LYS:HG2	1.91	0.53
8:X:6:A:HO2'	15:e:133:HIS:HD1	1.57	0.53
8:X:1444:C:H2'	8:X:1445:A:H8	1.72	0.53
8:X:2287:C:O2'	8:X:2456:C:OP2	2.23	0.53
8:X:2872:U:OP1	21:m:96:LYS:NZ	2.38	0.53
13:c:44:VAL:HG11	13:c:78:ARG:HB3	1.91	0.53
8:X:828:A:OP1	10:Z:217:ARG:NH2	2.40	0.53
8:X:2307:A:OP2	27:u:20:ASN:ND2	2.41	0.53
14:d:47:GLU:HB3	14:d:50:VAL:HB	1.91	0.53
37:A:263:G:OP1	53:Q:73:LYS:NZ	2.41	0.53
39:C:16:ARG:NH2	39:C:180:ASP:OD1	2.40	0.53
45:I:113:ARG:NH1	45:I:114:LYS:O	2.41	0.53
6:p:6:GLU:HA	6:p:9:LYS:HE2	1.89	0.53
8:X:2284:G:H21	27:u:16:GLY:HA3	1.71	0.53
8:X:2334:U:O4'	13:c:133:LYS:NZ	2.41	0.53
37:A:1161:A:OP1	46:J:72:ARG:NH2	2.42	0.53
40:D:88:ILE:HD12	40:D:180:PRO:HG2	1.91	0.53
48:L:52:THR:HG22	48:L:64:LYS:HA	1.89	0.53
20:l:97:ARG:HG3	20:l:99:GLY:H	1.73	0.53
35:4:18:ARG:HH12	35:4:21:GLY:HA2	1.73	0.53
37:A:1062:U:O2	37:A:1215:G:N2	2.36	0.53
41:E:152:ASP:OD1	41:E:155:LYS:NZ	2.42	0.53
3:W:12:A:N7	3:W:62:G:N2	2.57	0.53
37:A:412:G:O2'	37:A:448:U:O2	2.23	0.53
41:E:95:LEU:O	41:E:125:SER:HA	2.08	0.53
8:X:684:G:O6	8:X:698:C:N4	2.42	0.53
8:X:2108:U:O2'	28:v:23:ASN:OD1	2.23	0.53
23:o:59:THR:OG1	23:o:98:GLU:O	2.26	0.53
26:t:10:MET:HB2	26:t:71:LEU:HD11	1.91	0.53
37:A:1137:G:O6	37:A:1154:C:N4	2.41	0.53
43:G:31:MET:HE1	43:G:36:LYS:HA	1.90	0.53
45:I:31:ASN:O	45:I:33:ARG:NH1	2.41	0.53
53:Q:24:THR:HG22	53:Q:47:LYS:HD3	1.91	0.53
8:X:1885:A:H3'	8:X:1886:G:H21	1.74	0.53
39:C:11:ARG:HH12	39:C:179:ALA:HB3	1.74	0.53
48:L:26:LYS:O	48:L:72:ASN:ND2	2.40	0.53
7:q:59:SER:OG	7:q:67:THR:OG1	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:1112:U:O2	8:X:1115:A:C5	2.62	0.53
11:a:9:LYS:HB2	11:a:200:ILE:HD13	1.90	0.53
37:A:76:A:N6	37:A:78:G:O6	2.42	0.53
37:A:343:C:H2'	37:A:344:A:H8	1.74	0.53
15:e:96:ASN:O	15:e:127:ARG:NH2	2.42	0.53
39:C:42:ILE:O	39:C:46:LEU:HB2	2.09	0.53
8:X:2024:U:O2	16:f:3:GLN:NE2	2.39	0.52
13:c:37:ASN:HB2	13:c:153:ASP:HB2	1.90	0.52
21:m:109:ARG:NH1	37:A:1472:C:OP2	2.40	0.52
37:A:1275:G:N2	37:A:1278:A:OP2	2.42	0.52
7:q:29:GLY:HA2	7:q:35:ILE:HD11	1.91	0.52
8:X:2376:C:O2'	32:l:17:TYR:OH	2.23	0.52
18:j:51:ARG:HD3	18:j:66:ILE:HD11	1.91	0.52
37:A:1381:U:OP1	45:I:73:SER:N	2.43	0.52
4:g:67:LEU:CB	25:s:91:GLU:CG	2.88	0.52
8:X:6:A:N3	15:e:136:GLN:NE2	2.58	0.52
8:X:45:G:H5''	8:X:46:C:H5'	1.91	0.52
8:X:1321:U:H3	8:X:1325:A:H62	1.57	0.52
42:F:11:ARG:NH1	42:F:13:ASN:O	2.42	0.52
47:K:88:VAL:HG21	47:K:95:ARG:HE	1.75	0.52
3:W:153:U:O2	3:W:156:C:N4	2.42	0.52
8:X:1460:G:N7	8:X:1630:G:N1	2.56	0.52
37:A:353:C:O2	37:A:354:G:N2	2.42	0.52
38:B:196:ILE:HG12	38:B:198:VAL:H	1.73	0.52
43:G:72:VAL:HG12	43:G:73:LEU:HD12	1.91	0.52
8:X:2610:G:OP2	8:X:2610:G:N2	2.42	0.52
37:A:473:G:N2	37:A:476:U:OP1	2.43	0.52
3:W:72:U:OP2	3:W:256:A:N6	2.41	0.52
40:D:181:GLU:O	40:D:185:LEU:HB2	2.10	0.52
52:P:68:ASP:N	52:P:68:ASP:OD2	2.43	0.52
8:X:1829:C:HO2'	8:X:1847:U:H3	1.56	0.52
42:F:54:ASP:N	42:F:54:ASP:OD1	2.41	0.52
7:q:126:ARG:NH1	8:X:1127:U:OP1	2.43	0.52
8:X:47:C:N3	8:X:181:G:C2	2.78	0.52
8:X:733:U:O2'	33:2:4:THR:O	2.28	0.52
8:X:901:U:H2'	8:X:902:G:H8	1.75	0.52
8:X:931:C:N4	8:X:940:G:O6	2.41	0.52
8:X:1112:U:O2	8:X:1115:A:N7	2.43	0.52
8:X:2516:G:H2'	8:X:2517:A:H8	1.75	0.52
18:j:42:ILE:HD12	18:j:97:VAL:HG21	1.92	0.52
26:t:75:THR:HG23	26:t:77:GLU:H	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:O:25:PRO:HB3	51:O:66:LEU:HD22	1.92	0.52
24:r:82:LEU:HB3	24:r:84:ARG:HH11	1.75	0.52
37:A:682:G:H2'	37:A:683:G:C8	2.44	0.52
49:M:56:ILE:HA	49:M:59:ILE:HG22	1.91	0.52
8:X:309:U:O2'	8:X:406:G:N2	2.43	0.52
8:X:1112:U:N3	8:X:1115:A:OP2	2.43	0.52
29:w:19:LYS:HB3	29:w:19:LYS:HZ3	1.74	0.52
48:L:123:ARG:NH2	48:L:125:GLN:O	2.43	0.52
3:W:44:A:H2'	8:X:2690:G:H1	1.75	0.51
8:X:2544:C:H2'	8:X:2545:G:H8	1.75	0.51
11:a:183:ARG:HH21	21:m:8:ILE:HD13	1.73	0.51
21:m:6:GLU:O	21:m:10:LYS:HB2	2.10	0.51
37:A:1260:A:H1'	37:A:1379:G:H4'	1.92	0.51
37:A:1314:G:H22	37:A:1340:G:H2'	1.75	0.51
38:B:114:LEU:HD13	38:B:144:LEU:HD11	1.92	0.51
24:r:6:VAL:HG12	24:r:8:ARG:HG2	1.92	0.51
37:A:215:G:O6	37:A:224:U:O4	2.27	0.51
3:W:20:A:O2'	8:X:2689:A:O2'	2.28	0.51
8:X:1478:G:H2'	8:X:1479:G:C8	2.45	0.51
20:l:44:ILE:HD13	20:l:54:ALA:HB3	1.92	0.51
21:m:49:LYS:HG2	21:m:60:THR:HG22	1.92	0.51
37:A:62:A:H3'	56:T:5:LYS:HD2	1.92	0.51
37:A:1212:C:H2'	37:A:1213:A:H8	1.75	0.51
37:A:1416:C:H2'	37:A:1417:A:H8	1.75	0.51
7:q:56:VAL:HG22	7:q:70:THR:HG22	1.93	0.51
8:X:246:U:OP2	34:3:8:ARG:NH1	2.42	0.51
8:X:2716:U:H3	8:X:2751:G:H1	1.58	0.51
8:X:2721:C:O2	8:X:2872:U:O2'	2.29	0.51
14:d:3:ARG:HE	14:d:5:GLY:H	1.58	0.51
39:C:20:SER:OG	39:C:22:TRP:NE1	2.43	0.51
47:K:36:ILE:HG23	47:K:44:ILE:HB	1.92	0.51
8:X:1306:G:OP2	31:0:17:ARG:NH1	2.43	0.51
13:c:135:GLN:NE2	13:c:150:ARG:O	2.43	0.51
37:A:411:C:OP2	40:D:67:GLN:NE2	2.43	0.51
37:A:412:G:OP1	40:D:115:ASN:ND2	2.43	0.51
37:A:1275:G:H21	37:A:1277:G:H8	1.58	0.51
38:B:10:LEU:HD12	38:B:216:LYS:HE2	1.93	0.51
43:G:51:LYS:NZ	43:G:57:ASP:OD1	2.43	0.51
8:X:774:A:OP1	8:X:1477:A:O2'	2.22	0.51
8:X:2888:C:OP1	21:m:91:LYS:NZ	2.43	0.51
16:f:88:ARG:HD2	16:f:94:ARG:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:1157:U:O3'	45:I:11:ARG:NH2	2.44	0.51
39:C:70:ALA:HA	39:C:105:ILE:H	1.76	0.51
41:E:38:VAL:HG21	41:E:114:VAL:HG22	1.91	0.51
41:E:92:GLY:HA2	41:E:129:GLY:HA3	1.93	0.51
47:K:66:GLN:HG2	47:K:101:ALA:HB2	1.93	0.51
7:q:110:GLU:HA	7:q:113:MET:HG2	1.93	0.51
8:X:1528:U:O4	8:X:1557:G:O6	2.28	0.51
37:A:150:A:N6	37:A:169:U:C2	2.78	0.51
8:X:1713:A:N3	8:X:1715:C:N4	2.59	0.51
8:X:2123:A:H2'	8:X:2124:A:H8	1.76	0.51
8:X:2282:G:O6	27:u:12:LYS:NZ	2.44	0.51
38:B:49:LYS:HE3	38:B:201:PRO:HD2	1.92	0.51
49:M:9:ILE:HD12	49:M:10:PRO:HD2	1.92	0.51
50:N:40:CYS:O	50:N:44:PHE:CB	2.58	0.51
8:X:2357:A:H2'	8:X:2358:A:C8	2.46	0.51
8:X:2844:A:O2'	8:X:2846:A:N7	2.38	0.51
32:l:1:MET:HB3	32:l:23:LYS:HZ1	1.76	0.51
37:A:184:G:O6	37:A:206:A:N6	2.44	0.51
39:C:54:VAL:HG12	39:C:67:ILE:HG12	1.92	0.51
8:X:776:G:C5	10:Z:207:LYS:HB3	2.46	0.51
8:X:1106:U:H4'	8:X:1107:U:H3'	1.93	0.51
14:d:78:GLU:HB2	14:d:82:LYS:HZ1	1.75	0.51
15:e:53:ASP:OD1	15:e:53:ASP:N	2.44	0.51
40:D:44:LEU:HB2	40:D:49:LEU:HD12	1.93	0.51
3:W:178:U:OP2	3:W:180:A:N6	2.43	0.50
8:X:24:G:O2'	24:r:78:GLU:O	2.28	0.50
12:b:132:ASP:N	12:b:132:ASP:OD1	2.44	0.50
42:F:86:ILE:HG22	42:F:87:ARG:HG2	1.92	0.50
8:X:1094:A:OP2	8:X:1156:G:N2	2.37	0.50
8:X:2128:U:O2	8:X:2219:G:N2	2.44	0.50
8:X:2496:C:OP1	35:4:8:LYS:NZ	2.44	0.50
37:A:435:C:N4	37:A:436:G:O6	2.43	0.50
37:A:673:G:OP1	54:R:58:ARG:NH1	2.44	0.50
37:A:1023:G:O2'	37:A:1025:G:OP2	2.29	0.50
3:W:32:C:HO2'	3:W:75:A:HO2'	1.56	0.50
8:X:2153:G:N2	8:X:2204:U:OP2	2.44	0.50
23:o:21:TYR:OH	23:o:94:LYS:NZ	2.41	0.50
54:R:61:THR:OG1	54:R:65:LYS:NZ	2.44	0.50
8:X:1043:G:H5''	22:n:58:ARG:HH12	1.76	0.50
8:X:2856:G:N2	8:X:2909:U:OP2	2.43	0.50
37:A:691:C:H2'	37:A:692:G:H8	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:1081:C:H2'	37:A:1082:G:H8	1.76	0.50
39:C:71:LYS:NZ	39:C:74:MET:SD	2.85	0.50
30:x:23:VAL:HG21	30:x:53:LEU:HD22	1.92	0.50
37:A:1093:U:O2'	37:A:1112:A:OP2	2.28	0.50
43:G:98:THR:O	43:G:102:ARG:HB2	2.12	0.50
47:K:120:HIS:O	47:K:121:ASN:ND2	2.45	0.50
37:A:692:G:N2	47:K:41:GLY:O	2.44	0.50
37:A:1410:G:O6	37:A:1514:G:N2	2.45	0.50
41:E:83:HIS:HE1	41:E:85:ILE:HD13	1.77	0.50
46:J:11:LYS:HB3	46:J:71:LYS:HB3	1.93	0.50
8:X:514:G:O2'	8:X:843:C:O2'	2.26	0.50
8:X:527:A:O2'	26:t:42:LYS:O	2.29	0.50
8:X:1365:U:HO2'	8:X:2039:G:HO2'	1.58	0.50
8:X:2173:G:N2	8:X:2176:A:OP1	2.44	0.50
37:A:10:A:N6	40:D:196:GLU:O	2.41	0.50
37:A:1025:G:H2'	37:A:1026:A:C4	2.47	0.50
37:A:1248:A:H61	37:A:1305:C:H2'	1.77	0.50
43:G:145:ALA:O	43:G:149:LYS:HB3	2.12	0.50
55:S:27:LYS:NZ	55:S:46:GLY:O	2.44	0.50
56:T:35:VAL:HG11	56:T:79:LEU:HD21	1.94	0.50
6:p:67:ALA:HB1	6:p:72:LEU:HA	1.91	0.50
7:q:133:ARG:NH1	8:X:1124:C:OP1	2.45	0.50
8:X:790:A:O2'	8:X:1704:U:OP1	2.28	0.50
10:Z:158:ALA:HB1	10:Z:197:ASN:HB3	1.92	0.50
24:r:88:ARG:HB2	24:r:92:ARG:HB2	1.93	0.50
37:A:1108:C:H2'	37:A:1109:G:C8	2.47	0.50
39:C:12:ILE:HA	39:C:16:ARG:HB3	1.94	0.50
54:R:32:ASP:OD1	54:R:32:ASP:N	2.41	0.50
8:X:1546:G:O2'	10:Z:99:GLY:O	2.28	0.50
13:c:16:LEU:HD11	13:c:28:VAL:HG23	1.93	0.50
19:k:4:ARG:NH1	19:k:39:GLU:OE2	2.45	0.50
6:p:51:GLU:O	6:p:86:THR:OG1	2.30	0.49
8:X:1676:G:N1	8:X:1679:A:OP2	2.39	0.49
8:X:1683:C:O2	8:X:2727:U:O2'	2.30	0.49
8:X:1699:A:O2'	11:a:119:PHE:O	2.25	0.49
37:A:614:U:O2	37:A:641:G:O6	2.28	0.49
37:A:1195:G:N2	50:N:61:TRP:O	2.45	0.49
55:S:33:THR:OG1	55:S:35:SER:OG	2.30	0.49
8:X:747:G:O2'	8:X:1677:A:N3	2.40	0.49
13:c:159:THR:O	20:l:1:MET:N	2.45	0.49
37:A:668:C:OP1	51:O:5:GLN:NE2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:1426:G:O2'	37:A:1493:A:N6	2.45	0.49
8:X:869:U:H2'	8:X:870:A:H8	1.77	0.49
8:X:1657:C:O2'	33:2:5:PHE:O	2.29	0.49
8:X:2420:G:O2'	8:X:2458:G:N2	2.45	0.49
37:A:844:A:OP1	54:R:58:ARG:NH2	2.46	0.49
37:A:995:C:H2'	37:A:996:A:H8	1.77	0.49
8:X:1831:A:H2	8:X:1844:A:H62	1.59	0.49
37:A:150:A:N7	37:A:169:U:O4	2.44	0.49
37:A:600:U:H3	37:A:657:G:H1	1.59	0.49
37:A:1143:A:C6	37:A:1151:G:C6	3.00	0.49
37:A:1474:G:H22	37:A:1476:C:H41	1.59	0.49
40:D:81:LYS:O	40:D:85:ASN:HB2	2.13	0.49
40:D:116:HIS:O	40:D:125:ARG:NH2	2.45	0.49
53:Q:70:SER:HB3	53:Q:73:LYS:HB2	1.94	0.49
8:X:243:G:O2'	8:X:260:A:N6	2.45	0.49
8:X:2421:A:OP1	34:3:31:HIS:NE2	2.46	0.49
8:X:2882:G:N2	8:X:2885:A:OP2	2.44	0.49
37:A:262:G:H2'	37:A:263:G:C8	2.48	0.49
37:A:305:G:N2	37:A:308:A:OP2	2.37	0.49
37:A:1265:C:O2'	37:A:1287:C:N4	2.42	0.49
1:U:56:C:O3'	13:c:80:ARG:NH1	2.45	0.49
8:X:2507:A:OP2	35:4:2:LYS:NZ	2.44	0.49
13:c:109:PRO:HB2	36:6:35:ILE:HG23	1.95	0.49
37:A:900:G:O2'	37:A:916:G:O6	2.30	0.49
37:A:1070:U:H2'	37:A:1071:G:H8	1.77	0.49
37:A:1166:A:N6	37:A:1189:A:N7	2.60	0.49
42:F:4:TYR:HA	42:F:91:VAL:O	2.12	0.49
8:X:704:U:H2'	8:X:705:A:C8	2.48	0.49
8:X:2135:G:C2	8:X:2212:C:C2	3.00	0.49
37:A:722:G:H2'	37:A:723:G:C8	2.47	0.49
46:J:7:ARG:HB3	46:J:73:LEU:HD11	1.95	0.49
53:Q:30:TYR:HE2	53:Q:39:ARG:HG3	1.77	0.49
8:X:549:A:N3	8:X:551:A:O2'	2.43	0.49
8:X:633:U:H2'	8:X:634:A:H8	1.76	0.49
8:X:934:U:OP1	49:M:92:ARG:NH1	2.46	0.49
37:A:1067:G:H1'	39:C:194:LYS:HG2	1.95	0.49
37:A:1166:A:H62	37:A:1189:A:H62	1.61	0.49
45:I:51:PRO:HA	45:I:54:LEU:HG	1.94	0.49
46:J:63:GLU:OE2	50:N:58:LYS:NZ	2.46	0.49
37:A:662:U:O5'	44:H:56:LYS:NZ	2.46	0.49
37:A:1335:U:H2'	37:A:1336:G:H8	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C:9:GLY:HA3	50:N:49:TYR:HD1	1.78	0.49
41:E:13:GLU:HA	41:E:39:VAL:HG22	1.94	0.49
42:F:20:LYS:HA	42:F:23:ILE:HG12	1.95	0.49
3:W:147:G:N1	3:W:180:A:N7	2.60	0.49
8:X:1546:G:O3'	10:Z:101:LYS:NZ	2.43	0.49
8:X:2280:G:OP2	18:j:82:ARG:NH1	2.46	0.49
8:X:2859:G:N2	8:X:2908:A:H62	2.11	0.49
39:C:48:ASP:OD1	39:C:48:ASP:N	2.45	0.49
39:C:189:ASP:OD1	39:C:189:ASP:N	2.45	0.49
49:M:13:LYS:NZ	49:M:21:TYR:OH	2.41	0.49
49:M:68:ASP:HA	49:M:71:ARG:HG2	1.95	0.49
8:X:706:C:H2'	8:X:707:G:H8	1.78	0.48
8:X:1140:U:O2	8:X:1141:A:N6	2.46	0.48
8:X:2320:U:OP1	8:X:2409:U:O2'	2.31	0.48
49:M:91:HIS:CD2	49:M:97:VAL:HG21	2.48	0.48
8:X:2027:A:OP2	11:a:141:ARG:NH1	2.38	0.48
8:X:2227:A:H4'	8:X:2228:A:H5'	1.95	0.48
11:a:150:ASP:O	11:a:152:ASN:ND2	2.46	0.48
29:w:19:LYS:NZ	29:w:19:LYS:CB	2.73	0.48
37:A:554:C:OP1	40:D:54:LYS:NZ	2.46	0.48
37:A:874:A:H2'	37:A:875:A:C8	2.48	0.48
37:A:972:C:O2'	37:A:1210:A:N6	2.45	0.48
8:X:721:G:O2'	12:b:67:GLN:NE2	2.46	0.48
11:a:40:THR:OG1	11:a:42:GLU:OE1	2.31	0.48
11:a:54:ASP:HB3	11:a:78:ARG:HB3	1.95	0.48
46:J:46:LYS:HE3	46:J:68:ARG:HB3	1.95	0.48
3:W:81:G:N1	3:W:246:G:N7	2.51	0.48
8:X:277:C:H2'	8:X:278:A:H8	1.78	0.48
8:X:1159:U:OP1	14:d:2:SER:OG	2.29	0.48
8:X:1820:A:H61	8:X:1857:G:HO2'	1.58	0.48
15:e:13:GLU:O	15:e:42:LYS:NZ	2.45	0.48
37:A:238:G:H5''	52:P:32:ARG:HH12	1.79	0.48
37:A:551:U:H4'	40:D:33:PRO:HB3	1.95	0.48
37:A:954:G:N2	37:A:1348:A:C5	2.81	0.48
37:A:1114:G:OP1	38:B:110:ARG:NH2	2.40	0.48
11:a:70:ALA:HA	11:a:73:GLU:HB2	1.94	0.48
14:d:31:LYS:NZ	14:d:81:SER:O	2.45	0.48
14:d:65:LEU:HA	14:d:68:THR:HG22	1.95	0.48
37:A:510:C:OP1	48:L:127:ARG:NH2	2.37	0.48
46:J:92:LEU:HD12	46:J:96:VAL:HG21	1.95	0.48
3:W:38:C:N3	3:W:59:G:C6	2.82	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:d:99:LYS:NZ	14:d:101:GLY:O	2.45	0.48
37:A:1483:G:H2'	37:A:1484:G:C8	2.48	0.48
7:q:125:MET:HA	7:q:128:VAL:HG22	1.95	0.48
8:X:84:A:H4'	8:X:85:G:H5'	1.94	0.48
8:X:575:A:H62	8:X:2070:U:H3	1.60	0.48
8:X:2368:G:H2'	8:X:2369:A:H8	1.79	0.48
8:X:2502:U:OP1	8:X:2558:G:N2	2.46	0.48
9:Y:112:C:H2'	9:Y:113:A:H8	1.78	0.48
52:P:5:ILE:HG12	52:P:22:VAL:HG22	1.95	0.48
8:X:1111:U:O4	8:X:1120:G:N1	2.47	0.48
8:X:1306:G:O2'	8:X:2041:G:O6	2.29	0.48
10:Z:53:HIS:HA	10:Z:217:ARG:HB2	1.94	0.48
13:c:62:GLY:HA3	13:c:95:ARG:HH22	1.78	0.48
14:d:59:GLN:HE22	14:d:61:GLU:HG3	1.77	0.48
8:X:1152:G:H2'	8:X:1153:G:H8	1.78	0.48
13:c:4:LEU:HD12	13:c:97:TYR:HB3	1.95	0.48
37:A:384:G:H5''	52:P:6:ARG:HB2	1.95	0.48
41:E:120:VAL:HG21	41:E:123:ILE:HD12	1.95	0.48
3:W:15:C:H42	3:W:38:C:N4	2.09	0.48
8:X:1010:C:O2'	8:X:2302:A:N3	2.42	0.48
8:X:1130:A:H2	8:X:1152:G:H5'	1.79	0.48
27:u:75:VAL:HG12	27:u:89:VAL:HG22	1.95	0.48
37:A:1129:U:O4	37:A:1163:G:O6	2.31	0.48
41:E:82:PRO:HD2	41:E:147:LEU:HD23	1.96	0.48
1:U:49:G:O6	1:U:65:U:O4	2.32	0.47
7:q:101:LYS:H	7:q:104:LYS:HD2	1.79	0.47
8:X:28:A:N6	8:X:558:G:O2'	2.47	0.47
8:X:632:U:OP2	17:i:16:ARG:NH2	2.41	0.47
18:j:2:LEU:O	18:j:44:ASN:ND2	2.47	0.47
23:o:5:ILE:O	23:o:11:GLN:HA	2.14	0.47
37:A:1449:U:H3	37:A:1471:G:H1	1.62	0.47
43:G:20:SER:O	43:G:24:SER:HB3	2.13	0.47
51:O:36:ILE:O	51:O:40:ASN:HB2	2.13	0.47
8:X:2343:A:OP1	13:c:88:LYS:NZ	2.41	0.47
16:f:111:PHE:HD2	16:f:114:ILE:HD12	1.79	0.47
19:k:22:THR:O	19:k:26:ILE:HG12	2.13	0.47
37:A:224:U:O2'	37:A:477:A:N6	2.47	0.47
37:A:1384:A:OP1	43:G:9:LYS:NZ	2.36	0.47
37:A:1436:C:H2'	37:A:1437:A:H8	1.79	0.47
45:I:31:ASN:HB2	45:I:38:HIS:HE1	1.79	0.47
8:X:331:C:N4	8:X:332:G:O6	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:1216:C:H2'	8:X:1220:G:H22	1.79	0.47
8:X:1316:A:H2'	8:X:1317:G:C8	2.50	0.47
13:c:38:MET:SD	13:c:150:ARG:NH1	2.69	0.47
32:1:8:ALA:HA	32:1:15:ARG:HA	1.96	0.47
37:A:962:U:H2'	37:A:963:G:H8	1.79	0.47
38:B:207:ILE:HG13	38:B:208:ARG:HD3	1.96	0.47
3:W:105:U:O2	3:W:226:G:O6	2.32	0.47
8:X:310:C:H5''	8:X:406:G:H1	1.79	0.47
8:X:1137:G:H21	8:X:1139:G:H22	1.61	0.47
13:c:170:LEU:HD12	13:c:175:MET:HG2	1.96	0.47
17:i:96:LEU:HB3	17:i:102:ILE:HG12	1.97	0.47
37:A:525:U:O2'	37:A:528:C:N3	2.42	0.47
37:A:1351:C:H2'	37:A:1352:G:C8	2.49	0.47
39:C:59:ALA:HB3	39:C:62:ARG:HB2	1.95	0.47
43:G:49:ILE:O	43:G:53:ARG:HB2	2.14	0.47
1:U:38:C:H3'	1:U:39:G:H8	1.80	0.47
3:W:252:C:H2'	3:W:253:G:C8	2.50	0.47
6:p:31:ARG:NH2	6:p:109:LYS:O	2.47	0.47
10:Z:93:LEU:HD11	10:Z:101:LYS:HB3	1.94	0.47
24:r:24:ILE:HD11	24:r:32:ALA:HB1	1.95	0.47
37:A:995:C:H2'	37:A:996:A:C8	2.50	0.47
38:B:92:VAL:HG22	38:B:151:ILE:HD11	1.97	0.47
3:W:24:A:H1'	7:q:26:PRO:HG3	1.96	0.47
8:X:514:G:HO2'	8:X:843:C:HO2'	1.60	0.47
8:X:2320:U:O2'	8:X:2403:C:O2	2.32	0.47
8:X:2719:A:N6	19:k:39:GLU:OE1	2.40	0.47
8:X:2772:U:OP1	35:4:33:LYS:NZ	2.45	0.47
12:b:9:GLN:HA	12:b:126:LEU:HD11	1.96	0.47
37:A:989:C:OP1	37:A:1232:C:N4	2.47	0.47
38:B:27:MET:O	38:B:39:TYR:OH	2.29	0.47
3:W:66:C:H5'	3:W:67:C:H5	1.79	0.47
8:X:461:C:H2'	8:X:462:A:C8	2.49	0.47
8:X:1709:A:H61	8:X:2025:C:H5	1.63	0.47
8:X:2208:C:N4	8:X:2211:G:O6	2.46	0.47
8:X:2532:A:O2'	8:X:2534:G:OP2	2.31	0.47
13:c:58:THR:HB	36:6:7:PRO:HG3	1.97	0.47
16:f:34:ASN:OD1	16:f:35:ILE:N	2.45	0.47
37:A:320:C:H2'	37:A:321:A:H8	1.78	0.47
37:A:331:U:O3'	56:T:17:ARG:NH1	2.48	0.47
37:A:1259:A:H5'	45:I:69:GLY:HA2	1.97	0.47
39:C:178:ARG:NH1	39:C:206:VAL:O	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:E:14:ARG:NH2	41:E:116:GLU:OE1	2.43	0.47
45:I:51:PRO:HD3	45:I:80:ARG:HH12	1.80	0.47
11:a:69:VAL:HG21	11:a:76:PRO:HA	1.97	0.47
37:A:956:A:H2'	37:A:957:G:C8	2.50	0.47
37:A:1028:A:H2'	37:A:1029:G:C8	2.50	0.47
3:W:15:C:N4	3:W:38:C:H41	2.04	0.47
7:q:132:ALA:HB1	7:q:137:ILE:HB	1.96	0.47
8:X:302:A:H2'	8:X:303:G:H8	1.80	0.47
8:X:1116:A:C5	8:X:1142:A:H1'	2.50	0.47
8:X:1890:C:H2'	8:X:1891:G:H8	1.79	0.47
8:X:2012:C:H4'	8:X:2635:C:H4'	1.97	0.47
8:X:2498:A:O2'	18:j:56:ARG:NH1	2.48	0.47
16:f:88:ARG:NH1	16:f:92:SER:OG	2.48	0.47
16:f:92:SER:HB2	16:f:113:LYS:HD2	1.97	0.47
45:I:71:GLY:O	45:I:75:GLN:CB	2.62	0.47
8:X:776:G:H5'	8:X:777:C:H5''	1.96	0.47
8:X:1757:G:O6	8:X:1776:A:N6	2.48	0.47
8:X:1817:C:H5''	10:Z:224:VAL:HG11	1.97	0.47
8:X:2229:C:O2	8:X:2255:C:N4	2.48	0.47
8:X:2355:U:H3	8:X:2418:G:H1	1.62	0.47
10:Z:124:ILE:HG23	10:Z:192:ILE:HD13	1.96	0.47
20:l:33:VAL:HG11	20:l:106:VAL:HG12	1.96	0.47
37:A:1126:U:O4	37:A:1193:G:O6	2.33	0.47
37:A:1532:U:H2'	37:A:1533:G:H8	1.80	0.47
8:X:284:C:O2	8:X:287:G:N2	2.48	0.46
8:X:650:U:OP2	12:b:104:LYS:NZ	2.45	0.46
8:X:1136:U:C2	8:X:1148:C:C2	3.03	0.46
8:X:1516:A:H62	8:X:1569:A:H2	1.56	0.46
12:b:20:ASN:ND2	12:b:22:SER:OG	2.48	0.46
12:b:136:THR:HB	12:b:170:ILE:HD11	1.98	0.46
14:d:59:GLN:HE21	14:d:62:HIS:CG	2.33	0.46
14:d:81:SER:OG	14:d:82:LYS:NZ	2.42	0.46
23:o:27:ALA:O	23:o:65:GLN:NE2	2.48	0.46
37:A:1480:G:H2'	37:A:1481:G:H8	1.79	0.46
7:q:131:THR:HG22	8:X:1106:U:H5	1.81	0.46
8:X:2225:C:H2'	8:X:2226:U:C2	2.50	0.46
25:s:65:ARG:HA	25:s:69:TYR:O	2.15	0.46
39:C:68:HIS:HB3	39:C:105:ILE:HD11	1.97	0.46
8:X:2334:U:O5'	13:c:133:LYS:NZ	2.45	0.46
8:X:2685:U:H2'	8:X:2686:A:H8	1.81	0.46
12:b:34:PHE:HD1	17:i:6:LEU:HD22	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:124:LYS:NZ	17:i:144:GLU:OE2	2.42	0.46
41:E:11:LEU:HD23	41:E:40:GLY:HA2	1.97	0.46
49:M:34:LEU:HA	49:M:37:ALA:HB3	1.97	0.46
3:W:16:G:N2	3:W:34:U:O2	2.49	0.46
3:W:92:G:H2'	3:W:93:G:C8	2.50	0.46
8:X:253:G:OP1	34:3:13:ARG:NH1	2.37	0.46
8:X:286:U:H1'	8:X:287:G:H21	1.81	0.46
8:X:1090:U:H5'	8:X:1091:U:H5''	1.96	0.46
8:X:2154:G:H5''	8:X:2155:A:H5'	1.96	0.46
8:X:2275:G:H2'	8:X:2276:A:C8	2.50	0.46
43:G:11:ASP:N	43:G:11:ASP:OD1	2.49	0.46
6:p:61:ARG:NH1	8:X:1092:A:OP2	2.43	0.46
8:X:921:G:N2	8:X:950:U:O2	2.39	0.46
15:e:17:LEU:HD22	15:e:141:TYR:HB2	1.97	0.46
21:m:92:VAL:HG11	21:m:97:LEU:HD21	1.97	0.46
30:x:8:LEU:HG	30:x:28:LEU:HD23	1.97	0.46
36:6:14:VAL:HB	36:6:22:PHE:HB3	1.98	0.46
37:A:1119:C:OP2	39:C:175:HIS:ND1	2.46	0.46
37:A:1379:G:H2'	37:A:1380:G:H8	1.79	0.46
43:G:66:LEU:O	43:G:70:MET:HB2	2.14	0.46
50:N:6:MET:HB3	50:N:23:ARG:HH12	1.80	0.46
37:A:714:G:H21	47:K:33:ILE:HD11	1.80	0.46
37:A:1198:U:H4'	39:C:10:LEU:HD11	1.97	0.46
37:A:1323:C:H41	55:S:5:LEU:HG	1.80	0.46
37:A:1473:C:H5''	37:A:1475:C:H41	1.80	0.46
38:B:70:VAL:HA	38:B:92:VAL:HB	1.96	0.46
46:J:52:LEU:HB2	50:N:41:ARG:HD2	1.97	0.46
55:S:19:ILE:O	55:S:23:ASN:ND2	2.49	0.46
8:X:866:A:OP2	8:X:1228:G:N2	2.34	0.46
8:X:1136:U:C4	8:X:1148:C:N4	2.84	0.46
8:X:1615:A:OP1	10:Z:60:ARG:NH2	2.47	0.46
37:A:30:G:O2'	37:A:304:U:OP1	2.33	0.46
37:A:561:U:H2'	37:A:562:G:H8	1.80	0.46
37:A:992:U:H4'	37:A:993:A:H5'	1.97	0.46
37:A:1262:G:O6	37:A:1294:A:N6	2.49	0.46
44:H:10:MET:HG3	44:H:27:ILE:HG21	1.98	0.46
45:I:34:GLU:O	45:I:38:HIS:CB	2.63	0.46
21:m:71:GLU:OE1	21:m:101:ARG:NH1	2.49	0.46
37:A:541:A:H61	39:C:192:TYR:HA	1.81	0.46
52:P:70:VAL:HA	52:P:73:LEU:HG	1.97	0.46
8:X:328:G:H22	8:X:399:C:H1'	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:510:G:N2	8:X:513:A:OP2	2.43	0.46
8:X:563:C:O2'	24:r:18:ARG:NH2	2.48	0.46
11:a:130:ARG:HB2	11:a:141:ARG:H	1.81	0.46
41:E:42:LYS:HZ2	41:E:117:LEU:HA	1.80	0.46
8:X:500:A:N3	8:X:504:A:O2'	2.49	0.46
8:X:1634:U:H2'	8:X:1635:G:H8	1.81	0.46
37:A:10:A:H8	41:E:106:ILE:HG23	1.81	0.46
37:A:1091:G:OP2	41:E:52:LYS:NZ	2.36	0.46
37:A:1375:C:O3'	46:J:62:ARG:NH2	2.49	0.46
47:K:48:SER:H	47:K:51:ALA:HB3	1.81	0.46
8:X:87:U:OP2	26:t:29:LYS:NZ	2.49	0.45
8:X:602:G:H2'	8:X:603:G:H8	1.81	0.45
8:X:633:U:H2'	8:X:634:A:C8	2.51	0.45
8:X:2053:C:H5''	11:a:153:ARG:HD3	1.98	0.45
10:Z:8:PRO:HB3	10:Z:14:ARG:HA	1.98	0.45
18:j:37:LEU:HD11	18:j:130:LYS:HB2	1.98	0.45
37:A:24:G:O2'	37:A:923:A:N1	2.41	0.45
43:G:99:LEU:HB3	43:G:103:TRP:CZ3	2.52	0.45
8:X:2191:A:H61	8:X:2202:A:H62	1.64	0.45
14:d:90:LEU:HA	14:d:162:GLY:O	2.16	0.45
19:k:25:ILE:HG13	19:k:83:LEU:HD12	1.98	0.45
37:A:723:G:H2'	37:A:724:A:C8	2.52	0.45
42:F:28:ASN:HA	42:F:31:THR:HG22	1.98	0.45
8:X:719:C:H5	17:i:42:SER:HB2	1.82	0.45
8:X:867:A:H4'	8:X:883:G:H22	1.81	0.45
11:a:180:ASP:HB3	11:a:185:LEU:HB2	1.98	0.45
25:s:32:VAL:HG23	25:s:33:ARG:HG3	1.97	0.45
37:A:215:G:O6	37:A:225:A:N6	2.49	0.45
37:A:267:G:OP1	56:T:78:ARG:NH2	2.48	0.45
43:G:39:SER:O	43:G:43:LEU:HB2	2.16	0.45
53:Q:63:ILE:HD12	53:Q:75:PHE:HD1	1.81	0.45
8:X:342:A:N3	8:X:363:C:O2'	2.48	0.45
8:X:1823:U:HO2'	8:X:1929:A:HO2'	1.63	0.45
37:A:111:G:N3	37:A:361:A:O2'	2.49	0.45
37:A:209:A:O2'	37:A:210:A:N7	2.43	0.45
37:A:1056:A:N6	37:A:1220:U:O2	2.48	0.45
8:X:1854:G:N2	8:X:1930:A:OP1	2.49	0.45
8:X:1886:G:O2'	8:X:1887:G:O4'	2.24	0.45
17:i:1:MET:HE2	17:i:6:LEU:HA	1.99	0.45
35:4:20:LYS:O	35:4:22:LYS:NZ	2.49	0.45
37:A:181:G:H3'	37:A:208:A:H61	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:B:83:GLU:O	38:B:87:SER:OG	2.33	0.45
8:X:1001:U:OP1	18:j:87:LYS:NZ	2.40	0.45
37:A:381:A:H61	37:A:399:G:H1'	1.81	0.45
8:X:224:A:H1'	8:X:236:A:H1'	1.98	0.45
8:X:1516:A:N6	8:X:1569:A:C2	2.80	0.45
37:A:320:C:H2'	37:A:321:A:C8	2.51	0.45
8:X:676:G:O6	17:i:71:ARG:NH2	2.49	0.45
37:A:1017:A:N6	37:A:1032:C:N3	2.64	0.45
39:C:21:LYS:NZ	39:C:55:GLU:OE1	2.50	0.45
43:G:26:LEU:O	43:G:44:TYR:OH	2.33	0.45
8:X:603:G:N2	22:n:49:ASP:OD1	2.49	0.45
8:X:722:A:O2'	12:b:67:GLN:OE1	2.35	0.45
8:X:2362:A:N3	8:X:2364:A:N6	2.65	0.45
14:d:3:ARG:HG2	14:d:6:LYS:HE2	1.99	0.45
26:t:40:MET:SD	26:t:58:ASN:ND2	2.87	0.45
34:3:43:LYS:HA	34:3:43:LYS:HD3	1.80	0.45
37:A:1436:C:H2'	37:A:1437:A:C8	2.52	0.45
41:E:99:ALA:HB3	41:E:122:ASP:HB3	1.98	0.45
8:X:719:C:H5'	8:X:848:G:H22	1.82	0.45
8:X:1081:U:H2'	8:X:1082:G:H8	1.82	0.45
8:X:1088:G:H1	8:X:1159:U:H3	1.65	0.45
8:X:1855:C:OP1	10:Z:223:SER:OG	2.30	0.45
8:X:2320:U:H2'	8:X:2321:U:C6	2.52	0.45
8:X:2516:G:H2'	8:X:2517:A:C8	2.51	0.45
11:a:2:THR:OG1	11:a:85:GLY:O	2.30	0.45
30:x:24:ARG:O	30:x:24:ARG:NH1	2.37	0.45
37:A:552:G:H2'	37:A:553:G:H8	1.81	0.45
37:A:1421:C:H2'	37:A:1422:A:C8	2.52	0.45
45:I:92:PRO:HA	45:I:95:ARG:HB2	1.99	0.45
49:M:58:ASP:HA	49:M:61:ASP:HB2	1.97	0.45
6:p:92:PRO:HB2	6:p:96:LEU:HG	1.99	0.44
8:X:840:A:OP2	8:X:2100:A:O2'	2.35	0.44
8:X:2838:U:H2'	8:X:2839:C:H6	1.82	0.44
19:k:55:ASP:N	19:k:55:ASP:OD2	2.50	0.44
37:A:343:C:H2'	37:A:344:A:C8	2.52	0.44
37:A:957:G:O3'	49:M:108:THR:OG1	2.32	0.44
8:X:123:G:OP1	8:X:1415:C:O2'	2.32	0.44
37:A:416:G:O2'	40:D:105:ARG:NH1	2.46	0.44
37:A:490:G:O2'	37:A:492:C:N4	2.51	0.44
42:F:74:GLU:OE2	42:F:77:ARG:NH1	2.49	0.44
54:R:64:ILE:HG22	54:R:68:ARG:HD2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:70:ASP:OD1	20:l:71:THR:N	2.51	0.44
25:s:5:ARG:HH22	29:w:23:GLU:CG	2.24	0.44
32:1:31:GLU:OE1	32:1:46:ARG:NH1	2.50	0.44
37:A:424:G:H2'	37:A:425:G:H8	1.82	0.44
8:X:372:U:O2'	26:t:66:SER:OG	2.30	0.44
8:X:2334:U:O2'	8:X:2335:U:O2	2.30	0.44
37:A:97:U:O2'	37:A:98:U:O4'	2.30	0.44
37:A:1306:U:H4'	37:A:1307:C:H5'	1.99	0.44
41:E:39:VAL:HG21	41:E:64:VAL:HG23	1.99	0.44
48:L:112:ARG:HD3	48:L:117:THR:HB	1.98	0.44
3:W:26:C:O2'	3:W:53:A:OP2	2.35	0.44
8:X:302:A:H2'	8:X:303:G:C8	2.53	0.44
8:X:1112:U:C2	8:X:1115:A:N7	2.86	0.44
8:X:1942:A:H2'	37:A:1502:A:H62	1.83	0.44
10:Z:30:GLU:HG3	10:Z:32:SER:H	1.82	0.44
23:o:32:THR:HA	23:o:60:ALA:O	2.18	0.44
24:r:35:ILE:O	24:r:39:THR:OG1	2.26	0.44
37:A:553:G:OP1	40:D:55:GLN:NE2	2.51	0.44
37:A:954:G:O6	37:A:1349:A:N6	2.51	0.44
37:A:1231:G:OP2	37:A:1331:C:N4	2.43	0.44
3:W:24:A:N1	8:X:1142:A:N6	2.65	0.44
8:X:1065:U:OP1	8:X:1081:U:O2'	2.29	0.44
8:X:1321:U:H3	8:X:1325:A:N6	2.16	0.44
11:a:126:HIS:NE2	11:a:159:LEU:HD12	2.33	0.44
36:6:1:MET:N	36:6:1:MET:SD	2.85	0.44
40:D:128:ILE:HA	40:D:129:PRO:HD3	1.77	0.44
1:U:50:C:N4	1:U:51:G:O6	2.51	0.44
4:g:61:GLN:HA	4:g:64:MET:CB	2.47	0.44
7:q:101:LYS:HA	7:q:140:GLU:HB2	2.00	0.44
7:q:108:ILE:O	7:q:111:THR:OG1	2.36	0.44
8:X:294:G:H2'	8:X:295:G:C8	2.53	0.44
8:X:688:G:H21	8:X:692:A:H62	1.64	0.44
8:X:2041:G:OP1	24:r:11:ARG:NH2	2.39	0.44
10:Z:41:GLY:O	10:Z:43:ARG:NH1	2.51	0.44
23:o:96:THR:OG1	23:o:98:GLU:OE2	2.31	0.44
37:A:1158:C:O2'	37:A:1289:A:N1	2.46	0.44
39:C:111:ASP:OD1	39:C:111:ASP:N	2.48	0.44
39:C:150:THR:HG22	39:C:199:VAL:HG23	1.99	0.44
45:I:35:ILE:HD12	45:I:39:ILE:HG13	1.99	0.44
8:X:153:C:H2'	8:X:154:A:H8	1.83	0.44
8:X:296:G:O2'	8:X:297:G:O4'	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:2780:G:C5	14:d:2:SER:HA	2.53	0.44
31:0:10:LYS:H	31:0:10:LYS:HG2	1.63	0.44
31:0:13:LYS:HZ2	31:0:17:ARG:HE	1.65	0.44
25:s:14:THR:H	25:s:17:SER:HG	1.62	0.44
37:A:1055:C:N4	37:A:1220:U:O2'	2.50	0.44
38:B:77:GLN:NE2	38:B:93:ASN:O	2.35	0.44
45:I:27:ARG:O	45:I:62:ASP:HA	2.17	0.44
49:M:77:ILE:HD12	49:M:77:ILE:HA	1.88	0.44
55:S:39:THR:HA	55:S:70:LYS:HA	2.00	0.44
3:W:88:U:O2	3:W:240:A:N6	2.51	0.43
8:X:455:G:H2'	8:X:456:A:C8	2.53	0.43
8:X:1002:G:OP2	18:j:14:ARG:NH2	2.51	0.43
8:X:1017:C:O2'	8:X:1029:A:N3	2.44	0.43
8:X:1254:A:N6	8:X:1275:G:O2'	2.48	0.43
17:i:95:LEU:HA	17:i:98:GLU:HG3	2.00	0.43
29:w:8:ASP:OD1	29:w:9:LEU:N	2.50	0.43
39:C:152:VAL:HG22	39:C:197:VAL:HG22	1.99	0.43
11:a:178:LYS:HB3	11:a:187:LEU:HB2	2.00	0.43
12:b:32:VAL:HG13	12:b:105:VAL:HG13	1.99	0.43
13:c:30:LYS:H	13:c:159:THR:HG22	1.83	0.43
22:n:82:GLY:O	22:n:86:SER:CB	2.66	0.43
37:A:121:C:H2'	37:A:122:G:H8	1.82	0.43
53:Q:26:VAL:HA	53:Q:45:LYS:HA	2.00	0.43
3:W:6:C:H2'	3:W:7:G:C8	2.53	0.43
7:q:14:PRO:HA	7:q:53:ILE:HA	2.00	0.43
8:X:422:C:H2'	8:X:423:G:H8	1.83	0.43
10:Z:268:LYS:HB3	10:Z:268:LYS:HE2	1.82	0.43
16:f:63:VAL:HG13	16:f:102:VAL:HG13	1.98	0.43
29:w:42:ARG:NE	29:w:45:GLU:OE2	2.49	0.43
38:B:42:ASP:OD1	38:B:42:ASP:N	2.51	0.43
41:E:85:ILE:HG22	41:E:96:LEU:HB2	1.99	0.43
44:H:107:SER:HA	44:H:112:VAL:HA	2.01	0.43
55:S:50:ALA:HB1	55:S:57:HIS:HB3	2.00	0.43
7:q:79:LEU:HD22	7:q:100:VAL:HG21	2.01	0.43
8:X:1433:U:H3	25:s:16:ARG:HH22	1.66	0.43
8:X:1696:G:H3'	19:k:35:THR:HG21	2.00	0.43
22:n:58:ARG:O	22:n:62:ILE:HG12	2.18	0.43
37:A:854:C:H3'	37:A:855:G:H8	1.83	0.43
37:A:1351:C:H2'	37:A:1352:G:H8	1.84	0.43
42:F:44:GLY:O	42:F:59:PHE:HA	2.18	0.43
6:p:113:ILE:HD12	6:p:124:LYS:HD2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:2128:U:H2'	8:X:2129:G:C8	2.53	0.43
8:X:2169:G:N1	8:X:2180:U:O4	2.52	0.43
12:b:143:LEU:HD12	12:b:148:VAL:HB	2.00	0.43
13:c:22:TYR:OH	13:c:165:GLU:OE1	2.34	0.43
37:A:12:A:H2'	37:A:13:G:H8	1.84	0.43
37:A:150:A:N6	37:A:169:U:N3	2.62	0.43
37:A:671:A:H2'	37:A:672:A:C8	2.54	0.43
37:A:1128:A:H4'	45:I:85:ARG:HH22	1.83	0.43
37:A:1174:U:H3'	37:A:1175:G:H8	1.83	0.43
38:B:166:PRO:HG3	38:B:187:VAL:HG12	2.01	0.43
8:X:373:A:N6	26:t:15:LYS:H	2.16	0.43
8:X:1348:G:OP1	33:2:9:ASN:ND2	2.50	0.43
8:X:2368:G:H2'	8:X:2369:A:C8	2.52	0.43
10:Z:125:LYS:H	10:Z:128:ASN:HD22	1.65	0.43
12:b:68:LYS:HB3	12:b:68:LYS:HE3	1.80	0.43
21:m:25:THR:HA	21:m:46:VAL:HA	1.99	0.43
22:n:38:GLN:O	22:n:42:SER:N	2.45	0.43
24:r:9:THR:HG23	24:r:100:THR:HG21	2.01	0.43
37:A:209:A:H3'	56:T:63:LYS:HG3	2.01	0.43
43:G:116:MET:HA	43:G:119:ARG:HG2	2.00	0.43
8:X:1457:U:H5'	8:X:1458:U:H4'	2.01	0.43
8:X:1893:U:OP1	8:X:2439:G:O2'	2.29	0.43
8:X:2778:A:OP1	14:d:3:ARG:NH2	2.51	0.43
10:Z:155:VAL:HG21	10:Z:162:ALA:HB2	2.01	0.43
27:u:83:ASP:OD1	27:u:83:ASP:N	2.51	0.43
37:A:150:A:H62	37:A:169:U:H3	1.62	0.43
37:A:277:C:H2'	37:A:278:A:H8	1.84	0.43
45:I:88:LEU:HB2	45:I:95:ARG:HD2	1.99	0.43
55:S:50:ALA:HA	55:S:58:VAL:O	2.18	0.43
3:W:188:C:O2'	3:W:189:U:O4'	2.37	0.43
12:b:53:ASN:OD1	12:b:54:ARG:N	2.52	0.43
14:d:27:VAL:HB	14:d:76:MET:HE1	2.01	0.43
37:A:495:U:H2'	37:A:496:A:C8	2.54	0.43
37:A:956:A:O2'	37:A:1342:A:N3	2.47	0.43
37:A:1365:G:H2'	37:A:1366:A:C8	2.49	0.43
37:A:1380:G:OP1	45:I:14:SER:OG	2.35	0.43
40:D:22:THR:OG1	40:D:24:LYS:O	2.35	0.43
44:H:106:ILE:HG12	44:H:127:VAL:HA	2.00	0.43
3:W:38:C:N4	3:W:59:G:O6	2.51	0.43
8:X:29:U:O2	8:X:1255:G:O2'	2.37	0.43
8:X:1529:G:H2'	8:X:1530:G:H8	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:1634:U:H2'	8:X:1635:G:C8	2.54	0.43
8:X:2859:G:H21	8:X:2908:A:N6	2.15	0.43
8:X:2861:U:H2'	8:X:2862:A:C8	2.54	0.43
12:b:191:LYS:HD3	12:b:191:LYS:HA	1.86	0.43
38:B:108:GLN:HA	38:B:111:ILE:HG22	1.99	0.43
38:B:134:VAL:HG13	38:B:138:LYS:HD3	2.00	0.43
8:X:178:A:O2'	8:X:179:A:N7	2.50	0.43
8:X:2159:U:O2'	8:X:2187:A:N6	2.50	0.43
27:u:76:LYS:HE3	27:u:76:LYS:HB3	1.80	0.43
34:3:54:ASP:O	34:3:58:ILE:HG12	2.19	0.43
37:A:635:G:H2'	37:A:636:G:H8	1.84	0.43
37:A:646:U:H2'	37:A:647:G:H8	1.84	0.43
42:F:6:VAL:HG22	42:F:90:VAL:HG12	2.01	0.43
49:M:85:SER:O	49:M:87:ARG:N	2.47	0.43
50:N:3:LYS:HA	50:N:3:LYS:HD2	1.77	0.43
8:X:1141:A:H2'	8:X:1142:A:H8	1.83	0.42
37:A:1142:C:H2'	37:A:1143:A:C8	2.54	0.42
48:L:136:LYS:HA	48:L:136:LYS:HD3	1.80	0.42
56:T:51:LEU:HD22	56:T:83:VAL:HG11	2.00	0.42
6:p:18:LYS:HA	6:p:21:GLU:HB3	2.01	0.42
20:l:39:HIS:CE1	20:l:59:LEU:HB3	2.54	0.42
37:A:933:A:O2'	37:A:1408:C:OP2	2.27	0.42
39:C:118:ASN:ND2	39:C:136:GLN:OE1	2.52	0.42
1:U:23:A:H2'	1:U:24:A:H8	1.84	0.42
3:W:16:G:O6	3:W:34:U:O4	2.36	0.42
8:X:547:A:OP2	26:t:15:LYS:NZ	2.52	0.42
8:X:1516:A:N7	8:X:1569:A:N1	2.67	0.42
37:A:390:A:H2'	37:A:391:A:H8	1.84	0.42
37:A:689:C:H2'	37:A:690:A:C8	2.55	0.42
39:C:24:ALA:HB3	39:C:28:TYR:HD2	1.83	0.42
43:G:93:PRO:HA	43:G:96:ARG:HG3	2.01	0.42
44:H:4:THR:OG1	44:H:5:ASP:N	2.38	0.42
7:q:126:ARG:HB3	8:X:1126:A:H4'	2.01	0.42
8:X:1533:A:H2'	8:X:1534:A:C8	2.54	0.42
8:X:1712:G:H1'	8:X:1714:A:H62	1.83	0.42
8:X:2028:C:O2	8:X:2716:U:O2'	2.36	0.42
22:n:61:TRP:HB3	22:n:93:LYS:HB3	2.01	0.42
26:t:84:LYS:HD3	26:t:93:VAL:HG21	2.01	0.42
37:A:511:C:OP1	48:L:127:ARG:N	2.52	0.42
37:A:1450:G:H21	37:A:1470:A:H62	1.68	0.42
43:G:25:ARG:NH1	43:G:30:MET:SD	2.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:H:105:ILE:HB	44:H:129:ALA:HB3	2.01	0.42
49:M:12:ASP:OD1	49:M:46:ARG:NH1	2.52	0.42
8:X:1516:A:N6	8:X:1569:A:H2	2.17	0.42
8:X:2213:U:H2'	8:X:2214:G:C8	2.54	0.42
29:w:17:LYS:HB2	29:w:53:MET:HE1	2.01	0.42
37:A:277:C:H2'	37:A:278:A:C8	2.54	0.42
37:A:309:G:H2'	37:A:310:G:H8	1.85	0.42
37:A:371:A:C6	48:L:41:PRO:HD2	2.54	0.42
37:A:1084:G:H4'	38:B:102:THR:HB	2.00	0.42
37:A:1187:G:OP2	45:I:95:ARG:NH2	2.43	0.42
43:G:142:HIS:O	43:G:145:ALA:N	2.52	0.42
45:I:30:VAL:HG13	45:I:38:HIS:CE1	2.55	0.42
8:X:101:G:O6	26:t:89:LYS:NZ	2.52	0.42
8:X:217:G:N2	8:X:219:A:N3	2.67	0.42
8:X:1057:G:OP2	22:n:66:ASN:ND2	2.47	0.42
8:X:2138:U:H3	8:X:2172:C:HO2'	1.65	0.42
8:X:2861:U:H2'	8:X:2862:A:H8	1.84	0.42
17:i:120:LYS:NZ	17:i:140:GLY:O	2.47	0.42
18:j:31:GLU:HG3	18:j:107:SER:HA	2.01	0.42
37:A:512:A:OP1	48:L:129:LYS:NZ	2.39	0.42
37:A:962:U:H2'	37:A:963:G:C8	2.54	0.42
38:B:71:GLY:O	38:B:77:GLN:NE2	2.53	0.42
8:X:662:U:H2'	8:X:663:G:H8	1.84	0.42
8:X:910:A:H2'	8:X:911:G:C8	2.55	0.42
8:X:2874:G:O2'	8:X:2891:G:N2	2.53	0.42
10:Z:93:LEU:HB2	10:Z:103:TYR:HE1	1.85	0.42
11:a:14:GLN:NE2	11:a:22:LEU:HD13	2.34	0.42
13:c:42:ASP:OD2	13:c:148:LYS:NZ	2.46	0.42
18:j:65:TRP:HB3	18:j:105:GLU:HB2	2.02	0.42
23:o:53:VAL:HG12	23:o:56:ALA:HB3	2.02	0.42
25:s:20:LEU:HD22	25:s:25:LYS:HD2	2.02	0.42
36:6:26:SER:OG	36:6:27:VAL:N	2.53	0.42
37:A:1065:A:N6	37:A:1215:G:O6	2.52	0.42
37:A:1335:U:H2'	37:A:1336:G:C8	2.54	0.42
39:C:29:ALA:O	39:C:33:HIS:ND1	2.42	0.42
3:W:23:U:O2'	8:X:1141:A:N6	2.41	0.42
3:W:35:G:N7	3:W:36:U:O2'	2.52	0.42
8:X:670:C:O2'	8:X:704:U:OP1	2.36	0.42
8:X:904:A:N6	8:X:967:G:H1	2.17	0.42
8:X:1533:A:H2'	8:X:1534:A:H8	1.84	0.42
8:X:2873:G:H8	21:m:95:ALA:HB2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:22:LEU:HA	11:a:22:LEU:HD23	1.87	0.42
11:a:114:SER:OG	11:a:115:LYS:N	2.53	0.42
37:A:83:C:H2'	37:A:84:U:H2'	2.02	0.42
37:A:1400:U:H2'	37:A:1401:G:C8	2.54	0.42
6:p:94:LYS:HA	6:p:94:LYS:HD3	1.90	0.42
8:X:75:G:OP1	29:w:44:ARG:NH2	2.36	0.42
8:X:1314:A:N1	8:X:1334:C:O2'	2.49	0.42
8:X:2048:U:O3'	22:n:27:SER:OG	2.35	0.42
10:Z:191:SER:OG	10:Z:192:ILE:N	2.52	0.42
12:b:79:ARG:HA	12:b:79:ARG:HD3	1.79	0.42
13:c:158:THR:HG23	13:c:160:ALA:H	1.84	0.42
28:v:19:SER:OG	28:v:20:HIS:N	2.51	0.42
37:A:58:U:H2'	37:A:59:G:H8	1.85	0.42
37:A:551:U:O3'	40:D:14:ARG:NH2	2.44	0.42
37:A:1230:G:H4'	55:S:77:THR:HG21	2.02	0.42
37:A:1443:A:H62	37:A:1477:G:N2	2.18	0.42
52:P:76:SER:OG	52:P:77:GLN:OE1	2.37	0.42
3:W:17:G:H2'	3:W:18:G:C8	2.54	0.42
8:X:528:G:O5'	26:t:43:LYS:NZ	2.48	0.42
21:m:27:ARG:HB3	21:m:44:GLU:HG2	2.02	0.42
37:A:201:C:H2'	37:A:202:A:H8	1.85	0.42
37:A:1233:U:O2'	37:A:1331:C:OP1	2.33	0.42
37:A:1418:C:H2'	37:A:1419:A:H8	1.85	0.42
43:G:138:ARG:HD3	43:G:142:HIS:HE1	1.85	0.42
44:H:45:PHE:HE2	44:H:103:ILE:HG12	1.84	0.42
3:W:40:U:H2'	3:W:41:G:H8	1.84	0.41
6:p:52:PHE:HA	6:p:86:THR:H	1.85	0.41
8:X:277:C:H2'	8:X:278:A:C8	2.54	0.41
8:X:1184:G:N3	15:e:109:MET:HE2	2.35	0.41
8:X:1320:G:H2'	8:X:1321:U:C6	2.55	0.41
8:X:2397:C:H2'	8:X:2398:A:H8	1.85	0.41
17:i:1:MET:HE2	17:i:6:LEU:HD23	2.01	0.41
18:j:51:ARG:HG3	18:j:64:VAL:HG11	2.02	0.41
20:l:62:ASP:OD1	20:l:62:ASP:N	2.52	0.41
30:x:7:THR:HG22	30:x:34:THR:HG22	2.01	0.41
37:A:179:U:H2'	37:A:180:G:C8	2.54	0.41
37:A:368:G:H2'	37:A:369:G:C8	2.55	0.41
37:A:1023:G:OP2	37:A:1024:A:N6	2.53	0.41
38:B:109:LYS:HG3	38:B:113:ARG:HH22	1.83	0.41
53:Q:63:ILE:HA	53:Q:76:ARG:O	2.20	0.41
3:W:73:C:H5''	3:W:74:G:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:118:C:H3'	3:W:119:G:H8	1.85	0.41
6:p:106:LEU:HB3	6:p:107:GLU:H	1.64	0.41
8:X:973:G:H2'	8:X:974:A:C8	2.55	0.41
8:X:2162:G:H1'	8:X:2186:G:H4'	2.02	0.41
10:Z:39:LYS:HE2	10:Z:39:LYS:HB2	1.90	0.41
37:A:455:G:O6	37:A:494:G:O2'	2.36	0.41
37:A:568:A:OP2	41:E:126:LYS:NZ	2.53	0.41
37:A:942:C:H2'	37:A:943:G:C8	2.55	0.41
37:A:996:A:N3	55:S:52:TYR:OH	2.47	0.41
37:A:1463:A:H2'	37:A:1464:G:C8	2.55	0.41
40:D:182:ARG:HA	40:D:182:ARG:HD2	1.91	0.41
3:W:105:U:C2	3:W:226:G:O6	2.73	0.41
8:X:683:A:OP2	17:i:113:GLY:N	2.42	0.41
10:Z:2:ALA:HB3	10:Z:199:GLN:HE22	1.85	0.41
10:Z:247:MET:HE3	10:Z:247:MET:HB3	1.96	0.41
13:c:8:TYR:OH	13:c:29:PRO:O	2.38	0.41
37:A:267:G:H5'	56:T:78:ARG:HH22	1.85	0.41
37:A:282:A:H1'	37:A:283:G:N7	2.35	0.41
37:A:712:G:H4'	37:A:713:A:H5'	2.01	0.41
38:B:93:ASN:OD1	38:B:94:GLN:N	2.51	0.41
45:I:119:LYS:HA	45:I:119:LYS:HD2	1.85	0.41
47:K:57:SER:O	47:K:60:SER:OG	2.38	0.41
8:X:1117:G:N1	8:X:1137:G:O6	2.46	0.41
8:X:1469:G:H2'	8:X:1470:G:H8	1.85	0.41
13:c:36:ILE:HB	13:c:89:VAL:HG12	2.03	0.41
13:c:42:ASP:O	13:c:46:ASN:N	2.43	0.41
16:f:24:VAL:HG12	16:f:39:ILE:HG22	2.02	0.41
21:m:111:LYS:HE3	21:m:111:LYS:HB2	1.89	0.41
26:t:24:LEU:HD13	26:t:36:GLU:HB2	2.02	0.41
37:A:385:G:H2'	37:A:386:A:H8	1.85	0.41
37:A:417:U:H5'	40:D:105:ARG:HH22	1.85	0.41
37:A:683:G:H2'	37:A:684:A:C8	2.53	0.41
37:A:1495:U:H2'	37:A:1496:G:C8	2.55	0.41
39:C:174:LEU:HD21	39:C:200:TRP:HE1	1.85	0.41
43:G:42:ILE:HA	43:G:45:LYS:HG2	2.03	0.41
47:K:100:ARG:HA	47:K:103:GLN:HG3	2.03	0.41
54:R:31:VAL:HG22	54:R:72:LEU:HD23	2.03	0.41
8:X:613:U:O2'	8:X:1029:A:N1	2.45	0.41
8:X:1289:U:O2'	17:i:21:ARG:NH1	2.53	0.41
8:X:1444:C:H2'	8:X:1445:A:C8	2.53	0.41
8:X:1808:U:H5''	8:X:1809:A:H5''	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:1968:U:OP1	8:X:2633:U:O2'	2.36	0.41
8:X:2406:A:O2'	20:l:120:PHE:O	2.37	0.41
10:Z:145:GLU:HG2	10:Z:151:GLY:C	2.46	0.41
12:b:160:ASN:HB3	12:b:163:VAL:HG12	2.02	0.41
25:s:5:ARG:HH12	29:w:23:GLU:CG	2.33	0.41
32:1:10:THR:OG1	32:1:44:LEU:O	2.32	0.41
32:1:33:LYS:HE3	32:1:33:LYS:HB3	1.86	0.41
37:A:699:G:OP2	47:K:31:ASN:ND2	2.54	0.41
48:L:120:VAL:O	48:L:132:THR:OG1	2.28	0.41
3:W:182:U:H2'	3:W:183:G:C8	2.55	0.41
8:X:2164:A:N7	8:X:2165:A:O2'	2.51	0.41
15:e:106:ILE:HG21	15:e:123:LEU:HD22	2.02	0.41
37:A:417:U:H2'	37:A:418:G:C8	2.56	0.41
39:C:131:ARG:HH12	39:C:135:GLN:HB2	1.84	0.41
43:G:70:MET:HE1	43:G:97:THR:HA	2.03	0.41
45:I:85:ARG:HA	45:I:88:LEU:HG	2.01	0.41
46:J:80:THR:OG1	46:J:83:THR:OG1	2.35	0.41
1:U:49:G:N2	1:U:65:U:O2	2.34	0.41
6:p:43:LYS:HA	6:p:46:ARG:HD2	2.02	0.41
8:X:1485:A:H2	8:X:1600:G:H21	1.69	0.41
8:X:1823:U:H2'	8:X:1824:C:C6	2.56	0.41
13:c:144:ASP:N	13:c:144:ASP:OD1	2.52	0.41
20:l:14:ARG:HG3	20:l:99:GLY:HA3	2.02	0.41
30:x:47:ILE:O	30:x:51:SER:HB2	2.21	0.41
34:3:24:ARG:HD3	34:3:50:VAL:HG22	2.02	0.41
37:A:520:C:O3'	40:D:36:HIS:NE2	2.50	0.41
37:A:689:C:H2'	37:A:690:A:H8	1.85	0.41
45:I:31:ASN:HB2	45:I:38:HIS:CE1	2.55	0.41
8:X:1825:U:H2'	8:X:1826:C:H6	1.86	0.41
8:X:2060:A:N3	8:X:2484:G:O2'	2.41	0.41
8:X:2135:G:C2	8:X:2212:C:O2	2.74	0.41
10:Z:133:ILE:HD12	10:Z:133:ILE:HA	1.94	0.41
25:s:20:LEU:HB3	25:s:25:LYS:HG3	2.03	0.41
37:A:19:U:H2'	37:A:20:C:C6	2.56	0.41
37:A:552:G:H2'	37:A:553:G:C8	2.56	0.41
37:A:1188:A:H2'	37:A:1189:A:C8	2.56	0.41
37:A:1277:G:O2'	37:A:1278:A:O4'	2.32	0.41
43:G:138:ARG:O	43:G:141:THR:OG1	2.29	0.41
7:q:14:PRO:HB3	7:q:53:ILE:HG12	2.01	0.41
8:X:55:G:H2'	8:X:56:A:H8	1.86	0.41
8:X:662:U:H2'	8:X:663:G:C8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:757:C:H2'	8:X:758:A:C8	2.56	0.41
8:X:2021:G:N2	8:X:2025:C:O2'	2.54	0.41
8:X:2620:C:H2'	8:X:2621:G:H8	1.86	0.41
8:X:2778:A:H5'	14:d:3:ARG:HH22	1.85	0.41
10:Z:116:ILE:HD13	10:Z:116:ILE:HA	1.86	0.41
10:Z:144:ILE:HG21	10:Z:184:ILE:HD13	2.03	0.41
15:e:37:LEU:HD11	15:e:123:LEU:HB2	2.03	0.41
16:f:120:GLU:OE2	21:m:63:LYS:NZ	2.48	0.41
20:l:7:LYS:HE2	20:l:7:LYS:HB3	1.91	0.41
22:n:41:LYS:HA	22:n:41:LYS:HD3	1.84	0.41
37:A:181:G:H5''	37:A:182:U:H5	1.86	0.41
37:A:233:C:H2'	37:A:234:A:H8	1.85	0.41
37:A:332:G:OP1	56:T:17:ARG:NH2	2.54	0.41
37:A:837:A:H62	37:A:868:G:H21	1.68	0.41
37:A:848:G:H2'	37:A:849:G:C8	2.55	0.41
39:C:116:ALA:HB2	39:C:199:VAL:HG12	2.03	0.41
40:D:18:SER:OG	40:D:19:LEU:N	2.54	0.41
47:K:31:ASN:OD1	47:K:32:THR:N	2.53	0.41
48:L:81:PRO:HD2	48:L:112:ARG:HH21	1.85	0.41
49:M:59:ILE:HG23	49:M:60:ILE:HD12	2.03	0.41
51:O:33:THR:HG21	51:O:85:LEU:HD13	2.03	0.41
52:P:38:GLY:HA3	52:P:51:ILE:HA	2.03	0.41
3:W:138:G:N2	3:W:191:U:O2	2.45	0.41
8:X:461:C:H2'	8:X:462:A:H8	1.86	0.41
8:X:2048:U:OP2	31:O:6:ARG:NH2	2.52	0.41
8:X:2306:G:OP2	27:u:18:THR:OG1	2.39	0.41
12:b:142:ILE:HD13	12:b:142:ILE:HA	1.93	0.41
17:i:97:LEU:HD23	17:i:97:LEU:HA	1.89	0.41
27:u:80:PHE:HE1	27:u:86:LYS:HD3	1.85	0.41
37:A:98:U:O2'	37:A:99:A:O4'	2.37	0.41
37:A:724:A:H2'	37:A:725:A:C8	2.56	0.41
37:A:746:C:H2'	37:A:747:U:C6	2.56	0.41
37:A:1268:C:O2'	37:A:1292:C:O2	2.31	0.41
40:D:58:ARG:HH21	40:D:64:ASN:HA	1.86	0.41
44:H:32:LEU:HD12	44:H:32:LEU:HA	1.92	0.41
44:H:80:ILE:HD11	44:H:130:TYR:CG	2.56	0.41
10:Z:71:LYS:HG2	10:Z:74:ILE:HB	2.02	0.40
12:b:32:VAL:HG12	12:b:109:ALA:HB2	2.01	0.40
18:j:34:ILE:HB	18:j:118:LEU:HD12	2.02	0.40
37:A:1133:A:O2'	46:J:39:PRO:O	2.40	0.40
41:E:76:MET:HE1	41:E:120:VAL:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:52:U:O4	8:X:1113:A:N6	2.54	0.40
8:X:675:C:O2	8:X:685:U:O2'	2.40	0.40
14:d:24:THR:HG22	14:d:37:THR:HG23	2.02	0.40
15:e:33:VAL:HG13	15:e:55:VAL:HG11	2.02	0.40
32:1:12:CYS:SG	32:1:13:GLY:N	2.94	0.40
33:2:3:ARG:HA	33:2:3:ARG:HD3	1.75	0.40
37:A:432:G:H2'	37:A:433:A:H8	1.86	0.40
37:A:1053:G:H2'	37:A:1054:A:C8	2.56	0.40
42:F:16:GLU:OE1	42:F:20:LYS:NZ	2.33	0.40
43:G:76:LYS:HB3	43:G:76:LYS:HE2	1.87	0.40
8:X:47:C:O2	8:X:181:G:C2	2.71	0.40
8:X:1000:G:O6	8:X:1009:U:O2	2.39	0.40
8:X:1683:C:H5'	8:X:2739:C:H1'	2.02	0.40
10:Z:78:VAL:HG21	10:Z:110:ILE:HD11	2.03	0.40
32:1:31:GLU:HB3	32:1:44:LEU:HD11	2.02	0.40
37:A:1235:C:C5	49:M:103:LYS:HB3	2.55	0.40
37:A:1329:C:N3	55:S:36:ARG:HG2	2.36	0.40
44:H:48:ASP:HB3	44:H:63:PHE:HB2	2.02	0.40
48:L:95:ILE:HG12	48:L:110:ILE:HD13	2.04	0.40
4:g:60:GLY:O	4:g:64:MET:N	2.47	0.40
8:X:2901:G:H2'	8:X:2902:A:C8	2.57	0.40
8:X:2908:A:OP1	31:O:49:TYR:OH	2.28	0.40
9:Y:13:A:OP1	9:Y:105:A:O2'	2.39	0.40
20:l:19:ARG:HH12	20:l:30:ARG:CZ	2.35	0.40
24:r:21:MET:HA	24:r:24:ILE:HG22	2.02	0.40
37:A:587:C:O2'	37:A:737:A:N3	2.49	0.40
37:A:1070:U:H2'	37:A:1071:G:C8	2.56	0.40
37:A:1275:G:O2'	37:A:1277:G:O6	2.38	0.40
42:F:9:ILE:O	42:F:86:ILE:N	2.52	0.40
44:H:80:ILE:O	44:H:82:LYS:NZ	2.55	0.40
53:Q:30:TYR:HB2	53:Q:41:LYS:HA	2.04	0.40
4:g:261:ILE:O	4:g:262:ARG:C	2.65	0.40
6:p:4:ALA:O	6:p:7:THR:OG1	2.36	0.40
8:X:2448:U:OP1	34:3:41:LYS:NZ	2.40	0.40
13:c:161:ASN:HB3	20:l:1:MET:HG2	2.03	0.40
37:A:356:G:H2'	37:A:357:A:H8	1.86	0.40
37:A:461:C:OP1	52:P:72:ASN:ND2	2.54	0.40
37:A:787:G:H1'	47:K:123:CYS:HB2	2.03	0.40
37:A:1015:C:O2'	37:A:1048:A:O2'	2.35	0.40
38:B:204:ASP:N	38:B:204:ASP:OD1	2.53	0.40
40:D:112:GLN:HG3	40:D:116:HIS:NE2	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:E:32:ARG:HE	41:E:52:LYS:HE2	1.86	0.40
41:E:61:ARG:HA	41:E:64:VAL:HG12	2.02	0.40
53:Q:51:GLU:OE2	53:Q:51:GLU:N	2.52	0.40
56:T:31:ALA:O	56:T:35:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	g	399/447 (89%)	388 (97%)	10 (2%)	1 (0%)	36	65
5	h	39/96 (41%)	35 (90%)	2 (5%)	2 (5%)	1	11
6	p	121/166 (73%)	112 (93%)	6 (5%)	3 (2%)	4	24
7	q	131/141 (93%)	130 (99%)	1 (1%)	0	100	100
10	Z	270/277 (98%)	267 (99%)	3 (1%)	0	100	100
11	a	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
12	b	203/207 (98%)	199 (98%)	4 (2%)	0	100	100
13	c	174/179 (97%)	173 (99%)	1 (1%)	0	100	100
14	d	173/179 (97%)	170 (98%)	3 (2%)	0	100	100
15	e	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
16	f	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
17	i	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
18	j	133/144 (92%)	130 (98%)	3 (2%)	0	100	100
19	k	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
20	l	118/120 (98%)	118 (100%)	0	0	100	100
21	m	113/115 (98%)	113 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	n	115/119 (97%)	112 (97%)	2 (2%)	1 (1%)	14	43
23	o	99/102 (97%)	95 (96%)	4 (4%)	0	100	100
24	r	107/113 (95%)	101 (94%)	5 (5%)	1 (1%)	14	43
25	s	88/95 (93%)	88 (100%)	0	0	100	100
26	t	99/103 (96%)	95 (96%)	4 (4%)	0	100	100
27	u	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
28	v	56/62 (90%)	54 (96%)	2 (4%)	0	100	100
29	w	63/66 (96%)	63 (100%)	0	0	100	100
30	x	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
31	0	52/59 (88%)	50 (96%)	2 (4%)	0	100	100
32	1	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
33	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
34	3	62/66 (94%)	61 (98%)	1 (2%)	0	100	100
35	4	35/37 (95%)	35 (100%)	0	0	100	100
36	6	61/66 (92%)	60 (98%)	1 (2%)	0	100	100
38	B	216/246 (88%)	210 (97%)	6 (3%)	0	100	100
39	C	204/218 (94%)	202 (99%)	2 (1%)	0	100	100
40	D	193/200 (96%)	190 (98%)	3 (2%)	0	100	100
41	E	162/166 (98%)	160 (99%)	2 (1%)	0	100	100
42	F	90/95 (95%)	88 (98%)	2 (2%)	0	100	100
43	G	147/156 (94%)	145 (99%)	2 (1%)	0	100	100
44	H	129/132 (98%)	123 (95%)	5 (4%)	1 (1%)	16	46
45	I	123/130 (95%)	119 (97%)	4 (3%)	0	100	100
46	J	93/102 (91%)	90 (97%)	3 (3%)	0	100	100
47	K	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
48	L	134/138 (97%)	132 (98%)	2 (2%)	0	100	100
49	M	106/121 (88%)	102 (96%)	4 (4%)	0	100	100
50	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
51	O	83/89 (93%)	80 (96%)	3 (4%)	0	100	100
52	P	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
53	Q	82/87 (94%)	82 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R	62/79 (78%)	59 (95%)	3 (5%)	0	100	100
55	S	76/92 (83%)	75 (99%)	1 (1%)	0	100	100
56	T	81/88 (92%)	81 (100%)	0	0	100	100
All	All	5897/6367 (93%)	5764 (98%)	124 (2%)	9 (0%)	44	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	g	347	LEU
5	h	83	PRO
5	h	87	GLU
6	p	108	ILE
24	r	40	PRO
6	p	90	VAL
44	H	4	THR
22	n	92	ARG
6	p	113	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	g	4/381 (1%)	4 (100%)	0	100	100
5	h	3/85 (4%)	3 (100%)	0	100	100
6	p	105/139 (76%)	105 (100%)	0	100	100
7	q	103/110 (94%)	103 (100%)	0	100	100
10	Z	220/225 (98%)	220 (100%)	0	100	100
11	a	167/169 (99%)	167 (100%)	0	100	100
12	b	169/170 (99%)	168 (99%)	1 (1%)	78	81
13	c	151/154 (98%)	151 (100%)	0	100	100
14	d	148/151 (98%)	148 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	e	120/123 (98%)	120 (100%)	0	100	100
16	f	101/101 (100%)	101 (100%)	0	100	100
17	i	110/110 (100%)	110 (100%)	0	100	100
18	j	109/116 (94%)	109 (100%)	0	100	100
19	k	99/100 (99%)	99 (100%)	0	100	100
20	l	93/93 (100%)	93 (100%)	0	100	100
21	m	100/100 (100%)	100 (100%)	0	100	100
22	n	96/98 (98%)	96 (100%)	0	100	100
23	o	83/84 (99%)	83 (100%)	0	100	100
24	r	90/93 (97%)	90 (100%)	0	100	100
25	s	81/85 (95%)	81 (100%)	0	100	100
26	t	85/87 (98%)	85 (100%)	0	100	100
27	u	64/74 (86%)	64 (100%)	0	100	100
28	v	47/50 (94%)	47 (100%)	0	100	100
29	w	56/57 (98%)	50 (89%)	6 (11%)	6	25
30	x	52/53 (98%)	52 (100%)	0	100	100
31	0	48/53 (91%)	48 (100%)	0	100	100
32	1	46/47 (98%)	46 (100%)	0	100	100
33	2	39/39 (100%)	39 (100%)	0	100	100
34	3	54/56 (96%)	54 (100%)	0	100	100
35	4	35/35 (100%)	35 (100%)	0	100	100
36	6	53/55 (96%)	53 (100%)	0	100	100
38	B	189/212 (89%)	189 (100%)	0	100	100
39	C	168/178 (94%)	168 (100%)	0	100	100
40	D	169/173 (98%)	169 (100%)	0	100	100
41	E	128/130 (98%)	128 (100%)	0	100	100
42	F	81/84 (96%)	81 (100%)	0	100	100
43	G	125/132 (95%)	125 (100%)	0	100	100
44	H	111/112 (99%)	111 (100%)	0	100	100
45	I	98/102 (96%)	98 (100%)	0	100	100
46	J	86/92 (94%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	K	86/100 (86%)	86 (100%)	0	100	100
48	L	114/116 (98%)	114 (100%)	0	100	100
49	M	94/104 (90%)	94 (100%)	0	100	100
50	N	53/54 (98%)	53 (100%)	0	100	100
51	O	80/83 (96%)	80 (100%)	0	100	100
52	P	74/76 (97%)	74 (100%)	0	100	100
53	Q	77/80 (96%)	77 (100%)	0	100	100
54	R	56/64 (88%)	56 (100%)	0	100	100
55	S	70/81 (86%)	70 (100%)	0	100	100
56	T	66/70 (94%)	66 (100%)	0	100	100
All	All	4656/5336 (87%)	4649 (100%)	7 (0%)	85	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	b	82	GLN
29	w	19	LYS
29	w	21	LEU
29	w	22	LYS
29	w	24	GLU
29	w	25	LEU
29	w	28	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
6	p	73	ASN
10	Z	86	ASN
10	Z	153	GLN
10	Z	194	GLN
10	Z	226	ASN
11	a	19	ASN
11	a	43	ASN
11	a	120	GLN
11	a	152	ASN
11	a	168	GLN
12	b	29	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	c	27	GLN
13	c	135	GLN
14	d	20	ASN
14	d	23	ASN
14	d	59	GLN
15	e	78	HIS
17	i	70	ASN
18	j	46	GLN
23	o	45	ASN
26	t	53	GLN
29	w	27	ASN
33	2	26	ASN
34	3	38	GLN
38	B	24	ASN
38	B	59	ASN
38	B	226	GLN
39	C	101	ASN
42	F	33	ASN
43	G	19	ASN
43	G	28	ASN
44	H	68	GLN
46	J	56	HIS
48	L	42	GLN
50	N	19	GLN
51	O	18	HIS
54	R	57	GLN
55	S	23	ASN
56	T	34	GLN
56	T	41	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	76/77 (98%)	18 (23%)	0
2	V	7/8 (87%)	2 (28%)	0
3	W	265/266 (99%)	127 (47%)	2 (0%)
37	A	1532/1533 (99%)	433 (28%)	11 (0%)
8	X	2881/2887 (99%)	741 (25%)	25 (0%)
9	Y	111/112 (99%)	31 (27%)	2 (1%)
All	All	4872/4883 (99%)	1352 (27%)	40 (0%)

All (1352) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	8	U
1	U	16	U
1	U	17	U
1	U	18	G
1	U	38	C
1	U	42	G
1	U	46	G
1	U	47	U
1	U	48	C
1	U	49	G
1	U	51	G
1	U	55	U
1	U	56	C
1	U	57	G
1	U	59	G
1	U	60	U
1	U	61	C
1	U	76	A
2	V	14	G
2	V	15	A
3	W	6	C
3	W	11	U
3	W	14	G
3	W	16	G
3	W	20	A
3	W	21	G
3	W	24	A
3	W	25	G
3	W	26	C
3	W	30	G
3	W	35	G
3	W	36	U
3	W	37	A
3	W	38	C
3	W	40	U
3	W	44	A
3	W	45	U
3	W	46	C
3	W	47	C
3	W	49	C
3	W	51	C
3	W	52	U
3	W	54	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	W	55	C
3	W	61	C
3	W	62	G
3	W	63	A
3	W	64	A
3	W	65	U
3	W	68	C
3	W	70	U
3	W	71	C
3	W	74	G
3	W	76	G
3	W	79	U
3	W	80	C
3	W	81	G
3	W	83	U
3	W	84	U
3	W	85	A
3	W	88	U
3	W	94	C
3	W	95	C
3	W	98	C
3	W	103	A
3	W	104	G
3	W	108	G
3	W	111	G
3	W	113	G
3	W	115	U
3	W	116	G
3	W	117	A
3	W	118	C
3	W	120	U
3	W	126	U
3	W	127	C
3	W	128	C
3	W	130	G
3	W	132	G
3	W	133	C
3	W	134	A
3	W	135	A
3	W	136	U
3	W	139	G
3	W	142	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	W	145	A
3	W	148	A
3	W	149	A
3	W	150	C
3	W	151	C
3	W	153	U
3	W	154	G
3	W	156	C
3	W	157	A
3	W	159	G
3	W	164	G
3	W	165	A
3	W	166	A
3	W	167	G
3	W	170	A
3	W	171	G
3	W	172	C
3	W	173	A
3	W	174	G
3	W	177	U
3	W	180	A
3	W	181	G
3	W	185	A
3	W	187	C
3	W	195	G
3	W	198	C
3	W	200	G
3	W	204	G
3	W	205	G
3	W	207	U
3	W	208	G
3	W	209	C
3	W	210	C
3	W	211	U
3	W	213	G
3	W	214	G
3	W	215	C
3	W	222	A
3	W	223	A
3	W	228	U
3	W	230	A
3	W	231	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	W	235	A
3	W	236	C
3	W	237	G
3	W	238	C
3	W	239	U
3	W	241	G
3	W	242	G
3	W	243	G
3	W	245	A
3	W	246	G
3	W	249	A
3	W	250	A
3	W	254	A
3	W	255	C
3	W	256	A
3	W	257	G
3	W	258	A
3	W	260	G
3	W	263	G
3	W	268	G
8	X	4	U
8	X	5	A
8	X	11	G
8	X	15	G
8	X	19	G
8	X	27	G
8	X	34	U
8	X	35	G
8	X	36	G
8	X	46	C
8	X	49	A
8	X	58	G
8	X	60	G
8	X	61	A
8	X	62	C
8	X	63	G
8	X	71	A
8	X	74	U
8	X	75	G
8	X	76	C
8	X	77	U
8	X	78	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	84	A
8	X	85	G
8	X	86	C
8	X	91	A
8	X	92	G
8	X	93	C
8	X	94	A
8	X	95	A
8	X	96	G
8	X	100	U
8	X	101	G
8	X	106	G
8	X	117	A
8	X	118	A
8	X	119	U
8	X	122	G
8	X	124	A
8	X	125	A
8	X	126	A
8	X	127	C
8	X	130	A
8	X	140	A
8	X	150	A
8	X	160	G
8	X	162	A
8	X	164	U
8	X	165	C
8	X	169	G
8	X	175	G
8	X	176	A
8	X	177	G
8	X	178	A
8	X	179	A
8	X	183	A
8	X	184	G
8	X	189	G
8	X	199	A
8	X	200	A
8	X	202	A
8	X	204	C
8	X	207	A
8	X	216	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	218	G
8	X	219	A
8	X	224	A
8	X	225	A
8	X	226	A
8	X	229	A
8	X	231	A
8	X	232	U
8	X	233	G
8	X	234	C
8	X	236	A
8	X	244	A
8	X	251	G
8	X	252	C
8	X	253	G
8	X	258	A
8	X	264	G
8	X	268	A
8	X	270	C
8	X	272	C
8	X	275	A
8	X	276	C
8	X	279	A
8	X	282	G
8	X	284	C
8	X	286	U
8	X	287	G
8	X	288	C
8	X	291	C
8	X	294	G
8	X	295	G
8	X	296	G
8	X	297	G
8	X	298	U
8	X	302	A
8	X	305	A
8	X	306	C
8	X	307	A
8	X	308	C
8	X	309	U
8	X	310	C
8	X	329	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	330	A
8	X	332	G
8	X	334	G
8	X	336	U
8	X	337	A
8	X	338	G
8	X	345	A
8	X	346	G
8	X	355	A
8	X	366	A
8	X	367	G
8	X	373	A
8	X	374	A
8	X	376	A
8	X	379	C
8	X	389	A
8	X	395	C
8	X	396	G
8	X	397	U
8	X	399	C
8	X	407	A
8	X	410	G
8	X	411	G
8	X	412	A
8	X	417	G
8	X	418	A
8	X	419	G
8	X	430	C
8	X	433	G
8	X	434	U
8	X	442	C
8	X	448	A
8	X	451	C
8	X	452	C
8	X	453	G
8	X	458	G
8	X	459	A
8	X	467	C
8	X	471	G
8	X	487	G
8	X	491	C
8	X	495	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	499	G
8	X	502	C
8	X	504	A
8	X	514	G
8	X	528	G
8	X	537	A
8	X	548	A
8	X	550	G
8	X	551	A
8	X	552	G
8	X	554	U
8	X	555	C
8	X	556	C
8	X	557	U
8	X	558	G
8	X	564	G
8	X	568	G
8	X	573	C
8	X	574	A
8	X	575	A
8	X	576	G
8	X	577	U
8	X	578	A
8	X	590	U
8	X	592	A
8	X	593	A
8	X	594	C
8	X	595	G
8	X	607	G
8	X	617	G
8	X	619	A
8	X	644	G
8	X	646	A
8	X	647	A
8	X	648	G
8	X	673	A
8	X	680	G
8	X	683	A
8	X	684	G
8	X	691	U
8	X	697	G
8	X	698	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	699	A
8	X	700	U
8	X	701	G
8	X	702	A
8	X	715	A
8	X	716	G
8	X	717	A
8	X	718	C
8	X	729	G
8	X	733	U
8	X	762	A
8	X	763	A
8	X	766	C
8	X	777	C
8	X	785	C
8	X	787	C
8	X	788	G
8	X	794	U
8	X	795	G
8	X	809	U
8	X	810	G
8	X	811	A
8	X	812	G
8	X	822	G
8	X	823	G
8	X	824	G
8	X	829	A
8	X	830	A
8	X	831	U
8	X	832	G
8	X	837	U
8	X	840	A
8	X	847	A
8	X	852	G
8	X	858	U
8	X	859	C
8	X	866	A
8	X	874	U
8	X	875	U
8	X	892	U
8	X	893	A
8	X	904	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	906	G
8	X	913	A
8	X	923	C
8	X	924	U
8	X	929	G
8	X	930	C
8	X	933	C
8	X	934	U
8	X	935	A
8	X	936	C
8	X	937	C
8	X	940	G
8	X	943	A
8	X	949	U
8	X	957	A
8	X	959	C
8	X	964	A
8	X	980	C
8	X	987	A
8	X	991	A
8	X	992	G
8	X	996	G
8	X	999	A
8	X	1007	G
8	X	1019	A
8	X	1020	A
8	X	1029	A
8	X	1042	A
8	X	1049	G
8	X	1051	C
8	X	1058	U
8	X	1059	A
8	X	1062	C
8	X	1063	G
8	X	1068	G
8	X	1069	U
8	X	1072	A
8	X	1073	A
8	X	1079	U
8	X	1088	G
8	X	1091	U
8	X	1093	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	1102	G
8	X	1106	U
8	X	1108	G
8	X	1109	G
8	X	1113	A
8	X	1114	G
8	X	1116	A
8	X	1118	C
8	X	1119	A
8	X	1121	C
8	X	1122	C
8	X	1123	A
8	X	1124	C
8	X	1126	A
8	X	1127	U
8	X	1130	A
8	X	1131	A
8	X	1134	A
8	X	1136	U
8	X	1138	C
8	X	1139	G
8	X	1140	U
8	X	1141	A
8	X	1143	U
8	X	1144	A
8	X	1145	G
8	X	1146	C
8	X	1147	U
8	X	1148	C
8	X	1157	A
8	X	1158	G
8	X	1159	U
8	X	1160	G
8	X	1161	A
8	X	1172	A
8	X	1173	A
8	X	1174	A
8	X	1177	G
8	X	1178	U
8	X	1179	A
8	X	1180	C
8	X	1181	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	1182	G
8	X	1185	G
8	X	1187	U
8	X	1188	A
8	X	1202	A
8	X	1214	U
8	X	1216	C
8	X	1227	G
8	X	1236	G
8	X	1244	A
8	X	1248	C
8	X	1249	U
8	X	1251	U
8	X	1260	A
8	X	1272	G
8	X	1276	G
8	X	1277	A
8	X	1278	G
8	X	1280	G
8	X	1287	A
8	X	1293	A
8	X	1295	U
8	X	1296	G
8	X	1297	C
8	X	1311	G
8	X	1312	A
8	X	1314	A
8	X	1315	G
8	X	1339	A
8	X	1340	A
8	X	1353	C
8	X	1364	C
8	X	1366	C
8	X	1368	U
8	X	1369	C
8	X	1371	G
8	X	1380	U
8	X	1383	U
8	X	1387	G
8	X	1388	A
8	X	1389	C
8	X	1391	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	1401	C
8	X	1404	A
8	X	1417	A
8	X	1418	U
8	X	1425	C
8	X	1426	A
8	X	1427	G
8	X	1434	A
8	X	1435	U
8	X	1442	A
8	X	1450	C
8	X	1452	C
8	X	1453	A
8	X	1458	U
8	X	1460	G
8	X	1461	A
8	X	1464	A
8	X	1465	A
8	X	1466	U
8	X	1473	A
8	X	1474	C
8	X	1476	C
8	X	1481	G
8	X	1485	A
8	X	1489	U
8	X	1490	A
8	X	1499	A
8	X	1500	U
8	X	1507	U
8	X	1508	C
8	X	1514	C
8	X	1515	C
8	X	1516	A
8	X	1525	G
8	X	1526	G
8	X	1528	U
8	X	1529	G
8	X	1536	A
8	X	1537	G
8	X	1539	C
8	X	1540	A
8	X	1543	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	1552	C
8	X	1553	A
8	X	1557	G
8	X	1559	C
8	X	1563	G
8	X	1566	G
8	X	1568	G
8	X	1569	A
8	X	1601	A
8	X	1602	U
8	X	1615	A
8	X	1617	A
8	X	1621	G
8	X	1626	U
8	X	1631	A
8	X	1632	G
8	X	1653	A
8	X	1655	A
8	X	1661	A
8	X	1672	A
8	X	1676	G
8	X	1684	U
8	X	1692	U
8	X	1693	C
8	X	1694	G
8	X	1696	G
8	X	1705	C
8	X	1708	U
8	X	1717	C
8	X	1719	G
8	X	1738	U
8	X	1739	C
8	X	1741	G
8	X	1743	A
8	X	1745	A
8	X	1748	G
8	X	1757	G
8	X	1758	U
8	X	1759	U
8	X	1760	A
8	X	1765	G
8	X	1767	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	1774	A
8	X	1776	A
8	X	1779	G
8	X	1785	G
8	X	1792	G
8	X	1793	G
8	X	1802	A
8	X	1803	C
8	X	1810	G
8	X	1811	C
8	X	1828	G
8	X	1829	C
8	X	1830	G
8	X	1831	A
8	X	1832	A
8	X	1838	A
8	X	1841	G
8	X	1844	A
8	X	1845	A
8	X	1846	G
8	X	1848	A
8	X	1858	A
8	X	1877	A
8	X	1882	A
8	X	1883	A
8	X	1884	G
8	X	1887	G
8	X	1888	A
8	X	1899	U
8	X	1910	G
8	X	1914	A
8	X	1923	C
8	X	1925	A
8	X	1930	A
8	X	1935	G
8	X	1942	A
8	X	1943	C
8	X	1944	U
8	X	1948	A
8	X	1958	G
8	X	1959	G
8	X	1965	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	1967	A
8	X	1970	C
8	X	1971	C
8	X	1972	U
8	X	1984	U
8	X	1992	C
8	X	1993	G
8	X	1995	A
8	X	1996	C
8	X	1999	A
8	X	2000	A
8	X	2001	G
8	X	2020	U
8	X	2022	U
8	X	2025	C
8	X	2026	A
8	X	2050	G
8	X	2051	U
8	X	2052	A
8	X	2054	C
8	X	2060	A
8	X	2061	G
8	X	2062	A
8	X	2063	U
8	X	2064	G
8	X	2065	C
8	X	2068	G
8	X	2072	C
8	X	2078	A
8	X	2081	G
8	X	2084	C
8	X	2085	G
8	X	2088	A
8	X	2089	A
8	X	2090	G
8	X	2096	G
8	X	2097	U
8	X	2098	G
8	X	2121	U
8	X	2122	G
8	X	2123	A
8	X	2128	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	2129	G
8	X	2131	U
8	X	2132	A
8	X	2133	C
8	X	2134	A
8	X	2135	G
8	X	2138	U
8	X	2139	G
8	X	2140	U
8	X	2141	A
8	X	2143	A
8	X	2144	G
8	X	2145	G
8	X	2148	A
8	X	2149	G
8	X	2151	U
8	X	2152	A
8	X	2153	G
8	X	2154	G
8	X	2155	A
8	X	2157	C
8	X	2158	C
8	X	2159	U
8	X	2160	U
8	X	2161	G
8	X	2163	A
8	X	2165	A
8	X	2166	C
8	X	2168	G
8	X	2169	G
8	X	2171	G
8	X	2174	C
8	X	2175	C
8	X	2176	A
8	X	2179	U
8	X	2181	C
8	X	2186	G
8	X	2187	A
8	X	2190	C
8	X	2193	C
8	X	2194	G
8	X	2195	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	2199	G
8	X	2200	A
8	X	2201	U
8	X	2203	C
8	X	2204	U
8	X	2205	A
8	X	2206	C
8	X	2208	C
8	X	2210	G
8	X	2216	A
8	X	2217	U
8	X	2218	U
8	X	2222	C
8	X	2223	U
8	X	2227	A
8	X	2232	G
8	X	2233	C
8	X	2245	G
8	X	2246	G
8	X	2254	A
8	X	2267	G
8	X	2268	G
8	X	2272	U
8	X	2295	A
8	X	2297	A
8	X	2308	G
8	X	2312	C
8	X	2315	A
8	X	2316	A
8	X	2317	A
8	X	2318	G
8	X	2332	G
8	X	2334	U
8	X	2335	U
8	X	2336	G
8	X	2339	A
8	X	2340	A
8	X	2341	U
8	X	2348	C
8	X	2349	A
8	X	2350	G
8	X	2351	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	2356	A
8	X	2363	C
8	X	2364	A
8	X	2374	G
8	X	2376	C
8	X	2379	C
8	X	2387	A
8	X	2400	G
8	X	2408	G
8	X	2412	G
8	X	2414	C
8	X	2415	U
8	X	2418	G
8	X	2419	U
8	X	2420	G
8	X	2431	U
8	X	2432	C
8	X	2435	C
8	X	2451	C
8	X	2453	C
8	X	2454	A
8	X	2457	G
8	X	2458	G
8	X	2459	A
8	X	2460	U
8	X	2468	A
8	X	2469	C
8	X	2470	C
8	X	2474	G
8	X	2477	A
8	X	2494	C
8	X	2505	A
8	X	2507	A
8	X	2513	G
8	X	2527	C
8	X	2531	G
8	X	2532	A
8	X	2533	U
8	X	2534	G
8	X	2542	A
8	X	2547	A
8	X	2548	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	2554	G
8	X	2558	G
8	X	2560	A
8	X	2561	G
8	X	2563	C
8	X	2564	G
8	X	2571	A
8	X	2583	U
8	X	2584	U
8	X	2585	C
8	X	2595	A
8	X	2596	G
8	X	2602	C
8	X	2605	G
8	X	2611	G
8	X	2626	G
8	X	2628	G
8	X	2630	C
8	X	2631	A
8	X	2632	G
8	X	2637	G
8	X	2638	U
8	X	2640	C
8	X	2642	U
8	X	2644	U
8	X	2659	G
8	X	2661	A
8	X	2663	A
8	X	2670	A
8	X	2674	G
8	X	2675	C
8	X	2689	A
8	X	2690	G
8	X	2711	G
8	X	2714	G
8	X	2718	U
8	X	2719	A
8	X	2720	C
8	X	2743	G
8	X	2753	U
8	X	2755	U
8	X	2762	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	2764	G
8	X	2773	G
8	X	2777	A
8	X	2781	C
8	X	2785	U
8	X	2790	A
8	X	2793	A
8	X	2794	A
8	X	2795	G
8	X	2805	A
8	X	2806	G
8	X	2807	A
8	X	2808	U
8	X	2818	C
8	X	2819	A
8	X	2820	U
8	X	2822	C
8	X	2824	G
8	X	2826	A
8	X	2827	A
8	X	2830	A
8	X	2831	A
8	X	2837	A
8	X	2843	G
8	X	2845	A
8	X	2849	U
8	X	2850	G
8	X	2859	G
8	X	2860	A
8	X	2868	G
8	X	2873	G
8	X	2886	C
8	X	2891	G
8	X	2892	G
8	X	2893	A
8	X	2897	G
8	X	2898	A
8	X	2901	G
8	X	2905	C
8	X	2906	U
8	X	2908	A
8	X	2911	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	X	2916	A
8	X	2918	G
8	X	2919	A
8	X	2920	C
8	X	2925	C
9	Y	11	A
9	Y	12	U
9	Y	17	A
9	Y	18	A
9	Y	22	G
9	Y	23	U
9	Y	33	U
9	Y	34	C
9	Y	36	C
9	Y	39	A
9	Y	40	C
9	Y	41	C
9	Y	42	G
9	Y	49	G
9	Y	53	U
9	Y	54	U
9	Y	64	A
9	Y	65	G
9	Y	71	A
9	Y	75	U
9	Y	85	U
9	Y	86	U
9	Y	87	U
9	Y	88	C
9	Y	94	G
9	Y	97	A
9	Y	100	G
9	Y	101	U
9	Y	107	G
9	Y	108	C
9	Y	112	C
37	A	11	G
37	A	32	C
37	A	33	G
37	A	34	A
37	A	49	C
37	A	50	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	52	A
37	A	53	A
37	A	62	A
37	A	72	A
37	A	74	A
37	A	77	U
37	A	78	G
37	A	82	G
37	A	83	C
37	A	84	U
37	A	85	U
37	A	86	G
37	A	88	U
37	A	89	C
37	A	90	C
37	A	92	U
37	A	94	A
37	A	95	U
37	A	96	G
37	A	99	A
37	A	100	G
37	A	119	C
37	A	128	A
37	A	130	C
37	A	135	C
37	A	139	A
37	A	143	C
37	A	147	G
37	A	151	A
37	A	156	G
37	A	157	G
37	A	158	G
37	A	162	C
37	A	166	G
37	A	169	U
37	A	170	A
37	A	177	G
37	A	179	U
37	A	180	G
37	A	181	G
37	A	184	G
37	A	188	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	189	A
37	A	190	A
37	A	195	A
37	A	197	G
37	A	206	A
37	A	207	U
37	A	209	A
37	A	210	A
37	A	213	G
37	A	215	G
37	A	219	U
37	A	220	C
37	A	221	G
37	A	222	G
37	A	224	U
37	A	225	A
37	A	230	U
37	A	231	U
37	A	232	A
37	A	233	C
37	A	248	C
37	A	253	U
37	A	255	G
37	A	258	A
37	A	259	G
37	A	260	U
37	A	262	G
37	A	265	G
37	A	268	G
37	A	269	U
37	A	271	A
37	A	274	G
37	A	275	C
37	A	276	U
37	A	277	C
37	A	278	A
37	A	279	C
37	A	282	A
37	A	283	G
37	A	287	A
37	A	288	C
37	A	297	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	301	A
37	A	309	G
37	A	329	A
37	A	335	A
37	A	336	C
37	A	337	A
37	A	338	C
37	A	340	G
37	A	352	A
37	A	353	C
37	A	359	G
37	A	360	C
37	A	362	G
37	A	371	A
37	A	373	U
37	A	375	U
37	A	380	C
37	A	392	G
37	A	397	A
37	A	398	C
37	A	400	G
37	A	406	C
37	A	414	G
37	A	417	U
37	A	419	A
37	A	420	U
37	A	421	G
37	A	422	A
37	A	429	U
37	A	430	C
37	A	431	G
37	A	432	G
37	A	436	G
37	A	437	U
37	A	438	A
37	A	440	A
37	A	442	C
37	A	446	G
37	A	447	U
37	A	448	U
37	A	449	G
37	A	451	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	455	G
37	A	456	A
37	A	460	A
37	A	461	C
37	A	462	A
37	A	463	A
37	A	465	U
37	A	466	G
37	A	467	C
37	A	469	G
37	A	474	A
37	A	475	A
37	A	476	U
37	A	477	A
37	A	478	G
37	A	480	G
37	A	481	C
37	A	482	G
37	A	483	G
37	A	484	U
37	A	485	A
37	A	487	C
37	A	488	U
37	A	490	G
37	A	491	A
37	A	493	G
37	A	494	G
37	A	495	U
37	A	500	A
37	A	501	A
37	A	502	C
37	A	505	G
37	A	506	A
37	A	514	G
37	A	520	C
37	A	522	A
37	A	527	C
37	A	530	G
37	A	533	G
37	A	534	C
37	A	536	G
37	A	540	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	541	A
37	A	556	A
37	A	568	A
37	A	571	U
37	A	573	U
37	A	574	U
37	A	575	G
37	A	581	A
37	A	582	A
37	A	583	A
37	A	585	G
37	A	586	G
37	A	588	U
37	A	591	C
37	A	597	G
37	A	605	A
37	A	619	G
37	A	628	U
37	A	629	C
37	A	630	A
37	A	631	A
37	A	634	G
37	A	638	A
37	A	639	G
37	A	641	G
37	A	642	U
37	A	643	C
37	A	662	U
37	A	674	A
37	A	695	U
37	A	696	A
37	A	729	C
37	A	730	A
37	A	732	U
37	A	740	G
37	A	742	G
37	A	743	A
37	A	751	G
37	A	757	A
37	A	758	A
37	A	763	C
37	A	764	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	790	A
37	A	796	A
37	A	801	A
37	A	802	U
37	A	803	A
37	A	808	G
37	A	818	G
37	A	823	A
37	A	824	A
37	A	826	C
37	A	828	A
37	A	829	U
37	A	830	G
37	A	837	A
37	A	841	G
37	A	845	G
37	A	849	G
37	A	850	U
37	A	852	U
37	A	853	C
37	A	855	G
37	A	856	C
37	A	861	U
37	A	865	G
37	A	874	A
37	A	875	A
37	A	877	G
37	A	882	A
37	A	899	A
37	A	910	A
37	A	924	A
37	A	926	G
37	A	936	G
37	A	944	C
37	A	945	A
37	A	954	G
37	A	955	G
37	A	968	A
37	A	970	U
37	A	971	U
37	A	977	C
37	A	978	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	979	A
37	A	981	G
37	A	984	A
37	A	985	A
37	A	986	G
37	A	987	A
37	A	990	C
37	A	991	U
37	A	992	U
37	A	993	A
37	A	1002	U
37	A	1003	G
37	A	1006	A
37	A	1012	U
37	A	1013	G
37	A	1014	A
37	A	1019	C
37	A	1022	A
37	A	1023	G
37	A	1024	A
37	A	1025	G
37	A	1028	A
37	A	1031	A
37	A	1033	G
37	A	1034	U
37	A	1035	C
37	A	1036	C
37	A	1039	U
37	A	1041	C
37	A	1046	G
37	A	1048	A
37	A	1055	C
37	A	1058	G
37	A	1059	U
37	A	1060	G
37	A	1063	G
37	A	1064	C
37	A	1065	A
37	A	1067	G
37	A	1074	G
37	A	1076	C
37	A	1095	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	1096	U
37	A	1104	G
37	A	1105	U
37	A	1108	C
37	A	1109	G
37	A	1110	C
37	A	1111	A
37	A	1128	A
37	A	1134	G
37	A	1135	U
37	A	1136	U
37	A	1137	G
37	A	1139	C
37	A	1145	U
37	A	1146	C
37	A	1148	G
37	A	1149	U
37	A	1150	U
37	A	1151	G
37	A	1152	G
37	A	1155	A
37	A	1158	C
37	A	1165	G
37	A	1166	A
37	A	1167	C
37	A	1168	U
37	A	1169	G
37	A	1170	C
37	A	1176	A
37	A	1177	C
37	A	1185	A
37	A	1186	G
37	A	1187	G
37	A	1188	A
37	A	1192	U
37	A	1193	G
37	A	1205	A
37	A	1206	A
37	A	1210	A
37	A	1211	U
37	A	1215	G
37	A	1216	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	1220	U
37	A	1221	U
37	A	1222	A
37	A	1223	U
37	A	1224	G
37	A	1233	U
37	A	1235	C
37	A	1237	C
37	A	1247	A
37	A	1249	U
37	A	1250	G
37	A	1256	A
37	A	1257	A
37	A	1260	A
37	A	1261	A
37	A	1264	G
37	A	1265	C
37	A	1266	A
37	A	1267	G
37	A	1269	G
37	A	1277	G
37	A	1283	A
37	A	1284	A
37	A	1289	A
37	A	1290	U
37	A	1295	C
37	A	1296	A
37	A	1299	U
37	A	1305	C
37	A	1307	C
37	A	1308	A
37	A	1311	U
37	A	1314	G
37	A	1317	C
37	A	1329	C
37	A	1331	C
37	A	1332	G
37	A	1337	C
37	A	1340	G
37	A	1344	C
37	A	1345	U
37	A	1349	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	1354	U
37	A	1355	A
37	A	1356	G
37	A	1357	U
37	A	1362	G
37	A	1364	G
37	A	1373	U
37	A	1380	G
37	A	1383	A
37	A	1384	A
37	A	1386	A
37	A	1387	C
37	A	1388	G
37	A	1410	G
37	A	1414	G
37	A	1428	G
37	A	1435	A
37	A	1439	C
37	A	1443	A
37	A	1445	U
37	A	1446	C
37	A	1447	G
37	A	1448	G
37	A	1449	U
37	A	1451	A
37	A	1453	G
37	A	1455	A
37	A	1463	A
37	A	1464	G
37	A	1465	G
37	A	1466	A
37	A	1468	C
37	A	1472	C
37	A	1473	C
37	A	1474	G
37	A	1481	G
37	A	1485	G
37	A	1497	G
37	A	1500	U
37	A	1503	A
37	A	1504	G
37	A	1507	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	1512	A
37	A	1513	A
37	A	1515	G
37	A	1516	U
37	A	1529	A
37	A	1539	G
37	A	1540	G

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	W	63	A
3	W	259	A
8	X	62	C
8	X	125	A
8	X	164	U
8	X	252	C
8	X	307	A
8	X	396	G
8	X	441	C
8	X	450	U
8	X	549	A
8	X	831	U
8	X	1028	C
8	X	1176	U
8	X	1294	A
8	X	1451	U
8	X	1507	U
8	X	1525	G
8	X	1567	U
8	X	1671	G
8	X	1876	A
8	X	1882	A
8	X	2192	U
8	X	2459	A
8	X	2468	A
8	X	2805	A
8	X	2904	A
9	Y	33	U
9	Y	48	G
37	A	260	U
37	A	372	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	A	437	U
37	A	455	G
37	A	484	U
37	A	630	A
37	A	848	G
37	A	855	G
37	A	1157	U
37	A	1463	A
37	A	1480	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
57	G4P	g	501	-	36,38,38	3.12	16 (44%)	56,61,61	1.57	12 (21%)

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
57	G4P	g	501	-	-	2/27/43/43	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	g	501	G4P	O4'-C1'	8.91	1.62	1.42
57	g	501	G4P	C2'-C1'	-7.08	1.31	1.53
57	g	501	G4P	C4-N3	6.41	1.48	1.34
57	g	501	G4P	O4'-C4'	-5.84	1.32	1.45
57	g	501	G4P	C2-N3	5.09	1.45	1.33
57	g	501	G4P	C2-N2	4.75	1.45	1.34
57	g	501	G4P	PC-O3C	4.57	1.64	1.59
57	g	501	G4P	PA-O3A	3.01	1.62	1.59
57	g	501	G4P	C5-N7	-2.84	1.33	1.39
57	g	501	G4P	O2'-C2'	2.81	1.49	1.43
57	g	501	G4P	C5-C6	2.72	1.54	1.44
57	g	501	G4P	O6-C6	-2.45	1.18	1.23
57	g	501	G4P	C2-N1	2.39	1.43	1.37
57	g	501	G4P	O3'-C3'	-2.29	1.36	1.44
57	g	501	G4P	C6-N1	2.17	1.42	1.38
57	g	501	G4P	PC-O3'	2.05	1.65	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	g	501	G4P	C5-C4-N3	-5.23	120.06	128.39
57	g	501	G4P	C2-N3-C4	4.71	120.42	112.30
57	g	501	G4P	N9-C8-N7	-2.75	108.31	113.40
57	g	501	G4P	N9-C4-N3	2.58	131.11	125.95
57	g	501	G4P	C2-N1-C6	-2.44	120.68	125.11
57	g	501	G4P	C1'-N9-C4	-2.34	119.58	126.49
57	g	501	G4P	C8-N7-C5	2.28	108.32	104.26
57	g	501	G4P	C5-C6-N1	2.28	119.05	113.25
57	g	501	G4P	C4-C5-N7	-2.22	107.15	110.67
57	g	501	G4P	C1'-N9-C8	2.21	133.02	126.73
57	g	501	G4P	O3'-PC-O1C	2.08	116.47	109.81
57	g	501	G4P	C3'-C2'-C1'	2.05	104.40	99.89

There are no chirality outliers.

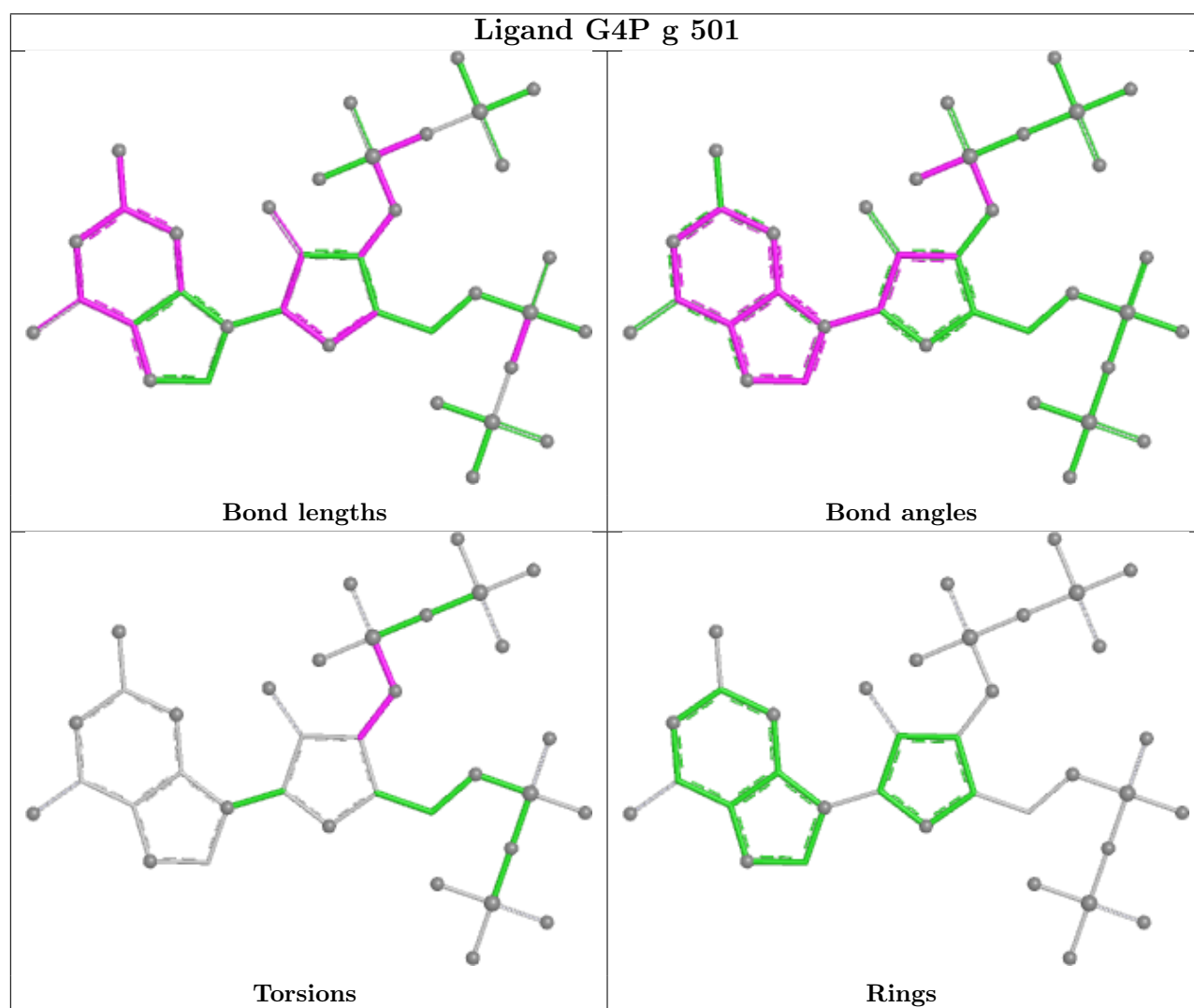
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	g	501	G4P	C4'-C3'-O3'-PC
57	g	501	G4P	C3'-O3'-PC-O2C

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	X	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	399:C	O3'	406:G	P	23.95
1	X	1577:C	O3'	1589:G	P	17.01
1	X	1553:A	O3'	1555:A	P	7.39

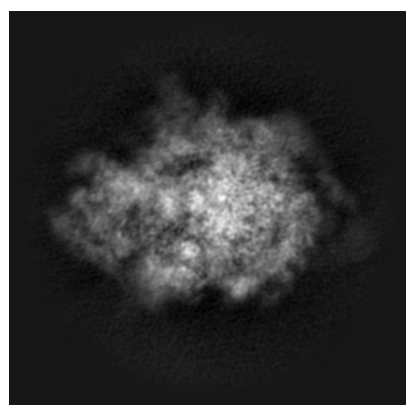
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12734. These allow visual inspection of the internal detail of the map and identification of artifacts.

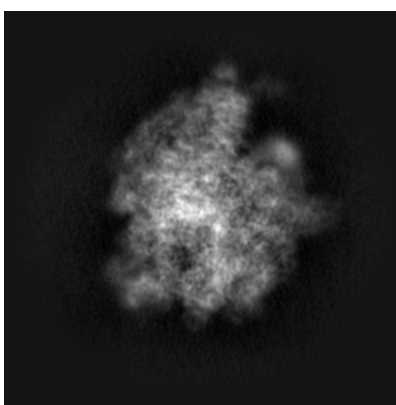
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

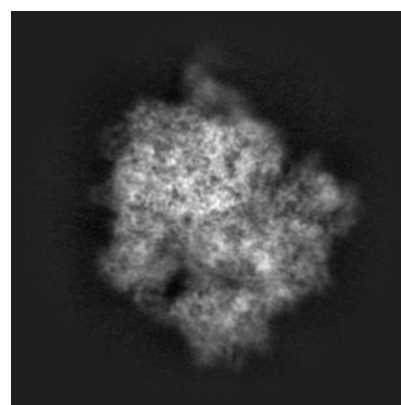
6.1.1 Primary map



X



Y

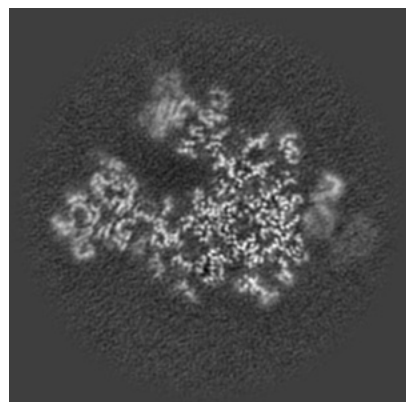


Z

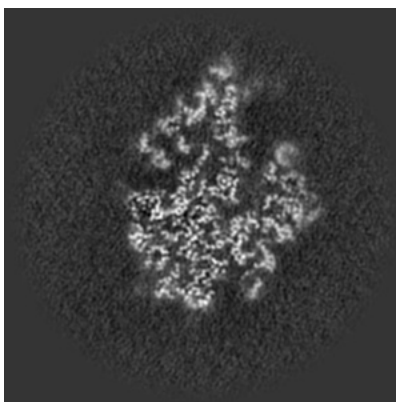
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

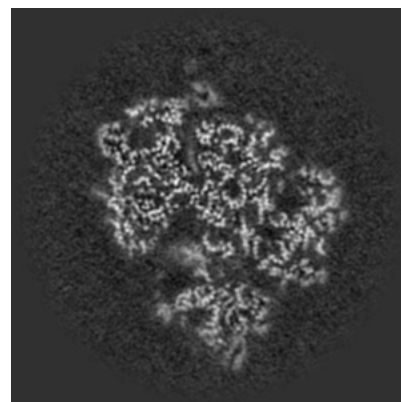
6.2.1 Primary map



X Index: 180



Y Index: 180

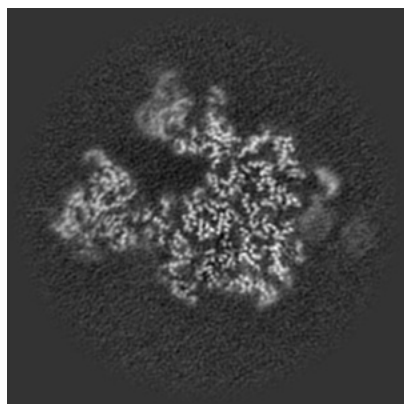


Z Index: 180

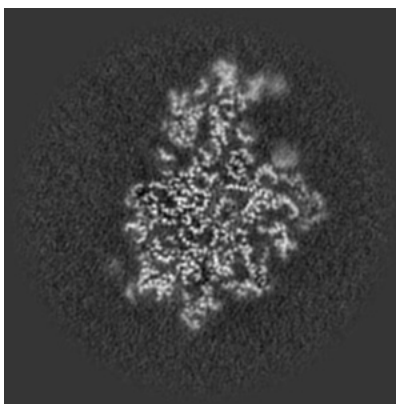
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

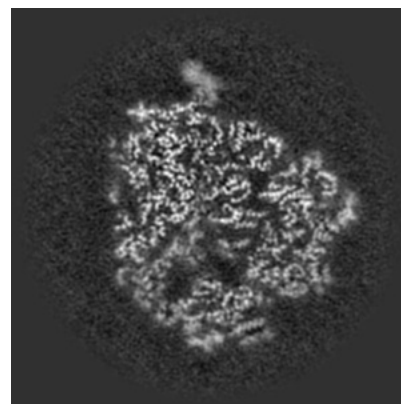
6.3.1 Primary map



X Index: 185



Y Index: 189

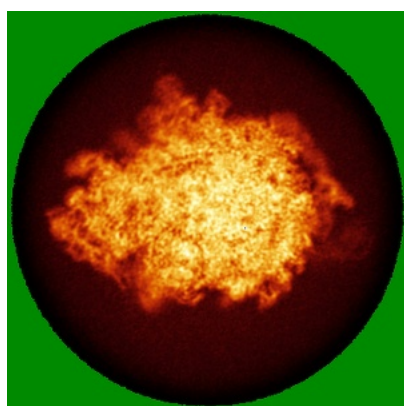


Z Index: 191

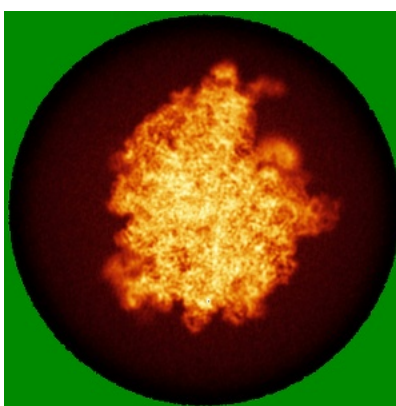
The images above show the largest variance slices of the map in three orthogonal directions.

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

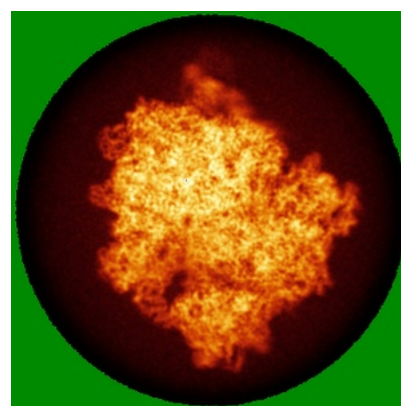
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.479. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

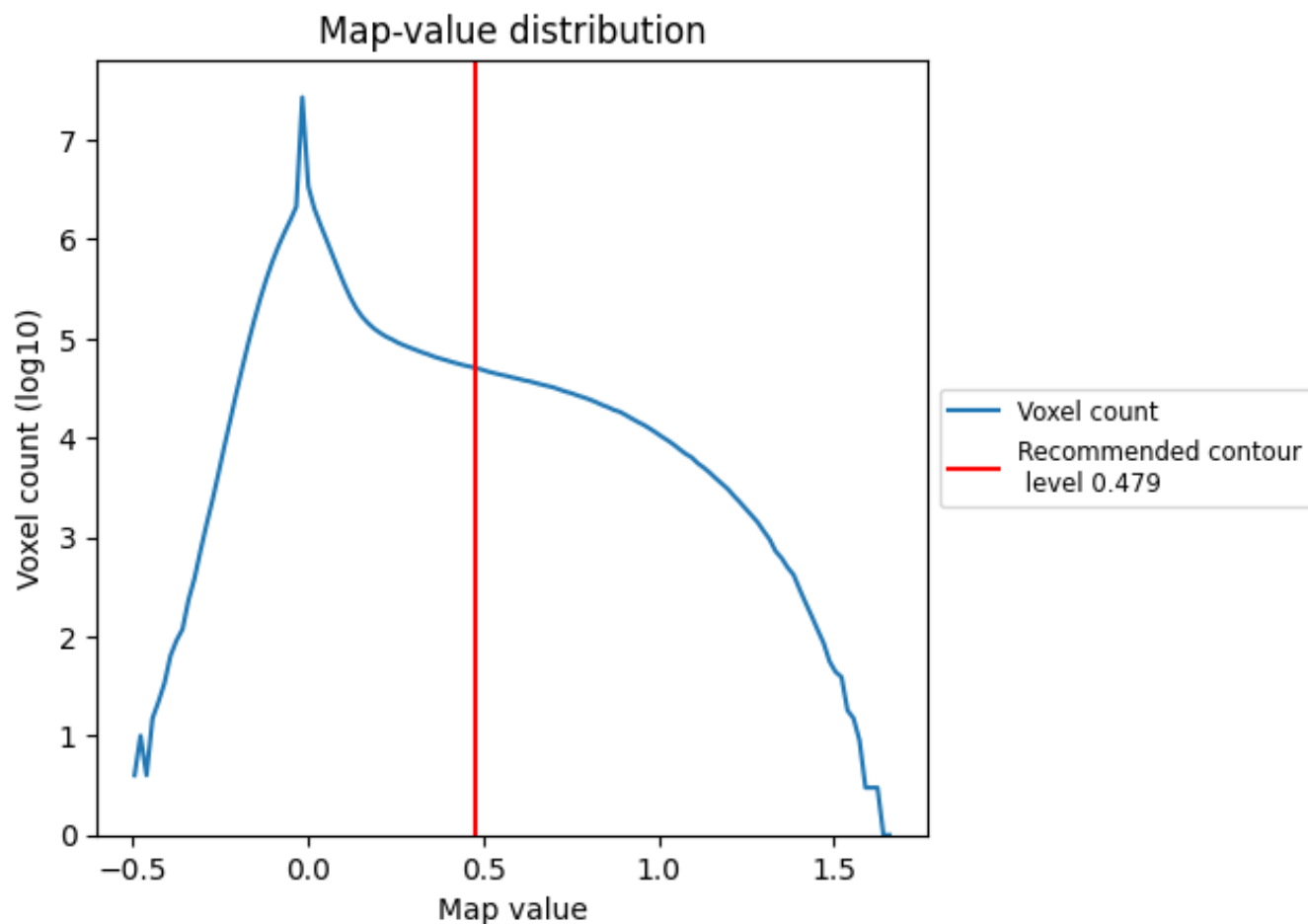
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

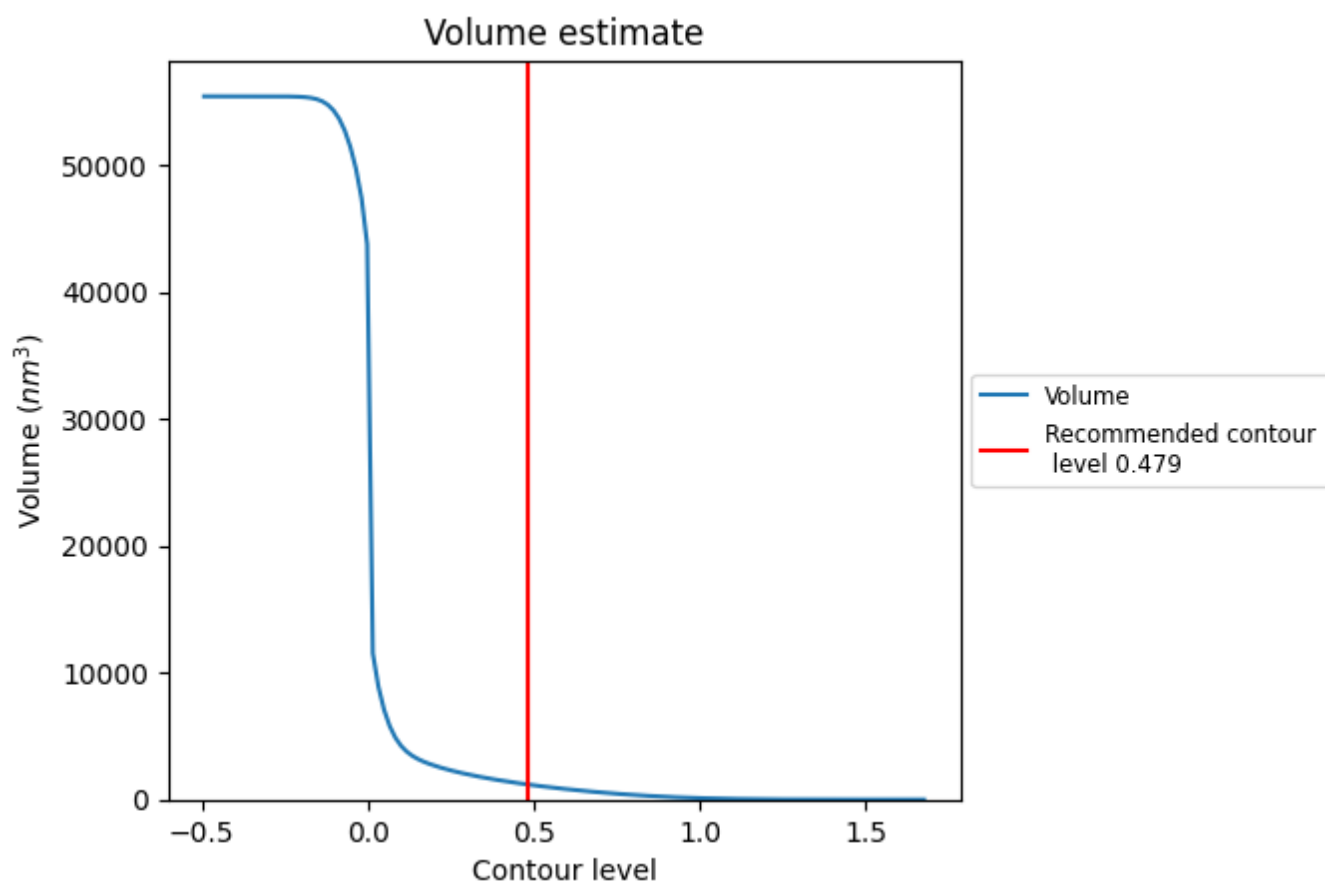
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

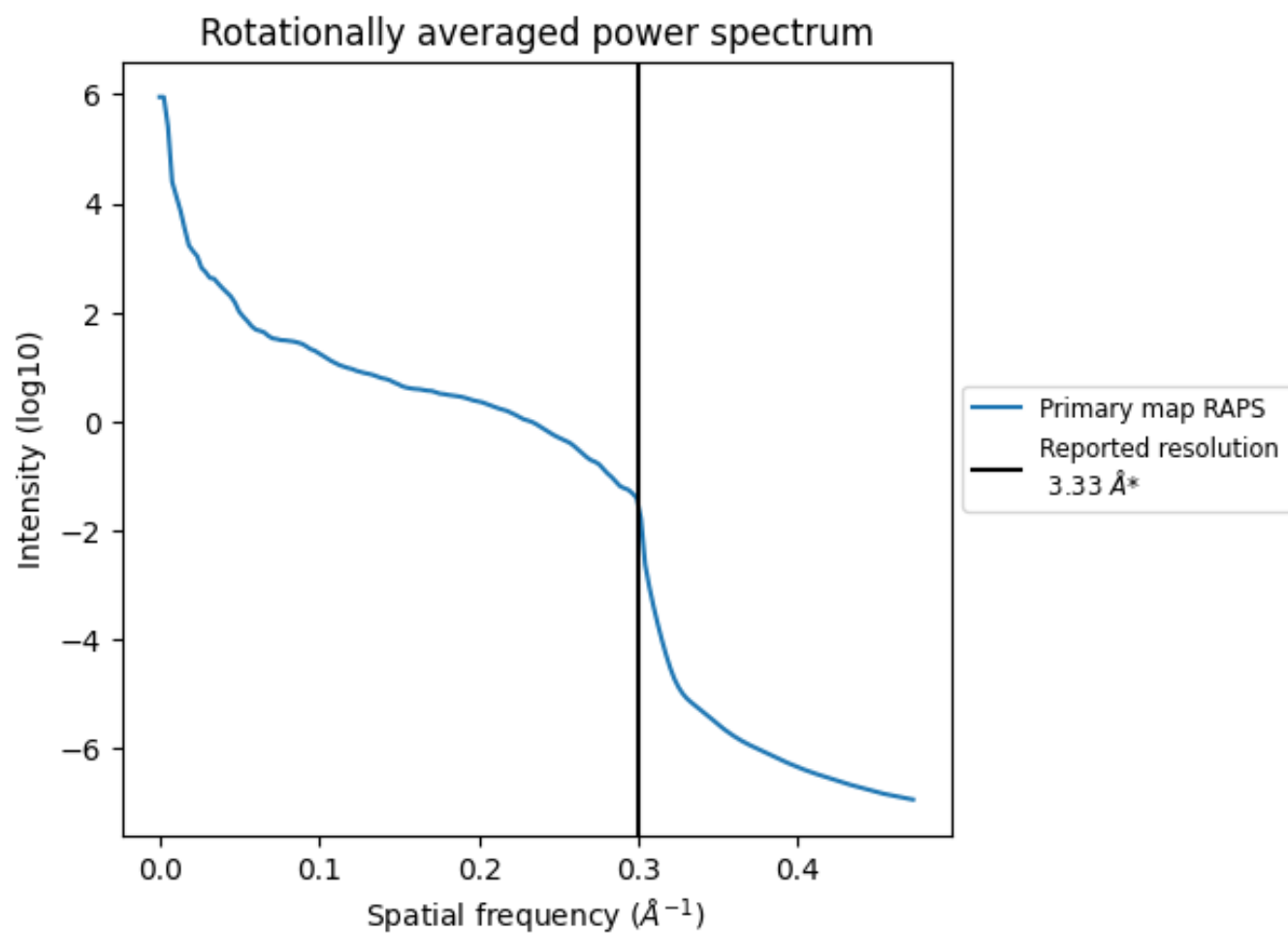
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1198 nm³; this corresponds to an approximate mass of 1082 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 0.300 Å⁻¹

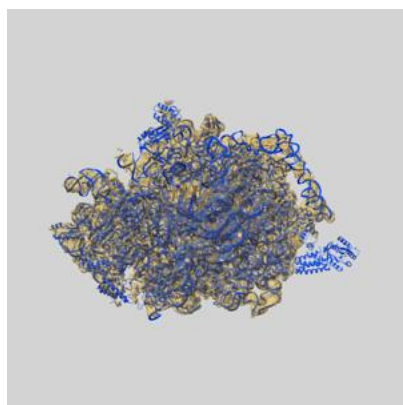
8 Fourier-Shell correlation ⓘ

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

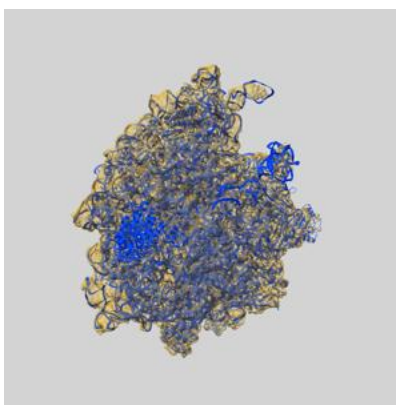
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12734 and PDB model 7O5B. Per-residue inclusion information can be found in section [3](#) on page [17](#).

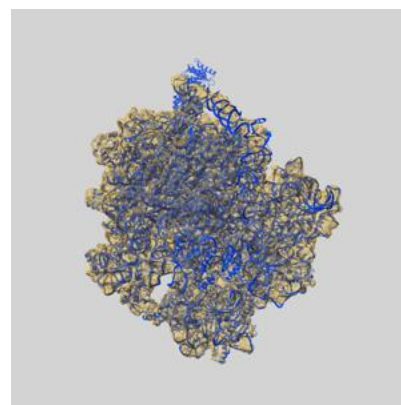
9.1 Map-model overlay [i](#)



X



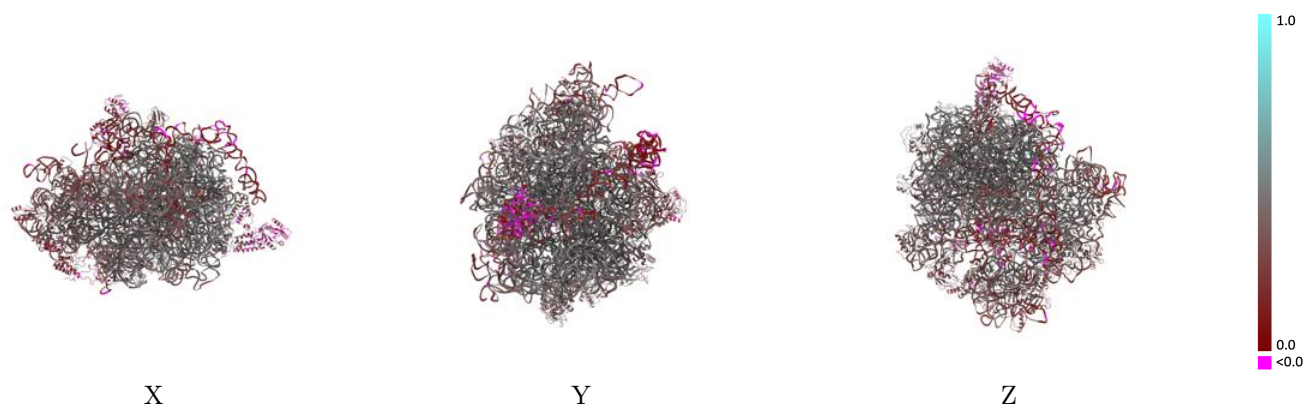
Y



Z

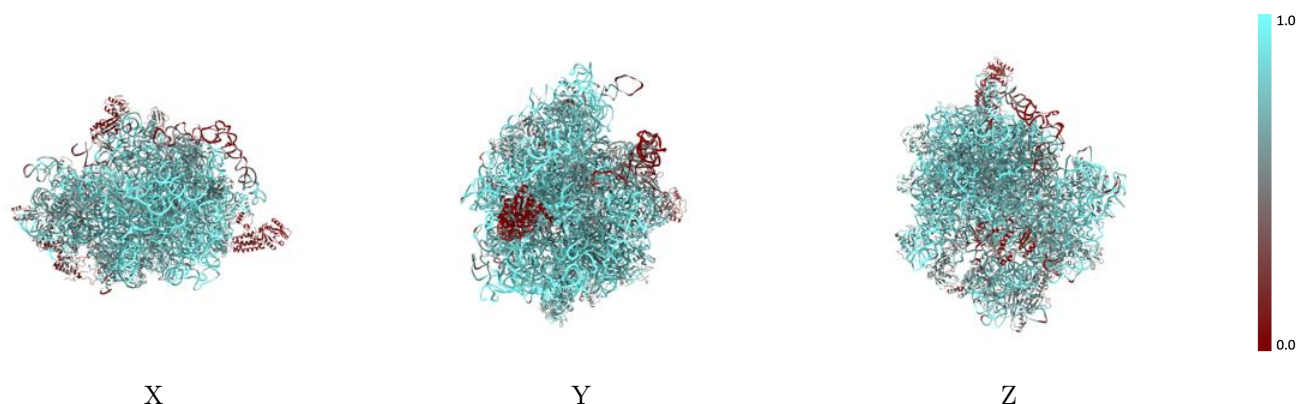
The images above show the 3D surface view of the map at the recommended contour level 0.479 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



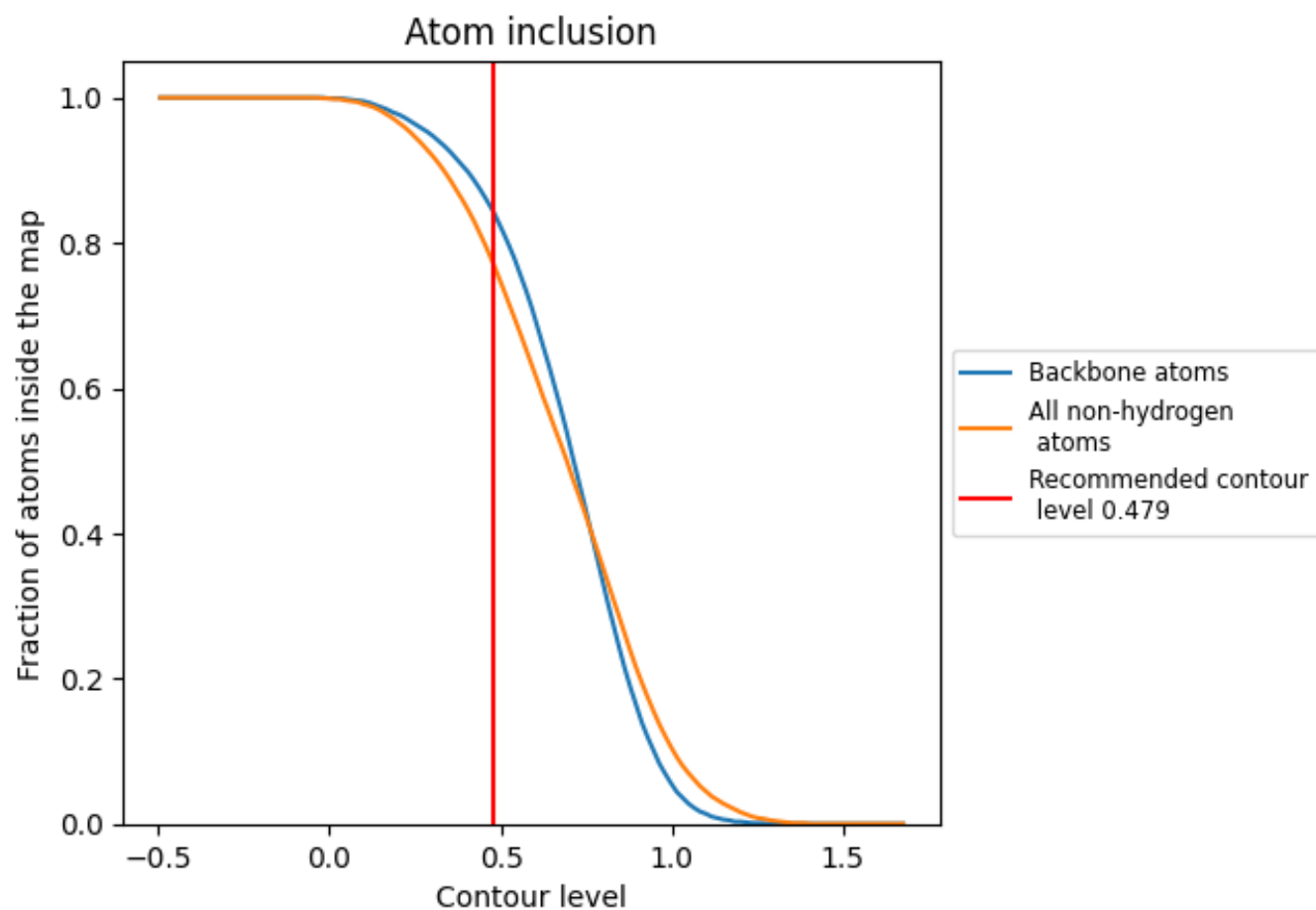
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.479).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 77% 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 (0.479) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.3810
0	 0.6710	 0.4440
1	 0.6360	 0.4280
2	 0.7420	 0.4780
3	 0.6290	 0.4670
4	 0.6280	 0.4410
6	 0.4760	 0.2500
A	 0.8830	 0.3860
B	 0.2370	 0.2130
C	 0.5480	 0.3360
D	 0.5540	 0.3150
E	 0.6060	 0.3980
F	 0.6290	 0.4070
G	 0.4570	 0.2340
H	 0.6380	 0.4010
I	 0.5310	 0.2700
J	 0.4920	 0.3060
K	 0.6050	 0.3750
L	 0.5730	 0.4190
M	 0.5410	 0.2990
N	 0.5980	 0.3800
O	 0.6530	 0.3940
P	 0.6560	 0.3750
Q	 0.5970	 0.4190
R	 0.6370	 0.4000
S	 0.5470	 0.3170
T	 0.6160	 0.3200
U	 0.7290	 0.3300
V	 0.5250	 0.3330
W	 0.4540	 0.1290
X	 0.8930	 0.4180
Y	 0.9030	 0.3790
Z	 0.6960	 0.4740
a	 0.6500	 0.4500
b	 0.6680	 0.4290



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	 0.5350	 0.3080
d	 0.5370	 0.3330
e	 0.6780	 0.4300
f	 0.5850	 0.4480
g	 0.1410	 0.1360
h	 0.0900	 0.1950
i	 0.6850	 0.4380
j	 0.6140	 0.4280
k	 0.6950	 0.4450
l	 0.6230	 0.3490
m	 0.6170	 0.4320
n	 0.7050	 0.4030
o	 0.6510	 0.4210
p	 0.1600	 0.1280
q	 0.1120	 0.1560
r	 0.6450	 0.4460
s	 0.6530	 0.4480
t	 0.6360	 0.4220
u	 0.6550	 0.4320
v	 0.5230	 0.4400
w	 0.6340	 0.3690
x	 0.6160	 0.4180