



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:50 PM UTC

PDB ID : 6VYZ / pdb_00006vyz
EMDB ID : EMD-21477
Title : Escherichia coli transcription-translation complex C6 (TTC-C6) containing mRNA with a 21 nt long spacer, NusA, and fMet-tRNAs at E-site and P-site
Authors : Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.H.
Deposited on : 2020-02-27
Resolution : 9.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

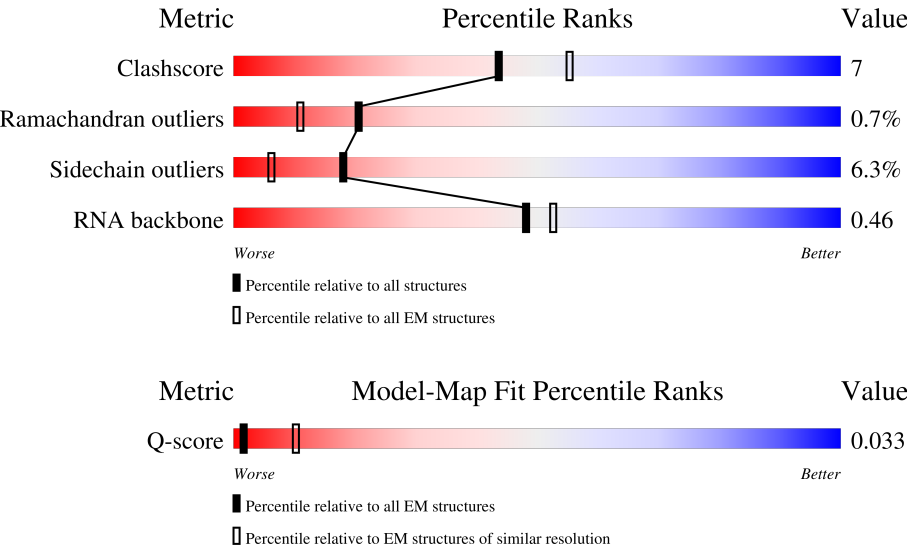
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 9.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	149 (9.40 - 10.40)

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

Mol	Chain	Length	Quality of chain
1	0	103	
2	1	110	
3	2	100	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	104	
5	4	94	
6	5	36	
7	6	36	
8	7	38	
9	A	76	
9	B	76	
10	AA	1342	
11	AB	181	
12	AC	329	
12	AD	329	
13	AE	1407	
14	AF	91	
15	C	75	
16	D	1542	
17	E	87	
18	F	71	
19	G	241	
20	H	557	
21	I	208	
22	J	206	
23	K	167	
24	L	135	
25	M	179	
26	N	130	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	O	130	36% 79% 18% ..
28	P	103	35% 79% 15% ...
29	Q	129	19% 82% 9% 9%
30	R	124	30% 86% 11% .
31	S	101	42% 89% 8% ...
32	T	89	17% 79% 18% ..
33	U	82	54% 88% 11% .
34	V	84	43% 87% 7% 5%
35	W	92	17% 82% 8% 10%
36	X	118	27% 75% 18% 5%
37	Y	3	100% 33% 67%
38	a	2904	21% 73% 23% ..
39	b	85	48% 85% 5% 11%
40	c	78	51% 88% 8% ..
41	d	120	38% 81% 18% .
42	e	62	32% 89% 10% .
43	f	59	64% 81% 15% ..
44	g	70	10% 80% 13% 6%
45	h	273	43% 85% 13% ..
46	i	57	46% 77% 19% ..
47	j	209	48% 88% 12%
48	k	55	25% 89% 5% 5%
49	l	201	38% 85% 14% .
50	m	46	61% 78% 17% .
51	n	179	16% 75% 20% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	o	65	
53	p	177	
54	q	38	
55	r	149	
56	s	142	
57	t	123	
58	u	144	
59	v	136	
60	w	127	
61	x	117	
62	y	115	
63	z	118	

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 297741 atoms, of which 124644 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	103	Total	C	H	N	O		0	0
			1632	498	844	148	142			

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	23	Total	C	H	N	O	P	0	0
			731	225	259	87	137	23		

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	27	Total	C	H	N	O	P	0	0
			847	259	305	89	167	27		

- Molecule 8 is a RNA chain called mRNA with 21 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	16	Total	C	H	N	O	P	0	0
			515	154	168	62	115	16		

- Molecule 9 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	A	76	Total	C	H	N	O	P	0	0
			2446	723	826	295	527	75		
9	B	76	Total	C	H	N	O	P	0	0
			2433	723	813	295	527	75		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AA	1223	Total	C	H	N	O	S	0	0
			19199	6029	9589	1672	1867	42		

- Molecule 11 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AB	98	Total	C	H	N	O	S	0	0
			1573	505	783	139	140	6		

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AC	230	Total	C	H	N	O	S	0	0
			3599	1112	1813	317	351	6		
12	AD	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AE	1335	Total	C	H	N	O	S	0	0
			20999	6526	10611	1854	1958	50		

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AF	83	Total	C	H	N	O	S	0	0
			1318	399	663	123	132	1		

- Molecule 15 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	C	66	Total	C	H	N	O	S	0	0
			1103	344	559	102	97	1		

- Molecule 16 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	D	1522	Total	C	H	N	O	P	0	0
			49076	14565	16420	5993	10576	1522		

- Molecule 17 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	E	86	Total	C	H	N	O	S	0	0
			1388	414	719	138	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 19 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 20 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 21 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 22 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 23 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 24 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 25 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 26 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 27 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

- Molecule 28 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

- Molecule 29 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 31 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 32 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 33 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 34 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 35 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 36 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 37 is a RNA chain called mRNA in the ribosomal RNA entrance pore.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	Y	3	Total	C	H	N	O	P	0	0
			90	27	30	6	24	3		

- Molecule 38 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	a	2880	Total	C	H	N	O	P	0	0
			92917	27587	31076	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 39 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 40 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	c	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 41 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	d	120	Total	C	H	N	O	P	0	0
			3870	1144	1301	468	837	120		

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	e	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 44 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

- Molecule 45 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 46 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

- Molecule 47 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	k	52	Total	C	H	N	O		0	0
			890	275	464	78	73			

- Molecule 49 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 53 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 55 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 56 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 57 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 58 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 59 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 60 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 61 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	x	116	Total	C	H	N	O	0	0
			1815	552	923	178	162		

- Molecule 62 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 63 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	z	117	Total	C	H	N	O	0	0
			1967	604	1020	192	151		

- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
64	AE	1	Total	Mg	0
			1	1	

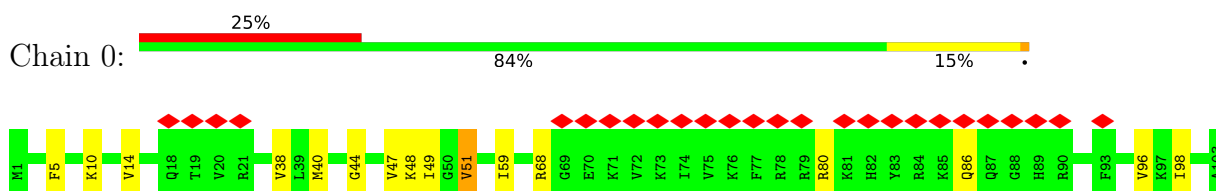
- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
65	AE	2	Total	Zn	0
			2	2	

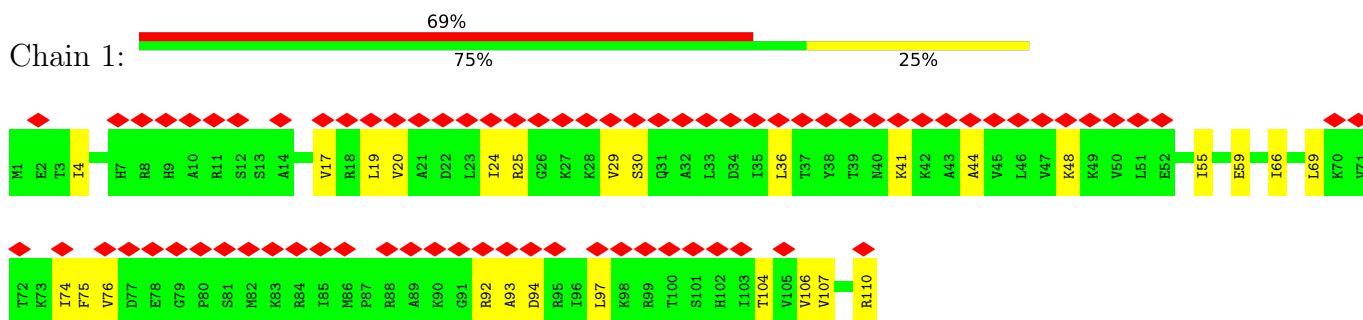
3 Residue-property plots [i](#)

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.

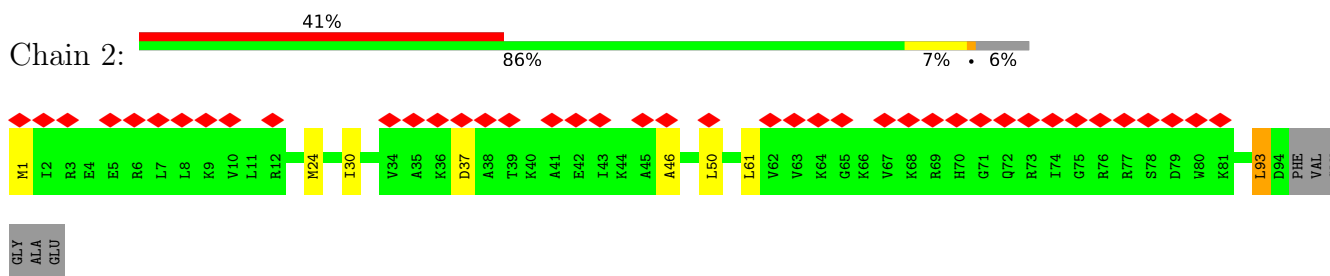
- Molecule 1: 50S ribosomal protein L21



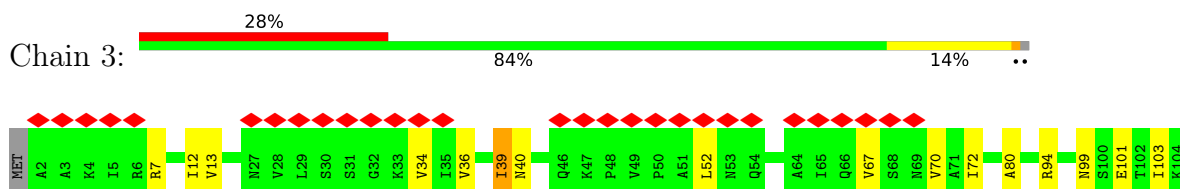
- Molecule 2: 50S ribosomal protein L22



- Molecule 3: 50S ribosomal protein L23



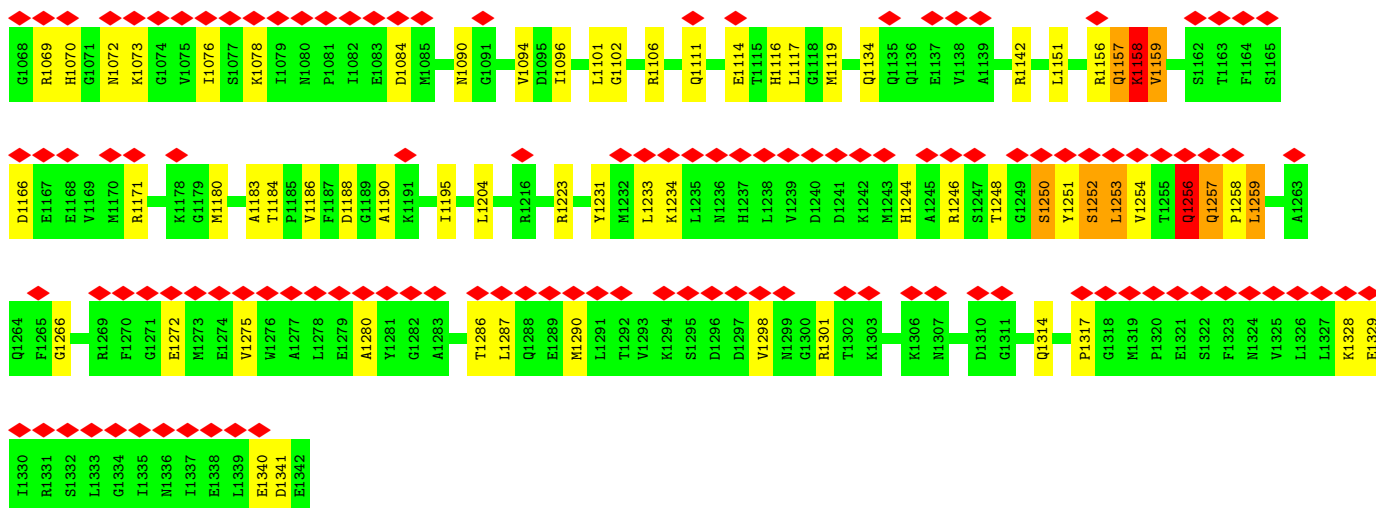
- Molecule 4: 50S ribosomal protein L24



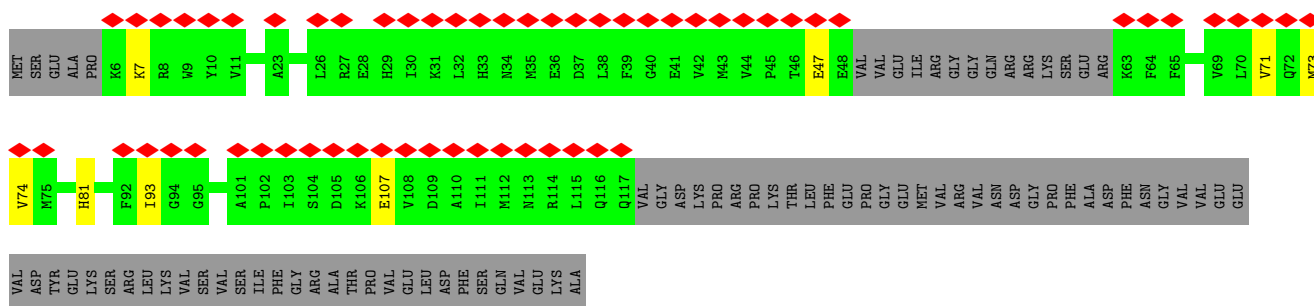
- Molecule 5: 50S ribosomal protein L25

Chain AA:

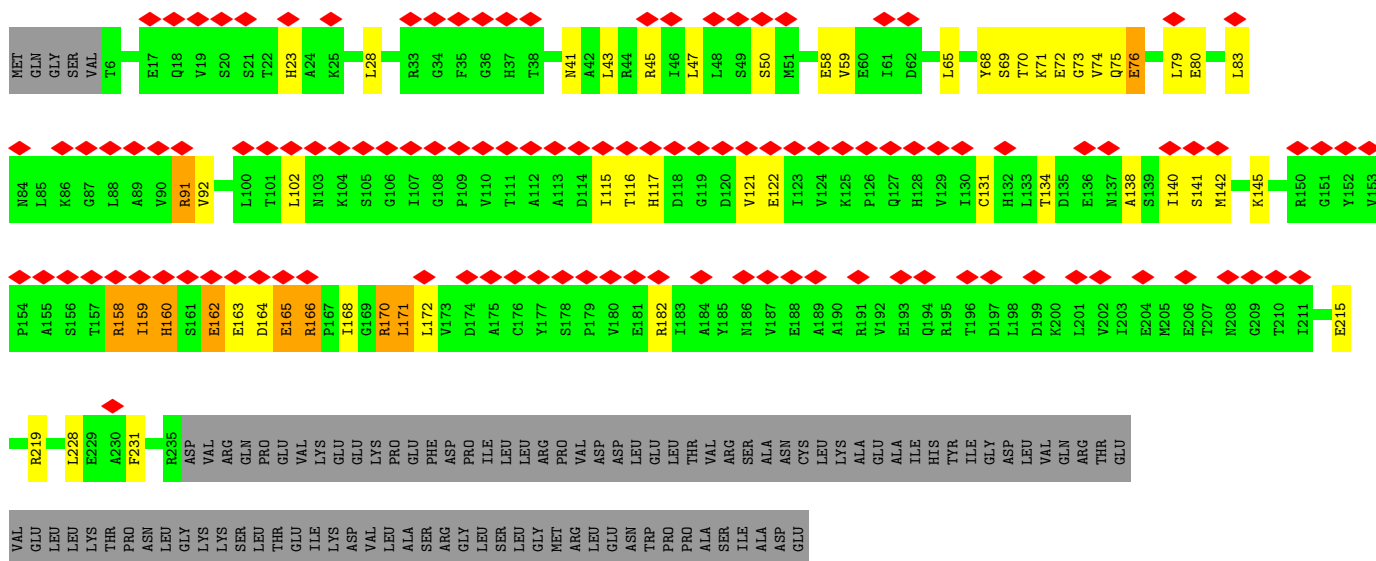




• Molecule 11: Transcription termination/antitermination protein NusG

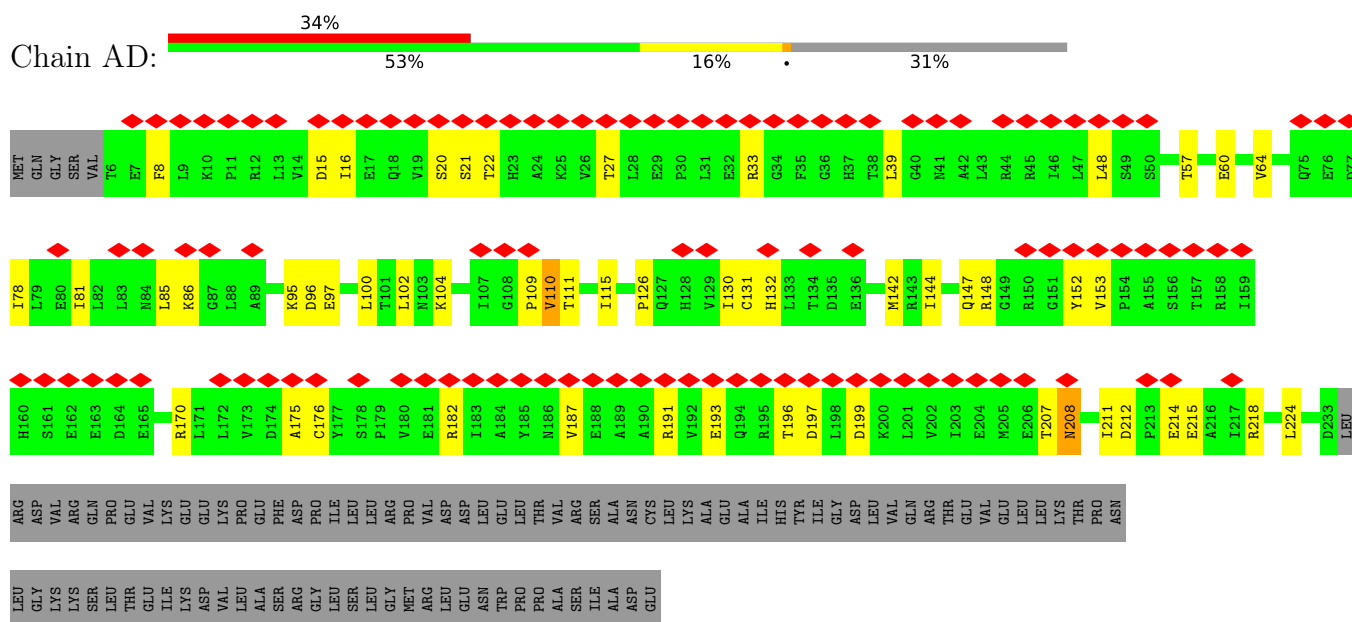


• Molecule 12: DNA-directed RNA polymerase subunit alpha



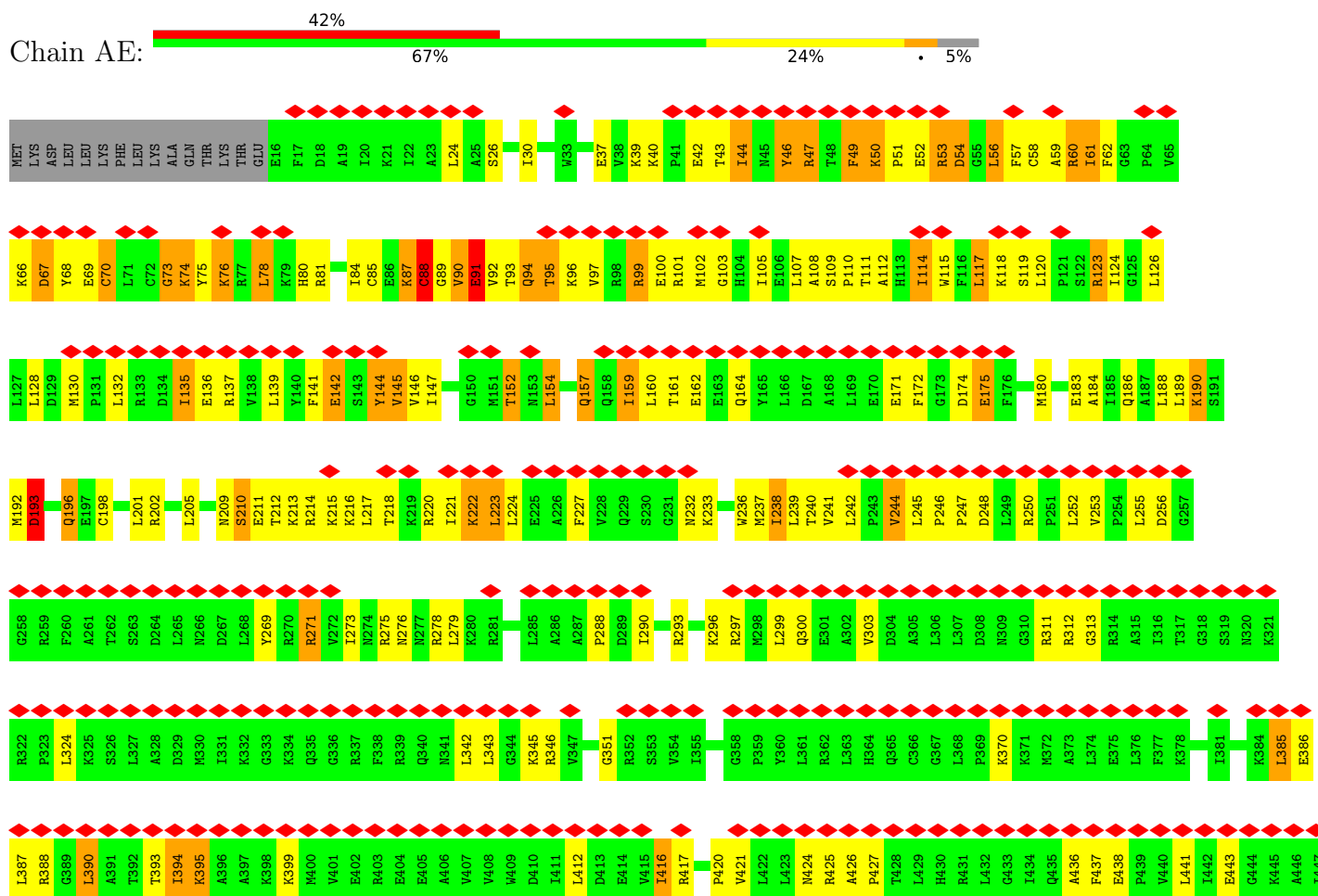
- Molecule 12: DNA-directed RNA polymerase subunit alpha

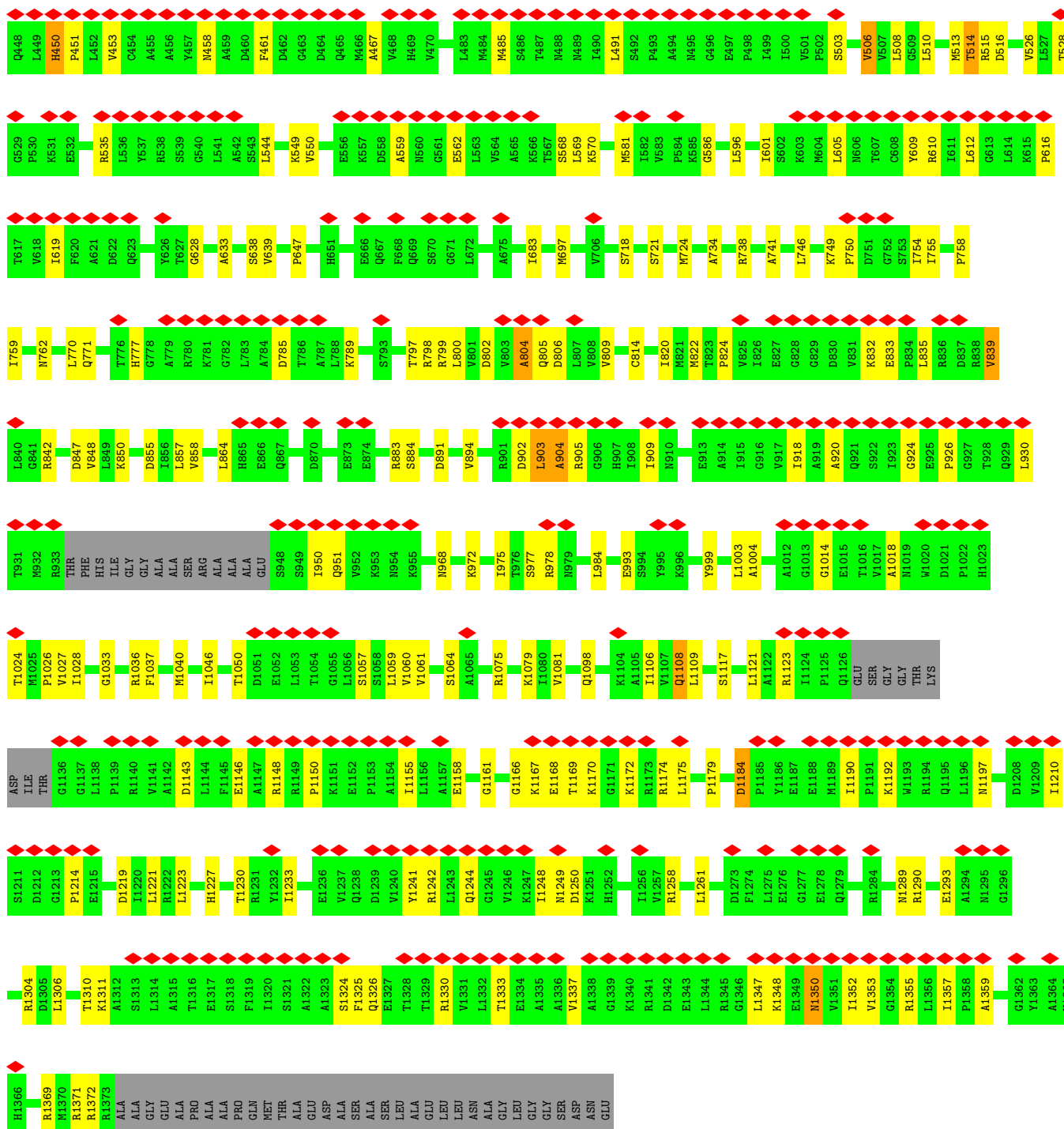
Chain AD:



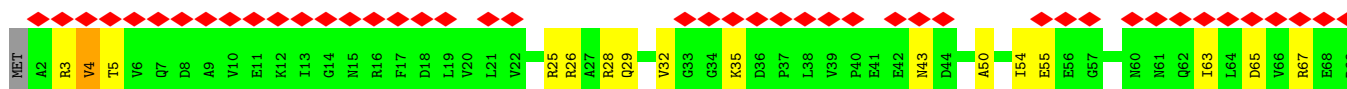
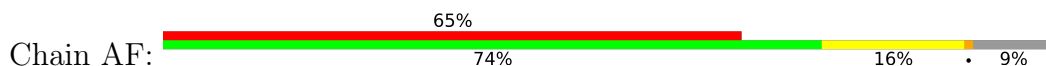
- Molecule 13: DNA-directed RNA polymerase subunit beta'

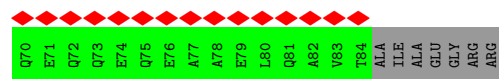
Chain AE:



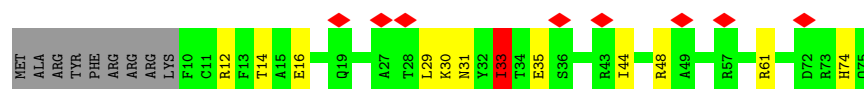
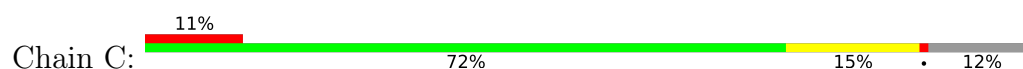


• Molecule 14: DNA-directed RNA polymerase subunit omega

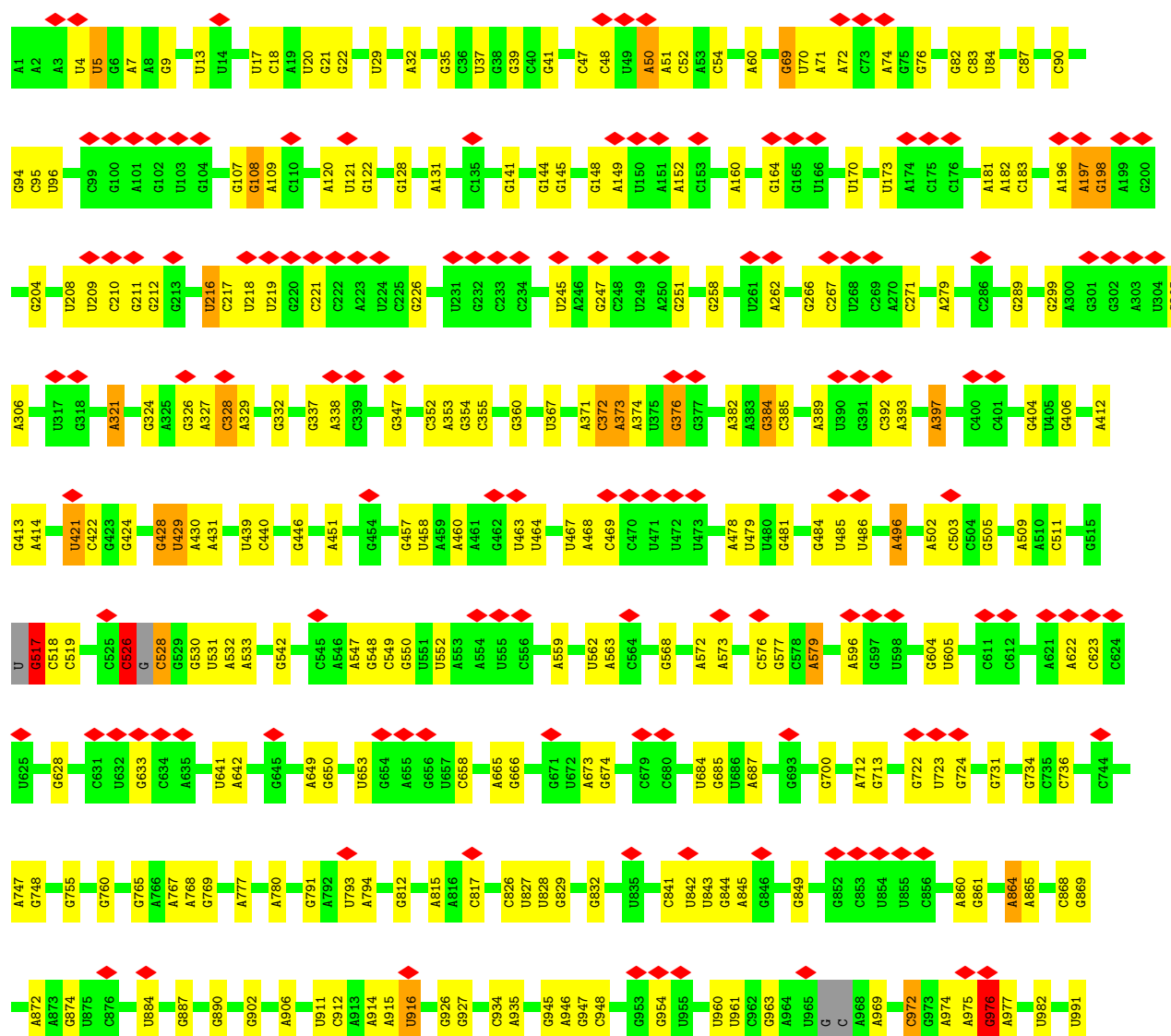


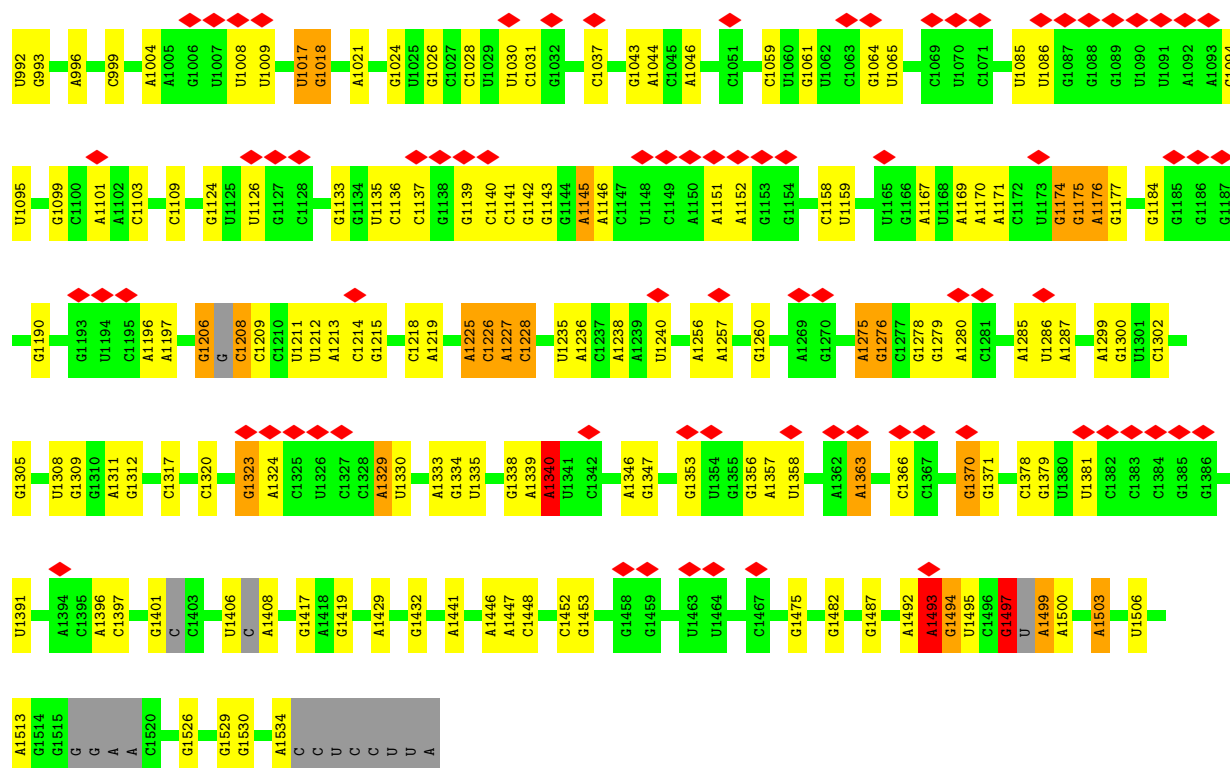


- Molecule 15: 30S ribosomal protein S18

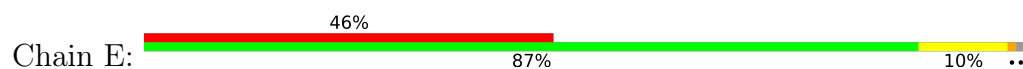


- Molecule 16: 16S rRNA

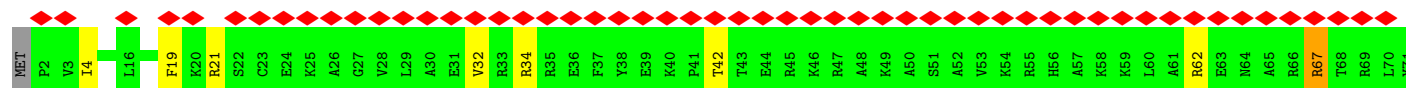
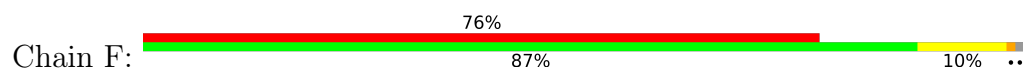




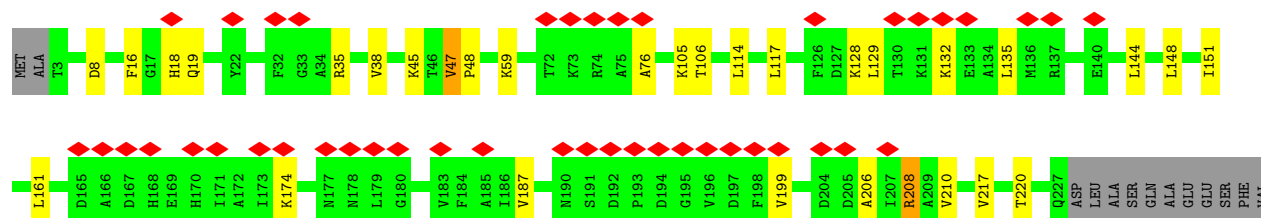
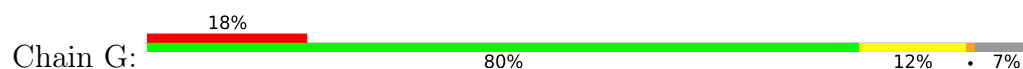
• Molecule 17: 30S ribosomal protein S20

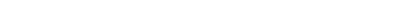


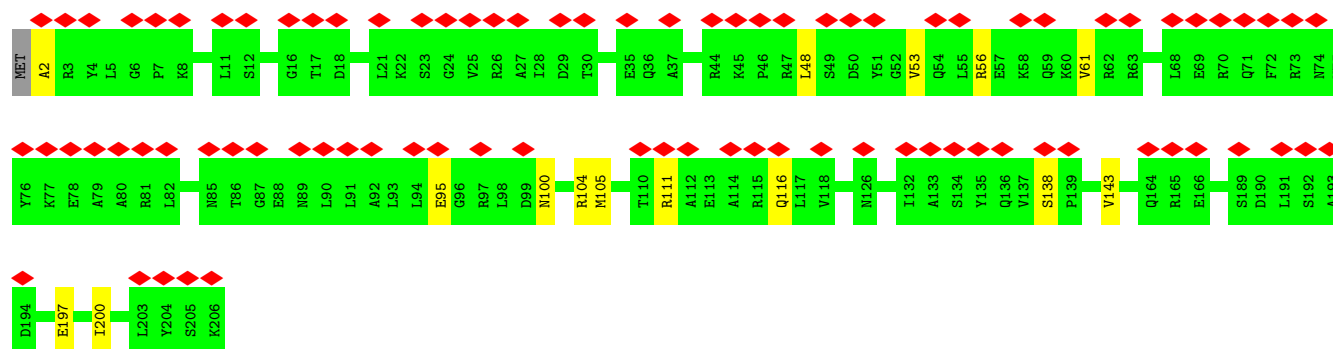
• Molecule 18: 30S ribosomal protein S21



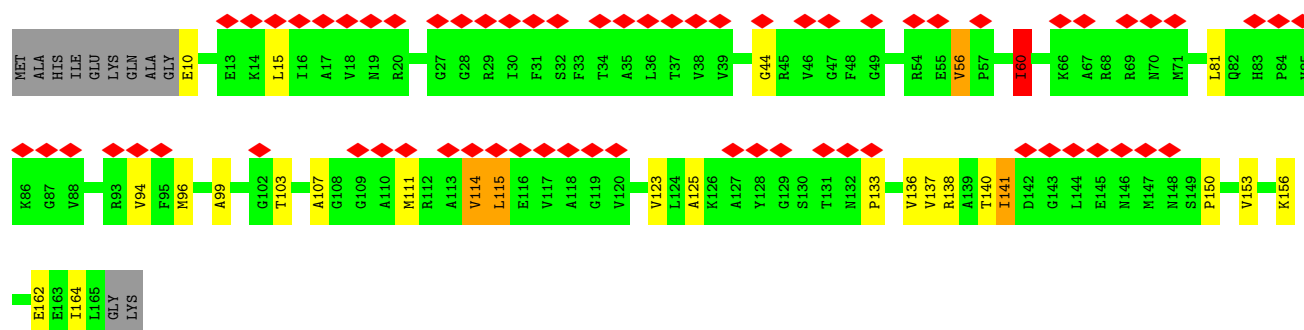
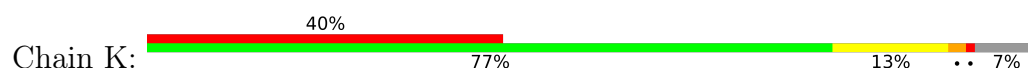
• Molecule 19: 30S ribosomal protein S2



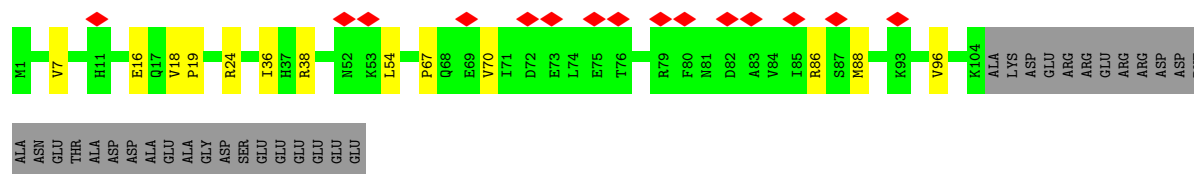
Chain J:  42% 92% 7%



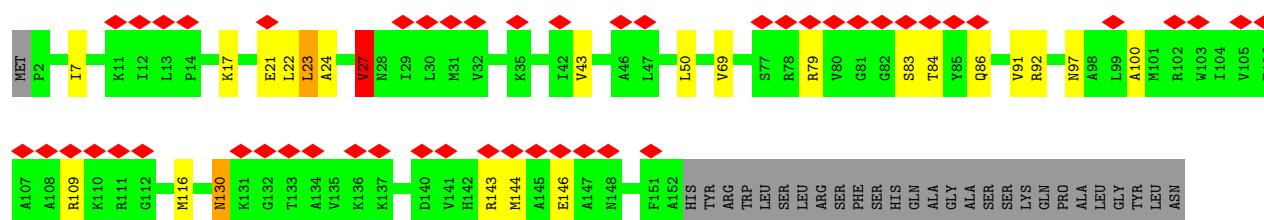
- Molecule 23: 30S ribosomal protein S5



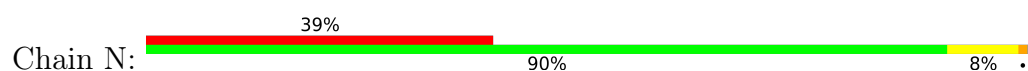
- Molecule 24: 30S ribosomal protein S6

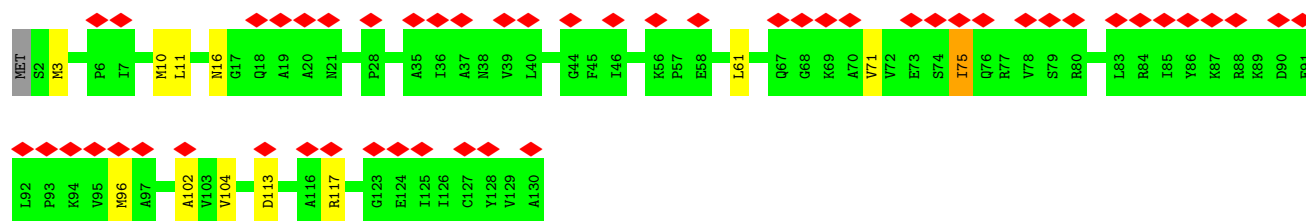


- Molecule 25: 30S ribosomal protein S7

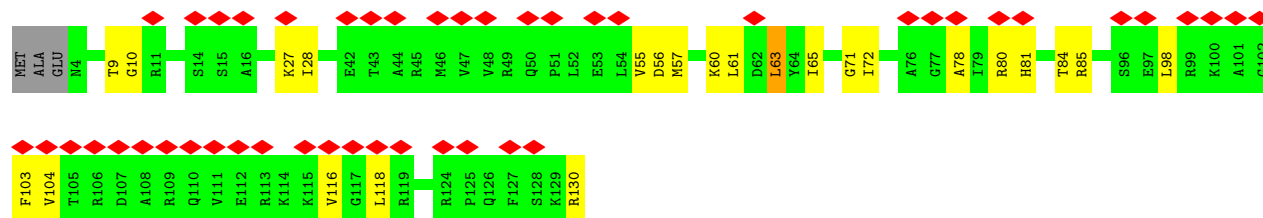
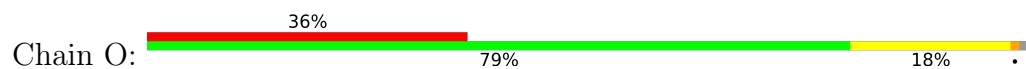


- Molecule 26: 30S ribosomal protein S8

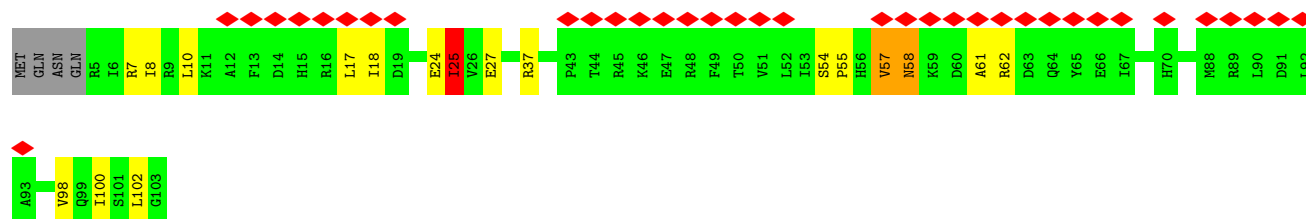
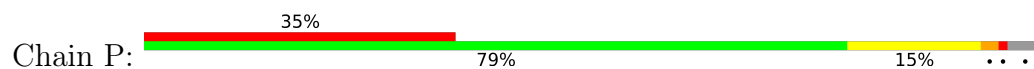




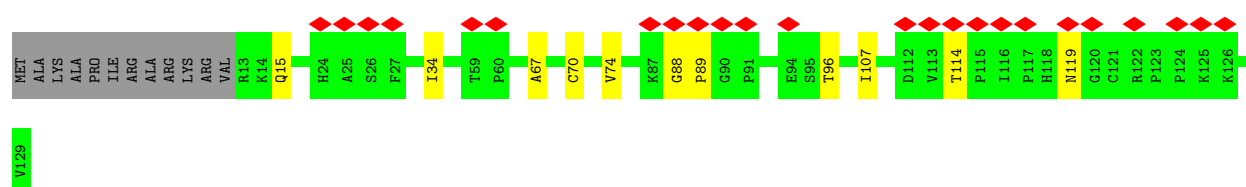
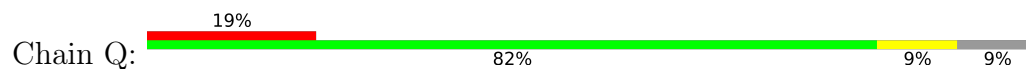
• Molecule 27: 30S ribosomal protein S9



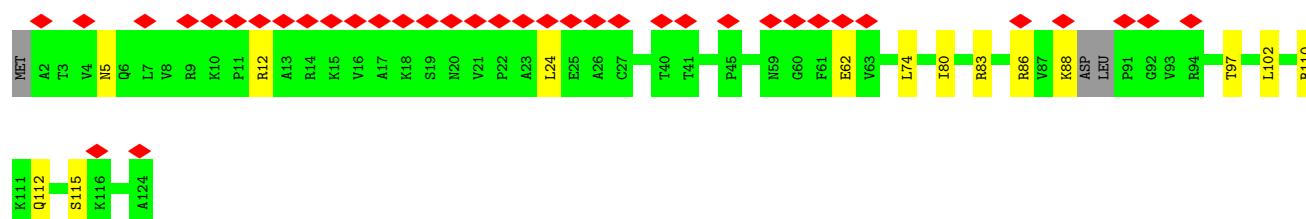
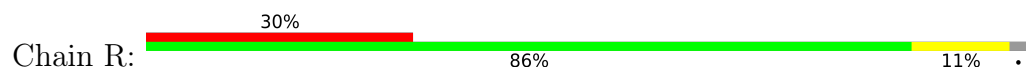
• Molecule 28: 30S ribosomal protein S10



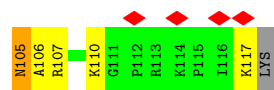
• Molecule 29: 30S ribosomal protein S11



• Molecule 30: 30S ribosomal protein S12



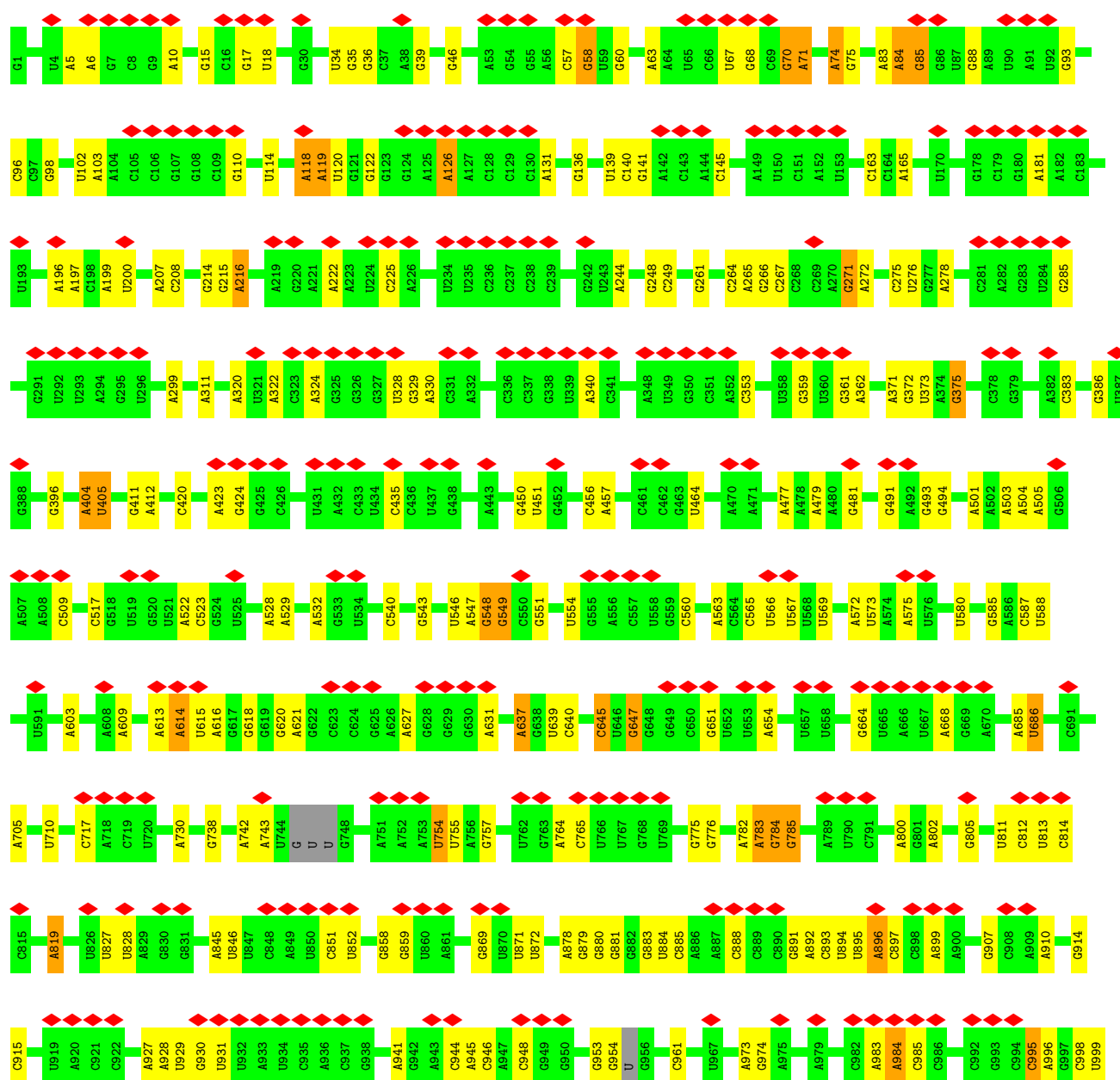
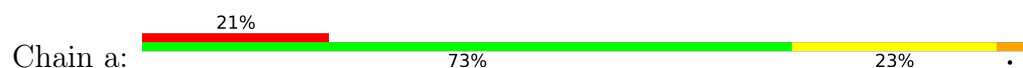
- [illegible]

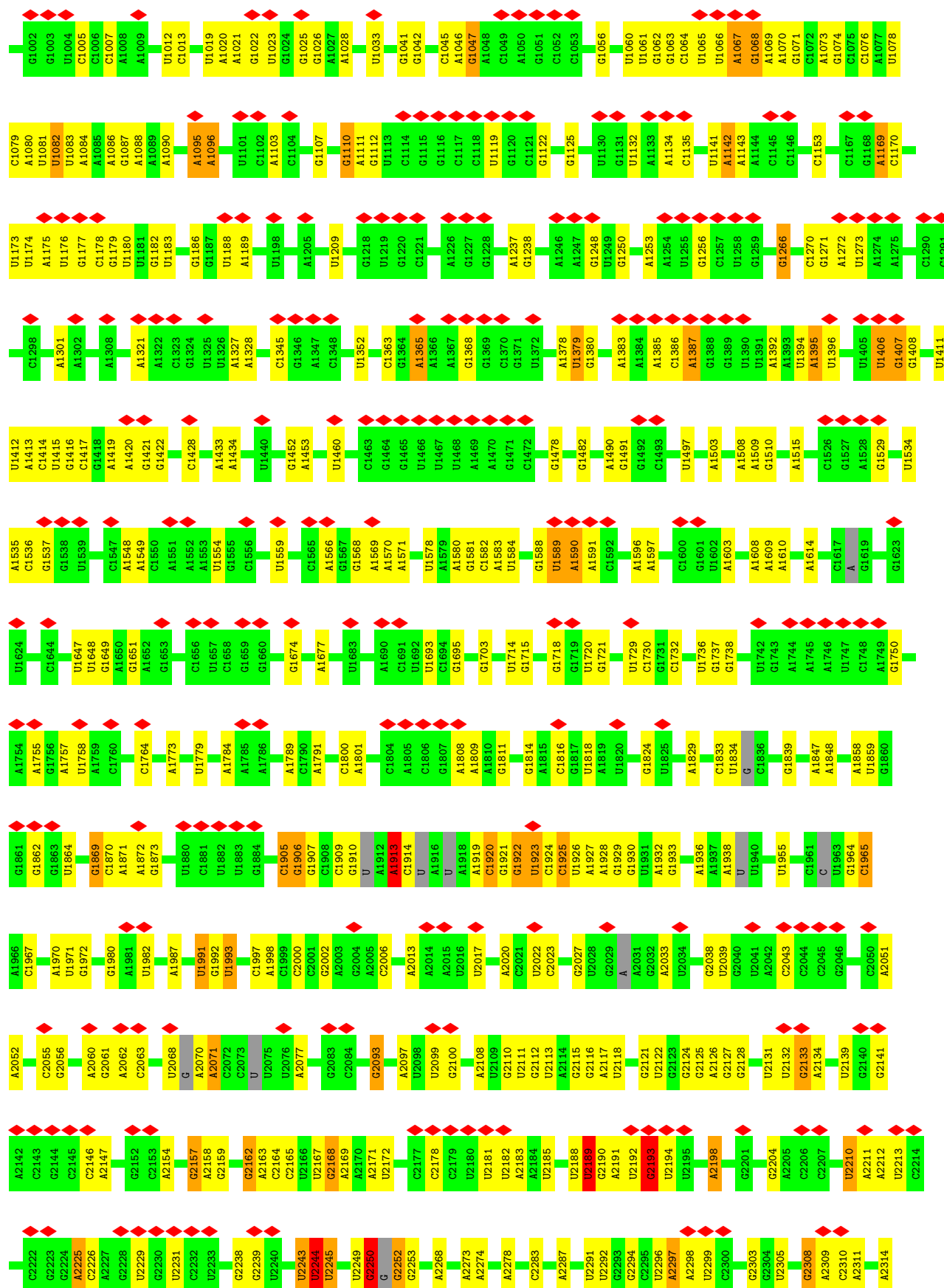


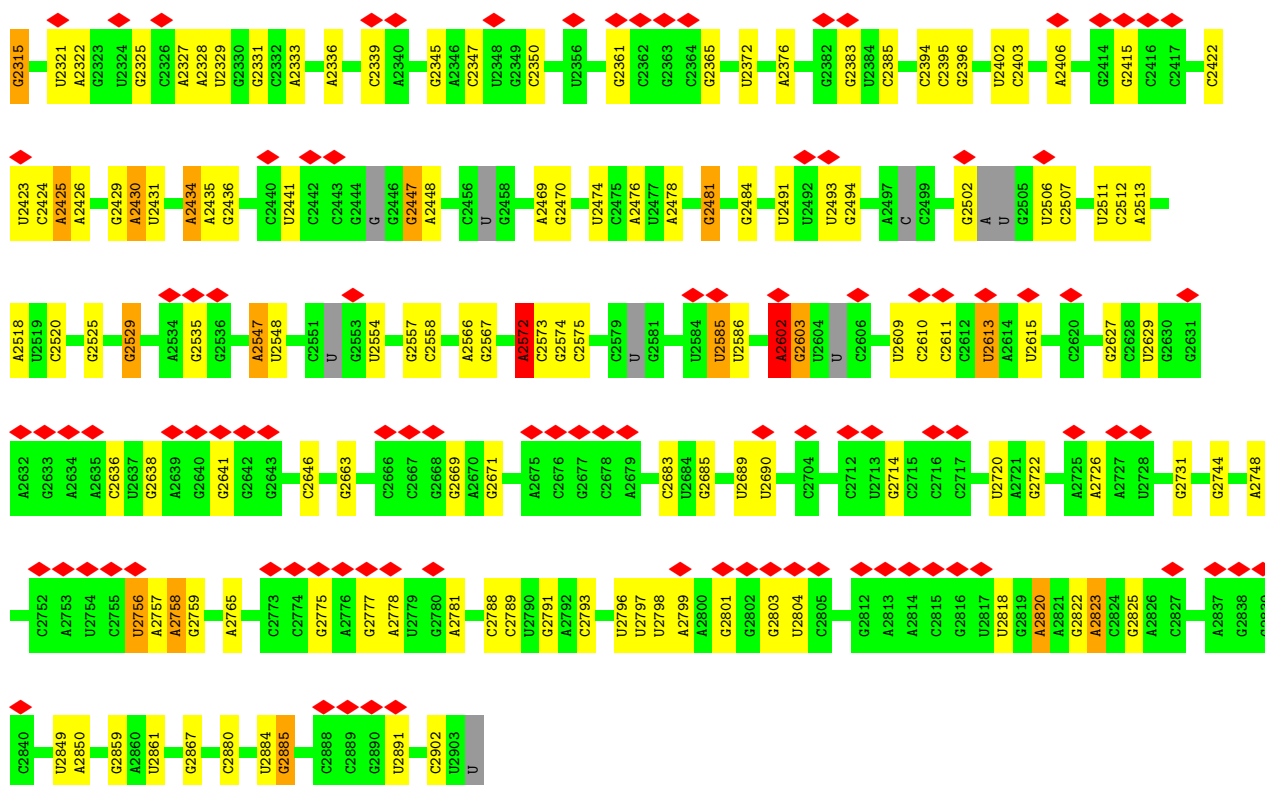
- Molecule 37: mRNA in the ribosomal RNA entrance pore



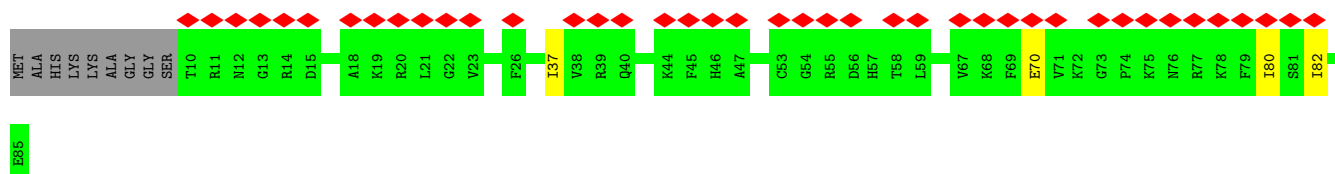
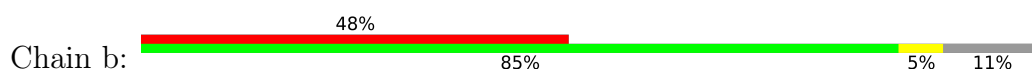
- Molecule 38: 23S rRNA



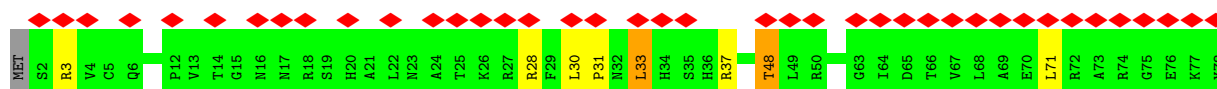
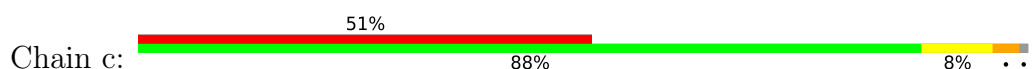




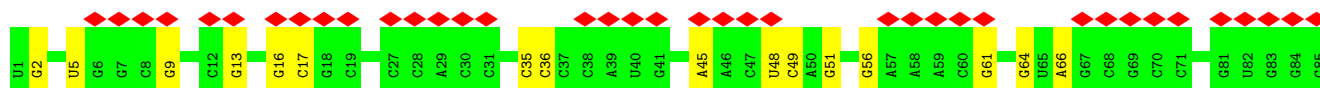
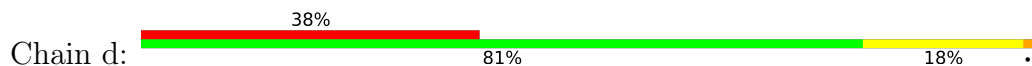
• Molecule 39: 50S ribosomal protein L27

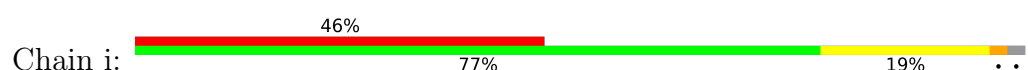


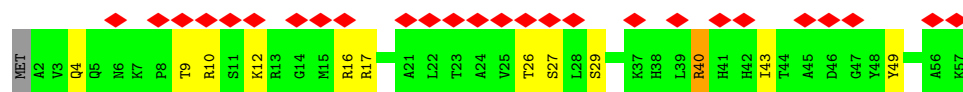
• Molecule 40: 50S ribosomal protein L28



• Molecule 41: 5S rRNA

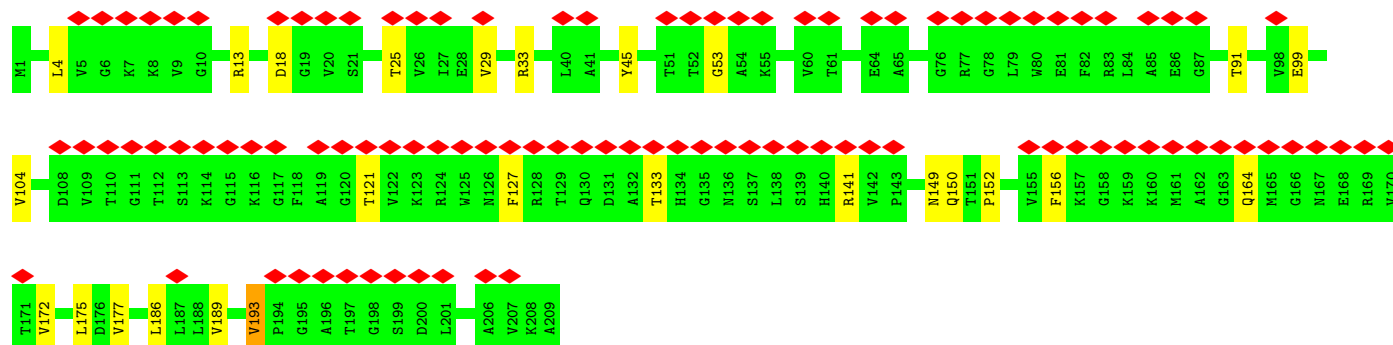






- Molecule 47: 50S ribosomal protein L3

Chain j: 48% 88% 12%



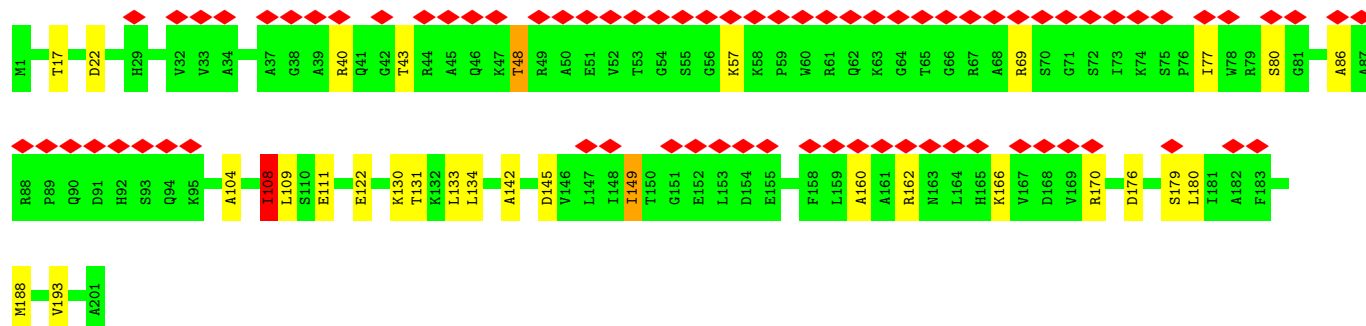
- Molecule 48: 50S ribosomal protein L33

Chain k: 25% 89% 5% 5%



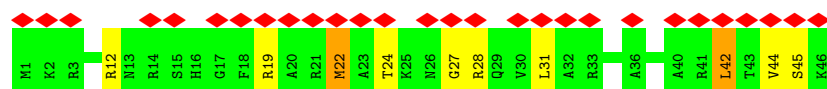
- Molecule 49: 50S ribosomal protein L4

Chain l: 38% 85% 14%

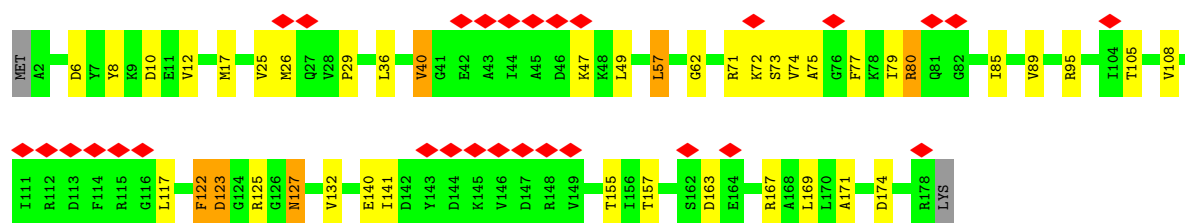
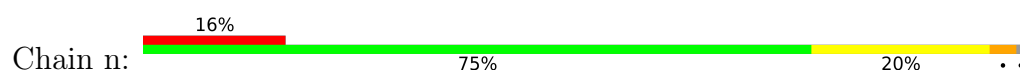


- Molecule 50: 50S ribosomal protein L34

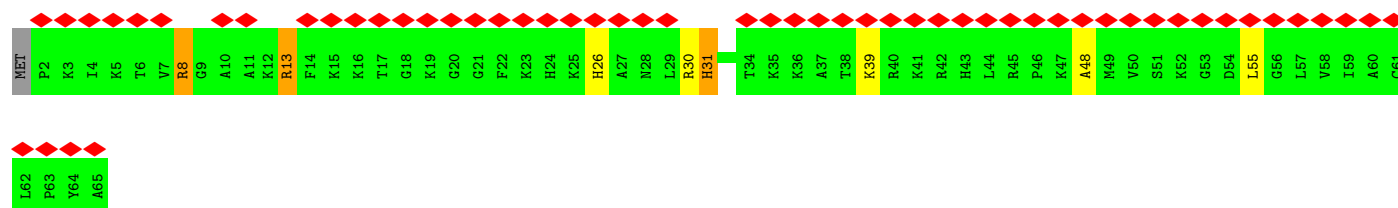
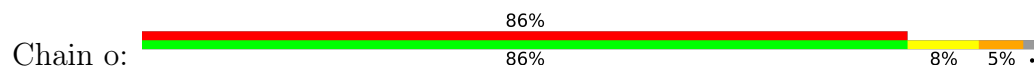
Chain m: 61% 78% 17%



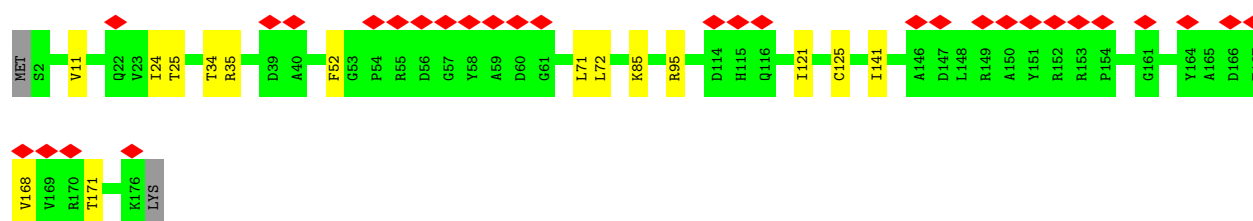
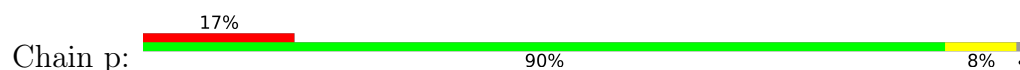
- Molecule 51: 50S ribosomal protein L5



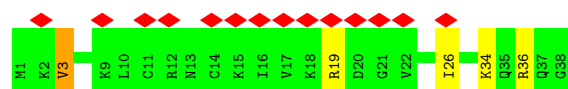
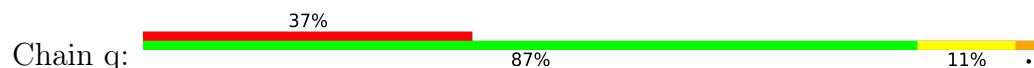
• Molecule 52: 50S ribosomal protein L35



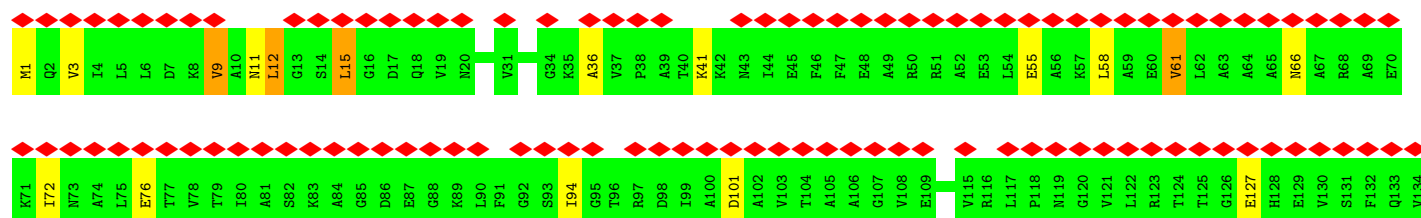
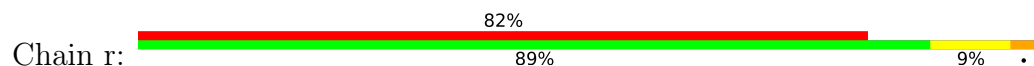
• Molecule 53: 50S ribosomal protein L6

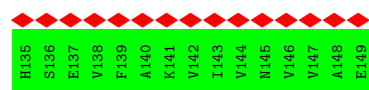


• Molecule 54: 50S ribosomal protein L36

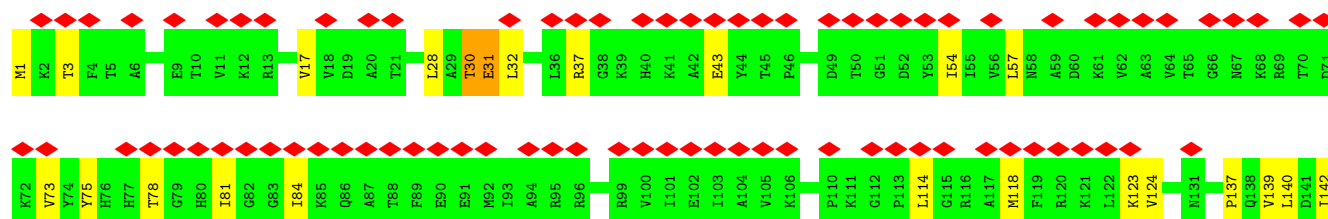
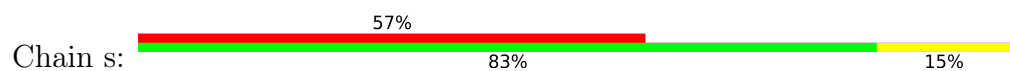


• Molecule 55: 50S ribosomal protein L9

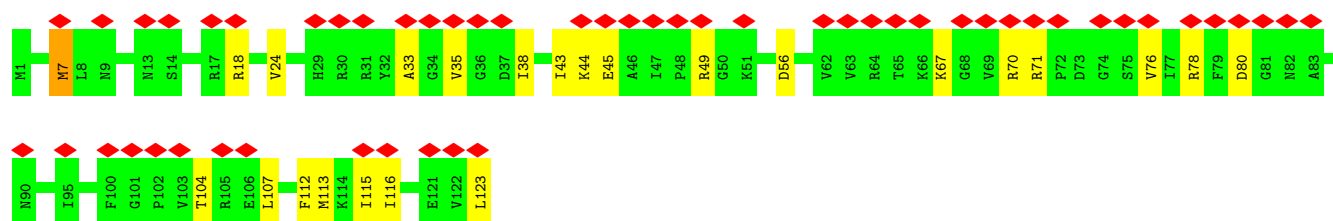
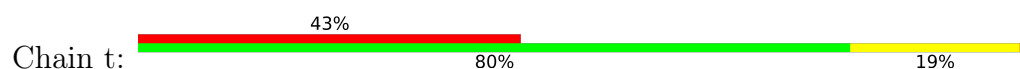




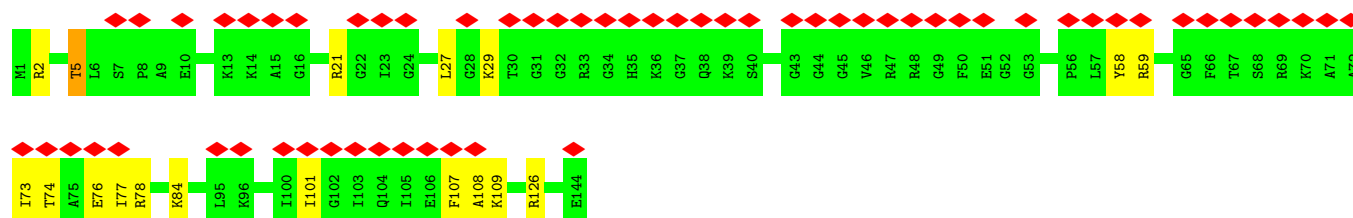
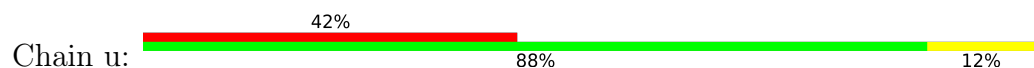
• Molecule 56: 50S ribosomal protein L13



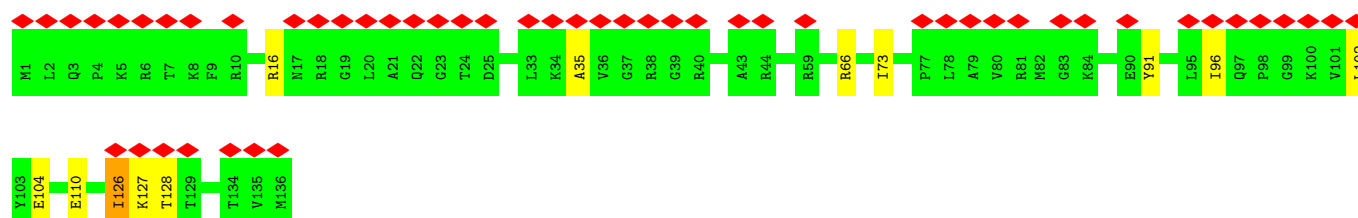
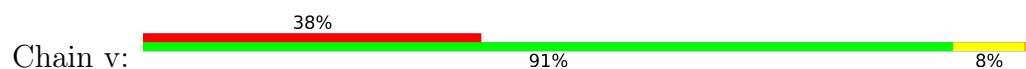
• Molecule 57: 50S ribosomal protein L14



• Molecule 58: 50S ribosomal protein L15

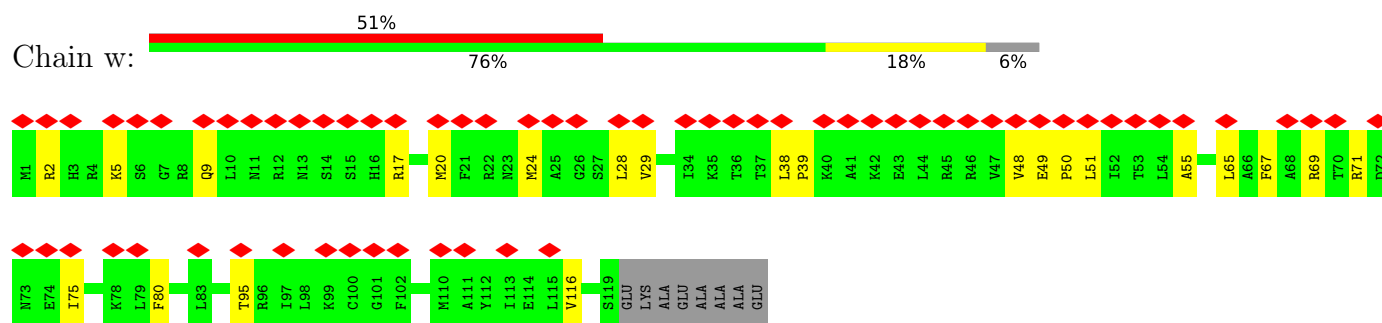


• Molecule 59: 50S ribosomal protein L16

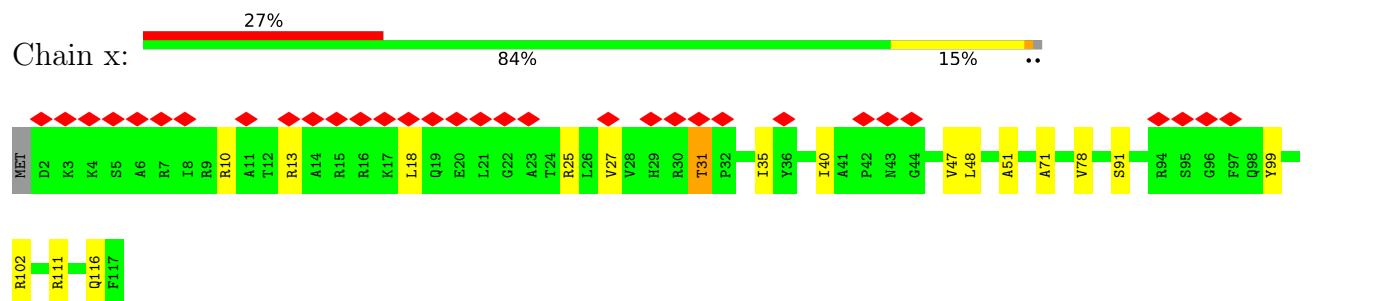


• Molecule 60: 50S ribosomal protein L17

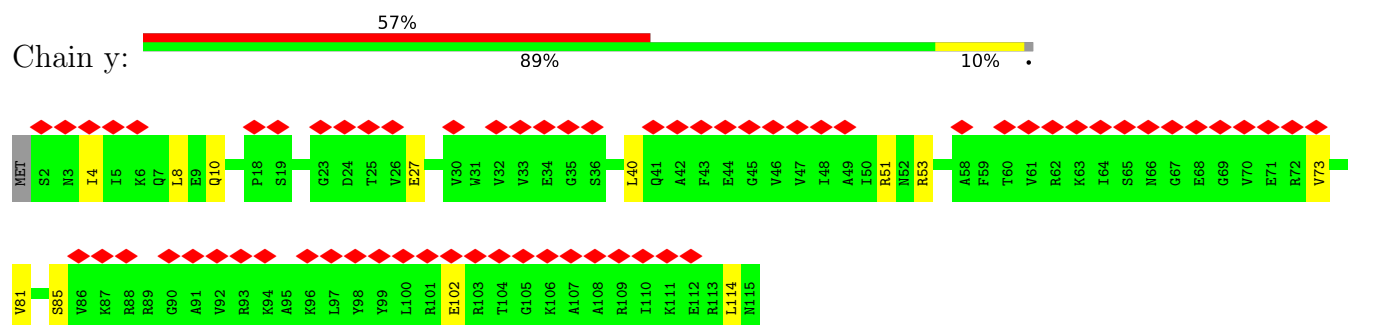




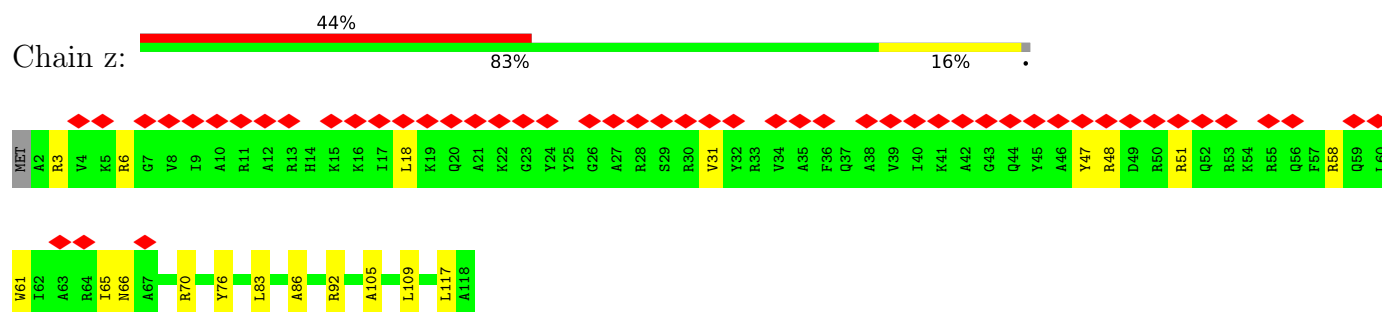
• Molecule 61: 50S ribosomal protein L18



• Molecule 62: 50S ribosomal protein L19



• Molecule 63: 50S ribosomal protein L20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5913	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.204	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	564.4608, 564.4608, 564.4608	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.9399002, 2.9399002, 2.9399002	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.49	0/829	0.74	0/1107
2	1	0.67	0/864	1.08	0/1156
3	2	0.54	0/752	0.89	0/1005
4	3	0.46	0/796	0.78	0/1062
5	4	0.52	0/766	0.88	0/1025
6	5	0.63	1/528 (0.2%)	0.55	0/810
7	6	0.56	1/603 (0.2%)	0.56	0/926
8	7	0.76	4/388 (1.0%)	0.55	0/604
9	A	0.35	0/1810	0.72	3/2821 (0.1%)
9	B	0.42	0/1810	0.86	8/2821 (0.3%)
10	AA	0.64	11/9768 (0.1%)	0.92	46/13191 (0.3%)
11	AB	0.42	0/808	0.70	2/1088 (0.2%)
12	AC	0.58	6/1808 (0.3%)	0.70	9/2450 (0.4%)
12	AD	0.39	0/1789	0.55	0/2425
13	AE	0.54	8/10545 (0.1%)	0.74	25/14236 (0.2%)
14	AF	0.48	0/657	0.73	0/886
15	C	0.66	0/553	1.14	2/743 (0.3%)
16	D	0.38	4/36557 (0.0%)	0.74	30/57006 (0.1%)
17	E	0.76	0/675	1.32	0/895
18	F	0.71	0/597	1.20	0/792
19	G	0.63	0/1791	1.06	1/2413 (0.0%)
20	H	0.76	4/1746 (0.2%)	1.58	34/2382 (1.4%)
21	I	0.57	0/1663	0.97	0/2241
22	J	0.61	0/1665	1.05	0/2227
23	K	0.64	1/1165 (0.1%)	1.06	2/1568 (0.1%)
24	L	0.58	0/867	0.94	0/1171
25	M	0.68	0/1195	1.19	3/1602 (0.2%)
26	N	0.55	0/989	0.91	0/1326
27	O	0.58	0/1034	1.02	1/1375 (0.1%)
28	P	0.54	0/800	1.06	4/1082 (0.4%)
29	Q	0.55	0/893	0.91	0/1205
30	R	0.49	0/952	0.81	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	S	0.64	0/817	1.11	1/1088 (0.1%)
32	T	0.69	0/722	1.21	0/964
33	U	0.57	0/659	0.99	0/884
34	V	0.45	0/657	0.73	0/881
35	W	0.51	0/680	0.83	0/915
36	X	0.67	0/909	1.21	3/1215 (0.2%)
37	Y	0.42	0/65	0.86	0/98
38	a	0.40	3/69247 (0.0%)	0.75	57/107985 (0.1%)
39	b	0.50	0/589	0.76	0/779
40	c	0.63	0/635	0.97	0/848
41	d	0.37	0/2872	0.69	0/4478
42	e	0.69	0/502	1.19	0/667
43	f	0.62	0/452	1.02	0/605
44	g	0.55	0/531	0.99	1/709 (0.1%)
45	h	0.53	0/2121	0.85	0/2852
46	i	0.52	0/450	0.94	0/599
47	j	0.60	0/1586	0.87	0/2134
48	k	0.46	0/433	0.80	0/576
49	l	0.60	0/1571	1.03	1/2113 (0.0%)
50	m	0.68	0/380	1.22	0/498
51	n	0.62	0/1434	1.18	10/1926 (0.5%)
52	o	0.63	0/513	1.11	1/676 (0.1%)
53	p	0.57	0/1333	0.89	0/1805
54	q	0.50	0/303	0.88	0/397
55	r	0.63	0/1122	0.97	1/1515 (0.1%)
56	s	0.68	0/1152	1.02	2/1551 (0.1%)
57	t	0.57	0/955	0.88	0/1279
58	u	0.54	0/1062	0.95	1/1413 (0.1%)
59	v	0.59	0/1093	0.96	0/1460
60	w	0.67	0/964	1.13	0/1289
61	x	0.60	0/902	1.09	0/1209
62	y	0.52	0/929	0.79	0/1242
63	z	0.80	0/960	1.25	0/1278
All	All	0.48	43/186263 (0.0%)	0.83	248/274843 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	A	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
9	B	0	2
10	AA	0	11
13	AE	0	5
14	AF	0	1
20	H	0	3
36	X	0	1
All	All	0	25

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	374	GLU	C-N	17.41	1.53	1.33
10	AA	850	ILE	N-CA	-13.14	1.29	1.46
13	AE	93	THR	CA-C	12.19	1.69	1.52
20	H	169	SER	N-CA	11.73	1.61	1.46
13	AE	70	CYS	CA-CB	-8.69	1.41	1.53
16	D	1339	A	O3'-P	8.39	1.73	1.61
10	AA	869	GLY	C-N	7.59	1.44	1.33
20	H	88	LYS	N-CA	7.04	1.55	1.46
8	7	69	G	C1'-N9	-6.91	1.37	1.48
12	AC	76	GLU	N-CA	-6.91	1.37	1.46
6	5	109	DT	O3'-P	6.84	1.71	1.61
16	D	196	A	O3'-P	6.63	1.71	1.61
16	D	145	G	O3'-P	6.45	1.70	1.61
20	H	168	VAL	C-N	6.39	1.42	1.33
8	7	59	U	C1'-N1	6.31	1.57	1.48
38	a	2434	A	O3'-P	6.09	1.70	1.61
16	D	1275	A	O3'-P	6.09	1.70	1.61
12	AC	75	GLN	CA-C	-6.00	1.45	1.53
8	7	60	U	C1'-N1	5.96	1.57	1.48
20	H	88	LYS	CA-C	5.85	1.60	1.52
13	AE	90	VAL	CA-C	5.70	1.60	1.52
8	7	64	U	C1'-N1	5.59	1.56	1.48
10	AA	885	GLY	C-O	-5.47	1.16	1.23
7	6	10	DG	C1'-N9	-5.42	1.35	1.46
38	a	2167	U	O3'-P	5.41	1.69	1.61
38	a	1905	C	O3'-P	5.28	1.69	1.61
13	AE	1350	ASN	CG-ND2	-5.21	1.22	1.33
10	AA	604	HIS	ND1-CE1	5.21	1.37	1.32
10	AA	1257	GLN	CD-OE1	5.18	1.33	1.23
10	AA	1157	GLN	CD-NE2	-5.16	1.22	1.33
12	AC	160	HIS	CD2-NE2	-5.14	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AE	777	HIS	ND1-CE1	5.14	1.37	1.32
13	AE	424	ASN	CG-ND2	-5.14	1.22	1.33
10	AA	1256	GLN	CD-OE1	5.11	1.33	1.23
10	AA	1116	HIS	CD2-NE2	-5.07	1.32	1.37
10	AA	604	HIS	CD2-NE2	-5.06	1.32	1.37
23	K	56	VAL	CA-CB	5.05	1.57	1.54
12	AC	41	ASN	CG-ND2	-5.02	1.22	1.33
10	AA	760	ASN	CG-ND2	-5.01	1.22	1.33
12	AC	23	HIS	CD2-NE2	-5.00	1.32	1.37
12	AC	23	HIS	ND1-CE1	5.00	1.37	1.32
13	AE	777	HIS	CD2-NE2	-5.00	1.32	1.37
13	AE	1108	GLN	CD-OE1	5.00	1.33	1.23

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	727	VAL	N-CA-C	-17.26	95.03	110.74
20	H	88	LYS	CA-C-N	16.98	143.64	120.38
20	H	88	LYS	C-N-CA	16.98	143.64	120.38
9	B	29	G	C3'-C2'-O2'	15.97	134.65	110.70
10	AA	1250	SER	CA-C-N	14.98	149.67	123.01
10	AA	1250	SER	C-N-CA	14.98	149.67	123.01
10	AA	374	GLU	CA-C-N	14.96	135.79	120.38
10	AA	374	GLU	C-N-CA	14.96	135.79	120.38
20	H	332	VAL	N-CA-C	13.70	124.59	110.62
20	H	169	SER	N-CA-C	12.75	137.96	110.80
20	H	330	VAL	N-CA-C	12.11	126.82	109.51
20	H	305	HIS	N-CA-C	11.96	131.10	111.37
13	AE	90	VAL	N-CA-C	9.89	122.19	107.75
38	a	2244	U	C1'-C2'-O2'	-9.77	93.75	108.40
10	AA	375	PRO	CA-N-CD	-9.73	98.37	112.00
51	n	73	SER	N-CA-CB	-9.57	94.59	110.47
16	D	1206	G	C4'-C3'-O3'	9.54	127.32	113.00
10	AA	935	THR	CA-CB-OG1	-9.45	95.43	109.60
28	P	54	SER	CA-C-N	9.36	129.05	118.85
28	P	54	SER	C-N-CA	9.36	129.05	118.85
38	a	2250	G	C4'-C3'-O3'	-9.29	95.47	109.40
10	AA	376	PRO	N-CA-CB	-9.13	93.66	103.25
16	D	1401	G	C4'-C3'-O3'	8.88	126.33	113.00
16	D	428	G	C4'-C3'-O3'	8.77	122.56	109.40
20	H	339	ARG	CA-C-N	8.57	137.91	121.54
20	H	339	ARG	C-N-CA	8.57	137.91	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	a	2296	U	C4'-C3'-O3'	8.46	122.08	109.40
31	S	45	VAL	N-CA-CB	8.45	120.44	110.55
10	AA	375	PRO	N-CA-C	8.37	120.91	110.70
10	AA	849	GLU	CA-C-N	8.36	137.02	121.97
10	AA	849	GLU	C-N-CA	8.36	137.02	121.97
28	P	57	VAL	N-CA-C	8.31	120.06	107.77
38	a	404	A	C2'-C3'-O3'	8.27	121.91	109.50
38	a	2252	G	N9-C1'-C2'	-8.19	99.72	112.00
16	D	1401	G	N9-C1'-C2'	-7.96	100.07	112.00
10	AA	1048	LYS	CA-C-N	-7.95	115.41	122.96
10	AA	1048	LYS	C-N-CA	-7.95	115.41	122.96
10	AA	859	GLU	CA-C-N	7.89	133.61	121.53
10	AA	859	GLU	C-N-CA	7.89	133.61	121.53
38	a	2425	A	C2'-C3'-O3'	7.86	121.29	109.50
10	AA	855	PRO	N-CA-CB	-7.85	95.01	103.25
20	H	155	LYS	CA-C-N	-7.75	110.97	121.66
20	H	155	LYS	C-N-CA	-7.75	110.97	121.66
38	a	2071	A	C4'-C3'-O3'	-7.72	101.42	113.00
20	H	168	VAL	CA-C-N	7.68	136.20	121.54
20	H	168	VAL	C-N-CA	7.68	136.20	121.54
13	AE	903	LEU	CA-C-N	7.66	136.16	121.54
13	AE	903	LEU	C-N-CA	7.66	136.16	121.54
20	H	52	GLN	N-CA-C	-7.64	104.10	113.50
16	D	1339	A	P-O3'-C3'	7.64	131.65	120.20
51	n	75	ALA	CA-C-N	7.63	129.68	120.14
51	n	75	ALA	C-N-CA	7.63	129.68	120.14
20	H	84	LEU	N-CA-C	7.63	120.99	110.24
16	D	1499	A	N9-C1'-C2'	-7.62	100.57	112.00
36	X	102	THR	CB-CA-C	7.57	123.41	110.84
16	D	528	C	N1-C1'-C2'	-7.57	100.65	112.00
23	K	60	ILE	N-CA-CB	7.56	119.40	110.55
51	n	108	VAL	O-C-N	7.50	125.39	120.07
10	AA	864	LYS	N-CA-C	-7.49	102.38	112.26
20	H	336	ASP	CB-CA-C	-7.43	98.69	110.79
23	K	56	VAL	O-C-N	7.42	125.17	120.42
51	n	73	SER	CB-CA-C	7.40	122.85	110.79
9	B	28	C	P-O3'-C3'	7.29	131.14	120.20
38	a	783	A	C4'-C3'-O3'	7.29	123.94	113.00
38	a	2602	A	C4'-C3'-O3'	7.28	120.33	109.40
19	G	47	VAL	O-C-N	7.22	125.04	120.42
10	AA	751	TYR	CA-C-N	7.18	132.13	121.72
10	AA	751	TYR	C-N-CA	7.18	132.13	121.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	196	A	P-O3'-C3'	7.15	130.93	120.20
38	a	2162	G	C4'-C3'-O3'	7.14	120.11	109.40
9	B	29	G	N9-C1'-C2'	-7.11	101.33	112.00
16	D	1497	G	C1'-C2'-O2'	-7.11	97.73	108.40
10	AA	375	PRO	CB-CA-C	-7.10	102.26	110.92
38	a	1379	U	C2'-C3'-O3'	7.02	124.23	113.70
38	a	896	A	C4'-C3'-O3'	7.02	119.93	109.40
25	M	27	VAL	N-CA-CB	6.98	118.72	110.55
38	a	2225	A	C4'-C3'-O3'	6.95	119.82	109.40
38	a	2244	U	C4'-C3'-O3'	6.90	123.34	113.00
20	H	340	ARG	CA-C-N	-6.87	112.45	123.23
20	H	340	ARG	C-N-CA	-6.87	112.45	123.23
20	H	140	PRO	N-CA-CB	6.86	110.45	103.25
38	a	2252	G	C4'-C3'-O3'	6.83	123.25	113.00
10	AA	604	HIS	CB-CG-CD2	-6.78	122.39	131.20
10	AA	728	ASP	N-CA-C	6.78	125.23	110.80
51	n	71	ARG	CA-C-N	6.76	134.00	122.37
51	n	71	ARG	C-N-CA	6.76	134.00	122.37
12	AC	160	HIS	CB-CG-CD2	-6.75	122.42	131.20
10	AA	855	PRO	CB-CA-C	-6.73	100.45	111.56
38	a	2243	U	C4'-C3'-O3'	6.66	122.99	113.00
12	AC	117	HIS	CB-CA-C	-6.63	97.91	109.64
20	H	170	ARG	N-CA-C	6.63	119.58	110.24
20	H	87	GLU	N-CA-C	-6.62	104.07	111.28
20	H	132	PRO	N-CA-CB	6.60	110.31	103.38
16	D	517	G	C5'-C4'-C3'	6.60	125.10	115.20
20	H	303	LEU	N-CA-C	6.59	121.16	112.13
52	o	13	ARG	N-CA-C	6.58	121.15	113.18
38	a	2189	U	C1'-C2'-O2'	-6.58	101.93	111.80
10	AA	869	GLY	CA-C-O	-6.57	109.14	120.57
10	AA	1116	HIS	CB-CG-CD2	-6.57	122.66	131.20
27	O	72	ILE	N-CA-C	-6.56	105.31	111.48
51	n	127	ASN	CB-CA-C	6.55	121.71	110.77
38	a	894	U	C2'-C3'-O3'	6.54	119.31	109.50
13	AE	450	HIS	CB-CG-CD2	-6.51	122.73	131.20
20	H	155	LYS	N-CA-C	-6.51	98.29	108.90
16	D	526	C	C4'-C3'-O3'	6.51	122.76	113.00
20	H	112	ILE	N-CA-C	6.51	117.07	106.72
55	r	61	VAL	N-CA-CB	6.49	118.15	110.55
51	n	127	ASN	CA-CB-CG	-6.48	106.12	112.60
12	AC	23	HIS	CB-CG-CD2	-6.47	122.79	131.20
38	a	2167	U	P-O3'-C3'	6.47	129.91	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	526	C	N1-C1'-C2'	-6.46	102.31	112.00
16	D	1340	A	C1'-C2'-O2'	6.45	118.07	108.40
16	D	69	G	C4'-C3'-O3'	-6.40	103.39	113.00
38	a	754	U	N1-C1'-C2'	6.40	121.60	112.00
11	AB	81	HIS	CB-CG-CD2	-6.39	122.90	131.20
13	AE	61	ILE	CA-C-N	-6.33	114.05	121.64
13	AE	61	ILE	C-N-CA	-6.33	114.05	121.64
13	AE	93	THR	CA-C-N	6.33	132.95	121.06
13	AE	93	THR	C-N-CA	6.33	132.95	121.06
10	AA	150	HIS	CB-CG-CD2	-6.32	122.98	131.20
13	AE	777	HIS	CB-CG-CD2	-6.31	123.00	131.20
16	D	1208	C	N1-C1'-C2'	-6.27	102.59	112.00
38	a	2434	A	P-O3'-C3'	6.26	129.59	120.20
10	AA	888	THR	CB-CA-C	-6.26	99.33	108.91
20	H	153	GLU	N-CA-C	-6.23	97.53	110.80
16	D	1206	G	N9-C1'-C2'	-6.23	102.66	112.00
20	H	113	ASN	N-CA-C	6.22	118.14	111.36
38	a	2425	A	C4'-C3'-O3'	6.19	118.69	109.40
10	AA	850	ILE	N-CA-CB	6.18	121.42	111.23
9	B	28	C	O3'-P-O5'	-6.17	94.75	104.00
15	C	33	ILE	CA-C-O	-6.16	115.03	121.93
10	AA	861	ALA	CA-C-N	6.13	133.25	121.54
10	AA	861	ALA	C-N-CA	6.13	133.25	121.54
13	AE	70	CYS	CB-CA-C	6.09	120.27	110.29
38	a	271	G	C4'-C3'-O3'	6.04	118.46	109.40
38	a	2210	U	C4'-C3'-O3'	6.00	118.40	109.40
38	a	2820	A	C4'-C3'-O3'	-5.99	104.02	113.00
16	D	1408	A	C4'-C3'-O3'	5.99	121.98	113.00
16	D	1275	A	P-O3'-C3'	5.95	129.12	120.20
38	a	1913	A	C2'-C3'-O3'	5.94	118.41	109.50
16	D	550	G	C3'-C2'-O2'	5.93	119.60	110.70
12	AC	74	VAL	N-CA-C	5.92	117.37	108.96
13	AE	90	VAL	CA-C-O	-5.92	114.24	120.39
25	M	92	ARG	CA-C-N	5.92	125.39	119.24
25	M	92	ARG	C-N-CA	5.92	125.39	119.24
12	AC	75	GLN	N-CA-CB	5.90	119.33	110.19
49	l	108	ILE	N-CA-CB	5.88	118.54	110.54
10	AA	604	HIS	CB-CG-ND1	5.88	131.51	122.70
38	a	2308	G	C2'-C3'-O3'	-5.86	104.91	113.70
10	AA	732	ILE	CB-CA-C	-5.85	103.55	111.15
20	H	109	THR	N-CA-C	-5.85	99.12	109.06
36	X	26	GLY	N-CA-C	-5.85	104.30	112.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	150	LYS	N-CA-C	5.82	118.21	110.53
51	n	72	LYS	N-CA-C	-5.80	99.19	109.06
9	B	29	G	O5'-C5'-C4'	-5.80	102.81	111.50
10	AA	936	ARG	CA-C-O	-5.79	114.03	120.70
10	AA	1116	HIS	CB-CG-ND1	5.79	131.38	122.70
38	a	1905	C	P-O3'-C3'	5.77	128.86	120.20
12	AC	76	GLU	N-CA-C	-5.77	101.75	110.28
38	a	2756	U	C4'-C3'-O3'	5.76	118.05	109.40
12	AC	160	HIS	CB-CG-ND1	5.76	131.34	122.70
9	A	48	C	N1-C1'-C2'	5.75	120.62	112.00
13	AE	91	GLU	N-CA-C	5.75	123.04	110.80
38	a	70	G	C4'-C3'-O3'	5.74	118.02	109.40
20	H	75	VAL	N-CA-C	5.74	116.39	108.12
9	B	48	C	N1-C1'-C2'	5.74	120.61	112.00
16	D	1493	A	C2'-C3'-O3'	5.74	118.11	109.50
16	D	1406	U	N1-C1'-C2'	-5.72	103.42	112.00
38	a	2168	G	C4'-C3'-O3'	-5.67	104.49	113.00
16	D	976	G	C4'-C3'-O3'	-5.67	104.50	113.00
38	a	2017	U	C2'-C3'-O3'	-5.65	105.22	113.70
16	D	1340	A	C5'-C4'-C3'	5.65	124.47	116.00
20	H	114	GLY	N-CA-C	5.62	121.26	111.14
38	a	1757	A	C4'-C3'-O3'	-5.62	104.56	113.00
13	AE	450	HIS	CB-CG-ND1	5.58	131.07	122.70
11	AB	81	HIS	CB-CG-ND1	5.57	131.06	122.70
10	AA	868	SER	N-CA-C	5.56	119.31	112.03
16	D	780	A	C4'-C3'-O3'	-5.56	104.66	113.00
38	a	1568	G	C4'-C3'-O3'	-5.54	104.69	113.00
12	AC	23	HIS	CB-CG-ND1	5.54	131.01	122.70
38	a	2447	G	C2'-C3'-O3'	-5.54	101.20	109.50
10	AA	853	ASP	CA-C-N	5.53	130.33	120.70
10	AA	853	ASP	C-N-CA	5.53	130.33	120.70
38	a	2731	G	C4'-C3'-O3'	-5.52	104.72	113.00
16	D	145	G	P-O3'-C3'	5.51	128.46	120.20
13	AE	69	GLU	CA-C-N	-5.49	113.76	121.72
13	AE	69	GLU	C-N-CA	-5.49	113.76	121.72
10	AA	150	HIS	CB-CG-ND1	5.45	130.88	122.70
38	a	2572	A	C4'-C3'-O3'	-5.40	101.30	109.40
38	a	2068	U	C4'-C3'-O3'	-5.39	104.91	113.00
38	a	2481	G	C4'-C3'-O3'	-5.39	104.92	113.00
13	AE	777	HIS	CB-CG-ND1	5.37	130.75	122.70
13	AE	93	THR	CB-CA-C	5.37	121.10	110.42
38	a	944	C	C4'-C3'-O3'	-5.36	104.96	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	864	A	N9-C1'-C2'	5.35	120.03	112.00
13	AE	90	VAL	O-C-N	-5.35	117.53	123.20
16	D	1499	A	C4'-C3'-O3'	5.34	121.00	113.00
13	AE	70	CYS	N-CA-C	-5.32	101.11	109.25
16	D	1145	A	C4'-C3'-O3'	-5.32	105.02	113.00
38	a	2231	U	C1'-C2'-O2'	5.32	116.38	108.40
38	a	2529	G	C4'-C3'-O3'	-5.31	105.03	113.00
10	AA	375	PRO	N-CA-CB	5.30	108.23	103.08
16	D	517	G	C4'-C3'-O3'	-5.30	101.45	109.40
38	a	1270	C	C2'-C3'-O3'	-5.30	105.76	113.70
58	u	101	ILE	N-CA-C	5.30	116.57	112.12
38	a	375	G	C2'-C3'-O3'	5.29	121.64	113.70
10	AA	1158	LYS	CA-C-N	5.28	131.48	121.97
10	AA	1158	LYS	C-N-CA	5.28	131.48	121.97
38	a	2020	A	C4'-C3'-O3'	-5.28	105.08	113.00
10	AA	732	ILE	N-CA-CB	5.28	116.28	110.53
44	g	5	ILE	N-CA-C	5.27	117.64	111.05
13	AE	73	GLY	N-CA-C	5.26	125.66	113.18
13	AE	88	CYS	N-CA-C	5.24	120.33	113.88
36	X	102	THR	CA-C-O	-5.23	114.90	121.02
38	a	423	A	C2'-C3'-O3'	-5.22	105.87	113.70
9	B	60	U	C2'-C3'-O3'	5.21	117.32	109.50
38	a	2245	U	N1-C1'-C2'	-5.21	104.18	112.00
10	AA	934	PHE	N-CA-C	-5.20	103.80	111.81
10	AA	859	GLU	O-C-N	5.20	129.51	122.59
9	A	60	U	C2'-C3'-O3'	5.18	117.27	109.50
16	D	1335	U	C4'-C3'-O3'	-5.17	105.25	113.00
38	a	528	A	C4'-C3'-O3'	-5.16	105.26	113.00
20	H	128	ARG	CA-C-N	-5.15	114.16	122.81
20	H	128	ARG	C-N-CA	-5.15	114.16	122.81
28	P	25	ILE	N-CA-CB	5.15	117.54	110.54
38	a	328	U	C4'-C3'-O3'	-5.14	105.29	113.00
38	a	1834	U	C4'-C3'-O3'	-5.14	105.30	113.00
56	s	28	LEU	CA-C-N	5.14	127.12	120.44
56	s	28	LEU	C-N-CA	5.14	127.12	120.44
20	H	154	PHE	N-CA-C	-5.13	100.34	109.06
38	a	126	A	C4'-C3'-O3'	-5.11	105.34	113.00
38	a	479	A	C4'-C3'-O3'	5.09	117.04	109.40
38	a	614	A	C2'-C3'-O3'	5.07	117.10	109.50
13	AE	89	GLY	CA-C-N	5.06	129.84	123.10
13	AE	89	GLY	C-N-CA	5.06	129.84	123.10
13	AE	61	ILE	CA-C-O	-5.05	115.69	120.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AC	117	HIS	N-CA-C	5.05	116.81	110.24
13	AE	1184	ASP	N-CA-C	5.05	120.96	109.81
38	a	2193	G	C2'-C3'-O3'	5.04	121.26	113.70
9	B	19	G	N9-C1'-C2'	5.04	119.55	112.00
9	A	19	G	N9-C1'-C2'	5.03	119.55	112.00
15	C	35	GLU	N-CA-C	-5.02	105.99	111.82
38	a	1025	G	C4'-C3'-O3'	5.02	116.93	109.40
20	H	108	VAL	N-CA-C	-5.02	98.90	109.34
38	a	1078	U	C2'-C3'-O3'	-5.02	106.18	113.70
38	a	1991	U	C3'-C2'-O2'	5.01	118.21	110.70
10	AA	377	THR	CA-C-N	5.00	126.95	120.44
10	AA	377	THR	C-N-CA	5.00	126.95	120.44

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	A	19	G	Sidechain
9	A	7	G	Sidechain
10	AA	1134	GLN	Peptide
10	AA	1157	GLN	Peptide
10	AA	1158	LYS	Peptide
10	AA	205	PRO	Peptide
10	AA	594	VAL	Peptide
10	AA	595	THR	Peptide
10	AA	596	ASP	Mainchain
10	AA	696	ASP	Peptide
10	AA	746	ALA	Peptide
10	AA	853	ASP	Mainchain
10	AA	859	GLU	Mainchain
13	AE	1184	ASP	Peptide
13	AE	1326	GLN	Peptide
13	AE	313	GLY	Peptide
13	AE	416	ILE	Peptide
13	AE	804	ALA	Peptide
14	AF	32	VAL	Peptide
9	B	19	G	Sidechain
9	B	7	G	Sidechain
20	H	274	TYR	Peptide
20	H	81	GLU	Peptide
20	H	82	THR	Peptide
36	X	100	GLN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	816	839	839	8	0
2	1	857	922	922	14	0
3	2	746	811	811	5	0
4	3	788	844	844	10	0
5	4	753	780	780	0	0
6	5	472	259	261	23	0
7	6	542	305	306	15	0
8	7	347	168	169	17	0
9	A	1620	826	826	174	0
9	B	1620	813	827	134	0
10	AA	9610	9589	9587	255	0
11	AB	790	783	783	7	0
12	AC	1786	1813	1813	46	0
12	AD	1767	1789	1789	46	0
13	AE	10388	10611	10611	358	0
14	AF	655	663	663	14	0
15	C	544	559	560	23	0
16	D	32656	16420	16438	178	0
17	E	669	719	719	4	0
18	F	589	629	629	8	0
19	G	1760	1785	1785	47	0
20	H	1730	1454	1454	211	0
21	I	1636	1710	1710	4	0
22	J	1643	1707	1707	8	0
23	K	1152	1196	1196	15	0
24	L	848	846	846	3	0
25	M	1181	1235	1235	33	0
26	N	979	1031	1031	6	0
27	O	1022	1070	1070	11	0
28	P	790	831	831	12	0
29	Q	877	887	887	4	0
30	R	939	1001	1001	7	0
31	S	805	844	844	5	0
32	T	714	734	734	8	0
33	U	649	666	666	3	0
34	V	648	691	691	4	0
35	W	663	688	688	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	X	900	964	964	58	0
37	Y	60	30	31	12	0
38	a	61841	31076	31124	279	0
39	b	582	599	599	2	0
40	c	625	652	652	4	0
41	d	2569	1301	1301	4	0
42	e	501	531	531	4	0
43	f	448	488	488	6	0
44	g	522	520	520	11	0
45	h	2082	2154	2154	18	0
46	i	444	459	458	6	0
47	j	1565	1617	1616	16	0
48	k	426	464	464	0	0
49	l	1552	1619	1619	14	0
50	m	377	418	418	10	0
51	n	1410	1443	1444	28	0
52	o	504	572	572	5	0
53	p	1313	1358	1358	7	0
54	q	302	343	343	2	0
55	r	1111	1148	1148	5	0
56	s	1129	1162	1162	13	0
57	t	946	1023	1023	11	0
58	u	1053	1129	1129	9	0
59	v	1074	1157	1157	5	0
60	w	951	994	994	9	0
61	x	892	923	923	8	0
62	y	917	962	962	4	0
63	z	947	1020	1019	13	0
64	AE	1	0	0	0	0
65	AE	2	0	0	0	0
All	All	173097	124644	124726	1930	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1930) 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)
20:H:131:LEU:CB	20:H:167:VAL:CA	1.78	1.61
15:C:12:ARG:HG3	20:H:264:GLU:CB	1.30	1.54
20:H:131:LEU:CB	20:H:167:VAL:HA	1.03	1.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:71:ALA:C	20:H:72:LEU:HD12	1.49	1.37
16:D:1358:U:O4	16:D:1363:A:N1	1.60	1.34
38:a:1839:G:H1'	38:a:1927:A:C8	1.62	1.33
20:H:118:GLY:O	20:H:133:GLY:CA	1.74	1.33
38:a:1021:A:N1	38:a:1141:U:O4	1.63	1.30
16:D:1308:U:H2'	36:X:98:ARG:NH2	1.47	1.26
16:D:1227:A:OP2	36:X:110:LYS:HE3	1.35	1.24
9:A:32:C:O4'	25:M:144:MET:HE1	1.09	1.23
15:C:12:ARG:CG	20:H:264:GLU:CB	2.15	1.22
9:A:18:G:N7	9:A:57:A:N6	1.87	1.21
16:D:948:C:OP2	36:X:105:ASN:OD1	1.53	1.21
16:D:1308:U:C2'	36:X:98:ARG:NH2	2.03	1.21
9:B:18:G:N7	9:B:57:A:N6	1.87	1.21
16:D:563:A:N1	16:D:884:U:O4	1.73	1.21
20:H:267:TRP:CZ2	20:H:340:ARG:HG2	1.75	1.20
16:D:1308:U:H3'	36:X:98:ARG:CZ	1.43	1.20
20:H:118:GLY:O	20:H:133:GLY:HA3	1.27	1.18
9:B:70:G:H2'	9:B:71:C:H5''	1.23	1.16
15:C:44:ILE:HD13	20:H:339:ARG:CG	1.78	1.13
20:H:135:LEU:CB	20:H:167:VAL:CB	2.27	1.12
16:D:1329:A:OP1	36:X:28:THR:HB	1.47	1.11
20:H:119:GLY:HA2	20:H:133:GLY:HA2	1.14	1.11
20:H:267:TRP:CE2	20:H:340:ARG:HG2	1.84	1.11
19:G:19:GLN:CD	20:H:76:GLU:CB	2.19	1.11
9:A:32:C:O4'	25:M:144:MET:CE	1.98	1.10
10:AA:735:LYS:NZ	37:Y:73:U:O4	1.83	1.10
19:G:19:GLN:CD	20:H:76:GLU:HB3	1.67	1.10
38:a:1839:G:C8	38:a:1927:A:H1'	1.87	1.10
9:A:70:G:H2'	9:A:71:C:H5''	1.22	1.09
16:D:1308:U:C3'	36:X:98:ARG:CZ	2.31	1.09
20:H:267:TRP:CH2	20:H:340:ARG:HG2	1.87	1.09
15:C:44:ILE:HD13	20:H:339:ARG:HG2	1.18	1.09
16:D:1308:U:C2'	36:X:98:ARG:HH21	1.63	1.08
19:G:19:GLN:CG	20:H:75:VAL:HG22	1.84	1.07
16:D:1308:U:C3'	36:X:98:ARG:NH2	2.16	1.07
13:AE:24:LEU:HG	13:AE:232:ASN:HD21	1.17	1.06
20:H:71:ALA:O	20:H:72:LEU:HD12	1.54	1.05
9:A:18:G:N2	9:A:55:U:O2	1.90	1.05
20:H:19:ARG:O	20:H:72:LEU:HB2	1.58	1.04
9:B:18:G:N2	9:B:55:U:O2	1.90	1.03
9:A:70:G:C2'	9:A:71:C:H5''	1.89	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:56:C:O4'	51:n:80:ARG:NH2	1.91	1.03
16:D:1227:A:OP2	36:X:110:LYS:CE	2.06	1.02
9:B:56:C:H5'	51:n:80:ARG:CZ	1.90	1.02
20:H:162:LYS:CB	20:H:298:GLU:CD	2.30	1.02
20:H:290:TYR:O	20:H:305:HIS:O	1.77	1.02
10:AA:735:LYS:NZ	37:Y:73:U:C4	2.28	1.02
9:B:70:G:C2'	9:B:71:C:H5''	1.89	1.02
16:D:1329:A:OP1	36:X:28:THR:CB	2.07	1.02
19:G:19:GLN:HG3	20:H:75:VAL:HG22	1.38	1.01
9:A:56:C:H2'	9:A:57:A:H5''	1.39	1.01
13:AE:111:THR:HG23	13:AE:300:GLN:CD	1.86	1.01
9:B:56:C:H2'	9:B:57:A:H5''	1.39	1.01
38:a:2297:A:N1	38:a:2321:U:C4	2.29	1.01
19:G:38:VAL:CG2	20:H:75:VAL:HG21	1.90	1.00
16:D:1308:U:H3'	36:X:98:ARG:NH2	1.76	0.99
16:D:13:U:O4	16:D:20:U:O4	1.79	0.99
16:D:13:U:N3	16:D:915:A:C6	2.29	0.99
20:H:131:LEU:CB	20:H:167:VAL:CB	2.40	0.98
19:G:38:VAL:HG22	20:H:75:VAL:HG21	1.44	0.98
9:A:32:C:C4'	25:M:144:MET:HE1	1.93	0.98
38:a:1839:G:O4'	38:a:1927:A:O4'	1.82	0.97
38:a:1839:G:C1'	38:a:1927:A:C8	2.47	0.97
9:A:32:C:O2'	25:M:86:GLN:CG	2.12	0.97
20:H:118:GLY:O	20:H:133:GLY:HA2	1.63	0.97
20:H:119:GLY:CA	20:H:133:GLY:HA2	1.95	0.97
7:6:15:DC:N4	7:6:16:DC:N4	2.15	0.95
12:AC:158:ARG:HB3	12:AC:158:ARG:HH11	1.32	0.95
13:AE:68:TYR:O	13:AE:75:TYR:CE2	2.20	0.95
8:7:60:U:OP1	13:AE:256:ASP:CG	2.09	0.94
38:a:1839:G:O4'	38:a:1927:A:C1'	2.15	0.94
9:B:72:A:H2'	9:B:73:A:H5''	1.49	0.94
16:D:13:U:C4	16:D:915:A:N6	2.36	0.94
38:a:67:U:N3	38:a:74:A:C6	2.36	0.94
16:D:13:U:N3	16:D:915:A:N6	2.16	0.94
9:B:68:C:H2'	9:B:69:C:H5''	1.50	0.93
10:AA:735:LYS:HD3	37:Y:73:U:H3	1.34	0.92
20:H:135:LEU:HA	20:H:157:ILE:CB	1.98	0.92
9:B:75:C:OP1	38:a:2602:A:C8	2.22	0.92
9:A:72:A:H2'	9:A:73:A:H5''	1.49	0.92
10:AA:878:THR:O	10:AA:920:VAL:HG11	1.68	0.92
10:AA:768:MET:CE	12:AC:80:GLU:OE1	2.17	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:a:2013:A:N6	38:a:2613:U:H3	1.68	0.91
38:a:1406:U:O2'	38:a:1407:G:C5'	2.19	0.91
9:A:56:C:H1'	38:a:2112:G:C6	2.06	0.91
6:5:113:DC:OP2	10:AA:163:LYS:HD3	1.71	0.90
9:A:32:C:O2'	25:M:86:GLN:HG3	1.68	0.90
10:AA:728:ASP:OD1	10:AA:769:PRO:HG2	1.71	0.90
9:B:18:G:N2	9:B:58:A:N7	2.19	0.90
16:D:13:U:C4	16:D:20:U:O4	2.24	0.90
20:H:119:GLY:HA3	20:H:131:LEU:O	1.68	0.90
20:H:279:LYS:HA	20:H:331:MET:HB3	1.54	0.90
20:H:119:GLY:HA2	20:H:133:GLY:CA	2.01	0.90
13:AE:24:LEU:HB2	13:AE:232:ASN:OD1	1.72	0.90
9:A:68:C:H2'	9:A:69:C:H5''	1.51	0.90
20:H:71:ALA:C	20:H:72:LEU:CD1	2.42	0.90
10:AA:870:ILE:HG23	10:AA:884:VAL:HG13	1.51	0.89
13:AE:136:GLU:OE1	13:AE:312:ARG:NH1	2.04	0.89
13:AE:202:ARG:HG2	13:AE:202:ARG:HH11	1.35	0.89
20:H:162:LYS:N	20:H:298:GLU:OE2	2.06	0.89
6:5:109:DT:H2''	10:AA:200:ARG:HG3	1.54	0.89
13:AE:68:TYR:C	13:AE:75:TYR:HE2	1.80	0.89
9:A:18:G:N2	9:A:58:A:N7	2.19	0.89
38:a:2314:A:H1'	51:n:155:THR:HG21	1.54	0.89
6:5:114:DC:H5''	13:AE:1148:ARG:NH2	1.87	0.88
12:AC:91:ARG:NE	12:AC:122:GLU:OE2	2.07	0.88
11:AB:107:GLU:CD	13:AE:288:PRO:HB3	1.99	0.88
44:g:16:CYS:CB	44:g:37:CYS:HB3	2.05	0.87
11:AB:107:GLU:OE1	13:AE:288:PRO:HB3	1.72	0.87
38:a:783:A:N3	38:a:783:A:H2'	1.89	0.87
9:A:33:U:H5''	25:M:84:THR:HG21	1.55	0.87
15:C:31:ASN:OD1	20:H:268:VAL:HG22	1.74	0.87
20:H:348:GLN:N	20:H:348:GLN:OE1	2.08	0.87
20:H:131:LEU:CB	20:H:167:VAL:N	2.37	0.86
13:AE:24:LEU:HG	13:AE:232:ASN:ND2	1.90	0.86
16:D:1308:U:H2'	36:X:98:ARG:HH21	1.06	0.86
10:AA:1090:ASN:O	12:AC:182:ARG:NH1	2.08	0.86
6:5:110:DA:N7	10:AA:183:TRP:CH2	2.43	0.86
16:D:197:A:C6	16:D:221:C:H4'	2.11	0.86
19:G:18:HIS:HA	20:H:43:LYS:HD2	1.55	0.85
9:B:18:G:N7	9:B:57:A:C6	2.44	0.85
20:H:332:VAL:HG11	20:H:335:ILE:HG13	1.57	0.85
22:J:61:VAL:HG21	22:J:200:ILE:HD11	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:a:67:U:N3	38:a:74:A:N6	2.25	0.85
23:K:111:MET:HE2	23:K:125:ALA:HB1	1.59	0.84
13:AE:26:SER:HB2	13:AE:236:TRP:CZ2	2.12	0.84
15:C:12:ARG:HH22	20:H:268:VAL:CG2	1.90	0.84
20:H:135:LEU:CB	20:H:167:VAL:C	2.50	0.84
13:AE:425:ARG:NH1	13:AE:458:ASN:O	2.09	0.84
19:G:16:PHE:HB3	20:H:43:LYS:HA	1.59	0.84
20:H:267:TRP:CD2	20:H:340:ARG:HG2	2.12	0.84
20:H:267:TRP:CH2	20:H:340:ARG:CG	2.61	0.84
13:AE:68:TYR:HB3	13:AE:75:TYR:OH	1.76	0.84
9:B:68:C:C2'	9:B:69:C:H5''	2.08	0.84
9:A:18:G:N7	9:A:57:A:C6	2.44	0.84
10:AA:1314:GLN:HB2	14:AF:28:ARG:HH12	1.43	0.84
9:A:16:C:O2	38:a:2181:U:H5'	1.76	0.84
38:a:2303:G:C2	38:a:2314:A:C2	2.66	0.84
9:A:68:C:C2'	9:A:69:C:H5''	2.08	0.84
14:AF:3:ARG:NH1	14:AF:55:GLU:OE2	2.09	0.83
20:H:267:TRP:CZ3	20:H:340:ARG:HG2	2.11	0.83
13:AE:68:TYR:O	13:AE:75:TYR:HE2	1.58	0.83
4:3:34:VAL:HG13	4:3:67:VAL:HG22	1.58	0.83
9:B:56:C:H5'	51:n:80:ARG:NE	1.93	0.83
20:H:131:LEU:CB	20:H:166:VAL:O	2.26	0.83
13:AE:141:PHE:HE2	13:AE:296:LYS:HB2	1.44	0.82
38:a:1019:U:H3	38:a:1142:A:N6	1.77	0.82
12:AD:86:LYS:CE	13:AE:528:THR:HB	2.09	0.82
19:G:19:GLN:OE1	20:H:75:VAL:O	1.85	0.82
9:A:54:U:H3	9:A:58:A:N6	1.77	0.82
9:A:72:A:C2'	9:A:73:A:H5''	2.08	0.82
10:AA:883:LEU:HD11	10:AA:920:VAL:HG22	1.59	0.82
16:D:37:U:N3	16:D:397:A:N6	2.28	0.82
38:a:1839:G:C1'	38:a:1927:A:N9	2.43	0.82
9:B:54:U:H3	9:B:58:A:N6	1.77	0.81
9:B:72:A:C2'	9:B:73:A:H5''	2.09	0.81
16:D:1227:A:H5'	36:X:110:LYS:NZ	1.94	0.81
6:5:110:DA:N7	10:AA:183:TRP:HH2	1.77	0.81
9:B:76:A:H1'	38:a:2494:G:P	2.20	0.81
20:H:267:TRP:CZ3	20:H:340:ARG:CG	2.63	0.81
38:a:1021:A:N6	38:a:1141:U:H3	1.77	0.81
20:H:305:HIS:CD2	20:H:306:VAL:H	1.98	0.81
10:AA:886:LYS:HE3	10:AA:886:LYS:O	1.80	0.81
9:B:22:G:H2'	9:B:23:C:C6	2.16	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AA:611:GLU:OE2	10:AA:637:ARG:NH2	2.13	0.81
13:AE:141:PHE:CE2	13:AE:296:LYS:HB2	2.15	0.81
20:H:155:LYS:CB	20:H:169:SER:CB	2.58	0.81
13:AE:144:TYR:HE1	13:AE:162:GLU:OE2	1.64	0.81
16:D:972:C:O2'	28:P:57:VAL:CG2	2.29	0.81
20:H:123:GLU:HA	20:H:128:ARG:HA	1.63	0.81
10:AA:1043:ALA:HB1	10:AA:1044:PRO:HD2	1.61	0.81
38:a:585:G:N7	63:z:6:ARG:NH1	2.29	0.81
51:n:125:ARG:O	51:n:127:ASN:ND2	2.14	0.81
13:AE:1169:THR:OG1	13:AE:1192:LYS:NZ	2.13	0.80
9:B:58:A:O2'	9:B:59:A:H3'	1.81	0.80
10:AA:118:LYS:NZ	10:AA:487:LEU:O	2.14	0.80
13:AE:37:GLU:O	13:AE:61:ILE:HD11	1.82	0.80
13:AE:90:VAL:HG13	13:AE:90:VAL:O	1.82	0.80
16:D:1329:A:P	36:X:28:THR:HB	2.22	0.80
13:AE:111:THR:HG23	13:AE:300:GLN:OE1	1.81	0.80
9:B:56:C:C2'	9:B:57:A:H5''	2.11	0.80
38:a:2298:A:C4	38:a:2321:U:C5	2.70	0.80
9:B:18:G:N2	9:B:58:A:C5	2.50	0.80
20:H:122:VAL:O	20:H:129:ALA:N	2.13	0.80
9:A:18:G:N2	9:A:58:A:C5	2.50	0.79
10:AA:724:VAL:CG1	10:AA:774:GLY:H	1.93	0.79
20:H:270:ILE:CG2	20:H:337:GLU:HB3	2.12	0.79
38:a:1019:U:H3	38:a:1142:A:H61	1.28	0.79
38:a:1406:U:O2'	38:a:1407:G:H5''	1.79	0.79
15:C:12:ARG:CB	20:H:264:GLU:CB	2.59	0.79
38:a:2297:A:N1	38:a:2321:U:O4	2.14	0.79
44:g:16:CYS:HB2	44:g:37:CYS:HB3	1.63	0.79
20:H:162:LYS:CA	20:H:298:GLU:OE2	2.17	0.79
9:A:22:G:H2'	9:A:23:C:C6	2.16	0.79
9:A:58:A:O2'	9:A:59:A:H3'	1.81	0.79
9:A:56:C:C2'	9:A:57:A:H5''	2.11	0.79
9:B:7:G:H4'	9:B:8:U:OP1	1.81	0.79
8:7:70:G:O2'	13:AE:425:ARG:NH2	2.15	0.79
9:A:7:G:H4'	9:A:8:U:OP1	1.81	0.79
44:g:18:CYS:HB3	44:g:40:CYS:CB	2.12	0.79
13:AE:87:LYS:HA	13:AE:87:LYS:HE3	1.64	0.79
38:a:1021:A:H61	38:a:1141:U:H3	1.29	0.79
9:A:5:G:H2'	9:A:6:G:H5'	1.66	0.78
19:G:16:PHE:CZ	20:H:41:GLY:O	2.36	0.78
10:AA:1257:GLN:HE22	13:AE:345:LYS:HA	1.48	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AE:186:GLN:HG3	13:AE:238:ILE:HG13	1.65	0.78
20:H:19:ARG:HD3	20:H:73:ASP:CG	2.09	0.78
38:a:2189:U:OP1	38:a:2189:U:O4'	2.00	0.78
9:A:76:A:H2'	38:a:2394:C:H42	1.48	0.78
9:B:5:G:H2'	9:B:6:G:H5'	1.66	0.78
19:G:35:ARG:HD2	20:H:14:LYS:HD3	1.66	0.78
10:AA:1257:GLN:OE1	13:AE:345:LYS:CG	2.32	0.78
12:AC:76:GLU:CD	12:AC:131:CYS:HA	2.09	0.78
9:A:33:U:O3'	25:M:84:THR:OG1	2.02	0.78
10:AA:858:GLY:O	10:AA:860:ALA:N	2.17	0.78
9:B:15:G:N1	9:B:20:U:O2	2.17	0.77
13:AE:1075:ARG:NH2	13:AE:1168:GLU:OE2	2.17	0.77
7:6:15:DC:C4	7:6:16:DC:N4	2.53	0.77
9:A:15:G:N1	9:A:20:U:O2	2.17	0.77
38:a:2756:U:N3	38:a:2758:A:C6	2.53	0.77
9:A:18:G:C5	9:A:57:A:C6	2.72	0.77
9:B:18:G:C5	9:B:57:A:C6	2.72	0.77
38:a:1406:U:O2'	38:a:1407:G:P	2.41	0.77
38:a:2756:U:N3	38:a:2758:A:N6	2.32	0.77
9:A:68:C:C3'	9:A:69:C:H5''	2.15	0.76
10:AA:1246:ARG:HH11	10:AA:1266:GLY:HA2	1.50	0.76
9:B:68:C:C3'	9:B:69:C:H5''	2.15	0.76
20:H:305:HIS:CD2	20:H:306:VAL:N	2.53	0.76
38:a:1406:U:O2'	38:a:1407:G:O5'	2.01	0.76
9:A:70:G:H2'	9:A:71:C:C5'	2.11	0.76
16:D:1358:U:C4	16:D:1363:A:N1	2.53	0.76
47:j:4:LEU:HD23	47:j:29:VAL:HG11	1.65	0.76
6:5:108:DT:H72	10:AA:199:ASP:HB3	1.67	0.76
16:D:197:A:N6	16:D:221:C:H4'	2.01	0.76
10:AA:1272:GLU:OE2	13:AE:798:ARG:NH1	2.19	0.75
13:AE:123:ARG:HG3	13:AE:1337:VAL:HG11	1.67	0.75
15:C:44:ILE:CD1	20:H:339:ARG:CG	2.62	0.75
20:H:109:THR:HA	20:H:153:GLU:HA	1.69	0.75
20:H:131:LEU:CB	20:H:166:VAL:C	2.60	0.75
9:A:41:C:H1'	25:M:143:ARG:HH12	1.52	0.75
9:A:41:C:O4'	25:M:143:ARG:NH1	2.20	0.75
61:x:31:THR:O	61:x:102:ARG:NH1	2.19	0.75
9:A:6:G:O2'	9:A:7:G:O5'	2.05	0.75
9:A:32:C:C1'	25:M:144:MET:HE1	2.16	0.75
10:AA:735:LYS:CD	37:Y:73:U:H3	2.00	0.75
16:D:1227:A:H5'	36:X:110:LYS:HZ2	1.49	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:1228:C:OP1	36:X:107:ARG:NH1	2.20	0.75
19:G:35:ARG:HG3	20:H:10:GLU:OE2	1.86	0.75
44:g:18:CYS:CB	44:g:40:CYS:HB3	2.16	0.75
38:a:2298:A:C4	38:a:2321:U:H5	2.04	0.74
10:AA:871:VAL:N	10:AA:883:LEU:O	2.18	0.74
13:AE:44:ILE:HD12	13:AE:252:LEU:CD2	2.18	0.74
13:AE:110:PRO:HG2	13:AE:183:GLU:HG3	1.68	0.74
12:AD:196:THR:HB	13:AE:443:GLU:HG3	1.68	0.74
9:B:18:G:H1'	9:B:58:A:C2	2.23	0.74
9:A:18:G:H1'	9:A:58:A:C2	2.23	0.74
9:B:6:G:O2'	9:B:7:G:O5'	2.05	0.74
9:B:76:A:H1'	38:a:2494:G:OP1	1.88	0.74
13:AE:202:ARG:HG2	13:AE:202:ARG:NH1	1.99	0.74
23:K:137:VAL:O	23:K:140:THR:OG1	2.04	0.74
20:H:109:THR:CA	20:H:153:GLU:HA	2.18	0.74
9:A:70:G:C3'	9:A:71:C:H5''	2.18	0.74
4:3:36:VAL:HG11	4:3:39:ILE:HD12	1.68	0.74
19:G:19:GLN:CG	20:H:76:GLU:HB2	2.18	0.74
13:AE:211:GLU:HG2	13:AE:215:LYS:HE3	1.70	0.73
9:B:76:A:H2'	9:B:76:A:N3	2.03	0.73
6:5:115:DA:OP1	13:AE:1148:ARG:NE	2.21	0.73
9:B:70:G:C3'	9:B:71:C:H5''	2.18	0.73
16:D:517:G:O2'	16:D:530:G:H4'	1.88	0.73
20:H:304:VAL:HG12	20:H:309:MET:SD	2.28	0.73
12:AC:158:ARG:HB3	12:AC:158:ARG:NH1	2.02	0.73
38:a:1021:A:N1	38:a:1141:U:C4	2.55	0.73
20:H:110:GLY:CA	20:H:153:GLU:O	2.36	0.73
13:AE:107:LEU:HD11	13:AE:242:LEU:HB2	1.70	0.73
10:AA:1047:LEU:O	10:AA:1049:ILE:HD12	1.89	0.73
10:AA:1253:LEU:HD12	13:AE:253:VAL:CG1	2.19	0.73
20:H:19:ARG:HB2	20:H:73:ASP:OD2	1.88	0.73
13:AE:120:LEU:O	13:AE:1330:ARG:NH1	2.21	0.73
9:B:70:G:H2'	9:B:71:C:C5'	2.11	0.72
15:C:44:ILE:HD13	20:H:339:ARG:HG3	1.70	0.72
38:a:67:U:C4	38:a:74:A:N6	2.57	0.72
9:A:18:G:O2'	9:A:60:U:C2	2.41	0.72
20:H:267:TRP:CE3	20:H:340:ARG:CG	2.72	0.72
9:A:33:U:H5''	25:M:84:THR:CG2	2.19	0.72
9:B:46:G:H1'	9:B:47:U:C5	2.25	0.72
16:D:827:U:H3	16:D:872:A:N6	1.87	0.72
38:a:1839:G:H1'	38:a:1927:A:N9	2.03	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:12:ARG:HB2	20:H:264:GLU:CB	2.20	0.72
20:H:70:VAL:HA	20:H:85:SER:CB	2.20	0.72
13:AE:1143:ASP:OD1	13:AE:1148:ARG:NH1	2.21	0.72
9:B:76:A:H2'	38:a:2493:U:H5''	1.72	0.72
38:a:1913:A:OP2	38:a:1913:A:H3'	1.89	0.72
10:AA:1043:ALA:HB1	10:AA:1044:PRO:CD	2.19	0.72
13:AE:157:GLN:OE1	13:AE:157:GLN:HA	1.88	0.72
13:AE:142:GLU:HG3	13:AE:142:GLU:O	1.89	0.72
19:G:16:PHE:CB	20:H:43:LYS:HA	2.20	0.72
38:a:1839:G:C1'	38:a:1927:A:C1'	2.67	0.72
13:AE:220:ARG:HG2	13:AE:220:ARG:HH11	1.55	0.71
9:B:18:G:O2'	9:B:60:U:C2	2.41	0.71
9:A:46:G:H1'	9:A:47:U:C5	2.25	0.71
10:AA:839:VAL:O	10:AA:886:LYS:HD3	1.90	0.71
20:H:267:TRP:CE3	20:H:340:ARG:HG2	2.25	0.71
44:g:18:CYS:CB	44:g:40:CYS:CB	2.69	0.71
13:AE:44:ILE:HD12	13:AE:252:LEU:HD21	1.71	0.71
16:D:1308:U:O5'	36:X:98:ARG:HG3	1.90	0.71
13:AE:210:SER:HB3	13:AE:213:LYS:HB2	1.71	0.71
9:B:72:A:C3'	9:B:73:A:H5''	2.20	0.71
20:H:86:ARG:O	20:H:89:ALA:HB3	1.91	0.71
9:A:72:A:C3'	9:A:73:A:H5''	2.20	0.71
10:AA:1257:GLN:OE1	13:AE:345:LYS:HD3	1.89	0.71
10:AA:19:PRO:HA	10:AA:1156:ARG:HD3	1.73	0.71
10:AA:207:THR:OG1	10:AA:354:ASP:OD2	2.09	0.71
36:X:96:PRO:HG2	36:X:102:THR:CG2	2.21	0.71
13:AE:128:LEU:HD11	13:AE:189:LEU:HG	1.73	0.71
27:O:84:THR:HG21	27:O:103:PHE:HB3	1.71	0.71
13:AE:105:ILE:HD12	13:AE:242:LEU:HD22	1.71	0.70
9:B:18:G:C5	9:B:57:A:N6	2.59	0.70
38:a:2013:A:N6	38:a:2613:U:N3	2.33	0.70
12:AD:86:LYS:HE3	13:AE:528:THR:HB	1.72	0.70
9:A:15:G:H2'	9:A:15:G:N3	2.06	0.70
16:D:1309:G:H8	36:X:98:ARG:NH2	1.89	0.70
20:H:70:VAL:HA	20:H:85:SER:CA	2.22	0.70
30:R:86:ARG:HG3	30:R:86:ARG:O	1.89	0.70
9:B:15:G:H2'	9:B:15:G:N3	2.06	0.70
10:AA:878:THR:HA	10:AA:925:SER:HA	1.73	0.70
19:G:19:GLN:CD	20:H:76:GLU:HB2	2.08	0.70
9:A:32:C:C4'	25:M:144:MET:CE	2.66	0.70
13:AE:68:TYR:C	13:AE:75:TYR:CE2	2.65	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:18:G:C5	9:A:57:A:N6	2.59	0.70
20:H:19:ARG:HD3	20:H:73:ASP:OD1	1.92	0.70
38:a:2310:C:O2'	51:n:74:VAL:CG1	2.40	0.70
1:0:80:ARG:NH2	38:a:572:A:OP2	2.25	0.70
10:AA:839:VAL:HA	10:AA:1048:LYS:O	1.91	0.70
9:A:11:A:H2'	9:A:12:G:O4'	1.92	0.69
38:a:742:A:H2'	38:a:743:A:C8	2.26	0.69
38:a:2314:A:C1'	51:n:155:THR:HG21	2.21	0.69
9:A:41:C:C1'	25:M:143:ARG:NH1	2.55	0.69
9:A:16:C:O2	38:a:2181:U:C5'	2.40	0.69
38:a:1021:A:H3'	38:a:1021:A:N3	2.07	0.69
38:a:1839:G:H8	38:a:1927:A:H1'	1.54	0.69
10:AA:878:THR:O	10:AA:920:VAL:CG1	2.40	0.69
10:AA:883:LEU:HD11	10:AA:920:VAL:CG2	2.21	0.69
10:AA:1047:LEU:O	10:AA:1049:ILE:CD1	2.40	0.69
13:AE:54:ASP:OD1	13:AE:54:ASP:N	2.24	0.69
16:D:915:A:N6	16:D:916:U:C4	2.60	0.69
13:AE:395:LYS:HZ2	13:AE:399:LYS:CD	2.06	0.69
9:A:32:C:C1'	25:M:144:MET:CE	2.69	0.69
45:h:146:MET:HE3	45:h:154:LEU:HD21	1.74	0.69
12:AC:76:GLU:OE1	12:AC:131:CYS:HA	1.92	0.69
16:D:1308:U:C3'	36:X:98:ARG:HH21	1.92	0.69
38:a:927:A:H2'	38:a:928:A:C8	2.28	0.69
38:a:1839:G:C4	38:a:1927:A:C4	2.81	0.69
13:AE:94:GLN:HB2	13:AE:97:VAL:HG23	1.76	0.69
20:H:110:GLY:HA3	20:H:153:GLU:O	1.93	0.69
10:AA:768:MET:HE1	12:AC:80:GLU:OE1	1.94	0.68
16:D:37:U:H3	16:D:397:A:N6	1.90	0.68
10:AA:935:THR:HA	10:AA:1049:ILE:HD12	1.74	0.68
13:AE:39:LYS:O	13:AE:273:ILE:CG2	2.41	0.68
13:AE:161:THR:HG22	13:AE:164:GLN:HB2	1.76	0.68
20:H:19:ARG:HD3	20:H:73:ASP:OD2	1.92	0.68
20:H:117:LYS:CB	20:H:279:LYS:O	2.41	0.68
13:AE:832:LYS:C	13:AE:1242:ARG:HH12	2.01	0.68
38:a:1153:C:OP1	63:z:92:ARG:NH1	2.27	0.68
38:a:2310:C:O2'	51:n:74:VAL:HG12	1.94	0.68
7:6:8:DC:C2'	7:6:9:DT:H71	2.24	0.68
16:D:13:U:O4	16:D:21:G:C2	2.46	0.68
38:a:1596:A:H2'	38:a:1597:A:C8	2.28	0.68
38:a:2756:U:C4	38:a:2758:A:N6	2.61	0.68
10:AA:802:VAL:HA	10:AA:1096:ILE:O	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:5:G:H2'	9:B:6:G:C5'	2.24	0.68
36:X:96:PRO:CG	36:X:102:THR:CG2	2.71	0.68
9:B:11:A:H2'	9:B:12:G:O4'	1.92	0.68
16:D:972:C:O2'	28:P:57:VAL:HG23	1.92	0.68
16:D:563:A:N1	16:D:884:U:C4	2.60	0.67
10:AA:768:MET:HE1	12:AC:80:GLU:CD	2.19	0.67
12:AC:76:GLU:OE2	12:AC:131:CYS:HA	1.95	0.67
13:AE:141:PHE:CD2	13:AE:293:ARG:O	2.47	0.67
10:AA:859:GLU:OE2	10:AA:859:GLU:N	2.21	0.67
10:AA:1253:LEU:HD12	13:AE:253:VAL:HG11	1.77	0.67
13:AE:111:THR:CG2	13:AE:300:GLN:CD	2.66	0.67
9:B:66:C:H5'	9:B:66:C:H6	1.60	0.67
20:H:70:VAL:HA	20:H:85:SER:HA	1.77	0.67
38:a:1920:C:O5'	38:a:1920:C:H6	1.77	0.67
36:X:96:PRO:CG	36:X:102:THR:HG22	2.25	0.67
10:AA:728:ASP:OD1	10:AA:769:PRO:CG	2.41	0.67
20:H:267:TRP:CD2	20:H:340:ARG:CG	2.76	0.67
38:a:1839:G:C8	38:a:1927:A:C1'	2.74	0.67
9:A:5:G:H2'	9:A:6:G:C5'	2.24	0.67
38:a:1779:U:H5	38:a:1784:A:N7	1.92	0.67
9:A:19:G:N2	38:a:2112:G:C8	2.62	0.67
13:AE:984:LEU:HB3	13:AE:993:GLU:HB2	1.77	0.67
16:D:1329:A:P	36:X:28:THR:CB	2.83	0.67
34:V:25:ILE:HD11	34:V:61:ILE:HD11	1.77	0.67
10:AA:339:ASN:HB3	10:AA:343:HIS:H	1.58	0.66
7:6:16:DC:H1'	13:AE:426:ALA:HB1	1.76	0.66
13:AE:108:ALA:CB	13:AE:279:LEU:HD22	2.25	0.66
20:H:110:GLY:H	20:H:153:GLU:CA	2.08	0.66
13:AE:117:LEU:HD12	13:AE:117:LEU:O	1.94	0.66
13:AE:1355:ARG:NH1	13:AE:1369:ARG:HH12	1.93	0.66
20:H:110:GLY:N	20:H:153:GLU:C	2.53	0.66
10:AA:1251:TYR:C	10:AA:1259:LEU:CD1	2.69	0.66
19:G:16:PHE:HZ	20:H:41:GLY:O	1.77	0.66
9:A:56:C:C5	38:a:2168:G:C6	2.83	0.66
9:A:66:C:H6	9:A:66:C:H5'	1.60	0.66
13:AE:193:ASP:HB3	13:AE:196:GLN:HB2	1.78	0.66
10:AA:9:LYS:HG2	10:AA:1171:ARG:NH1	2.11	0.66
12:AD:102:LEU:HB2	12:AD:115:ILE:HG13	1.77	0.66
20:H:162:LYS:CB	20:H:298:GLU:OE1	2.44	0.66
13:AE:1037:PHE:HB3	13:AE:1040:MET:HB2	1.78	0.65
9:B:21:A:H4'	9:B:21:A:OP1	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:270:ILE:HG23	20:H:337:GLU:HB3	1.78	0.65
10:AA:839:VAL:O	10:AA:886:LYS:CD	2.44	0.65
12:AD:86:LYS:HE3	13:AE:528:THR:CG2	2.26	0.65
13:AE:978:ARG:HG2	13:AE:1197:ASN:HD21	1.60	0.65
9:B:18:G:C8	9:B:57:A:C6	2.85	0.65
9:B:56:C:H5'	51:n:80:ARG:NH2	2.10	0.65
16:D:1308:U:H5''	36:X:98:ARG:HG2	1.77	0.65
20:H:85:SER:O	20:H:88:LYS:CB	2.45	0.65
9:A:21:A:H4'	9:A:21:A:OP1	1.95	0.65
10:AA:735:LYS:CE	37:Y:73:U:O4	2.44	0.65
9:B:76:A:H1'	38:a:2493:U:O3'	1.97	0.65
20:H:52:GLN:O	20:H:53:PHE:CD1	2.50	0.65
20:H:118:GLY:C	20:H:133:GLY:CA	2.67	0.65
38:a:1923:U:H2'	38:a:1923:U:OP2	1.96	0.65
13:AE:108:ALA:HB3	13:AE:279:LEU:HD22	1.77	0.65
16:D:197:A:C6	16:D:221:C:C4'	2.79	0.65
10:AA:735:LYS:NZ	37:Y:73:U:N3	2.41	0.65
13:AE:975:ILE:HG22	13:AE:977:SER:H	1.62	0.65
16:D:1227:A:OP2	36:X:110:LYS:NZ	2.29	0.65
20:H:72:LEU:HD12	20:H:72:LEU:N	2.11	0.65
20:H:267:TRP:CE3	20:H:340:ARG:HG3	2.32	0.65
9:A:3:C:H2'	9:A:4:G:H8	1.62	0.65
10:AA:852:ALA:O	10:AA:854:ILE:N	2.28	0.65
13:AE:68:TYR:HB3	13:AE:75:TYR:CE2	2.32	0.65
9:A:22:G:H2'	9:A:23:C:H6	1.62	0.65
10:AA:1257:GLN:OE1	13:AE:345:LYS:HG2	1.96	0.65
13:AE:162:GLU:OE1	13:AE:162:GLU:HA	1.97	0.65
53:p:24:ILE:HD13	53:p:72:LEU:HD21	1.77	0.65
9:A:18:G:C8	9:A:57:A:C6	2.85	0.64
10:AA:529:ARG:HH11	10:AA:572:ILE:HG22	1.62	0.64
9:B:3:C:H2'	9:B:4:G:H8	1.62	0.64
10:AA:9:LYS:HG2	10:AA:1171:ARG:HH12	1.61	0.64
13:AE:141:PHE:HD2	13:AE:293:ARG:O	1.80	0.64
16:D:1308:U:O5'	36:X:98:ARG:CG	2.45	0.64
38:a:1082:U:N3	38:a:1086:A:N6	2.45	0.64
9:B:75:C:OP1	38:a:2602:A:N9	2.30	0.64
36:X:96:PRO:HG3	36:X:102:THR:HG22	1.78	0.64
2:1:36:LEU:HD13	2:1:48:LYS:HA	1.80	0.64
10:AA:768:MET:HE3	12:AC:80:GLU:OE1	1.95	0.64
13:AE:67:ASP:OD1	13:AE:95:THR:OG1	2.15	0.64
38:a:1909:C:O5'	38:a:1909:C:H6	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AA:1257:GLN:OE1	13:AE:345:LYS:CD	2.44	0.64
16:D:1358:U:O4	16:D:1363:A:C2	2.47	0.64
19:G:18:HIS:HA	20:H:43:LYS:CD	2.28	0.64
38:a:1839:G:O4'	38:a:1927:A:H1'	1.97	0.64
52:o:26:HIS:CE1	52:o:48:ALA:HB2	2.32	0.64
9:B:50:U:H2'	9:B:51:C:C6	2.33	0.64
6:5:98:DA:C2'	6:5:99:DT:H72	2.28	0.64
9:A:50:U:H2'	9:A:51:C:C6	2.33	0.64
16:D:1309:G:C8	36:X:98:ARG:NH2	2.66	0.64
38:a:2303:G:N3	38:a:2314:A:C2	2.66	0.64
16:D:1358:U:N3	16:D:1363:A:N6	2.46	0.64
20:H:135:LEU:CA	20:H:157:ILE:CB	2.74	0.64
56:s:114:LEU:HG	56:s:118:MET:HE3	1.78	0.64
13:AE:84:ILE:O	13:AE:84:ILE:HG13	1.96	0.64
9:B:22:G:H2'	9:B:23:C:H6	1.62	0.64
38:a:2885:G:N7	46:i:40:ARG:NH2	2.46	0.64
11:AB:93:ILE:HG22	13:AE:290:ILE:CG2	2.27	0.63
13:AE:136:GLU:CD	13:AE:312:ARG:HH22	2.06	0.63
16:D:1059:C:O2	28:P:55:PRO:HG3	1.99	0.63
9:A:41:C:C4'	25:M:143:ARG:NH1	2.61	0.63
19:G:19:GLN:CG	20:H:76:GLU:CB	2.76	0.63
10:AA:1257:GLN:HE22	13:AE:345:LYS:CA	2.09	0.63
13:AE:128:LEU:HA	13:AE:192:MET:HE1	1.81	0.63
19:G:38:VAL:HG22	20:H:75:VAL:CG2	2.24	0.63
20:H:332:VAL:HG12	20:H:334:ASP:H	1.62	0.63
8:7:60:U:OP1	13:AE:256:ASP:N	2.31	0.63
9:A:37:A:O2'	9:A:38:A:H5'	1.99	0.63
10:AA:1251:TYR:C	10:AA:1259:LEU:HD13	2.24	0.63
6:5:101:DT:OP2	13:AE:275:ARG:NH2	2.31	0.63
10:AA:118:LYS:NZ	10:AA:485:ASP:OD1	2.25	0.63
12:AC:71:LYS:HZ1	12:AC:140:ILE:HB	1.62	0.63
13:AE:92:VAL:O	13:AE:92:VAL:HG12	1.99	0.63
14:AF:29:GLN:HB3	14:AF:35:LYS:HD2	1.80	0.63
19:G:35:ARG:HH21	20:H:10:GLU:HG2	1.62	0.63
9:A:69:C:H2'	9:A:70:G:O4'	1.99	0.63
10:AA:13:LYS:HB2	10:AA:1180:MET:HE2	1.81	0.63
13:AE:144:TYR:CE1	13:AE:162:GLU:OE2	2.51	0.63
53:p:121:ILE:HD12	53:p:141:ILE:HG22	1.79	0.63
20:H:49:PRO:CD	20:H:84:LEU:HD11	2.29	0.63
20:H:270:ILE:HG21	20:H:337:GLU:HB3	1.80	0.63
13:AE:1355:ARG:NH1	13:AE:1369:ARG:NH1	2.47	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:267:TRP:CZ2	20:H:340:ARG:CG	2.68	0.63
9:A:56:C:O2	38:a:2112:G:C4	2.52	0.62
10:AA:724:VAL:HG23	10:AA:734:ILE:HD13	1.80	0.62
13:AE:395:LYS:HZ2	13:AE:399:LYS:HD3	1.63	0.62
16:D:37:U:O2	16:D:548:G:C2	2.52	0.62
38:a:2189:U:O4'	38:a:2189:U:P	2.57	0.62
38:a:2297:A:C2	38:a:2321:U:C4	2.86	0.62
9:A:31:G:O2'	25:M:144:MET:SD	2.56	0.62
13:AE:245:LEU:HG	13:AE:246:PRO:HD2	1.80	0.62
20:H:270:ILE:CG2	20:H:337:GLU:CB	2.77	0.62
25:M:23:LEU:O	25:M:27:VAL:HG13	2.00	0.62
38:a:1998:A:OP2	47:j:141:ARG:NH2	2.32	0.62
13:AE:111:THR:CG2	13:AE:300:GLN:NE2	2.63	0.62
13:AE:201:LEU:HB2	13:AE:221:ILE:HD13	1.80	0.62
10:AA:850:ILE:O	10:AA:850:ILE:HG22	1.98	0.62
12:AD:176:CYS:SG	13:AE:535:ARG:NH2	2.72	0.62
16:D:1358:U:H3	16:D:1363:A:N6	1.96	0.62
38:a:1839:G:N9	38:a:1927:A:N9	2.48	0.62
9:A:54:U:N3	9:A:58:A:N6	2.47	0.62
10:AA:1328:LYS:HD2	13:AE:102:MET:SD	2.40	0.62
20:H:110:GLY:N	20:H:153:GLU:O	2.32	0.62
13:AE:395:LYS:NZ	13:AE:399:LYS:HD3	2.15	0.62
16:D:13:U:C5	16:D:20:U:O4	2.53	0.62
20:H:280:LEU:N	20:H:330:VAL:O	2.32	0.62
6:5:108:DT:O4	10:AA:199:ASP:OD2	2.18	0.62
10:AA:735:LYS:HD3	37:Y:73:U:N3	2.13	0.62
13:AE:44:ILE:CD1	13:AE:252:LEU:HD21	2.29	0.62
9:A:41:C:C1'	25:M:143:ARG:HH12	2.12	0.62
16:D:827:U:N3	16:D:872:A:N6	2.45	0.62
9:A:42:G:H2'	9:A:43:A:H8	1.65	0.62
1:0:40:MET:HE1	63:z:105:ALA:HB1	1.80	0.62
9:B:42:G:H2'	9:B:43:A:H8	1.65	0.62
9:B:56:C:C4'	51:n:80:ARG:NH2	2.63	0.62
36:X:101:ARG:O	36:X:101:ARG:HD3	2.00	0.62
3:2:50:LEU:HD23	42:e:26:PHE:CE1	2.35	0.61
9:B:69:C:H2'	9:B:70:G:O4'	1.99	0.61
15:C:29:LEU:O	15:C:33:ILE:HG23	2.00	0.61
15:C:44:ILE:CD1	20:H:339:ARG:HG2	2.12	0.61
19:G:18:HIS:CA	20:H:43:LYS:HD2	2.29	0.61
20:H:19:ARG:O	20:H:72:LEU:CB	2.41	0.61
28:P:57:VAL:O	28:P:58:ASN:CG	2.43	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:a:1789:A:OP2	45:h:221:ARG:NH1	2.32	0.61
10:AA:840:SER:O	10:AA:840:SER:OG	2.19	0.61
13:AE:223:LEU:HG	13:AE:223:LEU:O	2.00	0.61
16:D:13:U:O4	16:D:20:U:C4	2.51	0.61
13:AE:68:TYR:HB3	13:AE:75:TYR:CZ	2.35	0.61
13:AE:1161:GLY:HA3	13:AE:1179:PRO:HA	1.83	0.61
20:H:304:VAL:HG12	20:H:304:VAL:O	1.99	0.61
38:a:754:U:H2'	38:a:755:U:C6	2.35	0.61
9:A:6:G:HO2'	9:A:7:G:H8	1.47	0.61
9:A:33:U:H4'	25:M:84:THR:HB	1.82	0.61
9:B:54:U:N3	9:B:58:A:N6	2.47	0.61
16:D:658:C:H1'	32:T:22:THR:HG21	1.83	0.61
33:U:21:VAL:HG21	33:U:60:TRP:CD1	2.36	0.61
9:A:76:A:H2'	38:a:2394:C:N4	2.11	0.61
38:a:1406:U:HO2'	38:a:1407:G:C5'	2.09	0.61
10:AA:1223:ARG:NH2	13:AE:721:SER:OG	2.34	0.61
9:B:3:C:H2'	9:B:4:G:C8	2.36	0.61
13:AE:90:VAL:O	13:AE:90:VAL:CG1	2.48	0.61
9:B:65:C:H2'	9:B:66:C:H5'	1.82	0.61
20:H:84:LEU:HD22	20:H:84:LEU:N	2.16	0.61
7:6:15:DC:N4	7:6:16:DC:H41	1.96	0.61
19:G:19:GLN:CD	20:H:75:VAL:HG22	2.25	0.61
20:H:305:HIS:O	20:H:306:VAL:HB	2.00	0.61
38:a:2297:A:C2	38:a:2321:U:C5	2.89	0.60
13:AE:67:ASP:OD1	13:AE:67:ASP:N	2.34	0.60
7:6:15:DC:C4	7:6:16:DC:C4	2.88	0.60
13:AE:412:LEU:HD22	13:AE:441:LEU:HD21	1.84	0.60
13:AE:951:GLN:NE2	13:AE:1014:GLY:O	2.35	0.60
16:D:1218:C:H2'	16:D:1219:A:C8	2.36	0.60
9:A:3:C:H2'	9:A:4:G:C8	2.36	0.60
19:G:19:GLN:HG3	20:H:76:GLU:HB2	1.82	0.60
10:AA:374:GLU:HG3	10:AA:374:GLU:O	2.01	0.60
10:AA:478:ARG:NH1	10:AA:491:ASP:O	2.34	0.60
13:AE:118:LYS:HD2	13:AE:312:ARG:NH2	2.17	0.60
13:AE:154:LEU:HD21	13:AE:160:LEU:HD21	1.83	0.60
20:H:305:HIS:HD2	20:H:306:VAL:H	1.49	0.60
9:A:34:C:P	25:M:84:THR:OG1	2.60	0.60
9:A:41:C:H4'	25:M:143:ARG:CZ	2.32	0.60
10:AA:528:ARG:NH2	10:AA:576:SER:O	2.34	0.60
10:AA:660:VAL:HG13	10:AA:661:VAL:HG13	1.82	0.60
16:D:1308:U:H2'	36:X:98:ARG:HH22	1.61	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:a:1921:G:O5'	38:a:1921:G:H8	1.85	0.60
13:AE:514:THR:HG21	13:AE:596:LEU:HD12	1.84	0.60
13:AE:926:PRO:HG2	13:AE:1248:ILE:HD11	1.84	0.60
43:f:24:LEU:HD11	43:f:54:MET:HE2	1.83	0.60
13:AE:802:ASP:OD1	13:AE:1348:LYS:NZ	2.31	0.60
19:G:19:GLN:CG	20:H:75:VAL:CG2	2.70	0.60
19:G:19:GLN:HG3	20:H:75:VAL:CG2	2.23	0.60
31:S:47:LYS:O	31:S:50:THR:OG1	2.12	0.60
13:AE:201:LEU:HD11	13:AE:220:ARG:HH11	1.67	0.60
20:H:267:TRP:CE2	20:H:340:ARG:CG	2.73	0.60
38:a:2720:U:OP1	62:y:53:ARG:NH2	2.34	0.60
13:AE:342:LEU:HD23	13:AE:1352:ILE:HG23	1.83	0.60
9:B:6:G:HO2'	9:B:7:G:H8	1.50	0.60
20:H:284:VAL:HG12	20:H:294:VAL:HB	1.84	0.60
23:K:107:ALA:HB2	23:K:125:ALA:HB3	1.83	0.60
10:AA:888:THR:OG1	10:AA:889:PRO:HD2	2.02	0.59
12:AD:86:LYS:HE3	13:AE:528:THR:CB	2.32	0.59
9:B:47:U:O2'	9:B:50:U:P	2.60	0.59
38:a:70:G:H4'	38:a:71:A:OP1	2.02	0.59
9:A:47:U:O2'	9:A:50:U:P	2.60	0.59
9:A:65:C:H2'	9:A:66:C:H5'	1.82	0.59
4:3:36:VAL:CG1	4:3:39:ILE:HD12	2.32	0.59
10:AA:861:ALA:HA	10:AA:882:ILE:HD13	1.83	0.59
13:AE:99:ARG:HG3	13:AE:99:ARG:NH1	2.17	0.59
15:C:44:ILE:CD1	20:H:339:ARG:HG3	2.29	0.59
20:H:305:HIS:CD2	20:H:307:SER:H	2.19	0.59
25:M:69:VAL:HG23	25:M:100:ALA:HB1	1.83	0.59
9:A:35:A:H2'	9:A:36:U:C6	2.38	0.59
20:H:117:LYS:CB	20:H:278:THR:HG23	2.32	0.59
38:a:2683:C:OP1	62:y:51:ARG:NH2	2.31	0.59
13:AE:370:LYS:HG2	13:AE:441:LEU:HD23	1.84	0.59
14:AF:26:ARG:NH1	14:AF:67:ARG:HH12	2.00	0.59
17:E:25:ARG:HA	17:E:66:LEU:HD21	1.85	0.59
18:F:4:ILE:CD1	18:F:19:PHE:HA	2.33	0.59
20:H:270:ILE:HG21	20:H:337:GLU:CB	2.32	0.59
50:m:31:LEU:HD22	50:m:42:LEU:HD13	1.84	0.59
20:H:118:GLY:C	20:H:133:GLY:HA2	2.28	0.59
20:H:119:GLY:CA	20:H:131:LEU:O	2.46	0.59
10:AA:376:PRO:O	10:AA:376:PRO:HG2	2.02	0.59
10:AA:1184:THR:HG23	10:AA:1190:ALA:H	1.67	0.59
12:AD:81:ILE:HD13	12:AD:131:CYS:HB2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AE:416:ILE:HG13	13:AE:441:LEU:HD11	1.83	0.59
16:D:563:A:N6	16:D:884:U:N3	2.51	0.59
16:D:1308:U:C5'	36:X:98:ARG:HG2	2.32	0.59
10:AA:1256:GLN:OE1	10:AA:1256:GLN:HA	2.03	0.59
12:AC:76:GLU:OE1	12:AC:131:CYS:CA	2.51	0.59
13:AE:97:VAL:HG11	13:AE:101:ARG:NH2	2.18	0.59
38:a:2572:A:C8	47:j:149:ASN:OD1	2.56	0.59
10:AA:218:GLU:OE2	10:AA:300:ASP:N	2.28	0.59
20:H:119:GLY:HA3	20:H:132:PRO:C	2.28	0.59
6:5:99:DT:H2''	6:5:100:DA:H5''	1.85	0.58
10:AA:735:LYS:HZ2	37:Y:73:U:H3	1.50	0.58
16:D:404:G:N7	22:J:2:ALA:HB3	2.17	0.58
16:D:1225:A:H4'	35:W:78:ARG:NH1	2.17	0.58
19:G:35:ARG:HD2	20:H:14:LYS:CD	2.32	0.58
38:a:1021:A:C2	38:a:1141:U:O4	2.50	0.58
47:j:33:ARG:NH1	47:j:53:GLY:O	2.36	0.58
10:AA:1084:ASP:OD1	12:AC:45:ARG:NH1	2.32	0.58
9:A:58:A:H1'	9:A:60:U:C5	2.38	0.58
13:AE:438:GLU:HG3	13:AE:485:MET:HE1	1.85	0.58
33:U:4:ILE:HG12	33:U:21:VAL:HG22	1.84	0.58
13:AE:241:VAL:HG12	13:AE:241:VAL:O	2.04	0.58
20:H:331:MET:N	20:H:331:MET:SD	2.75	0.58
38:a:1590:A:H2'	38:a:1591:A:C8	2.38	0.58
13:AE:161:THR:HG23	13:AE:164:GLN:H	1.68	0.58
16:D:13:U:C2	16:D:915:A:N6	2.70	0.58
20:H:110:GLY:N	20:H:153:GLU:CA	2.67	0.58
13:AE:24:LEU:CG	13:AE:232:ASN:ND2	2.63	0.58
19:G:19:GLN:NE2	20:H:75:VAL:HG22	2.19	0.58
19:G:217:VAL:O	19:G:220:THR:HG22	2.02	0.58
36:X:104:THR:O	36:X:104:THR:HG22	2.03	0.58
10:AA:1142:ARG:NH2	10:AA:1166:ASP:OD1	2.36	0.58
13:AE:275:ARG:NH1	13:AE:278:ARG:NH1	2.51	0.58
22:J:48:LEU:HD23	22:J:53:VAL:HG12	1.84	0.58
9:B:58:A:H1'	9:B:60:U:C5	2.38	0.58
20:H:291:GLY:HA2	20:H:305:HIS:HA	1.86	0.58
11:AB:93:ILE:HG22	13:AE:290:ILE:HG22	1.85	0.58
9:B:60:U:P	9:B:61:C:H41	2.27	0.58
20:H:332:VAL:CG1	20:H:335:ILE:HG13	2.33	0.58
2:1:20:VAL:HG11	2:1:44:ALA:HA	1.86	0.57
8:7:60:U:OP2	13:AE:255:LEU:HA	2.04	0.57
8:7:70:G:H21	13:AE:427:PRO:HD3	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AE:160:LEU:HD22	13:AE:164:GLN:HB3	1.86	0.57
16:D:439:U:O2	16:D:440:C:C6	2.56	0.57
13:AE:1046:ILE:HD12	13:AE:1059:LEU:HB3	1.86	0.57
10:AA:10:ARG:NH1	10:AA:697:LYS:HD3	2.19	0.57
9:B:11:A:H2'	9:B:12:G:C8	2.40	0.57
38:a:2314:A:O2'	51:n:155:THR:CG2	2.52	0.57
9:A:76:A:C2'	38:a:2394:C:H42	2.16	0.57
20:H:110:GLY:H	20:H:153:GLU:C	2.11	0.57
20:H:267:TRP:CH2	20:H:340:ARG:CB	2.86	0.57
9:A:11:A:H2'	9:A:12:G:C8	2.40	0.57
13:AE:198:CYS:HA	13:AE:221:ILE:HD11	1.86	0.57
13:AE:510:LEU:HD22	13:AE:601:ILE:HD12	1.86	0.57
16:D:1329:A:P	36:X:28:THR:OG1	2.62	0.57
38:a:1839:G:N9	38:a:1927:A:C4	2.72	0.57
7:6:8:DC:H2'	7:6:9:DT:H71	1.86	0.57
8:7:63:G:H2'	8:7:64:U:C6	2.39	0.57
13:AE:37:GLU:O	13:AE:61:ILE:CD1	2.52	0.57
19:G:148:LEU:HD22	19:G:151:ILE:HD11	1.87	0.57
20:H:162:LYS:CB	20:H:298:GLU:OE2	2.45	0.57
2:1:93:ALA:HB2	38:a:1614:A:C2	2.40	0.57
10:AA:818:VAL:HG22	10:AA:1096:ILE:HG12	1.86	0.57
10:AA:1072:ASN:ND2	10:AA:1111:GLN:OE1	2.37	0.57
13:AE:124:ILE:HG22	13:AE:124:ILE:O	2.04	0.57
9:B:32:C:OP2	27:O:130:ARG:NH2	2.38	0.57
9:B:56:C:C5'	51:n:80:ARG:NH2	2.67	0.57
6:5:115:DA:OP2	13:AE:1148:ARG:HG3	2.04	0.57
12:AC:69:SER:OG	12:AC:70:THR:N	2.38	0.57
20:H:36:VAL:HB	20:H:48:ILE:HB	1.84	0.57
29:Q:67:ALA:HB2	29:Q:96:THR:HG23	1.86	0.57
58:u:77:ILE:HD11	58:u:108:ALA:HB1	1.87	0.57
13:AE:99:ARG:HH11	13:AE:99:ARG:CG	2.18	0.57
16:D:1526:G:OP2	18:F:42:THR:HG23	2.04	0.57
38:a:84:A:N1	38:a:98:G:O2'	2.33	0.57
38:a:2245:U:O2'	38:a:2436:G:OP2	2.22	0.57
9:A:50:U:H2'	9:A:51:C:H6	1.69	0.56
12:AD:81:ILE:HD11	12:AD:130:ILE:HG22	1.87	0.56
16:D:1227:A:P	36:X:110:LYS:HZ2	2.28	0.56
23:K:56:VAL:O	23:K:60:ILE:HG23	2.04	0.56
38:a:1818:U:OP2	45:h:156:ARG:NH1	2.38	0.56
13:AE:130:MET:HE2	13:AE:135:ILE:HG12	1.87	0.56
13:AE:343:LEU:HD11	13:AE:1324:SER:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AE:741:ALA:O	13:AE:762:ASN:ND2	2.38	0.56
9:B:18:G:C8	9:B:57:A:N6	2.69	0.56
9:B:60:U:O2'	9:B:61:C:OP1	2.23	0.56
20:H:330:VAL:HB	20:H:344:LEU:HD23	1.86	0.56
40:c:31:PRO:HG2	40:c:33:LEU:HD13	1.87	0.56
9:A:56:C:C6	38:a:2168:G:C6	2.94	0.56
10:AA:1257:GLN:OE1	13:AE:345:LYS:HB3	2.05	0.56
12:AD:15:ASP:HB3	12:AD:27:THR:HB	1.86	0.56
13:AE:74:LYS:HD2	13:AE:85:CYS:SG	2.45	0.56
13:AE:491:LEU:HB2	13:AE:904:ALA:HA	1.86	0.56
16:D:496:A:N3	16:D:496:A:H2'	2.18	0.56
32:T:5:THR:O	32:T:8:THR:OG1	2.18	0.56
10:AA:914:LYS:H	10:AA:914:LYS:HD3	1.68	0.56
13:AE:144:TYR:HE1	13:AE:162:GLU:CD	2.14	0.56
16:D:927:G:O2'	16:D:1503:A:N7	2.36	0.56
38:a:2000:C:OP1	60:w:5:LYS:NZ	2.36	0.56
10:AA:39:ILE:HD12	10:AA:75:LEU:HD22	1.88	0.56
13:AE:903:LEU:HD21	13:AE:1249:ASN:HD22	1.70	0.56
26:N:10:MET:HE3	26:N:61:LEU:HD11	1.87	0.56
10:AA:400:VAL:HG11	10:AA:452:ARG:HD2	1.86	0.56
13:AE:39:LYS:O	13:AE:273:ILE:HG21	2.06	0.56
16:D:528:C:H6	16:D:528:C:H5''	1.71	0.56
49:l:104:ALA:O	49:l:108:ILE:HG23	2.05	0.56
20:H:267:TRP:CH2	20:H:340:ARG:HB3	2.41	0.56
9:A:60:U:P	9:A:61:C:H41	2.27	0.56
10:AA:801:ARG:HG2	10:AA:1094:VAL:HG23	1.87	0.56
10:AA:855:PRO:O	10:AA:855:PRO:HG2	2.05	0.56
16:D:1227:A:H5'	36:X:110:LYS:HZ1	1.71	0.56
12:AC:91:ARG:HD2	12:AC:122:GLU:HB3	1.88	0.56
9:B:50:U:H2'	9:B:51:C:H6	1.69	0.56
20:H:49:PRO:HD3	20:H:84:LEU:HD11	1.87	0.56
38:a:580:U:O3'	63:z:31:VAL:HG13	2.05	0.56
44:g:16:CYS:CB	44:g:37:CYS:CB	2.82	0.56
10:AA:174:ALA:HB2	10:AA:432:LEU:HD13	1.88	0.55
10:AA:1251:TYR:C	10:AA:1259:LEU:HD11	2.31	0.55
9:B:11:A:H8	9:B:11:A:O5'	1.89	0.55
49:l:108:ILE:HD11	49:l:180:LEU:HD13	1.88	0.55
9:A:60:U:O2'	9:A:61:C:OP1	2.23	0.55
10:AA:241:LEU:HD21	10:AA:246:LEU:HD11	1.88	0.55
16:D:769:G:H4'	16:D:1513:A:H4'	1.88	0.55
9:A:11:A:O5'	9:A:11:A:H8	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AA:880:GLY:O	10:AA:919:ARG:HD3	2.06	0.55
13:AE:638:SER:OG	13:AE:639:VAL:N	2.36	0.55
13:AE:1175:LEU:HD22	13:AE:1190:ILE:HD11	1.88	0.55
38:a:2303:G:C4	38:a:2314:A:C2	2.95	0.55
7:6:26:DT:H2''	7:6:27:DG:H5'	1.89	0.55
10:AA:859:GLU:O	10:AA:859:GLU:HG2	2.06	0.55
10:AA:1246:ARG:NH1	10:AA:1266:GLY:HA2	2.19	0.55
13:AE:247:PRO:HA	13:AE:250:ARG:HG3	1.87	0.55
38:a:404:A:O2'	38:a:405:U:OP2	2.22	0.55
38:a:811:U:H2'	58:u:21:ARG:HA	1.89	0.55
10:AA:227:LYS:NZ	10:AA:298:ALA:HB1	2.21	0.55
13:AE:102:MET:HG2	13:AE:246:PRO:HG3	1.87	0.55
16:D:563:A:N6	16:D:884:U:H3	2.05	0.55
59:v:66:ARG:NH1	59:v:104:GLU:OE1	2.39	0.55
10:AA:699:LEU:HG	10:AA:799:ASN:HD22	1.72	0.55
13:AE:1166:GLY:HA3	13:AE:1174:ARG:HB2	1.88	0.55
20:H:154:PHE:CB	20:H:168:VAL:CB	2.85	0.55
44:g:18:CYS:HB3	44:g:40:CYS:HB2	1.88	0.55
10:AA:1046:VAL:HG22	10:AA:1049:ILE:HG13	1.88	0.55
10:AA:1252:SER:N	10:AA:1259:LEU:CD1	2.70	0.55
49:l:130:LYS:HB2	49:l:133:LEU:HD12	1.89	0.55
3:2:50:LEU:HD23	42:e:26:PHE:CZ	2.42	0.55
10:AA:724:VAL:HG12	10:AA:774:GLY:H	1.72	0.55
12:AD:142:MET:N	12:AD:142:MET:SD	2.80	0.55
12:AD:215:GLU:OE1	12:AD:218:ARG:NH1	2.40	0.55
13:AE:171:GLU:HA	13:AE:171:GLU:OE1	2.05	0.55
20:H:45:GLU:OE1	20:H:45:GLU:N	2.40	0.55
13:AE:58:CYS:SG	13:AE:59:ALA:N	2.80	0.55
38:a:523:C:O2	38:a:554:U:O2'	2.25	0.55
1:0:51:VAL:HG23	63:z:86:ALA:O	2.05	0.55
9:A:38:A:H2'	9:A:39:C:H5'	1.88	0.55
10:AA:449:GLY:HA3	10:AA:609:ILE:HG23	1.87	0.55
10:AA:1257:GLN:NE2	13:AE:346:ARG:H	2.04	0.55
16:D:13:U:C2	16:D:915:A:C6	2.95	0.55
20:H:52:GLN:OE1	20:H:86:ARG:CB	2.55	0.55
20:H:279:LYS:HA	20:H:331:MET:CB	2.33	0.55
13:AE:759:ILE:HG23	13:AE:771:GLN:HB3	1.89	0.54
20:H:22:SER:N	20:H:69:ASP:OD2	2.40	0.54
36:X:17:ILE:O	36:X:20:THR:OG1	2.22	0.54
38:a:2314:A:O2'	51:n:155:THR:HG21	2.07	0.54
16:D:439:U:O2	16:D:440:C:C5	2.61	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:961:U:O4	16:D:974:A:N1	2.40	0.54
13:AE:136:GLU:OE1	13:AE:312:ARG:CZ	2.55	0.54
13:AE:833:GLU:HB2	13:AE:1242:ARG:NH1	2.22	0.54
35:W:15:LEU:HD13	35:W:33:THR:HG21	1.88	0.54
13:AE:145:VAL:HG23	13:AE:159:ILE:HG22	1.89	0.54
14:AF:26:ARG:HH12	14:AF:67:ARG:HH12	1.55	0.54
38:a:2249:U:H3'	38:a:2250:G:C5'	2.36	0.54
10:AA:1275:VAL:HG13	10:AA:1287:LEU:HD11	1.90	0.54
10:AA:1070:HIS:NE2	10:AA:1114:GLU:OE1	2.36	0.54
28:P:8:ILE:HD12	28:P:25:ILE:HD11	1.89	0.54
61:x:27:VAL:HG21	61:x:40:ILE:HD12	1.89	0.54
10:AA:840:SER:HA	10:AA:886:LYS:HD2	1.89	0.54
13:AE:30:ILE:HG21	13:AE:241:VAL:O	2.08	0.54
20:H:84:LEU:HD22	20:H:84:LEU:H	1.72	0.54
20:H:84:LEU:H	20:H:84:LEU:CD2	2.21	0.54
55:r:58:LEU:O	55:r:61:VAL:HG22	2.08	0.54
10:AA:452:ARG:HH12	10:AA:458:GLU:CD	2.15	0.54
13:AE:814:CYS:SG	13:AE:883:ARG:NH2	2.81	0.54
44:g:16:CYS:HB3	44:g:37:CYS:HB3	1.86	0.54
7:6:2:DC:H2''	7:6:3:DC:C5	2.43	0.54
10:AA:628:HIS:HB3	10:AA:647:ARG:HH21	1.73	0.54
10:AA:1246:ARG:NH1	10:AA:1258:PRO:HB3	2.22	0.54
12:AD:196:THR:HB	13:AE:443:GLU:CG	2.36	0.54
13:AE:46:TYR:CD1	13:AE:46:TYR:C	2.85	0.54
13:AE:785:ASP:O	13:AE:789:LYS:HB2	2.08	0.54
16:D:13:U:C4	16:D:21:G:C2	2.96	0.54
23:K:99:ALA:HB1	23:K:103:THR:HG21	1.89	0.54
38:a:2636:C:HO2'	47:j:45:TYR:HH	1.56	0.54
13:AE:111:THR:HG22	13:AE:300:GLN:NE2	2.23	0.54
38:a:1056:G:O2'	38:a:1103:A:N6	2.41	0.54
8:7:58:A:H3'	8:7:58:A:N3	2.23	0.53
10:AA:738:GLU:HA	10:AA:741:MET:HE2	1.90	0.53
10:AA:835:GLU:OE2	10:AA:1051:LYS:HD3	2.08	0.53
11:AB:107:GLU:OE1	13:AE:288:PRO:CB	2.52	0.53
12:AC:140:ILE:HD11	12:AC:142:MET:HE3	1.89	0.53
13:AE:209:ASN:HA	13:AE:214:ARG:HH21	1.74	0.53
13:AE:746:LEU:HG	13:AE:758:PRO:HG3	1.90	0.53
13:AE:1155:ILE:HG13	13:AE:1210:ILE:HB	1.89	0.53
38:a:1906:G:H5''	38:a:1906:G:H8	1.73	0.53
38:a:2192:U:H2'	38:a:2193:G:C8	2.43	0.53
13:AE:124:ILE:HG23	13:AE:128:LEU:HD12	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:1228:C:OP2	36:X:110:LYS:NZ	2.41	0.53
16:D:1329:A:OP1	36:X:28:THR:N	2.41	0.53
20:H:321:VAL:HG13	20:H:322:VAL:HG23	1.90	0.53
30:R:80:ILE:HD12	30:R:97:THR:HG22	1.89	0.53
4:3:13:VAL:CG2	4:3:39:ILE:HD13	2.39	0.53
9:A:18:G:C8	9:A:57:A:N6	2.69	0.53
20:H:135:LEU:CB	20:H:167:VAL:CA	2.86	0.53
20:H:290:TYR:C	20:H:305:HIS:O	2.47	0.53
38:a:995:C:O2	56:s:3:THR:OG1	2.24	0.53
39:b:37:ILE:HD11	39:b:82:ILE:HD11	1.90	0.53
12:AD:109:PRO:HA	12:AD:132:HIS:HA	1.91	0.53
9:B:76:A:N3	38:a:2493:U:H4'	2.23	0.53
38:a:1839:G:N9	38:a:1927:A:H1'	2.23	0.53
2:1:59:GLU:CG	2:1:66:ILE:HD11	2.38	0.53
13:AE:26:SER:HB2	13:AE:236:TRP:CE2	2.42	0.53
9:B:18:G:C2	9:B:58:A:C5	2.96	0.53
20:H:135:LEU:CB	20:H:157:ILE:CB	2.87	0.53
57:t:7:MET:HE1	57:t:44:LYS:HD2	1.91	0.53
10:AA:724:VAL:CG1	10:AA:774:GLY:N	2.68	0.53
12:AD:33:ARG:HD3	12:AD:197:ASP:HB2	1.91	0.53
13:AE:39:LYS:O	13:AE:273:ILE:HG23	2.08	0.53
9:B:56:C:C5'	51:n:80:ARG:CZ	2.76	0.53
9:A:18:G:C2	9:A:58:A:C5	2.97	0.53
10:AA:884:VAL:HG11	10:AA:1050:VAL:HG11	1.91	0.53
12:AC:215:GLU:OE2	12:AC:219:ARG:NH2	2.41	0.53
13:AE:56:LEU:CD1	13:AE:273:ILE:HD12	2.39	0.53
9:B:12:G:H2'	9:B:13:C:OP1	2.08	0.53
16:D:1276:G:O5'	16:D:1276:G:H8	1.92	0.53
20:H:116:VAL:C	20:H:279:LYS:HB2	2.33	0.53
9:A:12:G:H2'	9:A:13:C:OP1	2.08	0.53
10:AA:726:TYR:HD2	10:AA:726:TYR:O	1.92	0.53
12:AC:171:LEU:HD23	12:AC:171:LEU:N	2.24	0.53
12:AD:22:THR:OG1	12:AD:207:THR:O	2.26	0.53
13:AE:78:LEU:O	13:AE:78:LEU:HD13	2.08	0.53
13:AE:111:THR:HG23	13:AE:300:GLN:NE2	2.24	0.53
13:AE:975:ILE:HD11	13:AE:1003:LEU:HD11	1.91	0.53
9:A:56:C:C2	38:a:2112:G:C8	2.96	0.53
10:AA:808:ASN:H	13:AE:633:ALA:HB2	1.74	0.53
13:AE:832:LYS:HB3	13:AE:1242:ARG:NH1	2.24	0.53
16:D:945:G:C2	16:D:946:A:C8	2.96	0.53
49:l:131:THR:HG22	49:l:160:ALA:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:16:C:O2	9:A:16:C:H2'	2.09	0.53
9:A:17:C:O2	9:A:17:C:H2'	2.08	0.53
21:I:77:ILE:HA	21:I:84:VAL:HG23	1.91	0.53
51:n:8:TYR:HA	51:n:12:VAL:HB	1.91	0.53
7:6:8:DC:H2''	7:6:9:DT:H71	1.91	0.52
13:AE:201:LEU:HD12	13:AE:224:LEU:HD12	1.91	0.52
20:H:49:PRO:HD2	20:H:84:LEU:CD1	2.40	0.52
37:Y:72:U:H6	37:Y:72:U:H3'	1.73	0.52
9:B:17:C:O2	9:B:17:C:H2'	2.08	0.52
16:D:767:A:H2'	16:D:768:A:O4'	2.08	0.52
16:D:864:A:C2	16:D:865:A:C2	2.98	0.52
9:A:38:A:C2'	9:A:39:C:H5'	2.39	0.52
10:AA:862:LEU:HD23	10:AA:862:LEU:H	1.74	0.52
13:AE:99:ARG:HG3	13:AE:99:ARG:HH11	1.74	0.52
13:AE:205:LEU:HG	13:AE:217:LEU:HB3	1.90	0.52
15:C:61:ARG:NH2	16:D:736:C:OP1	2.42	0.52
38:a:1209:U:O2'	38:a:1237:A:N1	2.40	0.52
10:AA:524:ILE:HG21	10:AA:708:VAL:HG13	1.91	0.52
10:AA:1257:GLN:OE1	13:AE:345:LYS:CB	2.57	0.52
27:O:98:LEU:HB3	27:O:104:VAL:HG13	1.91	0.52
9:A:22:G:O2'	9:A:23:C:P	2.68	0.52
10:AA:813:GLU:HB2	13:AE:461:PHE:HD2	1.74	0.52
13:AE:68:TYR:CA	13:AE:75:TYR:HE2	2.22	0.52
20:H:24:VAL:HG12	20:H:69:ASP:H	1.74	0.52
20:H:332:VAL:O	20:H:334:ASP:N	2.40	0.52
38:a:523:C:H4'	38:a:540:C:O2	2.10	0.52
9:A:15:G:N3	9:A:15:G:C2'	2.73	0.52
10:AA:862:LEU:HD23	10:AA:862:LEU:N	2.25	0.52
13:AE:112:ALA:HA	13:AE:238:ILE:HA	1.91	0.52
16:D:673:A:H2'	16:D:674:G:C8	2.44	0.52
20:H:267:TRP:CZ3	20:H:340:ARG:HG3	2.42	0.52
38:a:2298:A:C5	38:a:2321:U:O4	2.62	0.52
12:AD:182:ARG:CD	13:AE:581:MET:HE1	2.39	0.52
13:AE:88:CYS:HB3	13:AE:90:VAL:HG12	1.92	0.52
13:AE:144:TYR:CE1	13:AE:162:GLU:CD	2.88	0.52
16:D:1228:C:OP1	36:X:107:ARG:CZ	2.58	0.52
23:K:81:LEU:HD13	23:K:123:VAL:HG12	1.92	0.52
38:a:929:U:H1'	43:f:26:GLY:O	2.10	0.52
38:a:2328:A:H2'	38:a:2329:U:C6	2.44	0.52
61:x:35:ILE:HG21	61:x:71:ALA:HA	1.90	0.52
2:1:93:ALA:HB2	38:a:1614:A:N1	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:6:G:O2'	9:A:7:G:H8	1.92	0.52
9:B:16:C:O2	9:B:16:C:H2'	2.08	0.52
38:a:2315:G:O2'	51:n:125:ARG:HD3	2.09	0.52
60:w:38:LEU:N	60:w:39:PRO:CD	2.73	0.52
9:A:5:G:C2'	9:A:6:G:H5'	2.39	0.52
9:A:12:G:C2'	9:A:13:C:OP1	2.57	0.52
10:AA:1287:LEU:HD13	13:AE:1357:ILE:HD11	1.90	0.52
13:AE:99:ARG:HA	13:AE:248:ASP:HB2	1.92	0.52
13:AE:1167:LYS:HZ2	13:AE:1170:LYS:HB2	1.73	0.52
20:H:19:ARG:O	20:H:72:LEU:HD22	2.09	0.52
23:K:94:VAL:HG13	23:K:111:MET:HE1	1.91	0.52
9:A:34:C:P	25:M:84:THR:HG1	2.33	0.52
13:AE:390:LEU:N	13:AE:390:LEU:CD1	2.73	0.52
20:H:71:ALA:O	20:H:72:LEU:CD1	2.42	0.52
38:a:1910:G:O5'	38:a:1910:G:H8	1.93	0.52
10:AA:1045:GLY:O	10:AA:1047:LEU:HD13	2.10	0.51
13:AE:215:LYS:HA	13:AE:218:THR:HG22	1.91	0.51
9:B:6:G:O2'	9:B:7:G:H8	1.92	0.51
19:G:35:ARG:NH2	20:H:10:GLU:HG2	2.25	0.51
20:H:308:GLU:O	20:H:310:ASP:N	2.43	0.51
38:a:587:C:OP2	58:u:21:ARG:NH1	2.43	0.51
4:3:94:ARG:HB3	4:3:103:ILE:HD12	1.92	0.51
20:H:49:PRO:HD2	20:H:84:LEU:HD11	1.92	0.51
32:T:40:GLN:CA	32:T:40:GLN:HE21	2.23	0.51
38:a:783:A:N3	38:a:783:A:C2'	2.70	0.51
4:3:12:ILE:HG21	4:3:80:ALA:HB2	1.92	0.51
9:A:56:C:H1'	38:a:2112:G:C5	2.46	0.51
9:B:12:G:C2'	9:B:13:C:OP1	2.57	0.51
9:B:15:G:N3	9:B:15:G:C2'	2.73	0.51
16:D:1308:U:P	36:X:98:ARG:HG3	2.50	0.51
38:a:1693:U:O2'	45:h:14:ARG:NH2	2.43	0.51
13:AE:683:ILE:HD12	13:AE:754:ILE:HG21	1.93	0.51
16:D:1499:A:O2'	16:D:1500:A:H5'	2.10	0.51
38:a:118:A:C8	38:a:119:A:C8	2.99	0.51
9:A:56:C:C3'	9:A:57:A:H5''	2.40	0.51
10:AA:858:GLY:C	10:AA:860:ALA:H	2.14	0.51
12:AC:158:ARG:NH1	12:AC:158:ARG:CB	2.73	0.51
15:C:30:LYS:HA	15:C:33:ILE:HD13	1.92	0.51
38:a:639:U:H2'	38:a:640:C:C6	2.45	0.51
38:a:1814:G:H4'	45:h:51:THR:HG21	1.93	0.51
56:s:17:VAL:HG23	56:s:137:PRO:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:z:58:ARG:HA	63:z:61:TRP:CE3	2.45	0.51
9:A:19:G:C5	38:a:2112:G:H4'	2.44	0.51
10:AA:1244:HIS:NE2	10:AA:1266:GLY:O	2.35	0.51
9:B:22:G:O2'	9:B:23:C:P	2.68	0.51
9:B:24:U:O2'	38:a:1922:G:O3'	2.29	0.51
9:B:56:C:C3'	9:B:57:A:H5''	2.40	0.51
20:H:119:GLY:CA	20:H:133:GLY:CA	2.74	0.51
20:H:332:VAL:C	20:H:334:ASP:H	2.18	0.51
38:a:1980:G:O2'	38:a:1982:U:OP2	2.28	0.51
9:A:18:G:C2	9:A:58:A:C6	2.99	0.51
10:AA:880:GLY:C	10:AA:919:ARG:HD3	2.36	0.51
12:AD:182:ARG:HD3	13:AE:581:MET:HE1	1.91	0.51
38:a:1266:G:OP2	46:i:17:ARG:NE	2.43	0.51
9:A:15:G:H22	9:A:20:U:H3	1.59	0.51
9:A:76:A:O2'	38:a:2395:C:C2	2.64	0.51
10:AA:242:VAL:HB	10:AA:245:ARG:NH1	2.25	0.51
11:AB:71:VAL:HG12	11:AB:73:MET:HB2	1.93	0.51
13:AE:972:LYS:HD2	13:AE:1004:ALA:HA	1.93	0.51
41:d:106:G:H2'	41:d:107:G:O4'	2.10	0.51
53:p:121:ILE:HD12	53:p:141:ILE:CG2	2.41	0.51
57:t:71:ARG:NH2	57:t:123:LEU:O	2.42	0.51
10:AA:657:THR:HG21	10:AA:1188:ASP:HB2	1.92	0.51
10:AA:689:ALA:HB2	10:AA:1233:LEU:HD23	1.93	0.51
20:H:72:LEU:CD1	20:H:72:LEU:N	2.73	0.51
38:a:1964:G:H4'	38:a:1965:C:OP2	2.11	0.51
38:a:2243:U:H2'	38:a:2244:U:C6	2.46	0.51
9:A:48:C:H2'	9:A:48:C:O2	2.11	0.51
13:AE:850:LYS:HB2	13:AE:857:LEU:HB2	1.91	0.51
16:D:1366:C:O2'	28:P:62:ARG:NH2	2.44	0.51
28:P:57:VAL:O	28:P:57:VAL:HG13	2.11	0.51
6:5:101:DT:H72	13:AE:271:ARG:CZ	2.41	0.50
9:A:32:C:HO2'	25:M:86:GLN:HG3	1.74	0.50
9:A:56:C:C5	38:a:2168:G:O6	2.64	0.50
41:d:5:U:OP1	41:d:61:G:O2'	2.26	0.50
50:m:31:LEU:HD22	50:m:42:LEU:CD1	2.40	0.50
2:1:24:ILE:HD13	2:1:36:LEU:HD11	1.93	0.50
9:A:41:C:H4'	25:M:143:ARG:NH1	2.25	0.50
10:AA:694:ARG:NH2	12:AC:83:LEU:HD13	2.26	0.50
14:AF:25:ARG:NH2	14:AF:65:ASP:OD1	2.44	0.50
32:T:21:ASP:O	32:T:22:THR:HG22	2.12	0.50
38:a:1141:U:O2	38:a:1142:A:N6	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:a:1869:G:N2	38:a:1871:A:O2'	2.44	0.50
53:p:35:ARG:HD3	53:p:71:LEU:HD13	1.93	0.50
9:A:28:C:H2'	9:A:29:G:H8	1.76	0.50
10:AA:873:ILE:HG12	12:AC:65:LEU:HD13	1.93	0.50
9:B:18:G:C2	9:B:58:A:C6	2.99	0.50
56:s:30:THR:HG22	56:s:31:GLU:N	2.27	0.50
56:s:32:LEU:CD2	56:s:54:ILE:HG21	2.42	0.50
10:AA:1252:SER:HA	10:AA:1259:LEU:HD11	1.93	0.50
13:AE:749:LYS:HB3	13:AE:755:ILE:HD11	1.94	0.50
38:a:2627:G:O2'	38:a:2781:A:N1	2.37	0.50
45:h:107:PRO:HD2	45:h:110:LEU:HD22	1.94	0.50
13:AE:437:PHE:HZ	13:AE:453:VAL:HG11	1.76	0.50
20:H:52:GLN:O	20:H:53:PHE:HD1	1.95	0.50
57:t:43:ILE:HD12	57:t:56:ASP:HB2	1.93	0.50
6:5:96:DT:H2''	6:5:97:DC:C5	2.46	0.50
13:AE:804:ALA:O	13:AE:806:ASP:N	2.41	0.50
14:AF:26:ARG:NH1	14:AF:67:ARG:NH1	2.59	0.50
16:D:872:A:H2'	16:D:872:A:N3	2.27	0.50
27:O:81:HIS:O	27:O:84:THR:OG1	2.23	0.50
2:1:59:GLU:HG3	2:1:66:ILE:HD11	1.92	0.50
6:5:98:DA:N9	6:5:99:DT:H72	2.26	0.50
9:B:72:A:H2'	9:B:73:A:C5'	2.32	0.50
16:D:1356:G:H2'	16:D:1357:A:C8	2.47	0.50
12:AD:95:LYS:O	12:AD:148:ARG:NH2	2.42	0.50
9:B:39:C:O5'	9:B:39:C:H6	1.95	0.50
16:D:13:U:C4	16:D:915:A:C6	2.92	0.50
57:t:113:MET:O	57:t:116:ILE:HG13	2.11	0.50
60:w:55:ALA:HA	60:w:80:PHE:CE1	2.47	0.50
38:a:2557:G:H2'	38:a:2558:C:C6	2.47	0.50
16:D:108:G:H5''	16:D:108:G:N3	2.27	0.49
18:F:4:ILE:HD12	18:F:19:PHE:HA	1.93	0.49
38:a:742:A:C2	38:a:743:A:C6	3.00	0.49
60:w:67:PHE:O	60:w:71:ARG:N	2.45	0.49
10:AA:232:ILE:HD12	10:AA:331:LYS:HA	1.94	0.49
10:AA:733:VAL:HG22	10:AA:750:ILE:HG12	1.93	0.49
13:AE:275:ARG:HH12	13:AE:278:ARG:NH1	2.09	0.49
9:B:59:A:H2'	9:B:60:U:H5'	1.94	0.49
16:D:1329:A:OP1	36:X:28:THR:OG1	2.31	0.49
42:e:18:LEU:HB2	42:e:53:VAL:HG11	1.94	0.49
9:A:37:A:H2'	9:A:38:A:H8	1.77	0.49
10:AA:125:GLY:HA2	10:AA:499:SER:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AD:60:GLU:OE2	12:AD:170:ARG:NE	2.45	0.49
9:B:48:C:O2	9:B:48:C:H2'	2.11	0.49
20:H:117:LYS:CB	20:H:278:THR:CG2	2.90	0.49
38:a:2038:G:H2'	38:a:2039:U:O4'	2.13	0.49
10:AA:632:ASP:HA	10:AA:647:ARG:HB2	1.94	0.49
10:AA:817:LEU:HD12	10:AA:1078:LYS:HB3	1.93	0.49
13:AE:799:ARG:HG2	13:AE:1325:PHE:HZ	1.78	0.49
16:D:1208:C:H2'	16:D:1209:C:C6	2.47	0.49
16:D:1311:A:OP1	44:g:59:ARG:NH1	2.46	0.49
51:n:127:ASN:ND2	51:n:127:ASN:N	2.60	0.49
9:A:11:A:H2'	9:A:12:G:C1'	2.42	0.49
9:A:47:U:H2'	9:A:48:C:H4'	1.94	0.49
10:AA:1252:SER:CA	10:AA:1259:LEU:HD11	2.41	0.49
10:AA:1253:LEU:HD12	13:AE:253:VAL:HG13	1.90	0.49
13:AE:1371:ARG:HE	13:AE:1372:ARG:NH1	2.10	0.49
9:B:34:C:O2	9:B:34:C:H2'	2.11	0.49
23:K:114:VAL:HG21	23:K:141:ILE:HD12	1.94	0.49
26:N:3:MET:HA	26:N:3:MET:HE3	1.94	0.49
38:a:1824:G:O2'	45:h:252:THR:HG21	2.11	0.49
38:a:2646:C:O5'	38:a:2646:C:H6	1.95	0.49
63:z:47:TYR:CD1	63:z:47:TYR:C	2.90	0.49
1:O:14:VAL:HG21	1:O:98:ILE:HG13	1.94	0.49
10:AA:1047:LEU:O	10:AA:1049:ILE:HD11	2.13	0.49
12:AC:162:GLU:HG2	12:AC:162:GLU:O	2.04	0.49
13:AE:421:VAL:O	13:AE:436:ALA:HA	2.11	0.49
9:B:47:U:H2'	9:B:48:C:H4'	1.94	0.49
16:D:974:A:OP1	31:S:69:ARG:NH1	2.46	0.49
20:H:120:PHE:CB	20:H:136:VAL:CB	2.91	0.49
38:a:2303:G:C6	38:a:2314:A:N1	2.81	0.49
9:A:59:A:H2'	9:A:60:U:H5'	1.94	0.49
9:B:49:G:O5'	9:B:49:G:H8	1.96	0.49
16:D:50:A:O2'	16:D:360:G:N2	2.45	0.49
16:D:1308:U:OP1	36:X:100:GLN:OE1	2.22	0.49
16:D:1493:A:O2'	16:D:1494:G:P	2.71	0.49
47:j:156:PHE:CE1	56:s:81:ILE:HD13	2.48	0.49
2:1:55:ILE:HG23	2:1:66:ILE:HD12	1.93	0.49
10:AA:103:VAL:HG12	10:AA:117:ILE:HG22	1.94	0.49
10:AA:529:ARG:HH22	10:AA:687:ARG:NH1	2.11	0.49
10:AA:859:GLU:H	10:AA:859:GLU:CD	2.15	0.49
13:AE:201:LEU:HD11	13:AE:220:ARG:HG2	1.95	0.49
9:B:11:A:H2'	9:B:12:G:C1'	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:332:VAL:HG11	20:H:335:ILE:CG1	2.38	0.49
34:V:48:ASP:HB3	34:V:75:LEU:HD23	1.94	0.49
47:j:25:THR:HG21	47:j:193:VAL:HG22	1.94	0.49
10:AA:1102:GLY:HA2	10:AA:1106:ARG:NH1	2.28	0.49
12:AC:71:LYS:NZ	12:AC:140:ILE:HB	2.27	0.49
9:B:25:C:H2'	9:B:26:G:H5'	1.95	0.49
16:D:1017:U:O2'	16:D:1018:G:O4'	2.31	0.49
20:H:132:PRO:N	20:H:167:VAL:CB	2.75	0.49
38:a:464:U:O3'	50:m:12:ARG:NH2	2.45	0.49
38:a:1412:U:C4	38:a:1413:A:N7	2.81	0.49
61:x:51:ALA:HB3	61:x:78:VAL:HB	1.95	0.49
2:1:29:VAL:HB	2:1:55:ILE:HD11	1.95	0.48
10:AA:14:ASP:HA	10:AA:1183:ALA:HB3	1.94	0.48
10:AA:24:VAL:HG22	10:AA:578:TYR:HE1	1.78	0.48
10:AA:728:ASP:HA	10:AA:731:ARG:O	2.12	0.48
10:AA:1069:ARG:NH2	10:AA:1114:GLU:OE2	2.30	0.48
12:AD:96:ASP:OD1	12:AD:96:ASP:N	2.46	0.48
13:AE:99:ARG:NH1	13:AE:99:ARG:CG	2.76	0.48
13:AE:809:VAL:HG21	13:AE:909:ILE:HG12	1.95	0.48
9:B:18:G:C5	9:B:57:A:C5	3.01	0.48
16:D:1499:A:H3'	16:D:1499:A:OP2	2.12	0.48
38:a:2297:A:C6	38:a:2321:U:O4	2.65	0.48
38:a:2298:A:N3	38:a:2321:U:C5	2.80	0.48
4:3:7:ARG:HB2	38:a:85:G:OP2	2.13	0.48
13:AE:220:ARG:HG2	13:AE:220:ARG:NH1	2.26	0.48
47:j:121:THR:HB	47:j:127:PHE:CD2	2.49	0.48
50:m:24:THR:HG23	50:m:27:GLY:H	1.78	0.48
55:r:3:VAL:HG22	55:r:36:ALA:HB1	1.95	0.48
10:AA:618:GLN:HG3	13:AE:770:LEU:HD13	1.96	0.48
13:AE:117:LEU:HG	13:AE:118:LYS:HG3	1.95	0.48
13:AE:152:THR:HB	13:AE:172:PHE:CZ	2.48	0.48
16:D:13:U:O4	16:D:21:G:N3	2.46	0.48
32:T:4:SER:O	32:T:8:THR:HG23	2.12	0.48
43:f:24:LEU:HD11	43:f:54:MET:CE	2.42	0.48
9:A:42:G:H2'	9:A:43:A:C8	2.47	0.48
10:AA:935:THR:HA	10:AA:1049:ILE:CD1	2.41	0.48
19:G:38:VAL:CG2	20:H:75:VAL:CG2	2.77	0.48
20:H:318:PRO:HA	20:H:321:VAL:HG12	1.95	0.48
38:a:1839:G:N9	38:a:1927:A:C1'	2.77	0.48
45:h:210:ALA:HA	45:h:213:TRP:CE3	2.48	0.48
50:m:22:MET:O	50:m:28:ARG:NH1	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:4:ILE:HG12	2:1:106:VAL:HG22	1.95	0.48
9:A:18:G:C5	9:A:57:A:C5	3.01	0.48
9:A:49:G:H8	9:A:49:G:O5'	1.96	0.48
10:AA:227:LYS:HZ2	10:AA:298:ALA:HB1	1.77	0.48
12:AD:20:SER:OG	12:AD:21:SER:N	2.46	0.48
24:L:18:VAL:N	24:L:19:PRO:CD	2.76	0.48
38:a:1067:A:O2'	38:a:1068:G:O4'	2.31	0.48
2:1:25:ARG:NH1	2:1:74:ILE:O	2.46	0.48
9:A:15:G:C2	9:A:20:U:O2	2.66	0.48
10:AA:914:LYS:NZ	10:AA:914:LYS:HB2	2.28	0.48
12:AC:71:LYS:NZ	12:AC:140:ILE:CG1	2.76	0.48
13:AE:102:MET:HG2	13:AE:246:PRO:HD3	1.95	0.48
13:AE:190:LYS:HB2	13:AE:190:LYS:HE3	1.41	0.48
16:D:35:G:N3	30:R:115:SER:OG	2.47	0.48
23:K:99:ALA:CB	23:K:103:THR:HG21	2.43	0.48
9:A:58:A:OP2	9:A:58:A:C8	2.67	0.48
9:A:68:C:H3'	9:A:69:C:H5''	1.96	0.48
10:AA:618:GLN:OE1	10:AA:635:THR:OG1	2.32	0.48
10:AA:857:VAL:CG1	10:AA:861:ALA:HB2	2.43	0.48
10:AA:1101:LEU:HD21	13:AE:508:LEU:HD22	1.95	0.48
10:AA:1314:GLN:HA	14:AF:28:ARG:HH22	1.78	0.48
13:AE:114:ILE:HG12	13:AE:311:ARG:HD2	1.95	0.48
9:B:18:G:N3	9:B:58:A:C6	2.82	0.48
16:D:1169:A:H2'	16:D:1170:A:C8	2.48	0.48
16:D:1174:G:H2'	16:D:1175:G:H5'	1.95	0.48
20:H:330:VAL:HG12	20:H:345:GLY:O	2.14	0.48
38:a:565:C:H2'	38:a:566:U:O4'	2.13	0.48
38:a:1588:G:C6	38:a:1589:U:O4	2.67	0.48
1:0:14:VAL:CG2	1:0:98:ILE:HG13	2.43	0.48
3:2:61:LEU:C	3:2:61:LEU:HD12	2.39	0.48
9:A:18:G:N3	9:A:58:A:C6	2.82	0.48
9:A:76:A:N6	38:a:2422:C:O4'	2.46	0.48
10:AA:866:ASP:OD2	10:AA:869:GLY:O	2.31	0.48
13:AE:47:ARG:CZ	13:AE:47:ARG:HB2	2.44	0.48
13:AE:800:LEU:HB3	13:AE:920:ALA:HB1	1.95	0.48
13:AE:1027:VAL:HB	13:AE:1121:LEU:HB2	1.96	0.48
22:J:61:VAL:HG21	22:J:200:ILE:CD1	2.35	0.48
39:b:37:ILE:HG21	39:b:80:ILE:HG21	1.95	0.48
12:AD:191:ARG:NH2	12:AD:193:GLU:O	2.47	0.48
13:AE:53:ARG:HA	13:AE:54:ASP:HA	1.55	0.48
9:B:11:A:C2'	9:B:12:G:O4'	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:15:G:C2	9:B:20:U:O2	2.66	0.48
9:B:42:G:H2'	9:B:43:A:C8	2.47	0.48
16:D:1064:G:O2'	16:D:1190:G:N2	2.47	0.48
20:H:23:ILE:N	20:H:69:ASP:OD2	2.47	0.48
38:a:1433:A:H2'	38:a:1434:A:O4'	2.13	0.48
40:c:3:ARG:HD2	40:c:30:LEU:HD22	1.94	0.48
53:p:24:ILE:CD1	53:p:72:LEU:HD21	2.43	0.48
9:A:25:C:H2'	9:A:26:G:H5'	1.95	0.48
9:A:60:U:H4'	9:A:61:C:OP2	2.14	0.48
9:A:72:A:H2'	9:A:73:A:C5'	2.32	0.48
10:AA:936:ARG:O	10:AA:936:ARG:HD3	2.13	0.48
13:AE:145:VAL:HG12	13:AE:184:ALA:HB1	1.94	0.48
16:D:604:G:H2'	16:D:605:U:O4'	2.14	0.48
61:x:27:VAL:CG2	61:x:40:ILE:HD12	2.44	0.48
13:AE:550:VAL:O	13:AE:569:LEU:HA	2.13	0.47
13:AE:1036:ARG:HE	13:AE:1081:VAL:HG11	1.79	0.47
9:B:58:A:C8	9:B:58:A:OP2	2.67	0.47
9:B:68:C:C4	9:B:69:C:C5	3.02	0.47
16:D:911:U:H2'	16:D:912:C:C6	2.49	0.47
1:0:40:MET:HE3	1:0:49:ILE:CD1	2.44	0.47
9:A:68:C:C4	9:A:69:C:C5	3.02	0.47
10:AA:845:LEU:HD23	10:AA:845:LEU:N	2.28	0.47
12:AC:102:LEU:HB2	12:AC:115:ILE:HG12	1.95	0.47
13:AE:108:ALA:HB1	13:AE:279:LEU:HD22	1.96	0.47
13:AE:1221:LEU:HD22	13:AE:1306:LEU:HB2	1.97	0.47
13:AE:1261:LEU:HD12	13:AE:1304:ARG:HH21	1.78	0.47
9:B:9:G:H5''	9:B:10:G:OP2	2.15	0.47
9:B:76:A:N3	9:B:76:A:C2'	2.74	0.47
19:G:35:ARG:CD	20:H:14:LYS:HD3	2.40	0.47
13:AE:1347:LEU:HG	13:AE:1357:ILE:HG23	1.96	0.47
16:D:5:U:O2	16:D:5:U:O4'	2.29	0.47
16:D:371:A:H2'	16:D:372:C:O4'	2.14	0.47
38:a:1993:U:H4'	47:j:133:THR:HG22	1.96	0.47
10:AA:1119:MET:HG3	10:AA:1204:LEU:HD13	1.97	0.47
10:AA:1280:ALA:HB1	13:AE:918:ILE:HG22	1.96	0.47
13:AE:968:ASN:HA	13:AE:1117:SER:HB2	1.96	0.47
9:B:60:U:H4'	9:B:61:C:OP2	2.14	0.47
1:0:5:PHE:HB3	1:0:59:ILE:HD12	1.96	0.47
10:AA:27:LEU:O	10:AA:528:ARG:NH1	2.42	0.47
12:AC:159:ILE:HA	12:AC:159:ILE:HD13	1.69	0.47
12:AD:100:LEU:O	12:AD:144:ILE:N	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AE:115:TRP:O	13:AE:1333:THR:HG21	2.13	0.47
13:AE:833:GLU:N	13:AE:1242:ARG:HH12	2.12	0.47
13:AE:1146:GLU:OE2	13:AE:1310:THR:HG22	2.14	0.47
14:AF:4:VAL:HG22	14:AF:5:THR:HG23	1.96	0.47
9:A:41:C:H5'	25:M:143:ARG:HD2	1.96	0.47
13:AE:103:GLY:H	13:AE:244:VAL:HG22	1.78	0.47
9:B:18:G:C6	9:B:57:A:N7	2.83	0.47
16:D:526:C:P	30:R:88:LYS:HE3	2.55	0.47
16:D:1308:U:P	36:X:98:ARG:CG	3.03	0.47
9:A:9:G:H5''	9:A:10:G:OP2	2.14	0.47
10:AA:243:PRO:HB2	10:AA:274:ILE:HG23	1.96	0.47
10:AA:859:GLU:N	10:AA:859:GLU:CD	2.73	0.47
12:AC:43:LEU:O	12:AC:47:LEU:HB2	2.14	0.47
12:AC:166:ARG:HB3	12:AC:166:ARG:NH1	2.30	0.47
12:AD:48:LEU:HD22	13:AE:535:ARG:HG3	1.96	0.47
13:AE:842:ARG:HH22	13:AE:1250:ASP:HB2	1.80	0.47
14:AF:26:ARG:HH12	14:AF:67:ARG:NH1	2.12	0.47
9:B:5:G:C2'	9:B:6:G:H5'	2.40	0.47
17:E:54:MET:O	17:E:57:ILE:HG22	2.15	0.47
20:H:135:LEU:CB	20:H:167:VAL:O	2.63	0.47
24:L:67:PRO:O	24:L:70:VAL:HG22	2.15	0.47
26:N:102:ALA:HB3	26:N:113:ASP:HB3	1.96	0.47
36:X:16:VAL:HG23	36:X:17:ILE:HD12	1.97	0.47
38:a:1020:A:C6	38:a:1141:U:O2	2.68	0.47
38:a:1406:U:H3	38:a:1596:A:H2	1.58	0.47
52:o:13:ARG:HD3	58:u:58:TYR:O	2.14	0.47
9:A:11:A:C2'	9:A:12:G:O4'	2.60	0.47
10:AA:685:MET:SD	10:AA:1073:LYS:HG2	2.55	0.47
10:AA:1257:GLN:CD	13:AE:345:LYS:HB3	2.40	0.47
13:AE:420:PRO:HA	13:AE:437:PHE:O	2.15	0.47
13:AE:1150:PRO:HG3	13:AE:1214:PRO:HB2	1.96	0.47
16:D:1103:C:O2	19:G:106:THR:HG21	2.15	0.47
16:D:1225:A:OP1	36:X:101:ARG:HB2	2.15	0.47
38:a:2303:G:C2	38:a:2314:A:N3	2.82	0.47
9:A:14:A:H2'	9:A:14:A:N3	2.29	0.47
9:A:18:G:C6	9:A:57:A:N7	2.83	0.47
9:A:37:A:H2'	9:A:38:A:C8	2.48	0.47
10:AA:93:SER:HA	10:AA:128:PRO:HA	1.97	0.47
10:AA:841:ARG:HB2	10:AA:841:ARG:NH1	2.30	0.47
10:AA:1072:ASN:OD1	10:AA:1072:ASN:N	2.47	0.47
12:AD:104:LYS:HG2	12:AD:110:VAL:HB	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AE:395:LYS:NZ	13:AE:399:LYS:CE	2.77	0.47
13:AE:891:ASP:OD2	13:AE:1290:ARG:NH2	2.47	0.47
9:B:15:G:H22	9:B:20:U:H3	1.59	0.47
16:D:13:U:O2	16:D:915:A:N7	2.47	0.47
16:D:946:A:H2'	16:D:947:G:C8	2.50	0.47
38:a:2685:G:OP1	57:t:78:ARG:NH2	2.47	0.47
38:a:2756:U:C4	38:a:2759:G:C6	3.03	0.47
10:AA:549:ASP:OD2	13:AE:750:PRO:HB3	2.15	0.47
9:B:14:A:N3	9:B:14:A:H2'	2.29	0.47
20:H:69:ASP:O	20:H:85:SER:CB	2.63	0.47
34:V:75:LEU:C	34:V:75:LEU:HD12	2.38	0.47
38:a:742:A:C2	38:a:755:U:N3	2.81	0.47
38:a:2315:G:H5'	51:n:157:THR:HG23	1.97	0.47
8:7:60:U:OP1	13:AE:256:ASP:CB	2.62	0.46
9:A:33:U:H2'	9:A:35:A:OP2	2.14	0.46
9:A:56:C:H2'	9:A:57:A:C5'	2.27	0.46
9:A:60:U:OP2	9:A:61:C:N4	2.45	0.46
10:AA:735:LYS:NZ	37:Y:73:U:H3	2.10	0.46
10:AA:829:THR:HG23	10:AA:1059:ARG:HA	1.97	0.46
10:AA:1046:VAL:CG2	10:AA:1049:ILE:HG13	2.45	0.46
12:AD:86:LYS:HE3	13:AE:528:THR:HG21	1.98	0.46
12:AD:109:PRO:HB3	12:AD:132:HIS:CD2	2.50	0.46
12:AD:199:ASP:N	12:AD:199:ASP:OD1	2.47	0.46
13:AE:1167:LYS:NZ	13:AE:1170:LYS:HB2	2.30	0.46
9:B:18:G:C8	9:B:57:A:N1	2.83	0.46
16:D:373:A:C2	16:D:374:A:C8	3.03	0.46
34:V:8:LEU:HD23	34:V:25:ILE:HG21	1.97	0.46
38:a:2168:G:H8	38:a:2168:G:OP1	1.97	0.46
38:a:2168:G:OP1	38:a:2168:G:C8	2.68	0.46
47:j:152:PRO:HG3	47:j:156:PHE:CZ	2.50	0.46
13:AE:198:CYS:HA	13:AE:221:ILE:CD1	2.45	0.46
13:AE:1219:ASP:O	13:AE:1223:LEU:HB2	2.15	0.46
16:D:1228:C:P	36:X:107:ARG:HH12	2.38	0.46
20:H:291:GLY:HA2	20:H:305:HIS:O	2.15	0.46
38:a:686:U:O4	50:m:12:ARG:HB2	2.14	0.46
38:a:1814:G:C4'	45:h:51:THR:HG21	2.44	0.46
10:AA:588:GLU:HA	10:AA:606:LEU:O	2.15	0.46
12:AC:73:GLY:HA3	12:AC:138:ALA:CB	2.46	0.46
13:AE:902:ASP:OD2	13:AE:905:ARG:HB2	2.15	0.46
13:AE:1060:VAL:HG13	13:AE:1106:ILE:HG12	1.96	0.46
16:D:429:U:N3	16:D:431:A:N6	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:526:C:OP2	30:R:88:LYS:HE3	2.15	0.46
16:D:868:C:H2'	16:D:869:G:O4'	2.15	0.46
23:K:96:MET:CE	23:K:115:LEU:HD11	2.46	0.46
51:n:36:LEU:HB3	51:n:57:LEU:HD21	1.97	0.46
56:s:84:ILE:HG23	56:s:84:ILE:O	2.14	0.46
59:v:96:ILE:HG21	59:v:126:ILE:HD12	1.97	0.46
3:2:30:ILE:HD13	3:2:93:LEU:HD12	1.97	0.46
9:A:76:A:C2'	38:a:2394:C:N4	2.75	0.46
13:AE:24:LEU:CB	13:AE:232:ASN:OD1	2.54	0.46
13:AE:128:LEU:HD21	13:AE:188:LEU:HB3	1.97	0.46
13:AE:526:VAL:HG12	13:AE:549:LYS:HB2	1.96	0.46
15:C:12:ARG:NH2	20:H:268:VAL:CG2	2.71	0.46
15:C:33:ILE:O	15:C:33:ILE:HG12	2.15	0.46
16:D:915:A:C8	16:D:915:A:H3'	2.51	0.46
38:a:784:G:H5'	38:a:785:G:OP1	2.15	0.46
38:a:2291:U:H2'	38:a:2292:U:C6	2.51	0.46
45:h:76:ALA:HB2	45:h:96:TYR:CD1	2.51	0.46
60:w:28:LEU:HD23	60:w:48:VAL:HG21	1.98	0.46
4:3:94:ARG:CB	4:3:103:ILE:HD12	2.46	0.46
9:A:18:G:C8	9:A:57:A:N1	2.83	0.46
10:AA:559:CYS:HB2	10:AA:662:SER:HB3	1.97	0.46
13:AE:417:ARG:HH12	14:AF:43:ASN:HB2	1.80	0.46
25:M:24:ALA:O	25:M:27:VAL:HG22	2.16	0.46
38:a:2298:A:C6	38:a:2299:U:C2	3.04	0.46
9:A:5:G:C2'	9:A:6:G:C5'	2.93	0.46
9:A:29:G:H2'	9:A:30:G:O4'	2.15	0.46
10:AA:756:TYR:CD2	12:AC:68:TYR:O	2.68	0.46
12:AC:141:SER:O	12:AC:141:SER:OG	2.33	0.46
9:B:56:C:H2'	9:B:57:A:C5'	2.27	0.46
20:H:309:MET:HE2	20:H:318:PRO:HB3	1.97	0.46
38:a:517:C:OP2	46:i:10:ARG:NH2	2.48	0.46
9:A:58:A:C1'	9:A:60:U:C5	2.99	0.46
12:AD:96:ASP:HB3	12:AD:148:ARG:HE	1.81	0.46
13:AE:141:PHE:CE2	13:AE:296:LYS:CB	2.94	0.46
16:D:321:A:N7	16:D:328:C:O2'	2.35	0.46
21:I:117:ALA:HB2	21:I:200:VAL:CG1	2.46	0.46
32:T:21:ASP:OD1	32:T:22:THR:N	2.49	0.46
56:s:30:THR:CG2	56:s:31:GLU:N	2.79	0.46
8:7:58:A:N3	8:7:58:A:H5''	2.31	0.46
8:7:66:A:OP2	10:AA:540:ARG:NH2	2.49	0.46
9:A:14:A:H1'	9:A:22:G:N2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AC:228:LEU:HD11	12:AD:224:LEU:HD23	1.98	0.46
9:B:48:C:N4	9:B:59:A:C5	2.84	0.46
16:D:1176:A:H2'	16:D:1177:G:O4'	2.16	0.46
38:a:1394:U:H4'	38:a:1603:A:H4'	1.97	0.46
57:t:18:ARG:HB2	57:t:45:GLU:HB3	1.97	0.46
12:AD:131:CYS:SG	12:AD:132:HIS:N	2.89	0.46
9:B:58:A:C1'	9:B:60:U:C5	2.99	0.46
16:D:1175:G:N3	16:D:1176:A:C8	2.83	0.46
19:G:114:LEU:HD13	19:G:144:LEU:CB	2.46	0.46
28:P:8:ILE:HD12	28:P:25:ILE:CD1	2.46	0.46
49:l:149:ILE:CD1	49:l:188:MET:HE3	2.46	0.46
8:7:69:G:C6	8:7:70:G:C5	3.04	0.46
9:A:6:G:O2'	9:A:7:G:C5'	2.64	0.46
9:A:48:C:N4	9:A:59:A:C5	2.84	0.46
10:AA:446:ASP:HA	10:AA:451:ARG:HH21	1.81	0.46
10:AA:641:GLU:OE2	13:AE:749:LYS:NZ	2.47	0.46
18:F:67:ARG:HD3	18:F:67:ARG:N	2.31	0.46
38:a:1695:G:N7	45:h:14:ARG:NH2	2.64	0.46
38:a:2070:A:H2'	38:a:2071:A:O4'	2.16	0.46
38:a:2585:U:O2	38:a:2585:U:O4'	2.31	0.46
1:O:51:VAL:HG22	1:O:51:VAL:O	2.15	0.45
10:AA:318:SER:H	10:AA:321:LEU:HD12	1.80	0.45
10:AA:1252:SER:N	10:AA:1259:LEU:HD11	2.31	0.45
16:D:1240:U:OP1	25:M:116:MET:HB2	2.16	0.45
20:H:332:VAL:HG13	20:H:342:ILE:HG23	1.98	0.45
36:X:96:PRO:HG2	36:X:102:THR:HG23	1.97	0.45
8:7:60:U:C5	8:7:61:U:N3	2.84	0.45
8:7:63:G:H2'	8:7:64:U:H6	1.81	0.45
10:AA:1340:GLU:HB3	10:AA:1341:ASP:H	1.58	0.45
13:AE:43:THR:HG22	13:AE:57:PHE:HE1	1.80	0.45
13:AE:109:SER:HB2	13:AE:296:LYS:HG2	1.98	0.45
13:AE:395:LYS:NZ	13:AE:399:LYS:CD	2.74	0.45
16:D:17:U:H2'	16:D:18:C:C6	2.52	0.45
43:f:25:LEU:C	43:f:25:LEU:HD13	2.41	0.45
7:6:15:DC:N3	7:6:16:DC:C4	2.84	0.45
10:AA:914:LYS:HD3	10:AA:914:LYS:N	2.31	0.45
13:AE:105:ILE:HD12	13:AE:242:LEU:CD2	2.44	0.45
13:AE:115:TRP:HB3	13:AE:1333:THR:CG2	2.47	0.45
25:M:27:VAL:HG12	25:M:43:VAL:HG11	1.98	0.45
29:Q:34:ILE:HG12	29:Q:70:CYS:SG	2.56	0.45
38:a:2822:G:OP1	47:j:164:GLN:NE2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AA:724:VAL:HG13	10:AA:774:GLY:H	1.76	0.45
10:AA:726:TYR:O	10:AA:726:TYR:CD2	2.69	0.45
15:C:12:ARG:CZ	20:H:264:GLU:HA	2.46	0.45
20:H:316:ILE:HD11	20:H:321:VAL:HG11	1.97	0.45
27:O:63:LEU:HD13	27:O:65:ILE:HD11	1.97	0.45
38:a:1327:A:H2'	38:a:1328:A:O4'	2.17	0.45
47:j:186:LEU:HD21	62:y:4:ILE:HG21	1.98	0.45
51:n:29:PRO:HB2	51:n:169:LEU:HD22	1.99	0.45
51:n:57:LEU:HD22	51:n:89:VAL:CG2	2.47	0.45
9:A:41:C:C5'	25:M:143:ARG:HD2	2.46	0.45
10:AA:735:LYS:HA	10:AA:748:ILE:HG22	1.97	0.45
13:AE:201:LEU:CD1	13:AE:224:LEU:HD12	2.46	0.45
13:AE:1158:GLU:HA	13:AE:1223:LEU:HD21	1.99	0.45
17:E:55:GLN:N	17:E:56:PRO:HD2	2.32	0.45
6:5:116:DG:OP1	13:AE:1311:LYS:NZ	2.46	0.45
9:A:49:G:C2'	9:A:50:U:H5'	2.47	0.45
10:AA:538:LEU:HD11	10:AA:571:LEU:HD22	1.97	0.45
10:AA:933:VAL:O	10:AA:933:VAL:HG12	2.16	0.45
12:AD:16:ILE:HD13	12:AD:214:GLU:HG2	1.99	0.45
12:AD:212:ASP:O	12:AD:215:GLU:N	2.48	0.45
13:AE:213:LYS:HA	13:AE:213:LYS:HE3	1.99	0.45
9:B:48:C:C5	9:B:59:A:C8	3.05	0.45
15:C:61:ARG:HG2	24:L:88:MET:HE1	1.98	0.45
16:D:337:G:H2'	16:D:338:A:C8	2.52	0.45
16:D:1340:A:H8	16:D:1340:A:O5'	1.99	0.45
19:G:16:PHE:CD2	20:H:42:LEU:O	2.69	0.45
38:a:39:G:H1'	49:l:43:THR:HG21	1.99	0.45
10:AA:176:ILE:HD12	10:AA:184:LEU:HD23	1.99	0.45
10:AA:933:VAL:HG22	10:AA:935:THR:CG2	2.47	0.45
13:AE:209:ASN:HA	13:AE:214:ARG:NH2	2.31	0.45
9:B:49:G:C2'	9:B:50:U:H5'	2.47	0.45
9:B:68:C:H3'	9:B:69:C:H5''	1.96	0.45
20:H:33:LYS:HA	20:H:34:ASP:HA	1.61	0.45
38:a:1007:C:OP1	56:s:37:ARG:NH2	2.50	0.45
38:a:1720:U:H2'	38:a:1721:G:O4'	2.16	0.45
13:AE:211:GLU:CG	13:AE:215:LYS:HE3	2.44	0.45
19:G:114:LEU:HA	19:G:144:LEU:HD13	1.98	0.45
20:H:19:ARG:O	20:H:72:LEU:HD13	2.16	0.45
38:a:954:G:OP2	59:v:16:ARG:NH2	2.50	0.45
6:5:114:DC:H5''	13:AE:1148:ARG:CZ	2.46	0.45
10:AA:803:ALA:HB2	10:AA:1094:VAL:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:197:GLU:HA	22:J:200:ILE:HD12	1.99	0.45
38:a:340:A:O2'	49:l:162:ARG:NH1	2.50	0.45
38:a:2547:A:H2'	38:a:2548:U:C6	2.52	0.45
9:A:48:C:C5	9:A:59:A:C8	3.05	0.45
12:AC:79:LEU:HD23	12:AC:79:LEU:HA	1.86	0.45
9:B:5:G:C2'	9:B:6:G:C5'	2.93	0.45
9:B:6:G:O2'	9:B:7:G:C5'	2.64	0.45
9:B:14:A:H1'	9:B:22:G:N2	2.31	0.45
9:B:34:C:C5	9:B:34:C:OP1	2.70	0.45
16:D:563:A:C2	16:D:884:U:O4	2.62	0.45
16:D:915:A:H8	16:D:915:A:O5'	2.00	0.45
19:G:76:ALA:CB	19:G:210:VAL:HG11	2.47	0.45
21:I:155:GLY:HA2	21:I:163:ALA:HB1	1.99	0.45
36:X:106:ALA:HB3	36:X:110:LYS:HD2	1.98	0.45
47:j:4:LEU:HD23	47:j:29:VAL:CG1	2.39	0.45
51:n:77:PHE:N	51:n:77:PHE:CD1	2.82	0.45
10:AA:844:LYS:HD3	10:AA:844:LYS:HA	1.48	0.44
10:AA:939:VAL:HG12	10:AA:939:VAL:O	2.17	0.44
12:AC:59:VAL:O	12:AC:171:LEU:HG	2.17	0.44
13:AE:50:LYS:HD3	13:AE:50:LYS:HA	1.72	0.44
13:AE:126:LEU:HD12	13:AE:223:LEU:HD22	1.99	0.44
13:AE:213:LYS:HE3	13:AE:213:LYS:CA	2.47	0.44
16:D:13:U:C2	16:D:915:A:C5	3.05	0.44
38:a:645:C:H2'	38:a:647:G:C8	2.52	0.44
55:r:55:GLU:HA	55:r:58:LEU:HD12	1.99	0.44
7:6:15:DC:C4	7:6:16:DC:C5	3.05	0.44
10:AA:32:LEU:HD23	10:AA:32:LEU:HA	1.83	0.44
10:AA:95:PRO:HB3	10:AA:123:TYR:HE1	1.83	0.44
12:AD:64:VAL:HG11	12:AD:78:ILE:HG21	1.99	0.44
9:B:60:U:OP2	9:B:61:C:N4	2.45	0.44
16:D:198:G:OP2	16:D:198:G:C8	2.70	0.44
16:D:397:A:H3'	16:D:397:A:N3	2.33	0.44
16:D:1308:U:O5'	36:X:98:ARG:HG2	2.16	0.44
20:H:38:VAL:HG22	20:H:48:ILE:HD11	1.99	0.44
20:H:84:LEU:N	20:H:84:LEU:CD2	2.78	0.44
20:H:294:VAL:HG21	20:H:330:VAL:HG21	1.99	0.44
61:x:18:LEU:HD23	61:x:25:ARG:HD2	1.99	0.44
6:5:115:DA:P	13:AE:1148:ARG:HG3	2.58	0.44
10:AA:724:VAL:HG12	10:AA:774:GLY:N	2.31	0.44
10:AA:850:ILE:HD12	10:AA:1048:LYS:HG2	1.99	0.44
13:AE:123:ARG:HD3	13:AE:123:ARG:HA	1.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AE:1033:GLY:HA3	13:AE:1081:VAL:O	2.18	0.44
9:B:9:G:O2'	9:B:45:G:H2'	2.18	0.44
36:X:75:MET:HA	36:X:75:MET:HE3	1.99	0.44
36:X:106:ALA:HB3	36:X:110:LYS:CD	2.47	0.44
38:a:68:G:N2	38:a:74:A:OP2	2.49	0.44
38:a:2093:G:O2'	38:a:2198:A:N1	2.41	0.44
41:d:48:U:H2'	41:d:49:C:C6	2.52	0.44
10:AA:800:MET:HE3	10:AA:800:MET:HB2	1.60	0.44
12:AD:211:ILE:HD11	12:AD:215:GLU:HG3	1.99	0.44
13:AE:385:LEU:HD23	13:AE:390:LEU:HB2	1.98	0.44
13:AE:847:ASP:N	13:AE:847:ASP:OD1	2.49	0.44
13:AE:978:ARG:HD3	13:AE:999:TYR:H	1.82	0.44
13:AE:1227:HIS:HA	13:AE:1230:THR:HG22	1.99	0.44
9:B:34:C:O5'	9:B:34:C:C6	2.70	0.44
9:B:57:A:O5'	9:B:58:A:P	2.76	0.44
38:a:57:C:H2'	38:a:58:G:O4'	2.17	0.44
38:a:1047:G:N2	38:a:1110:G:O2'	2.50	0.44
45:h:6:CYS:SG	45:h:13:ARG:NH1	2.89	0.44
57:t:24:VAL:HG13	57:t:33:ALA:HB2	2.00	0.44
9:A:56:C:OP1	38:a:2168:G:C4	2.71	0.44
13:AE:62:PHE:N	13:AE:62:PHE:CD1	2.86	0.44
13:AE:161:THR:H	13:AE:164:GLN:HB2	1.82	0.44
13:AE:395:LYS:NZ	13:AE:399:LYS:HE2	2.32	0.44
13:AE:894:VAL:HG22	13:AE:1258:ARG:HH11	1.83	0.44
9:B:25:C:C2'	9:B:26:G:H5'	2.48	0.44
36:X:23:TYR:CD2	36:X:69:LEU:HD23	2.53	0.44
38:a:2395:C:H2'	38:a:2396:G:O4'	2.18	0.44
9:A:57:A:O5'	9:A:58:A:P	2.76	0.44
13:AE:128:LEU:CD2	13:AE:188:LEU:HB3	2.47	0.44
13:AE:141:PHE:HE2	13:AE:296:LYS:CB	2.22	0.44
13:AE:222:LYS:HA	13:AE:222:LYS:HD2	1.32	0.44
16:D:376:G:C2	16:D:389:A:C2	3.06	0.44
38:a:1906:G:H4'	38:a:1906:G:OP1	2.16	0.44
42:e:59:GLU:O	42:e:63:ALA:HB3	2.18	0.44
9:A:22:G:H2'	9:A:23:C:C5	2.52	0.44
10:AA:75:LEU:HD23	10:AA:94:ALA:HB3	2.00	0.44
10:AA:469:VAL:HA	10:AA:472:GLU:HG2	2.00	0.44
10:AA:857:VAL:HG11	10:AA:861:ALA:HB2	1.99	0.44
12:AC:71:LYS:HZ1	12:AC:140:ILE:HD12	1.82	0.44
13:AE:515:ARG:NH2	13:AE:718:SER:O	2.48	0.44
13:AE:926:PRO:HB2	13:AE:1241:TYR:HE1	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AE:1108:GLN:HG3	13:AE:1109:LEU:HD12	1.99	0.44
9:B:22:G:O2'	9:B:23:C:O5'	2.36	0.44
16:D:109:A:C6	16:D:326:G:C6	3.05	0.44
16:D:842:U:H3'	16:D:843:U:C5'	2.48	0.44
19:G:206:ALA:O	19:G:210:VAL:HG23	2.18	0.44
20:H:290:TYR:O	20:H:305:HIS:C	2.56	0.44
38:a:930:G:H1'	43:f:25:LEU:HD11	1.98	0.44
56:s:73:VAL:HG11	56:s:75:TYR:CZ	2.53	0.44
6:5:116:DG:C6	6:5:117:DA:C6	3.06	0.44
12:AC:71:LYS:NZ	12:AC:140:ILE:HG13	2.32	0.44
12:AC:92:VAL:HG12	12:AC:121:VAL:HG12	1.98	0.44
13:AE:67:ASP:CG	13:AE:95:THR:HG1	2.25	0.44
13:AE:111:THR:CG2	13:AE:300:GLN:HA	2.48	0.44
13:AE:824:PRO:HD3	13:AE:835:LEU:HD12	2.00	0.44
13:AE:1026:PRO:HB2	13:AE:1028:ILE:HG23	2.00	0.44
19:G:114:LEU:HD13	19:G:144:LEU:HB3	1.99	0.44
20:H:136:VAL:HA	20:H:168:VAL:O	2.18	0.44
23:K:156:LYS:HG2	26:N:71:VAL:HG13	2.00	0.44
38:a:1589:U:C2	38:a:1590:A:C8	3.06	0.44
38:a:1925:C:C5	38:a:1925:C:OP2	2.70	0.44
51:n:17:MET:HE2	51:n:25:VAL:HA	1.98	0.44
7:6:12:DC:O5'	7:6:12:DC:H6	2.01	0.44
10:AA:717:VAL:HG22	10:AA:782:VAL:HG12	2.00	0.44
10:AA:1117:LEU:HD12	10:AA:1195:ILE:HG12	2.00	0.44
12:AD:57:THR:HG21	12:AD:147:GLN:HB2	1.99	0.44
13:AE:75:TYR:CD2	13:AE:75:TYR:O	2.70	0.44
13:AE:245:LEU:CG	13:AE:246:PRO:HD2	2.47	0.44
13:AE:388:ARG:HG2	13:AE:388:ARG:NH1	2.32	0.44
13:AE:506:VAL:HG23	13:AE:628:GLY:HA3	1.99	0.44
9:B:18:G:O2'	9:B:60:U:N3	2.48	0.44
15:C:12:ARG:HD3	15:C:16:GLU:OE1	2.18	0.44
16:D:1417:G:C6	16:D:1482:G:C6	3.06	0.44
18:F:21:ARG:HH22	20:H:341:ARG:HD2	1.82	0.44
22:J:61:VAL:CG2	22:J:200:ILE:HD11	2.39	0.44
38:a:74:A:N7	38:a:88:G:C5	2.86	0.44
58:u:2:ARG:H	58:u:5:THR:HG1	1.64	0.44
63:z:76:TYR:OH	63:z:92:ARG:NH1	2.51	0.44
2:1:17:VAL:HG12	2:1:76:VAL:HG21	1.98	0.43
9:A:76:A:C2	52:o:31:HIS:NE2	2.85	0.43
12:AD:86:LYS:NZ	13:AE:528:THR:HB	2.33	0.43
16:D:324:G:N2	16:D:327:A:C8	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:208:ARG:HH12	20:H:29:VAL:HG11	1.82	0.43
27:O:80:ARG:O	27:O:84:THR:HG23	2.18	0.43
38:a:813:U:H2'	38:a:814:C:C6	2.53	0.43
38:a:1385:A:O2'	38:a:1396:U:O2	2.35	0.43
38:a:2252:G:O2'	38:a:2253:G:H5'	2.18	0.43
40:c:37:ARG:HG2	40:c:48:THR:HG23	2.00	0.43
59:v:35:ALA:HB2	59:v:102:LEU:HD11	2.00	0.43
9:A:25:C:C2'	9:A:26:G:H5'	2.48	0.43
13:AE:68:TYR:O	13:AE:75:TYR:CD2	2.70	0.43
13:AE:1079:LYS:HD3	13:AE:1098:GLN:HB3	2.00	0.43
9:B:1:C:C5	9:B:2:G:N7	2.86	0.43
16:D:1499:A:O2'	16:D:1500:A:C5'	2.67	0.43
20:H:61:GLU:HG2	20:H:62:ILE:HG23	2.00	0.43
38:a:214:G:N2	38:a:216:A:N3	2.66	0.43
38:a:1386:C:H2'	38:a:1387:A:C8	2.53	0.43
38:a:2133:G:O2'	38:a:2157:G:N2	2.51	0.43
9:A:22:G:O2'	9:A:23:C:O5'	2.36	0.43
10:AA:524:ILE:HB	10:AA:712:SER:HB2	1.99	0.43
12:AC:58:GLU:HB3	12:AC:170:ARG:HG2	1.99	0.43
20:H:76:GLU:HA	20:H:76:GLU:OE2	2.19	0.43
23:K:153:VAL:HG23	23:K:164:ILE:HD13	2.00	0.43
55:r:15:LEU:HD13	55:r:15:LEU:C	2.42	0.43
6:5:113:DC:P	10:AA:163:LYS:HD3	2.55	0.43
10:AA:870:ILE:HG12	10:AA:884:VAL:HG12	1.98	0.43
16:D:684:U:H2'	16:D:685:G:O4'	2.18	0.43
16:D:976:G:C8	16:D:1358:U:O2	2.71	0.43
20:H:302:GLY:HA3	20:H:344:LEU:HD13	2.00	0.43
33:U:6:LEU:HG	33:U:17:TYR:HB3	2.00	0.43
38:a:1142:A:H2'	38:a:1142:A:N3	2.34	0.43
38:a:1266:G:OP1	46:i:16:ARG:NE	2.45	0.43
38:a:1927:A:C8	38:a:1927:A:O5'	2.70	0.43
38:a:2469:A:N6	38:a:2481:G:O2'	2.52	0.43
8:7:56:U:O2	8:7:56:U:H2'	2.17	0.43
10:AA:318:SER:OG	10:AA:320:ASP:OD1	2.31	0.43
10:AA:623:LEU:HD13	10:AA:627:GLY:HA2	2.01	0.43
12:AC:145:LYS:HE3	12:AC:145:LYS:HB2	1.83	0.43
13:AE:58:CYS:SG	13:AE:60:ARG:HG2	2.59	0.43
13:AE:201:LEU:HD11	13:AE:220:ARG:NH1	2.31	0.43
13:AE:417:ARG:NH1	14:AF:43:ASN:O	2.51	0.43
13:AE:568:SER:HB3	13:AE:570:LYS:NZ	2.34	0.43
16:D:384:G:H2'	16:D:385:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:1371:G:O3'	27:O:71:GLY:HA3	2.19	0.43
38:a:998:C:OP2	63:z:58:ARG:NH2	2.49	0.43
9:A:9:G:O2'	9:A:45:G:H2'	2.18	0.43
9:A:49:G:O5'	9:A:49:G:C8	2.71	0.43
9:B:49:G:O5'	9:B:49:G:C8	2.71	0.43
23:K:111:MET:CE	23:K:125:ALA:HB1	2.39	0.43
38:a:631:A:N3	38:a:2415:G:O2'	2.48	0.43
8:7:60:U:H2'	8:7:61:U:O4'	2.19	0.43
9:A:1:C:C5	9:A:2:G:N7	2.86	0.43
9:A:18:G:N3	9:A:58:A:C5	2.87	0.43
9:A:34:C:OP1	25:M:84:THR:OG1	2.35	0.43
13:AE:107:LEU:HA	13:AE:276:ASN:ND2	2.33	0.43
13:AE:111:THR:HG21	13:AE:303:VAL:HB	2.00	0.43
13:AE:395:LYS:HB3	13:AE:395:LYS:HE3	1.45	0.43
13:AE:450:HIS:HA	13:AE:451:PRO:HD3	1.91	0.43
13:AE:1046:ILE:HG22	13:AE:1061:VAL:HA	2.00	0.43
20:H:109:THR:C	20:H:153:GLU:HA	2.43	0.43
20:H:280:LEU:HB2	20:H:330:VAL:O	2.19	0.43
28:P:10:LEU:HG	28:P:98:VAL:HG12	1.99	0.43
29:Q:88:GLY:H	29:Q:114:THR:HG22	1.84	0.43
38:a:1095:A:H2'	38:a:1096:A:C8	2.53	0.43
57:t:76:VAL:HG12	62:y:73:VAL:HB	2.01	0.43
57:t:107:LEU:HD21	57:t:115:ILE:HG21	2.01	0.43
10:AA:796:LEU:N	10:AA:1231:TYR:OH	2.52	0.43
10:AA:805:MET:HE3	10:AA:805:MET:HB2	1.87	0.43
13:AE:76:LYS:HB3	13:AE:76:LYS:NZ	2.32	0.43
13:AE:244:VAL:HA	13:AE:269:TYR:OH	2.19	0.43
13:AE:850:LYS:HB3	13:AE:855:ASP:HB2	2.00	0.43
9:B:53:G:C2	9:B:54:U:C5	3.07	0.43
16:D:1333:A:H2'	16:D:1334:G:O4'	2.19	0.43
38:a:126:A:O5'	50:m:19:ARG:HG3	2.19	0.43
50:m:12:ARG:HG3	50:m:44:VAL:HG11	2.00	0.43
4:3:12:ILE:CG2	4:3:80:ALA:HB2	2.49	0.43
9:A:26:G:N2	9:A:45:G:N2	2.66	0.43
9:A:53:G:C2	9:A:54:U:C5	3.07	0.43
10:AA:873:ILE:O	10:AA:928:VAL:HB	2.18	0.43
10:AA:1329:GLU:HA	13:AE:245:LEU:HD13	2.01	0.43
12:AC:50:SER:HB3	12:AD:8:PHE:HZ	1.84	0.43
13:AE:126:LEU:CD1	13:AE:223:LEU:HD22	2.49	0.43
9:B:18:G:N3	9:B:58:A:C5	2.87	0.43
9:B:22:G:H2'	9:B:23:C:C5	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:26:G:N2	9:B:45:G:N2	2.66	0.43
9:B:46:G:O2'	9:B:47:U:H5''	2.19	0.43
16:D:60:A:N1	16:D:107:G:O2'	2.42	0.43
19:G:35:ARG:CG	20:H:10:GLU:OE2	2.63	0.43
38:a:705:A:O4'	45:h:9:THR:HG21	2.18	0.43
38:a:819:A:C4	38:a:1189:A:C2	3.07	0.43
38:a:2602:A:H5''	38:a:2603:G:C5'	2.49	0.43
13:AE:609:TYR:HD2	13:AE:610:ARG:NH1	2.17	0.43
13:AE:1024:THR:HG23	13:AE:1123:ARG:HA	2.00	0.43
16:D:421:U:O2	16:D:421:U:O4'	2.37	0.43
16:D:826:C:O2	26:N:16:ASN:ND2	2.52	0.43
19:G:16:PHE:CG	20:H:43:LYS:HA	2.53	0.43
19:G:47:VAL:N	19:G:48:PRO:HD2	2.34	0.43
20:H:274:TYR:HD1	20:H:335:ILE:HD12	1.84	0.43
27:O:55:VAL:O	27:O:57:MET:N	2.52	0.43
38:a:2511:U:O4	38:a:2575:C:N3	2.52	0.43
9:A:36:U:H2'	9:A:37:A:O4'	2.19	0.42
9:A:46:G:O2'	9:A:47:U:H5''	2.19	0.42
38:a:2365:G:N7	52:o:39:LYS:NZ	2.59	0.42
63:z:83:LEU:HD23	63:z:83:LEU:HA	1.92	0.42
4:3:39:ILE:HG22	4:3:40:ASN:N	2.34	0.42
12:AD:207:THR:OG1	12:AD:208:ASN:N	2.52	0.42
13:AE:388:ARG:HG2	13:AE:388:ARG:HH11	1.84	0.42
13:AE:515:ARG:HH12	13:AE:724:MET:HG2	1.83	0.42
16:D:37:U:O2	16:D:548:G:N2	2.53	0.42
19:G:208:ARG:NH1	20:H:29:VAL:HG11	2.34	0.42
27:O:28:ILE:HD12	27:O:28:ILE:N	2.35	0.42
38:a:879:G:H2'	38:a:880:G:O4'	2.19	0.42
38:a:1019:U:N3	38:a:1142:A:N6	2.49	0.42
38:a:1250:G:OP2	58:u:21:ARG:NH2	2.52	0.42
38:a:1394:U:C4	38:a:1395:A:C6	3.07	0.42
54:q:3:VAL:HA	54:q:36:ARG:O	2.19	0.42
6:5:109:DT:H2''	10:AA:200:ARG:CG	2.37	0.42
9:A:47:U:O2'	9:A:50:U:OP1	2.37	0.42
10:AA:666:SER:HB2	10:AA:1186:VAL:HG21	2.00	0.42
10:AA:1043:ALA:CB	10:AA:1044:PRO:CD	2.91	0.42
18:F:67:ARG:HD3	18:F:67:ARG:H	1.85	0.42
20:H:152:LEU:CB	20:H:171:ARG:H	2.32	0.42
38:a:299:A:N1	38:a:322:A:O2'	2.47	0.42
38:a:637:A:N1	38:a:651:G:O2'	2.51	0.42
38:a:2615:U:C2	46:i:4:GLN:HA	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:h:240:PHE:CD2	45:h:240:PHE:O	2.73	0.42
57:t:38:ILE:HD11	57:t:112:PHE:CZ	2.55	0.42
9:A:58:A:OP2	9:A:58:A:H8	2.02	0.42
10:AA:395:TYR:HE2	10:AA:420:LEU:HG	1.84	0.42
10:AA:529:ARG:HH22	10:AA:687:ARG:HH11	1.66	0.42
13:AE:141:PHE:CD2	13:AE:297:ARG:HB2	2.54	0.42
13:AE:144:TYR:CE1	13:AE:162:GLU:OE1	2.73	0.42
13:AE:586:GLY:HA3	13:AE:612:LEU:HD11	2.01	0.42
13:AE:1350:ASN:HA	13:AE:1353:VAL:HG12	2.02	0.42
16:D:622:A:C8	16:D:623:C:C6	3.08	0.42
20:H:119:GLY:CA	20:H:132:PRO:C	2.92	0.42
38:a:973:A:O4'	38:a:1188:U:C6	2.72	0.42
38:a:1021:A:N3	38:a:1021:A:C3'	2.78	0.42
38:a:1082:U:H3	38:a:1086:A:N6	2.15	0.42
38:a:2638:G:O2'	38:a:2775:G:N2	2.42	0.42
61:x:99:TYR:OH	61:x:111:ARG:NH1	2.53	0.42
10:AA:562:GLU:OE1	10:AA:662:SER:OG	2.31	0.42
10:AA:914:LYS:C	10:AA:914:LYS:HE3	2.44	0.42
11:AB:7:LYS:HG2	11:AB:74:VAL:HG13	2.01	0.42
13:AE:647:PRO:HG3	13:AE:697:MET:HB3	2.01	0.42
13:AE:820:ILE:HG12	13:AE:884:SER:HB2	2.02	0.42
13:AE:1357:ILE:HG22	13:AE:1359:ALA:H	1.83	0.42
9:B:15:G:H1	9:B:20:U:H3	1.68	0.42
15:C:44:ILE:HG21	20:H:339:ARG:HA	2.01	0.42
23:K:150:PRO:O	23:K:153:VAL:HG22	2.19	0.42
38:a:126:A:OP1	50:m:45:SER:OG	2.38	0.42
38:a:948:C:H1'	38:a:984:A:C8	2.55	0.42
38:a:1028:A:N6	38:a:1125:G:H2'	2.34	0.42
38:a:1363:C:O2'	38:a:1809:A:N3	2.46	0.42
38:a:2756:U:C4	38:a:2759:G:O6	2.72	0.42
45:h:37:ASN:HB2	45:h:62:TYR:HB2	2.01	0.42
57:t:113:MET:HE3	57:t:116:ILE:HD11	2.01	0.42
58:u:109:LYS:HG2	58:u:126:ARG:HB2	2.02	0.42
12:AC:47:LEU:HD23	12:AC:47:LEU:HA	1.88	0.42
16:D:1323:G:H2'	16:D:1324:A:C8	2.54	0.42
19:G:187:VAL:HG21	19:G:199:VAL:HG23	2.02	0.42
37:Y:72:U:C3'	37:Y:72:U:C6	3.02	0.42
38:a:1932:A:H2'	38:a:1933:G:O4'	2.19	0.42
38:a:2252:G:H2'	38:a:2253:G:H8	1.84	0.42
46:i:43:ILE:HG22	46:i:49:TYR:HB2	2.01	0.42
49:l:170:ARG:NH2	49:l:176:ASP:OD1	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:w:49:GLU:HB2	60:w:50:PRO:HD3	2.01	0.42
10:AA:68:LEU:HD11	10:AA:100:LEU:HB3	2.01	0.42
10:AA:565:GLU:HA	10:AA:569:ILE:HG12	2.01	0.42
10:AA:596:ASP:N	10:AA:596:ASP:OD1	2.49	0.42
13:AE:616:PRO:HA	13:AE:619:ILE:HG22	2.02	0.42
16:D:429:U:O2	16:D:430:A:C8	2.72	0.42
16:D:552:U:O2'	30:R:83:ARG:O	2.27	0.42
19:G:19:GLN:OE1	20:H:76:GLU:HB3	2.12	0.42
21:I:9:GLY:HA3	31:S:89:MET:HE3	2.01	0.42
28:P:57:VAL:O	28:P:58:ASN:ND2	2.53	0.42
38:a:984:A:N3	38:a:984:A:H2'	2.35	0.42
38:a:1020:A:C2	38:a:1141:U:C2	3.07	0.42
38:a:1082:U:N3	38:a:1086:A:C6	2.87	0.42
38:a:1082:U:C4	38:a:1086:A:N6	2.88	0.42
56:s:32:LEU:HD23	56:s:54:ILE:HD13	2.01	0.42
63:z:65:ILE:CD1	63:z:92:ARG:HB2	2.49	0.42
10:AA:104:ILE:HD11	10:AA:116:ASP:HB2	2.01	0.42
10:AA:300:ASP:OD1	10:AA:313:ALA:N	2.52	0.42
13:AE:797:THR:HG22	13:AE:924:GLY:HA3	2.01	0.42
13:AE:839:VAL:HG12	13:AE:864:LEU:HD12	2.01	0.42
16:D:216:U:H2'	16:D:217:C:C6	2.55	0.42
16:D:1126:U:OP1	28:P:7:ARG:NH2	2.51	0.42
49:l:134:LEU:HB2	49:l:160:ALA:HB1	2.02	0.42
10:AA:830:THR:HG22	10:AA:1234:LYS:NZ	2.34	0.42
12:AC:231:PHE:HE2	12:AD:39:LEU:HD13	1.85	0.42
13:AE:390:LEU:N	13:AE:390:LEU:HD13	2.35	0.42
13:AE:394:ILE:O	13:AE:394:ILE:HG13	2.18	0.42
16:D:1235:U:H2'	16:D:1236:A:O4'	2.20	0.42
20:H:19:ARG:CD	20:H:73:ASP:OD1	2.66	0.42
20:H:335:ILE:HG12	20:H:342:ILE:HG23	2.00	0.42
38:a:1921:G:C2'	38:a:1922:G:H5'	2.49	0.42
38:a:2273:A:H2'	38:a:2274:A:C8	2.55	0.42
38:a:2788:C:H2'	38:a:2789:C:C6	2.55	0.42
6:5:98:DA:C2'	6:5:99:DT:C7	2.96	0.42
9:A:18:G:O2'	9:A:60:U:N3	2.48	0.42
9:A:56:C:OP1	38:a:2168:G:N3	2.53	0.42
10:AA:55:SER:CB	10:AA:465:ARG:HH12	2.32	0.42
10:AA:888:THR:HG22	10:AA:914:LYS:HD2	2.02	0.42
13:AE:24:LEU:CD1	13:AE:232:ASN:ND2	2.82	0.42
13:AE:102:MET:HG2	13:AE:246:PRO:CG	2.49	0.42
13:AE:279:LEU:HD13	13:AE:299:LEU:HD13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AE:513:MET:HG3	13:AE:544:LEU:HD11	2.01	0.42
13:AE:848:VAL:HB	13:AE:858:VAL:HG22	2.02	0.42
13:AE:950:ILE:HB	13:AE:1018:ALA:HB3	2.01	0.42
14:AF:50:ALA:O	14:AF:54:ILE:HG12	2.19	0.42
16:D:1061:G:H5'	28:P:61:ALA:HB2	2.02	0.42
30:R:110:ARG:NH1	30:R:112:GLN:O	2.53	0.42
38:a:2331:G:O2'	38:a:2336:A:N1	2.47	0.42
45:h:76:ALA:HB2	45:h:96:TYR:CE1	2.55	0.42
47:j:172:VAL:HG11	47:j:175:LEU:HD21	2.01	0.42
56:s:114:LEU:HD12	56:s:114:LEU:HA	1.86	0.42
7:6:27:DG:H1'	7:6:28:DA:C5	2.55	0.41
8:7:55:U:O5'	8:7:55:U:H6	2.03	0.41
10:AA:230:PHE:HB2	10:AA:333:ILE:HB	2.01	0.41
10:AA:242:VAL:HA	10:AA:243:PRO:HD3	1.94	0.41
10:AA:452:ARG:NH1	10:AA:458:GLU:OE2	2.52	0.41
10:AA:685:MET:HE3	10:AA:685:MET:HB2	1.84	0.41
10:AA:1252:SER:N	10:AA:1259:LEU:HD13	2.35	0.41
13:AE:1106:ILE:O	13:AE:1123:ARG:N	2.46	0.41
9:B:26:G:H1	9:B:44:A:N6	2.18	0.41
9:B:58:A:OP2	9:B:58:A:H8	2.02	0.41
15:C:12:ARG:O	15:C:16:GLU:HG3	2.19	0.41
16:D:1208:C:H2'	16:D:1209:C:H6	1.85	0.41
20:H:292:CYS:SG	20:H:304:VAL:HB	2.60	0.41
25:M:22:LEU:HD13	25:M:97:ASN:ND2	2.35	0.41
38:a:1406:U:O2'	38:a:1407:G:OP2	2.38	0.41
38:a:1548:A:H2'	38:a:1549:A:C8	2.55	0.41
38:a:1925:C:OP2	38:a:1925:C:C6	2.73	0.41
49:l:149:ILE:HD11	49:l:188:MET:HE3	2.02	0.41
50:m:12:ARG:CG	50:m:44:VAL:HG11	2.50	0.41
51:n:123:ASP:OD1	51:n:123:ASP:C	2.62	0.41
53:p:25:THR:HG22	53:p:34:THR:HG23	2.02	0.41
59:v:73:ILE:HG21	59:v:91:TYR:CZ	2.55	0.41
10:AA:257:ALA:HB2	10:AA:285:ILE:HG22	2.02	0.41
13:AE:515:ARG:HG2	13:AE:516:ASP:H	1.85	0.41
13:AE:559:ALA:HB3	13:AE:562:GLU:HB3	2.01	0.41
9:B:22:G:HO2'	9:B:23:C:P	2.41	0.41
18:F:32:VAL:HG11	29:Q:89:PRO:HG3	2.01	0.41
23:K:133:PRO:HA	23:K:136:VAL:HG12	2.02	0.41
38:a:197:A:N6	38:a:2430:A:H2'	2.36	0.41
38:a:2006:C:O2'	38:a:2823:A:N3	2.47	0.41
9:A:56:C:C2	38:a:2112:G:C5	3.07	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AA:218:GLU:HG2	10:AA:299:LYS:HA	2.02	0.41
10:AA:593:LYS:HB3	10:AA:602:GLU:HG3	2.02	0.41
10:AA:1046:VAL:HG22	10:AA:1049:ILE:CG1	2.50	0.41
10:AA:1251:TYR:CE2	10:AA:1301:ARG:NH1	2.88	0.41
12:AC:28:LEU:HD23	12:AC:28:LEU:HA	1.87	0.41
13:AE:47:ARG:HA	13:AE:47:ARG:NE	2.34	0.41
9:B:26:G:C2	9:B:45:G:N2	2.88	0.41
16:D:860:A:H2'	16:D:861:G:O4'	2.21	0.41
22:J:48:LEU:HD21	22:J:56:ARG:HG3	2.02	0.41
38:a:67:U:C4	38:a:74:A:C6	3.04	0.41
38:a:207:A:H2'	38:a:208:C:O4'	2.21	0.41
38:a:320:A:H2'	49:l:131:THR:HG21	2.01	0.41
38:a:493:G:H2'	38:a:494:G:O4'	2.21	0.41
38:a:560:C:O2	63:z:48:ARG:NH1	2.41	0.41
38:a:567:U:OP2	58:u:29:LYS:NZ	2.53	0.41
38:a:1570:A:H2'	38:a:1571:A:C8	2.55	0.41
38:a:2803:G:H2'	38:a:2804:U:C5	2.55	0.41
44:g:18:CYS:HB2	44:g:40:CYS:HB3	1.96	0.41
60:w:9:GLN:O	60:w:17:ARG:NH2	2.51	0.41
63:z:66:ASN:OD1	63:z:70:ARG:NE	2.54	0.41
10:AA:839:VAL:O	10:AA:886:LYS:HD2	2.19	0.41
13:AE:137:ARG:HA	13:AE:142:GLU:HG2	2.02	0.41
13:AE:1064:SER:OG	13:AE:1168:GLU:OE1	2.31	0.41
15:C:14:THR:CG2	15:C:48:ARG:HE	2.33	0.41
16:D:429:U:O2	16:D:430:A:N7	2.53	0.41
16:D:502:A:H2'	16:D:503:C:O4'	2.20	0.41
16:D:977:A:H1'	16:D:982:U:O4	2.20	0.41
20:H:110:GLY:H	20:H:153:GLU:N	2.17	0.41
36:X:4:ILE:CG1	36:X:9:ILE:HD12	2.50	0.41
49:l:145:ASP:HA	49:l:166:LYS:HB3	2.01	0.41
2:1:92:ARG:NE	2:1:94:ASP:OD1	2.53	0.41
7:6:21:DA:H5''	10:AA:141:THR:HG21	2.03	0.41
9:A:15:G:H1	9:A:20:U:H3	1.68	0.41
9:A:34:C:H41	25:M:83:SER:HA	1.86	0.41
10:AA:56:VAL:HG11	10:AA:468:LEU:HD13	2.03	0.41
13:AE:144:TYR:N	13:AE:144:TYR:CD1	2.88	0.41
13:AE:201:LEU:HD23	13:AE:201:LEU:HA	1.92	0.41
13:AE:242:LEU:C	13:AE:242:LEU:HD23	2.44	0.41
20:H:342:ILE:HG22	20:H:344:LEU:HD12	2.01	0.41
38:a:36:G:N3	38:a:450:G:O2'	2.53	0.41
38:a:548:G:H3'	38:a:549:G:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:a:2311:A:C2	51:n:85:ILE:HD11	2.55	0.41
47:j:175:LEU:CD1	47:j:193:VAL:HG12	2.51	0.41
49:l:48:THR:HG23	49:l:86:ALA:HB3	2.02	0.41
53:p:52:PHE:CZ	53:p:72:LEU:HD22	2.56	0.41
6:5:98:DA:H2'	6:5:99:DT:H72	2.01	0.41
9:A:8:U:O2'	9:A:47:U:C4	2.72	0.41
10:AA:26:TYR:HE2	10:AA:32:LEU:HD12	1.86	0.41
12:AC:158:ARG:HH12	12:AC:172:LEU:HD23	1.86	0.41
16:D:218:U:H2'	16:D:219:U:O4'	2.21	0.41
16:D:712:A:H2'	16:D:713:G:O4'	2.21	0.41
16:D:1227:A:C5'	36:X:110:LYS:HZ2	2.27	0.41
19:G:38:VAL:HG23	20:H:75:VAL:HG21	1.92	0.41
20:H:155:LYS:O	20:H:169:SER:CB	2.69	0.41
38:a:1839:G:C4	38:a:1927:A:C5	3.08	0.41
9:A:26:G:C2	9:A:45:G:N2	2.89	0.41
9:A:46:G:H2'	9:A:47:U:OP2	2.21	0.41
10:AA:400:VAL:HG21	10:AA:452:ARG:HE	1.84	0.41
13:AE:136:GLU:OE1	13:AE:312:ARG:NH2	2.53	0.41
13:AE:1289:ASN:O	13:AE:1293:GLU:HB2	2.20	0.41
32:T:43:PHE:CE2	32:T:56:LEU:HD22	2.55	0.41
38:a:1021:A:N6	38:a:1141:U:N3	2.47	0.41
38:a:2294:G:OP1	61:x:10:ARG:HD3	2.21	0.41
10:AA:850:ILE:HG21	10:AA:870:ILE:HD11	2.03	0.41
13:AE:820:ILE:HD11	13:AE:822:MET:HE2	2.02	0.41
16:D:37:U:C4	16:D:397:A:N6	2.87	0.41
16:D:548:G:C6	16:D:549:C:C4	3.08	0.41
16:D:765:G:H1	16:D:812:G:HO2'	1.68	0.41
38:a:17:G:H2'	38:a:18:U:C6	2.56	0.41
38:a:742:A:N1	38:a:755:U:O4	2.53	0.41
38:a:1169:A:H5''	38:a:1169:A:N3	2.36	0.41
38:a:2602:A:H5''	38:a:2603:G:H5''	2.03	0.41
38:a:2641:G:OP1	56:s:78:THR:HG22	2.21	0.41
45:h:119:GLY:O	45:h:130:LEU:HB3	2.20	0.41
60:w:67:PHE:O	60:w:71:ARG:HG2	2.21	0.41
8:7:66:A:O2'	10:AA:513:GLN:OE1	2.33	0.41
9:A:7:G:O6	9:A:49:G:O6	2.39	0.41
9:A:22:G:HO2'	9:A:23:C:P	2.44	0.41
10:AA:46:GLN:HA	10:AA:47:TYR:HA	1.77	0.41
10:AA:812:PHE:HZ	13:AE:503:SER:HB2	1.85	0.41
12:AD:152:TYR:HE2	13:AE:535:ARG:HH21	1.68	0.41
12:AD:153:VAL:HG23	12:AD:175:ALA:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AE:44:ILE:CD1	13:AE:252:LEU:CD2	2.94	0.41
13:AE:109:SER:CB	13:AE:296:LYS:HG2	2.51	0.41
13:AE:201:LEU:CB	13:AE:221:ILE:HD13	2.47	0.41
13:AE:351:GLY:O	13:AE:467:ALA:HA	2.21	0.41
16:D:107:G:N7	17:E:10:ARG:NH2	2.60	0.41
16:D:1330:U:OP2	36:X:26:GLY:HA3	2.21	0.41
16:D:1526:G:P	18:F:42:THR:HG23	2.61	0.41
38:a:5:A:H2'	38:a:6:A:C8	2.56	0.41
38:a:1095:A:O2'	38:a:1096:A:O4'	2.33	0.41
38:a:1182:G:H2'	38:a:1183:U:O4'	2.20	0.41
38:a:1365:A:O5'	40:c:28:ARG:NH2	2.51	0.41
38:a:1839:G:C1'	38:a:1927:A:H1'	2.46	0.41
49:l:188:MET:HE2	49:l:193:VAL:HA	2.03	0.41
51:n:122:PHE:CZ	51:n:167:ARG:HA	2.56	0.41
55:r:9:VAL:HG11	55:r:12:LEU:HD21	2.03	0.41
10:AA:241:LEU:N	10:AA:283:LYS:O	2.51	0.41
10:AA:1253:LEU:CD1	13:AE:253:VAL:CG1	2.95	0.41
12:AD:97:GLU:HG3	12:AD:147:GLN:HG2	2.03	0.41
12:AD:111:THR:OG1	12:AD:126:PRO:O	2.35	0.41
13:AE:385:LEU:CD2	13:AE:390:LEU:HB2	2.50	0.41
13:AE:930:LEU:HA	13:AE:1244:GLN:HG3	2.02	0.41
20:H:54:LYS:HE3	20:H:54:LYS:HB3	1.91	0.41
27:O:9:THR:O	27:O:85:ARG:HD2	2.21	0.41
27:O:10:GLY:HA3	27:O:78:ALA:O	2.21	0.41
31:S:41:ARG:O	31:S:45:VAL:HG12	2.20	0.41
43:f:27:LEU:O	43:f:38:ARG:NE	2.46	0.41
60:w:29:VAL:HG11	60:w:75:ILE:HG23	2.03	0.41
3:2:46:ALA:O	3:2:50:LEU:HB2	2.20	0.40
9:A:8:U:H6	9:A:8:U:OP2	2.04	0.40
9:A:26:G:H1	9:A:44:A:N6	2.18	0.40
10:AA:933:VAL:O	10:AA:933:VAL:CG1	2.68	0.40
12:AC:116:THR:O	12:AC:116:THR:OG1	2.35	0.40
13:AE:68:TYR:HB3	13:AE:75:TYR:HE2	1.81	0.40
9:B:7:G:O6	9:B:49:G:O6	2.39	0.40
16:D:915:A:C6	16:D:916:U:C4	3.08	0.40
16:D:1370:G:C2	16:D:1371:G:C8	3.09	0.40
20:H:119:GLY:O	20:H:120:PHE:C	2.62	0.40
22:J:100:ASN:OD1	22:J:111:ARG:NH1	2.54	0.40
36:X:16:VAL:O	36:X:20:THR:HG23	2.21	0.40
38:a:1421:G:C2	38:a:1422:G:C8	3.09	0.40
38:a:2572:A:N7	47:j:150:GLN:NE2	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:h:175:ARG:NH1	45:h:181:MET:HE2	2.36	0.40
10:AA:6:THR:HA	10:AA:9:LYS:HG3	2.03	0.40
10:AA:801:ARG:HH12	10:AA:1119:MET:HE1	1.86	0.40
10:AA:1102:GLY:HA2	10:AA:1106:ARG:HH11	1.85	0.40
13:AE:1050:THR:HG23	13:AE:1057:SER:HB3	2.03	0.40
14:AF:3:ARG:HH12	14:AF:55:GLU:CD	2.27	0.40
16:D:579:A:O2'	32:T:54:ARG:NH1	2.54	0.40
37:Y:72:U:H3'	37:Y:72:U:C6	2.56	0.40
38:a:244:A:OP2	52:o:8:ARG:NH2	2.50	0.40
38:a:851:C:H2'	38:a:852:U:C6	2.55	0.40
38:a:1406:U:C2'	38:a:1407:G:OP2	2.69	0.40
38:a:2298:A:C5	38:a:2321:U:C4	3.09	0.40
41:d:89:U:O2	41:d:89:U:O4'	2.40	0.40
44:g:37:CYS:N	44:g:40:CYS:SG	2.78	0.40
9:A:15:G:N2	9:A:20:U:C2	2.88	0.40
10:AA:488:MET:O	10:AA:490:GLN:N	2.47	0.40
10:AA:731:ARG:HH11	10:AA:731:ARG:HG3	1.86	0.40
13:AE:395:LYS:HZ2	13:AE:399:LYS:CE	2.33	0.40
13:AE:605:LEU:HD23	13:AE:605:LEU:HA	1.93	0.40
16:D:152:A:N6	16:D:170:U:C2	2.89	0.40
31:S:16:LEU:HD13	31:S:54:ASP:HB2	2.03	0.40
38:a:2315:G:C5'	51:n:157:THR:HG23	2.52	0.40
2:1:75:PHE:CZ	2:1:104:THR:HG21	2.56	0.40
12:AD:81:ILE:O	12:AD:85:LEU:HB2	2.22	0.40
13:AE:47:ARG:NE	13:AE:47:ARG:CA	2.83	0.40
13:AE:108:ALA:HB2	13:AE:276:ASN:OD1	2.22	0.40
13:AE:117:LEU:HD22	13:AE:139:LEU:CD1	2.52	0.40
13:AE:734:ALA:O	13:AE:738:ARG:HB2	2.22	0.40
9:B:25:C:H2'	9:B:26:G:C5'	2.51	0.40
16:D:791:G:N2	16:D:1497:G:O3'	2.53	0.40
16:D:890:G:O2'	16:D:906:A:N6	2.55	0.40
36:X:16:VAL:HG13	36:X:34:LEU:CD1	2.51	0.40
38:a:2756:U:OP2	54:q:19:ARG:NE	2.54	0.40
51:n:171:ALA:O	51:n:174:ASP:N	2.54	0.40
58:u:74:THR:HG22	58:u:107:PHE:HB2	2.04	0.40
10:AA:1286:THR:O	10:AA:1290:MET:HB2	2.21	0.40
13:AE:68:TYR:CB	13:AE:75:TYR:HE2	2.34	0.40
16:D:1225:A:H2'	16:D:1226:C:C5	2.56	0.40
26:N:11:LEU:HD22	26:N:75:ILE:HD11	2.03	0.40
38:a:871:U:H2'	38:a:872:U:C6	2.56	0.40
38:a:1736:U:H2'	38:a:1737:G:O4'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	12	49
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
3	2	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
4	3	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	12	49
5	4	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
10	AA	1217/1342 (91%)	1071 (88%)	124 (10%)	22 (2%)	6	34
11	AB	94/181 (52%)	88 (94%)	6 (6%)	0	100	100
12	AC	228/329 (69%)	214 (94%)	12 (5%)	2 (1%)	14	51
12	AD	226/329 (69%)	211 (93%)	15 (7%)	0	100	100
13	AE	1329/1407 (94%)	1199 (90%)	121 (9%)	9 (1%)	18	56
14	AF	81/91 (89%)	74 (91%)	7 (9%)	0	100	100
15	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
17	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
18	F	68/71 (96%)	68 (100%)	0	0	100	100
19	G	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
20	H	255/557 (46%)	189 (74%)	54 (21%)	12 (5%)	2	16
21	I	206/208 (99%)	196 (95%)	9 (4%)	1 (0%)	24	63
22	J	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
23	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	21	59
24	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	12	49
25	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	18	56
26	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	16	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	16	54
28	P	97/103 (94%)	89 (92%)	7 (7%)	1 (1%)	12	49
29	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	7	36
30	R	117/124 (94%)	116 (99%)	1 (1%)	0	100	100
31	S	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
32	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
33	U	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	9	42
34	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
35	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
36	X	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	6	34
39	b	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
40	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
42	e	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
43	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
44	g	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
45	h	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	30	67
46	i	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
47	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
48	k	50/55 (91%)	50 (100%)	0	0	100	100
49	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	24	63
50	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
51	n	175/179 (98%)	162 (93%)	11 (6%)	2 (1%)	11	46
52	o	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
53	p	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
54	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
55	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
56	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
57	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
58	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
59	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
60	w	117/127 (92%)	107 (92%)	10 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	x	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
62	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
63	z	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	51
All	All	9035/10123 (89%)	8383 (93%)	588 (6%)	64 (1%)	20	56

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	AA	596	ASP
10	AA	853	ASP
10	AA	859	GLU
10	AA	862	LEU
10	AA	937	ASP
20	H	139	ARG
20	H	153	GLU
20	H	169	SER
20	H	306	VAL
20	H	340	ARG
27	O	56	ASP
36	X	103	LYS
10	AA	375	PRO
10	AA	856	ASN
10	AA	870	ILE
10	AA	873	ILE
10	AA	1158	LYS
13	AE	175	GLU
20	H	108	VAL
20	H	309	MET
20	H	333	LEU
45	h	158	ALA
49	l	142	ALA
63	z	3	ARG
10	AA	376	PRO
10	AA	723	VAL
10	AA	728	ASP
10	AA	935	THR
10	AA	1045	GLY
12	AC	164	ASP
12	AC	165	GLU
13	AE	51	PRO
13	AE	805	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	H	76	GLU
20	H	142	ARG
25	M	130	ASN
28	P	58	ASN
29	Q	119	ASN
36	X	105	ASN
10	AA	850	ILE
13	AE	174	ASP
13	AE	193	ASP
20	H	82	THR
21	I	80	LYS
51	n	40	VAL
10	AA	917	SER
10	AA	1044	PRO
13	AE	91	GLU
20	H	70	VAL
4	3	39	ILE
13	AE	49	PHE
13	AE	73	GLY
13	AE	904	ALA
24	L	96	VAL
1	0	44	GLY
10	AA	697	LYS
10	AA	1159	VAL
10	AA	1317	PRO
23	K	44	GLY
29	Q	74	VAL
33	U	64	GLY
10	AA	933	VAL
26	N	75	ILE
51	n	62	GLY

5.3.2 Protein sidechains ⓘ

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	84/84 (100%)	76 (90%)	8 (10%)	8	25
2	1	93/93 (100%)	86 (92%)	7 (8%)	12	33
3	2	81/84 (96%)	77 (95%)	4 (5%)	22	43
4	3	84/85 (99%)	79 (94%)	5 (6%)	17	39
5	4	78/78 (100%)	75 (96%)	3 (4%)	29	50
10	AA	1054/1157 (91%)	998 (95%)	56 (5%)	20	41
11	AB	86/158 (54%)	85 (99%)	1 (1%)	63	75
12	AC	198/286 (69%)	185 (93%)	13 (7%)	15	37
12	AD	196/286 (68%)	193 (98%)	3 (2%)	57	72
13	AE	1120/1168 (96%)	1046 (93%)	74 (7%)	15	37
14	AF	70/75 (93%)	68 (97%)	2 (3%)	37	58
15	C	57/65 (88%)	55 (96%)	2 (4%)	32	53
17	E	65/66 (98%)	61 (94%)	4 (6%)	16	38
18	F	60/61 (98%)	57 (95%)	3 (5%)	22	43
19	G	187/199 (94%)	175 (94%)	12 (6%)	16	37
20	H	137/461 (30%)	124 (90%)	13 (10%)	8	25
21	I	171/171 (100%)	164 (96%)	7 (4%)	27	49
22	J	172/173 (99%)	166 (96%)	6 (4%)	32	53
23	K	119/126 (94%)	111 (93%)	8 (7%)	15	36
24	L	91/116 (78%)	84 (92%)	7 (8%)	12	32
25	M	124/147 (84%)	113 (91%)	11 (9%)	9	28
26	N	104/105 (99%)	101 (97%)	3 (3%)	37	58
27	O	105/107 (98%)	99 (94%)	6 (6%)	18	40
28	P	86/90 (96%)	78 (91%)	8 (9%)	8	26
29	Q	90/99 (91%)	88 (98%)	2 (2%)	45	64
30	R	101/104 (97%)	95 (94%)	6 (6%)	18	39
31	S	83/84 (99%)	79 (95%)	4 (5%)	23	44
32	T	76/77 (99%)	65 (86%)	11 (14%)	3	13
33	U	65/65 (100%)	60 (92%)	5 (8%)	12	32
34	V	74/78 (95%)	71 (96%)	3 (4%)	27	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	W	72/79 (91%)	66 (92%)	6 (8%)	10	30
36	X	94/96 (98%)	87 (93%)	7 (7%)	13	33
39	b	58/63 (92%)	57 (98%)	1 (2%)	53	69
40	c	67/68 (98%)	64 (96%)	3 (4%)	24	46
42	e	54/54 (100%)	51 (94%)	3 (6%)	19	40
43	f	48/49 (98%)	43 (90%)	5 (10%)	7	22
44	g	59/62 (95%)	54 (92%)	5 (8%)	10	29
45	h	216/218 (99%)	199 (92%)	17 (8%)	11	32
46	i	47/48 (98%)	41 (87%)	6 (13%)	4	15
47	j	164/164 (100%)	156 (95%)	8 (5%)	22	43
48	k	47/49 (96%)	44 (94%)	3 (6%)	16	37
49	l	165/165 (100%)	151 (92%)	14 (8%)	10	29
50	m	38/38 (100%)	36 (95%)	2 (5%)	20	41
51	n	148/150 (99%)	130 (88%)	18 (12%)	5	17
52	o	51/52 (98%)	47 (92%)	4 (8%)	11	32
53	p	136/138 (99%)	130 (96%)	6 (4%)	25	47
54	q	34/34 (100%)	31 (91%)	3 (9%)	9	28
55	r	114/114 (100%)	102 (90%)	12 (10%)	6	21
56	s	116/116 (100%)	106 (91%)	10 (9%)	10	29
57	t	104/104 (100%)	97 (93%)	7 (7%)	15	36
58	u	103/103 (100%)	96 (93%)	7 (7%)	14	36
59	v	109/109 (100%)	105 (96%)	4 (4%)	30	51
60	w	99/103 (96%)	91 (92%)	8 (8%)	11	31
61	x	86/87 (99%)	80 (93%)	6 (7%)	14	35
62	y	99/100 (99%)	91 (92%)	8 (8%)	11	31
63	z	89/90 (99%)	85 (96%)	4 (4%)	24	46
All	All	7528/8401 (90%)	7054 (94%)	474 (6%)	18	37

All (474) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	38	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	47	VAL
1	0	48	LYS
1	0	51	VAL
1	0	68	ARG
1	0	86	GLN
1	0	96	VAL
2	1	19	LEU
2	1	30	SER
2	1	41	LYS
2	1	69	LEU
2	1	97	LEU
2	1	107	VAL
2	1	110	ARG
3	2	1	MET
3	2	24	MET
3	2	37	ASP
3	2	93	LEU
4	3	52	LEU
4	3	70	VAL
4	3	72	ILE
4	3	99	ASN
4	3	101	GLU
5	4	40	ILE
5	4	69	GLU
5	4	71	LYS
10	AA	39	ILE
10	AA	145	ILE
10	AA	376	PRO
10	AA	615	VAL
10	AA	723	VAL
10	AA	727	VAL
10	AA	728	ASP
10	AA	731	ARG
10	AA	732	ILE
10	AA	752	ASN
10	AA	753	LEU
10	AA	802	VAL
10	AA	817	LEU
10	AA	840	SER
10	AA	844	LYS
10	AA	845	LEU
10	AA	851	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	AA	854	ILE
10	AA	855	PRO
10	AA	857	VAL
10	AA	862	LEU
10	AA	864	LYS
10	AA	865	LEU
10	AA	866	ASP
10	AA	867	GLU
10	AA	868	SER
10	AA	871	VAL
10	AA	872	TYR
10	AA	873	ILE
10	AA	884	VAL
10	AA	886	LYS
10	AA	887	VAL
10	AA	890	LYS
10	AA	911	SER
10	AA	913	VAL
10	AA	914	LYS
10	AA	918	LEU
10	AA	933	VAL
10	AA	936	ARG
10	AA	939	VAL
10	AA	1041	ASP
10	AA	1042	LEU
10	AA	1046	VAL
10	AA	1047	LEU
10	AA	1048	LYS
10	AA	1076	ILE
10	AA	1151	LEU
10	AA	1159	VAL
10	AA	1248	THR
10	AA	1250	SER
10	AA	1252	SER
10	AA	1253	LEU
10	AA	1254	VAL
10	AA	1256	GLN
10	AA	1259	LEU
10	AA	1298	VAL
11	AB	47	GLU
12	AC	72	GLU
12	AC	91	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	AC	134	THR
12	AC	158	ARG
12	AC	159	ILE
12	AC	160	HIS
12	AC	162	GLU
12	AC	163	GLU
12	AC	165	GLU
12	AC	166	ARG
12	AC	168	ILE
12	AC	170	ARG
12	AC	171	LEU
12	AD	110	VAL
12	AD	187	VAL
12	AD	208	ASN
13	AE	40	LYS
13	AE	42	GLU
13	AE	44	ILE
13	AE	46	TYR
13	AE	47	ARG
13	AE	49	PHE
13	AE	50	LYS
13	AE	52	GLU
13	AE	53	ARG
13	AE	54	ASP
13	AE	56	LEU
13	AE	60	ARG
13	AE	66	LYS
13	AE	67	ASP
13	AE	70	CYS
13	AE	74	LYS
13	AE	76	LYS
13	AE	78	LEU
13	AE	80	HIS
13	AE	81	ARG
13	AE	87	LYS
13	AE	88	CYS
13	AE	91	GLU
13	AE	94	GLN
13	AE	95	THR
13	AE	96	LYS
13	AE	99	ARG
13	AE	100	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AE	114	ILE
13	AE	117	LEU
13	AE	119	SER
13	AE	123	ARG
13	AE	132	LEU
13	AE	135	ILE
13	AE	142	GLU
13	AE	144	TYR
13	AE	145	VAL
13	AE	146	VAL
13	AE	147	ILE
13	AE	152	THR
13	AE	154	LEU
13	AE	157	GLN
13	AE	159	ILE
13	AE	175	GLU
13	AE	180	MET
13	AE	190	LYS
13	AE	193	ASP
13	AE	196	GLN
13	AE	210	SER
13	AE	212	THR
13	AE	216	LYS
13	AE	222	LYS
13	AE	223	LEU
13	AE	227	PHE
13	AE	233	LYS
13	AE	237	MET
13	AE	238	ILE
13	AE	239	LEU
13	AE	240	THR
13	AE	244	VAL
13	AE	271	ARG
13	AE	324	LEU
13	AE	385	LEU
13	AE	386	GLU
13	AE	387	LEU
13	AE	390	LEU
13	AE	393	THR
13	AE	394	ILE
13	AE	395	LYS
13	AE	506	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AE	514	THR
13	AE	839	VAL
13	AE	1172	LYS
13	AE	1233	ILE
14	AF	4	VAL
14	AF	63	ILE
15	C	33	ILE
15	C	74	HIS
17	E	6	SER
17	E	10	ARG
17	E	48	GLN
17	E	64	LYS
18	F	34	ARG
18	F	62	ARG
18	F	67	ARG
19	G	8	ASP
19	G	45	LYS
19	G	59	LYS
19	G	105	LYS
19	G	117	LEU
19	G	128	LYS
19	G	129	LEU
19	G	132	LYS
19	G	135	LEU
19	G	161	LEU
19	G	174	LYS
19	G	208	ARG
20	H	9	PHE
20	H	31	ILE
20	H	43	LYS
20	H	54	LYS
20	H	62	ILE
20	H	70	VAL
20	H	294	VAL
20	H	305	HIS
20	H	336	ASP
20	H	337	GLU
20	H	338	GLU
20	H	339	ARG
20	H	340	ARG
21	I	14	ILE
21	I	21	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	I	33	LEU
21	I	89	LYS
21	I	175	LEU
21	I	178	LEU
21	I	200	VAL
22	J	95	GLU
22	J	104	ARG
22	J	105	MET
22	J	116	GLN
22	J	138	SER
22	J	143	VAL
23	K	10	GLU
23	K	15	LEU
23	K	60	ILE
23	K	114	VAL
23	K	115	LEU
23	K	138	ARG
23	K	141	ILE
23	K	162	GLU
24	L	7	VAL
24	L	16	GLU
24	L	24	ARG
24	L	36	ILE
24	L	38	ARG
24	L	54	LEU
24	L	86	ARG
25	M	7	ILE
25	M	17	LYS
25	M	21	GLU
25	M	23	LEU
25	M	27	VAL
25	M	50	LEU
25	M	79	ARG
25	M	91	VAL
25	M	109	ARG
25	M	130	ASN
25	M	146	GLU
26	N	96	MET
26	N	104	VAL
26	N	117	ARG
27	O	27	LYS
27	O	60	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	O	61	LEU
27	O	63	LEU
27	O	116	VAL
27	O	118	LEU
28	P	17	LEU
28	P	18	ILE
28	P	24	GLU
28	P	25	ILE
28	P	27	GLU
28	P	37	ARG
28	P	100	ILE
28	P	102	LEU
29	Q	15	GLN
29	Q	107	ILE
30	R	5	ASN
30	R	12	ARG
30	R	24	LEU
30	R	62	GLU
30	R	74	LEU
30	R	102	LEU
31	S	45	VAL
31	S	46	LEU
31	S	89	MET
31	S	92	GLU
32	T	10	LYS
32	T	22	THR
32	T	39	LEU
32	T	40	GLN
32	T	64	ARG
32	T	66	LEU
32	T	67	LEU
32	T	70	LEU
32	T	73	LYS
32	T	84	ARG
32	T	85	LEU
33	U	1	MET
33	U	2	VAL
33	U	6	LEU
33	U	19	VAL
33	U	50	THR
34	V	46	VAL
34	V	75	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	V	81	LYS
35	W	21	LYS
35	W	33	THR
35	W	49	ILE
35	W	58	VAL
35	W	79	THR
35	W	81	ARG
36	X	16	VAL
36	X	25	VAL
36	X	29	ARG
36	X	59	GLU
36	X	93	ARG
36	X	101	ARG
36	X	117	LYS
39	b	70	GLU
40	c	33	LEU
40	c	48	THR
40	c	71	LEU
42	e	18	LEU
42	e	58	ASN
42	e	60	LYS
43	f	3	LYS
43	f	11	ARG
43	f	25	LEU
43	f	45	ARG
43	f	55	VAL
44	g	3	LYS
44	g	16	CYS
44	g	24	ILE
44	g	36	VAL
44	g	47	LYS
45	h	51	THR
45	h	94	VAL
45	h	105	LEU
45	h	118	SER
45	h	125	LYS
45	h	130	LEU
45	h	141	VAL
45	h	156	ARG
45	h	183	LYS
45	h	187	ASP
45	h	195	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	h	202	LEU
45	h	203	ARG
45	h	204	VAL
45	h	205	LEU
45	h	242	LYS
45	h	271	ARG
46	i	9	THR
46	i	12	LYS
46	i	26	THR
46	i	27	SER
46	i	29	SER
46	i	40	ARG
47	j	13	ARG
47	j	18	ASP
47	j	91	THR
47	j	99	GLU
47	j	104	VAL
47	j	177	VAL
47	j	189	VAL
47	j	193	VAL
48	k	5	ILE
48	k	17	THR
48	k	24	THR
49	l	17	THR
49	l	22	ASP
49	l	40	ARG
49	l	48	THR
49	l	57	LYS
49	l	69	ARG
49	l	77	ILE
49	l	80	SER
49	l	108	ILE
49	l	109	LEU
49	l	111	GLU
49	l	122	GLU
49	l	149	ILE
49	l	179	SER
50	m	22	MET
50	m	42	LEU
51	n	6	ASP
51	n	10	ASP
51	n	26	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	n	40	VAL
51	n	47	LYS
51	n	49	LEU
51	n	57	LEU
51	n	79	ILE
51	n	80	ARG
51	n	95	ARG
51	n	105	THR
51	n	117	LEU
51	n	122	PHE
51	n	123	ASP
51	n	132	VAL
51	n	140	GLU
51	n	141	ILE
51	n	163	ASP
52	o	8	ARG
52	o	30	ARG
52	o	31	HIS
52	o	55	LEU
53	p	11	VAL
53	p	85	LYS
53	p	95	ARG
53	p	125	CYS
53	p	168	VAL
53	p	171	THR
54	q	3	VAL
54	q	26	ILE
54	q	34	LYS
55	r	1	MET
55	r	9	VAL
55	r	11	ASN
55	r	12	LEU
55	r	15	LEU
55	r	41	LYS
55	r	66	ASN
55	r	72	ILE
55	r	76	GLU
55	r	94	ILE
55	r	101	ASP
55	r	127	GLU
56	s	1	MET
56	s	30	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	s	31	GLU
56	s	43	GLU
56	s	57	LEU
56	s	123	LYS
56	s	124	VAL
56	s	139	VAL
56	s	140	LEU
56	s	142	ILE
57	t	7	MET
57	t	35	VAL
57	t	49	ARG
57	t	67	LYS
57	t	70	ARG
57	t	80	ASP
57	t	104	THR
58	u	5	THR
58	u	27	LEU
58	u	59	ARG
58	u	73	ILE
58	u	76	GLU
58	u	78	ARG
58	u	84	LYS
59	v	110	GLU
59	v	126	ILE
59	v	127	LYS
59	v	128	THR
60	w	2	ARG
60	w	20	MET
60	w	24	MET
60	w	51	LEU
60	w	65	LEU
60	w	69	ARG
60	w	95	THR
60	w	116	VAL
61	x	13	ARG
61	x	31	THR
61	x	47	VAL
61	x	48	LEU
61	x	91	SER
61	x	116	GLN
62	y	8	LEU
62	y	10	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
62	y	27	GLU
62	y	40	LEU
62	y	81	VAL
62	y	85	SER
62	y	102	GLU
62	y	114	LEU
63	z	18	LEU
63	z	51	ARG
63	z	109	LEU
63	z	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	86	GLN
2	1	61	ASN
3	2	28	ASN
3	2	59	ASN
4	3	54	GLN
10	AA	193	ASN
10	AA	273	HIS
10	AA	761	GLN
10	AA	808	ASN
10	AA	1157	GLN
10	AA	1236	ASN
12	AC	41	ASN
12	AC	66	HIS
12	AC	132	HIS
12	AD	41	ASN
12	AD	93	GLN
12	AD	103	ASN
13	AE	196	GLN
13	AE	469	HIS
13	AE	865	HIS
13	AE	1195	GLN
13	AE	1238	GLN
13	AE	1249	ASN
13	AE	1259	GLN
14	AF	29	GLN
14	AF	62	GLN
17	E	3	ASN
17	E	55	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	E	61	GLN
19	G	18	HIS
19	G	58	ASN
19	G	94	HIS
19	G	177	ASN
21	I	3	GLN
21	I	6	HIS
21	I	123	GLN
22	J	36	GLN
22	J	40	GLN
22	J	41	HIS
23	K	97	GLN
24	L	11	HIS
24	L	37	HIS
24	L	63	ASN
24	L	94	HIS
25	M	97	ASN
25	M	148	ASN
27	O	81	HIS
28	P	58	ASN
30	R	6	GLN
30	R	72	HIS
31	S	60	GLN
32	T	40	GLN
33	U	59	HIS
36	X	105	ASN
44	g	33	ASN
44	g	41	HIS
45	h	70	ASN
45	h	163	GLN
46	i	5	GLN
48	k	26	ASN
51	n	63	GLN
52	o	28	ASN
53	p	88	GLN
54	q	35	GLN
55	r	11	ASN
55	r	20	ASN
57	t	88	ASN
62	y	15	GLN
62	y	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	D	1513/1542 (98%)	285 (18%)	33 (2%)
37	Y	2/3 (66%)	2 (100%)	0
38	a	2859/2904 (98%)	542 (18%)	0
41	d	119/120 (99%)	17 (14%)	0
8	7	15/38 (39%)	7 (46%)	0
9	A	75/76 (98%)	29 (38%)	6 (8%)
9	B	75/76 (98%)	34 (45%)	5 (6%)
All	All	4658/4759 (97%)	916 (19%)	44 (0%)

All (916) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	56	U
8	7	57	G
8	7	58	A
8	7	59	U
8	7	60	U
8	7	62	G
8	7	63	G
9	A	2	G
9	A	6	G
9	A	7	G
9	A	8	U
9	A	10	G
9	A	13	C
9	A	14	A
9	A	15	G
9	A	16	C
9	A	17	C
9	A	18	G
9	A	19	G
9	A	20	U
9	A	21	A
9	A	22	G
9	A	23	C
9	A	46	G
9	A	47	U
9	A	48	C
9	A	49	G
9	A	52	G
9	A	57	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	58	A
9	A	59	A
9	A	61	C
9	A	66	C
9	A	69	C
9	A	71	C
9	A	73	A
9	B	2	G
9	B	6	G
9	B	7	G
9	B	8	U
9	B	10	G
9	B	13	C
9	B	14	A
9	B	15	G
9	B	16	C
9	B	17	C
9	B	18	G
9	B	19	G
9	B	20	U
9	B	21	A
9	B	22	G
9	B	23	C
9	B	30	G
9	B	31	G
9	B	32	C
9	B	37	A
9	B	38	A
9	B	46	G
9	B	47	U
9	B	48	C
9	B	49	G
9	B	52	G
9	B	57	A
9	B	58	A
9	B	59	A
9	B	61	C
9	B	66	C
9	B	69	C
9	B	71	C
9	B	73	A
16	D	4	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	D	5	U
16	D	9	G
16	D	22	G
16	D	29	U
16	D	32	A
16	D	39	G
16	D	41	G
16	D	47	C
16	D	48	C
16	D	50	A
16	D	51	A
16	D	52	C
16	D	54	C
16	D	69	G
16	D	70	U
16	D	71	A
16	D	72	A
16	D	74	A
16	D	76	G
16	D	82	G
16	D	83	C
16	D	84	U
16	D	87	C
16	D	90	C
16	D	94	G
16	D	95	C
16	D	96	U
16	D	108	G
16	D	120	A
16	D	122	G
16	D	128	G
16	D	131	A
16	D	141	G
16	D	144	G
16	D	148	G
16	D	149	A
16	D	160	A
16	D	164	G
16	D	173	U
16	D	181	A
16	D	182	A
16	D	197	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	D	198	G
16	D	204	G
16	D	208	U
16	D	209	U
16	D	210	C
16	D	211	G
16	D	212	G
16	D	216	U
16	D	226	G
16	D	245	U
16	D	247	G
16	D	251	G
16	D	258	G
16	D	262	A
16	D	266	G
16	D	267	C
16	D	271	C
16	D	279	A
16	D	289	G
16	D	299	G
16	D	306	A
16	D	321	A
16	D	328	C
16	D	329	A
16	D	332	G
16	D	347	G
16	D	352	C
16	D	353	A
16	D	354	G
16	D	355	C
16	D	367	U
16	D	372	C
16	D	373	A
16	D	376	G
16	D	382	A
16	D	384	G
16	D	392	C
16	D	393	A
16	D	397	A
16	D	406	G
16	D	412	A
16	D	413	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	D	414	A
16	D	421	U
16	D	422	C
16	D	424	G
16	D	429	U
16	D	446	G
16	D	451	A
16	D	457	G
16	D	458	U
16	D	460	A
16	D	463	U
16	D	464	U
16	D	467	U
16	D	468	A
16	D	469	C
16	D	478	A
16	D	479	U
16	D	481	G
16	D	484	G
16	D	485	U
16	D	486	U
16	D	505	G
16	D	509	A
16	D	511	C
16	D	518	C
16	D	519	C
16	D	526	C
16	D	531	U
16	D	532	A
16	D	533	A
16	D	542	G
16	D	547	A
16	D	559	A
16	D	562	U
16	D	568	G
16	D	572	A
16	D	573	A
16	D	576	C
16	D	577	G
16	D	579	A
16	D	596	A
16	D	628	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	D	633	G
16	D	641	U
16	D	642	A
16	D	649	A
16	D	650	G
16	D	653	U
16	D	665	A
16	D	666	G
16	D	687	A
16	D	700	G
16	D	723	U
16	D	724	G
16	D	731	G
16	D	734	G
16	D	747	A
16	D	748	G
16	D	755	G
16	D	760	G
16	D	777	A
16	D	793	U
16	D	794	A
16	D	815	A
16	D	817	C
16	D	828	U
16	D	829	G
16	D	832	G
16	D	841	C
16	D	844	G
16	D	845	A
16	D	849	G
16	D	874	G
16	D	887	G
16	D	902	G
16	D	914	A
16	D	916	U
16	D	926	G
16	D	934	C
16	D	935	A
16	D	954	G
16	D	960	U
16	D	963	G
16	D	969	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	D	972	C
16	D	975	A
16	D	976	G
16	D	991	U
16	D	992	U
16	D	993	G
16	D	996	A
16	D	999	C
16	D	1004	A
16	D	1008	U
16	D	1009	U
16	D	1017	U
16	D	1018	G
16	D	1021	A
16	D	1024	G
16	D	1026	G
16	D	1028	C
16	D	1030	U
16	D	1031	C
16	D	1037	C
16	D	1043	G
16	D	1044	A
16	D	1046	A
16	D	1065	U
16	D	1085	U
16	D	1086	U
16	D	1094	G
16	D	1095	U
16	D	1099	G
16	D	1101	A
16	D	1124	G
16	D	1133	G
16	D	1135	U
16	D	1136	C
16	D	1137	C
16	D	1139	G
16	D	1140	C
16	D	1141	C
16	D	1142	G
16	D	1143	G
16	D	1145	A
16	D	1146	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	D	1151	A
16	D	1152	A
16	D	1158	C
16	D	1159	U
16	D	1167	A
16	D	1171	A
16	D	1174	G
16	D	1175	G
16	D	1176	A
16	D	1184	G
16	D	1196	A
16	D	1197	A
16	D	1206	G
16	D	1211	U
16	D	1212	U
16	D	1213	A
16	D	1214	C
16	D	1215	G
16	D	1226	C
16	D	1227	A
16	D	1228	C
16	D	1238	A
16	D	1256	A
16	D	1257	A
16	D	1260	G
16	D	1275	A
16	D	1276	G
16	D	1278	G
16	D	1279	G
16	D	1280	A
16	D	1285	A
16	D	1286	U
16	D	1287	A
16	D	1299	A
16	D	1300	G
16	D	1302	C
16	D	1305	G
16	D	1312	G
16	D	1317	C
16	D	1320	C
16	D	1323	G
16	D	1329	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	D	1338	G
16	D	1340	A
16	D	1346	A
16	D	1347	G
16	D	1353	G
16	D	1363	A
16	D	1370	G
16	D	1378	C
16	D	1379	G
16	D	1381	U
16	D	1391	U
16	D	1396	A
16	D	1397	C
16	D	1419	G
16	D	1429	A
16	D	1441	A
16	D	1446	A
16	D	1447	A
16	D	1448	C
16	D	1452	C
16	D	1453	G
16	D	1475	G
16	D	1487	G
16	D	1492	A
16	D	1494	G
16	D	1495	U
16	D	1497	G
16	D	1503	A
16	D	1506	U
16	D	1529	G
16	D	1530	G
16	D	1534	A
37	Y	72	U
37	Y	73	U
38	a	10	A
38	a	15	G
38	a	34	U
38	a	35	G
38	a	46	G
38	a	58	G
38	a	60	G
38	a	63	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	71	A
38	a	74	A
38	a	75	G
38	a	83	A
38	a	84	A
38	a	85	G
38	a	93	G
38	a	96	C
38	a	102	U
38	a	103	A
38	a	110	G
38	a	114	U
38	a	118	A
38	a	119	A
38	a	120	U
38	a	122	G
38	a	131	A
38	a	136	G
38	a	139	U
38	a	140	C
38	a	141	G
38	a	145	C
38	a	163	C
38	a	165	A
38	a	181	A
38	a	196	A
38	a	199	A
38	a	200	U
38	a	215	G
38	a	216	A
38	a	222	A
38	a	225	C
38	a	248	G
38	a	249	C
38	a	261	G
38	a	264	C
38	a	265	A
38	a	266	G
38	a	267	C
38	a	271	G
38	a	272	A
38	a	275	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	276	U
38	a	278	A
38	a	285	G
38	a	311	A
38	a	324	A
38	a	329	G
38	a	330	A
38	a	353	C
38	a	359	G
38	a	361	G
38	a	362	A
38	a	371	A
38	a	372	G
38	a	373	U
38	a	375	G
38	a	383	C
38	a	386	G
38	a	396	G
38	a	405	U
38	a	411	G
38	a	412	A
38	a	420	C
38	a	424	G
38	a	435	C
38	a	451	U
38	a	456	C
38	a	457	A
38	a	477	A
38	a	481	G
38	a	491	G
38	a	501	A
38	a	503	A
38	a	504	A
38	a	505	A
38	a	509	C
38	a	522	A
38	a	529	A
38	a	532	A
38	a	543	G
38	a	546	U
38	a	547	A
38	a	548	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	549	G
38	a	551	G
38	a	563	A
38	a	569	U
38	a	573	U
38	a	575	A
38	a	588	U
38	a	603	A
38	a	609	A
38	a	613	A
38	a	614	A
38	a	615	U
38	a	616	A
38	a	618	G
38	a	620	G
38	a	621	A
38	a	627	A
38	a	637	A
38	a	645	C
38	a	647	G
38	a	654	A
38	a	664	G
38	a	668	A
38	a	685	A
38	a	686	U
38	a	710	U
38	a	717	C
38	a	730	A
38	a	738	G
38	a	757	G
38	a	764	A
38	a	765	C
38	a	775	G
38	a	776	G
38	a	782	A
38	a	784	G
38	a	785	G
38	a	800	A
38	a	802	A
38	a	805	G
38	a	812	C
38	a	819	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	827	U
38	a	828	U
38	a	845	A
38	a	846	U
38	a	858	G
38	a	859	G
38	a	869	G
38	a	878	A
38	a	881	G
38	a	883	G
38	a	884	U
38	a	885	C
38	a	888	C
38	a	891	G
38	a	892	A
38	a	893	C
38	a	895	U
38	a	896	A
38	a	897	C
38	a	899	A
38	a	907	G
38	a	910	A
38	a	914	G
38	a	915	C
38	a	931	U
38	a	941	A
38	a	945	A
38	a	946	C
38	a	953	G
38	a	961	C
38	a	974	G
38	a	983	A
38	a	984	A
38	a	985	C
38	a	995	C
38	a	996	A
38	a	999	U
38	a	1005	C
38	a	1012	U
38	a	1013	C
38	a	1022	G
38	a	1023	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	1026	G
38	a	1033	U
38	a	1041	G
38	a	1042	G
38	a	1045	C
38	a	1046	A
38	a	1047	G
38	a	1060	U
38	a	1061	U
38	a	1062	G
38	a	1063	G
38	a	1064	C
38	a	1065	U
38	a	1066	U
38	a	1067	A
38	a	1068	G
38	a	1069	A
38	a	1070	A
38	a	1071	G
38	a	1073	A
38	a	1074	G
38	a	1076	C
38	a	1079	C
38	a	1080	A
38	a	1081	U
38	a	1082	U
38	a	1083	U
38	a	1084	A
38	a	1087	G
38	a	1088	A
38	a	1090	A
38	a	1095	A
38	a	1096	A
38	a	1107	G
38	a	1110	G
38	a	1111	A
38	a	1112	G
38	a	1119	U
38	a	1122	G
38	a	1132	U
38	a	1134	A
38	a	1135	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	1142	A
38	a	1143	A
38	a	1169	A
38	a	1170	C
38	a	1173	U
38	a	1174	U
38	a	1175	A
38	a	1176	U
38	a	1177	G
38	a	1178	C
38	a	1179	G
38	a	1180	U
38	a	1186	G
38	a	1238	G
38	a	1248	G
38	a	1253	A
38	a	1256	G
38	a	1266	G
38	a	1271	G
38	a	1272	A
38	a	1273	U
38	a	1301	A
38	a	1321	A
38	a	1345	C
38	a	1352	U
38	a	1365	A
38	a	1368	G
38	a	1378	A
38	a	1379	U
38	a	1380	G
38	a	1383	A
38	a	1387	A
38	a	1392	A
38	a	1395	A
38	a	1406	U
38	a	1407	G
38	a	1408	G
38	a	1411	U
38	a	1414	C
38	a	1415	U
38	a	1416	G
38	a	1417	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	1419	A
38	a	1420	A
38	a	1428	C
38	a	1452	G
38	a	1453	A
38	a	1460	U
38	a	1478	G
38	a	1482	G
38	a	1490	A
38	a	1491	G
38	a	1497	U
38	a	1503	A
38	a	1508	A
38	a	1509	A
38	a	1510	G
38	a	1515	A
38	a	1529	G
38	a	1534	U
38	a	1535	A
38	a	1536	C
38	a	1537	G
38	a	1554	U
38	a	1559	U
38	a	1566	A
38	a	1569	A
38	a	1578	U
38	a	1580	A
38	a	1581	G
38	a	1582	C
38	a	1583	A
38	a	1584	U
38	a	1589	U
38	a	1590	A
38	a	1608	A
38	a	1609	A
38	a	1610	A
38	a	1647	U
38	a	1648	U
38	a	1649	G
38	a	1651	G
38	a	1674	G
38	a	1677	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	1703	G
38	a	1714	U
38	a	1715	G
38	a	1718	G
38	a	1729	U
38	a	1730	C
38	a	1732	C
38	a	1738	G
38	a	1750	G
38	a	1755	A
38	a	1758	U
38	a	1764	C
38	a	1773	A
38	a	1791	A
38	a	1800	C
38	a	1801	A
38	a	1808	A
38	a	1811	G
38	a	1816	C
38	a	1829	A
38	a	1833	C
38	a	1847	A
38	a	1848	A
38	a	1858	A
38	a	1859	U
38	a	1862	G
38	a	1864	U
38	a	1869	G
38	a	1870	C
38	a	1872	A
38	a	1873	G
38	a	1905	C
38	a	1906	G
38	a	1907	G
38	a	1913	A
38	a	1914	C
38	a	1919	A
38	a	1920	C
38	a	1922	G
38	a	1923	U
38	a	1924	C
38	a	1925	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	1926	U
38	a	1928	A
38	a	1929	G
38	a	1930	G
38	a	1936	A
38	a	1938	A
38	a	1955	U
38	a	1965	C
38	a	1967	C
38	a	1970	A
38	a	1971	U
38	a	1972	G
38	a	1987	A
38	a	1991	U
38	a	1992	G
38	a	1993	U
38	a	1997	C
38	a	2002	G
38	a	2022	U
38	a	2023	C
38	a	2027	G
38	a	2033	A
38	a	2043	C
38	a	2051	A
38	a	2052	A
38	a	2055	C
38	a	2056	G
38	a	2060	A
38	a	2061	G
38	a	2062	A
38	a	2063	C
38	a	2077	A
38	a	2093	G
38	a	2097	A
38	a	2099	U
38	a	2100	G
38	a	2108	A
38	a	2110	G
38	a	2111	U
38	a	2113	U
38	a	2115	G
38	a	2116	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	2117	A
38	a	2118	U
38	a	2121	G
38	a	2122	U
38	a	2124	G
38	a	2125	G
38	a	2126	A
38	a	2127	G
38	a	2128	G
38	a	2131	U
38	a	2132	U
38	a	2133	G
38	a	2134	A
38	a	2139	U
38	a	2141	G
38	a	2146	C
38	a	2147	A
38	a	2154	A
38	a	2157	G
38	a	2158	A
38	a	2159	G
38	a	2162	G
38	a	2163	A
38	a	2164	C
38	a	2165	C
38	a	2169	A
38	a	2171	A
38	a	2172	U
38	a	2178	C
38	a	2182	U
38	a	2183	A
38	a	2185	U
38	a	2188	U
38	a	2189	U
38	a	2190	G
38	a	2191	A
38	a	2193	G
38	a	2194	U
38	a	2198	A
38	a	2204	G
38	a	2210	U
38	a	2211	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	2212	A
38	a	2213	U
38	a	2225	A
38	a	2226	C
38	a	2229	U
38	a	2238	G
38	a	2239	G
38	a	2244	U
38	a	2250	G
38	a	2268	A
38	a	2278	A
38	a	2283	C
38	a	2287	A
38	a	2297	A
38	a	2305	U
38	a	2308	G
38	a	2309	A
38	a	2315	G
38	a	2322	A
38	a	2325	G
38	a	2327	A
38	a	2333	A
38	a	2339	C
38	a	2345	G
38	a	2347	C
38	a	2350	C
38	a	2361	G
38	a	2372	U
38	a	2376	A
38	a	2383	G
38	a	2385	C
38	a	2402	U
38	a	2403	C
38	a	2406	A
38	a	2423	U
38	a	2424	C
38	a	2425	A
38	a	2426	A
38	a	2429	G
38	a	2430	A
38	a	2431	U
38	a	2434	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	2435	A
38	a	2441	U
38	a	2447	G
38	a	2448	A
38	a	2470	G
38	a	2474	U
38	a	2476	A
38	a	2478	A
38	a	2484	G
38	a	2491	U
38	a	2502	G
38	a	2506	U
38	a	2507	C
38	a	2512	C
38	a	2513	A
38	a	2518	A
38	a	2520	C
38	a	2525	G
38	a	2529	G
38	a	2535	G
38	a	2547	A
38	a	2554	U
38	a	2566	A
38	a	2567	G
38	a	2572	A
38	a	2573	C
38	a	2574	G
38	a	2585	U
38	a	2586	U
38	a	2602	A
38	a	2603	G
38	a	2609	U
38	a	2610	C
38	a	2611	C
38	a	2613	U
38	a	2629	U
38	a	2663	G
38	a	2669	G
38	a	2671	G
38	a	2689	U
38	a	2690	U
38	a	2714	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	a	2722	G
38	a	2726	A
38	a	2744	G
38	a	2748	A
38	a	2757	A
38	a	2758	A
38	a	2765	A
38	a	2777	G
38	a	2778	A
38	a	2791	G
38	a	2793	C
38	a	2796	U
38	a	2797	U
38	a	2798	U
38	a	2799	A
38	a	2801	G
38	a	2818	U
38	a	2820	A
38	a	2823	A
38	a	2825	G
38	a	2849	U
38	a	2850	A
38	a	2859	G
38	a	2861	U
38	a	2867	G
38	a	2880	C
38	a	2884	U
38	a	2885	G
38	a	2891	U
38	a	2902	C
41	d	2	G
41	d	9	G
41	d	13	G
41	d	16	G
41	d	17	C
41	d	35	C
41	d	36	C
41	d	45	A
41	d	51	G
41	d	56	G
41	d	64	G
41	d	66	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	d	88	C
41	d	89	U
41	d	90	C
41	d	99	A
41	d	109	A

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	6	G
9	A	7	G
9	A	9	G
9	A	22	G
9	A	60	U
9	A	70	G
9	B	6	G
9	B	7	G
9	B	9	G
9	B	22	G
9	B	60	U
16	D	7	A
16	D	70	U
16	D	121	U
16	D	181	A
16	D	183	C
16	D	197	A
16	D	209	U
16	D	305	G
16	D	328	C
16	D	428	G
16	D	496	A
16	D	517	G
16	D	531	U
16	D	532	A
16	D	562	U
16	D	641	U
16	D	722	G
16	D	793	U
16	D	991	U
16	D	992	U
16	D	1109	C
16	D	1145	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	D	1196	A
16	D	1211	U
16	D	1212	U
16	D	1213	A
16	D	1214	C
16	D	1225	A
16	D	1299	A
16	D	1396	A
16	D	1432	G
16	D	1447	A
16	D	1493	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

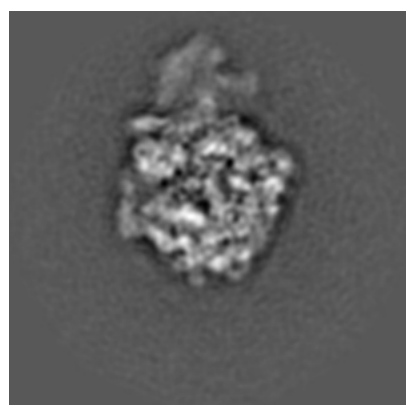
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21477. These allow visual inspection of the internal detail of the map and identification of artifacts.

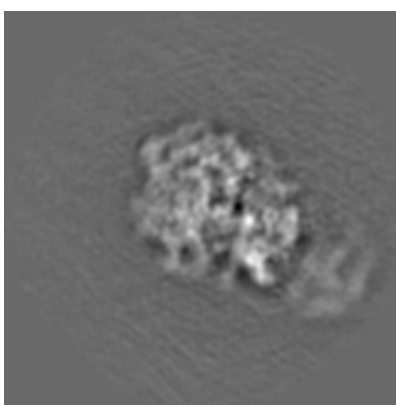
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

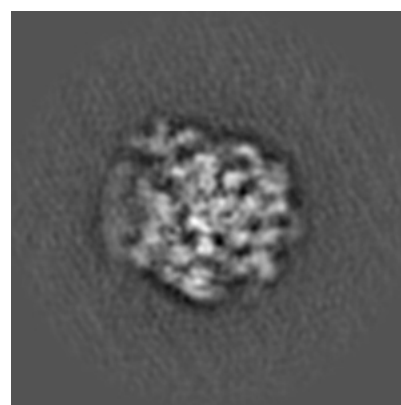
6.1.1 Primary map



X



Y

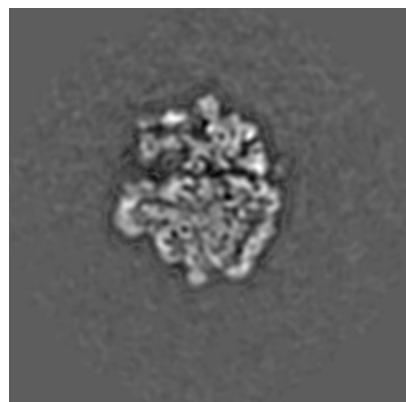


Z

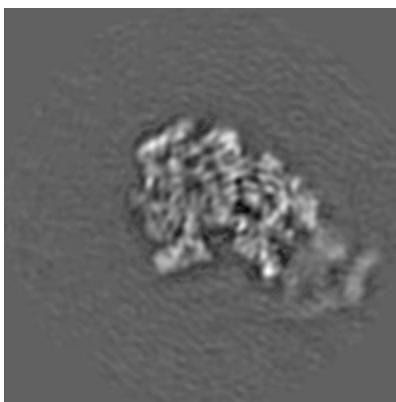
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

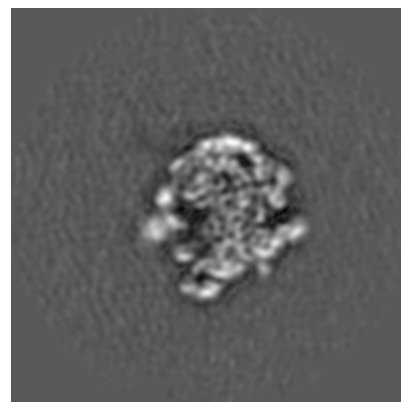
6.2.1 Primary map



X Index: 96



Y Index: 96

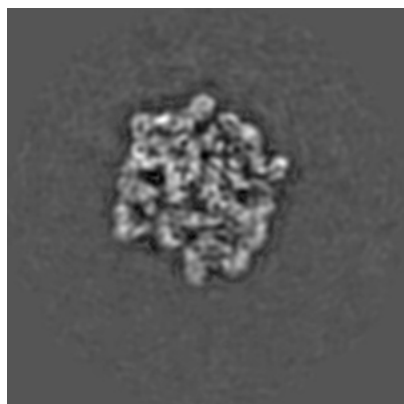


Z Index: 96

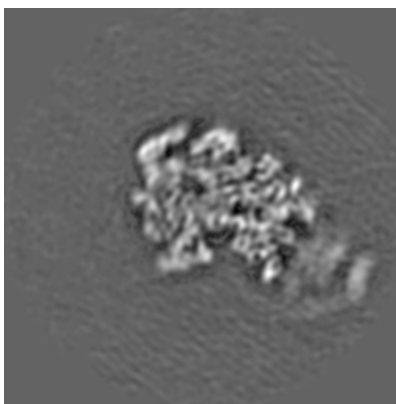
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

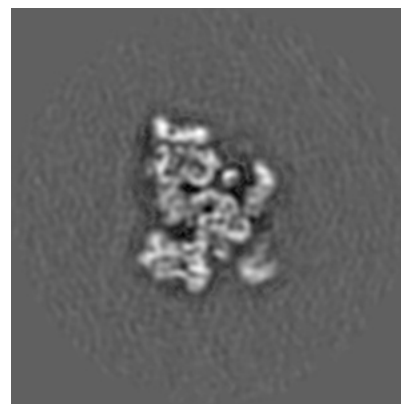
6.3.1 Primary map



X Index: 91



Y Index: 98

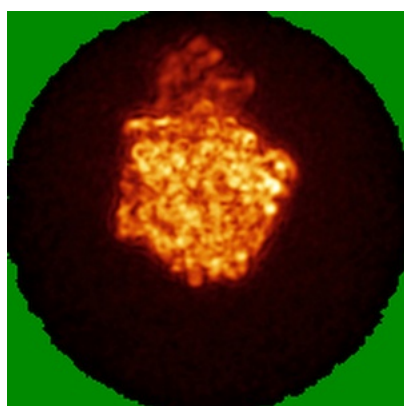


Z Index: 117

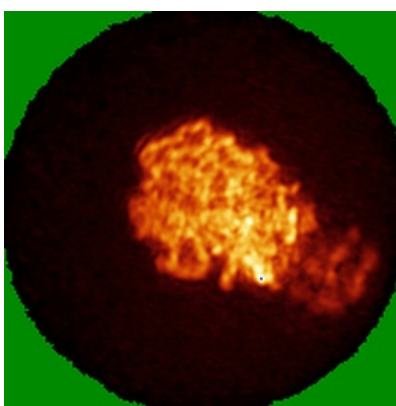
The images above show the largest variance slices of the map in three orthogonal directions.

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

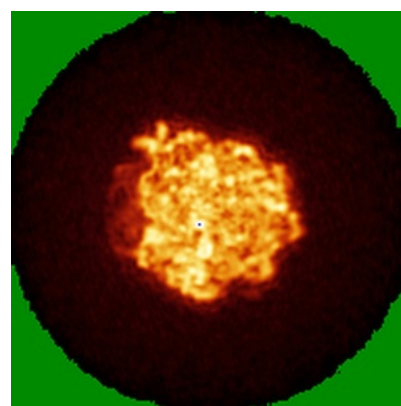
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

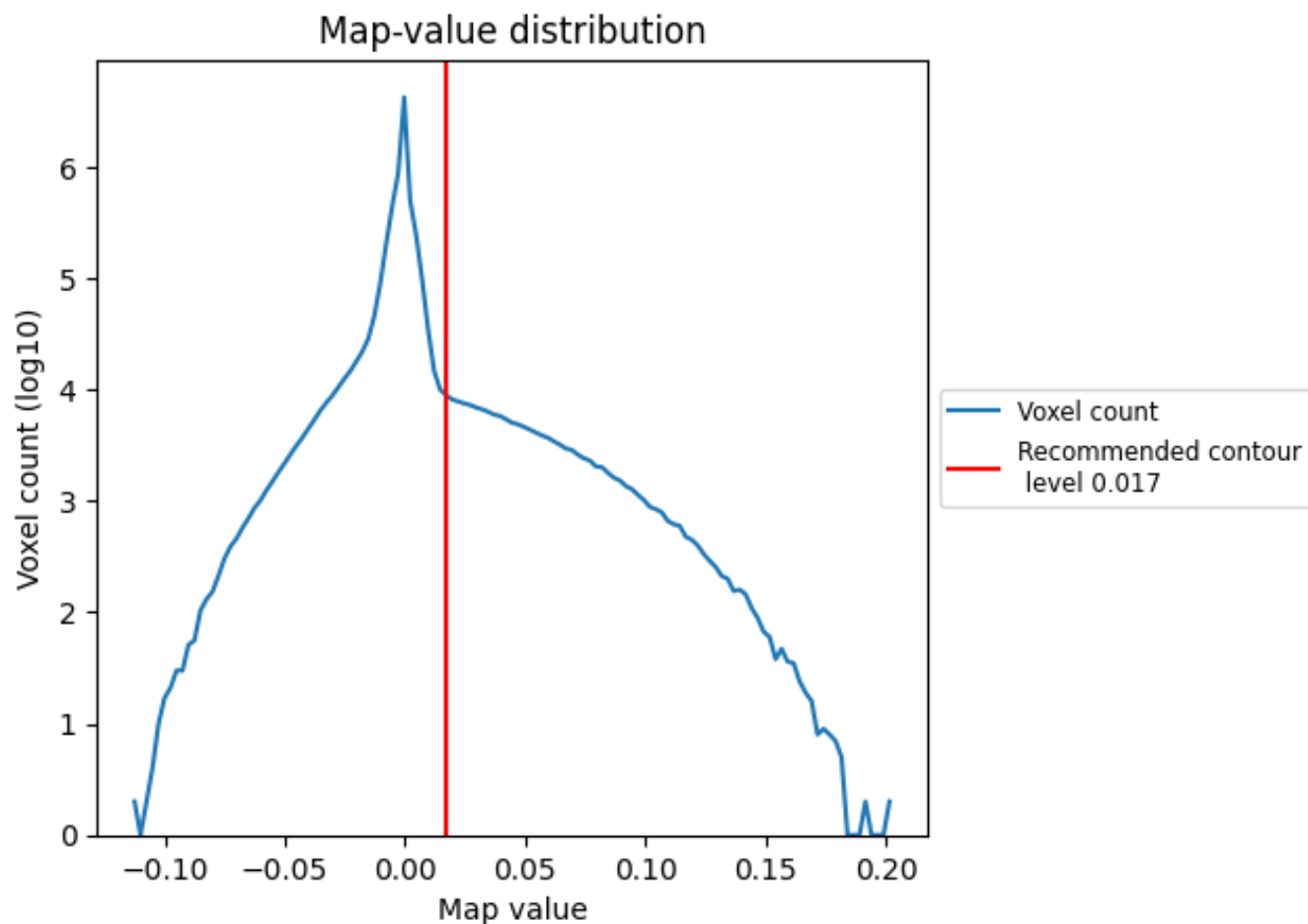
6.6 Mask visualisation

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

7 Map analysis [i](#)

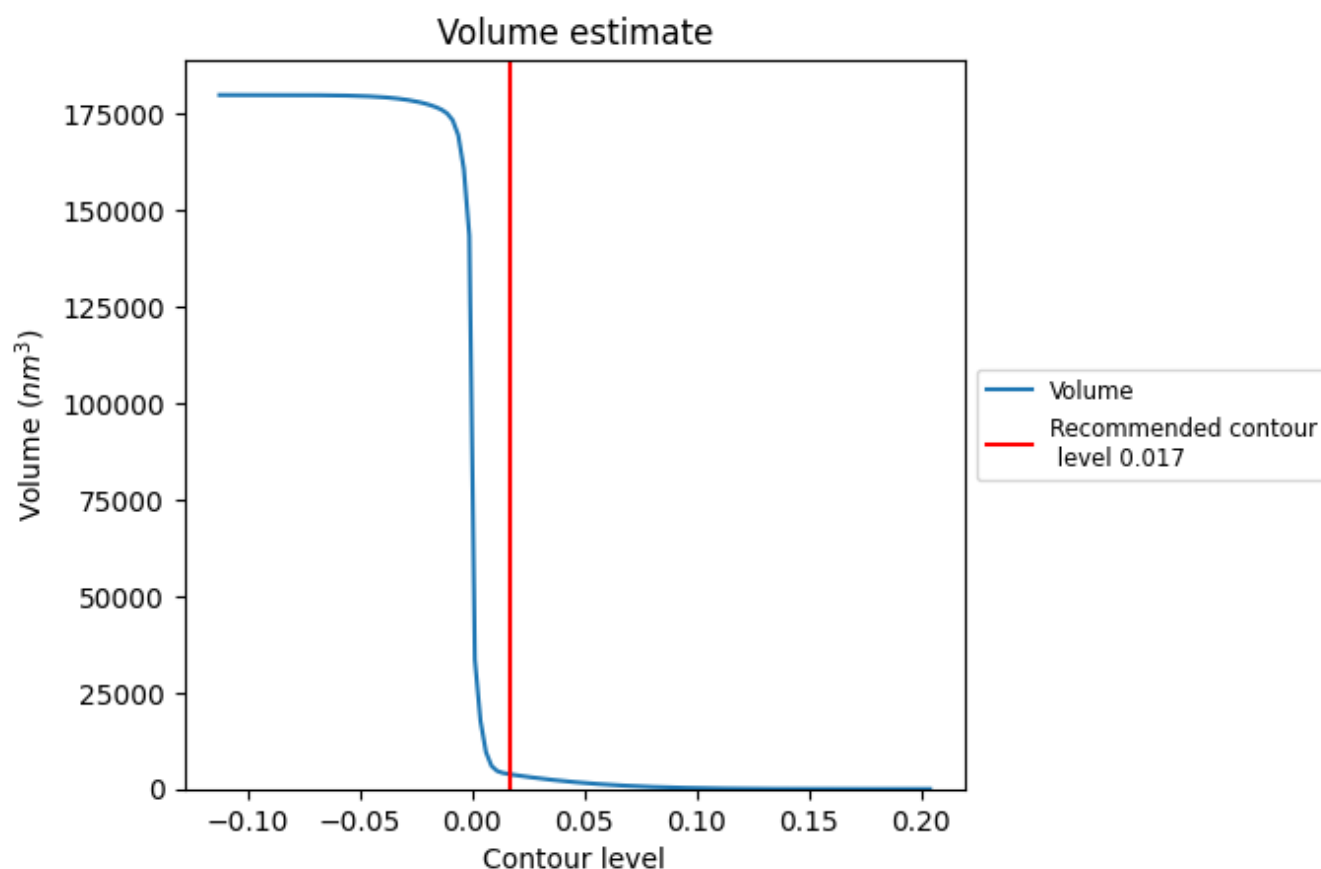
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

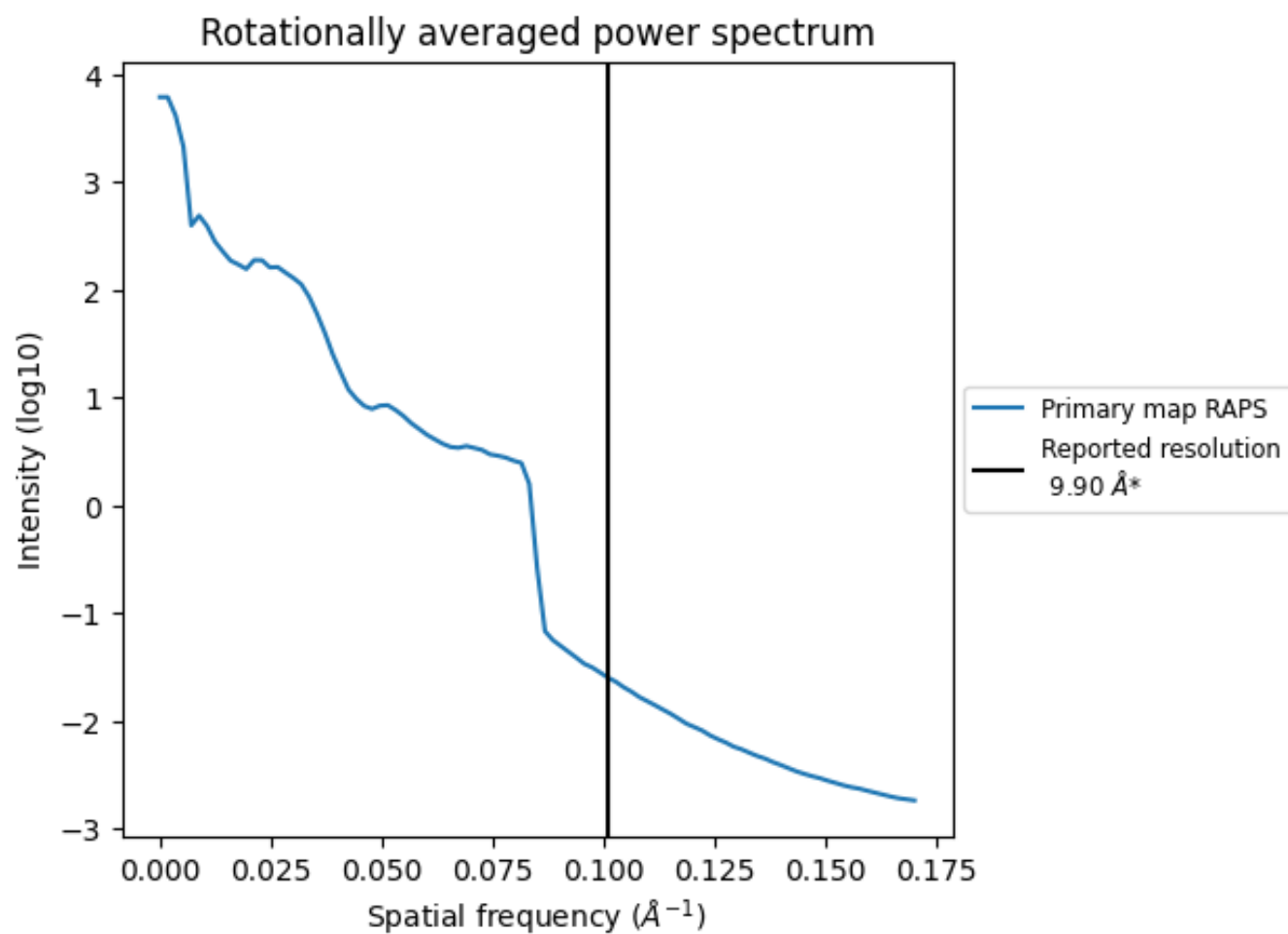
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3791 nm^3 ; this corresponds to an approximate mass of 3425 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 0.101 Å⁻¹

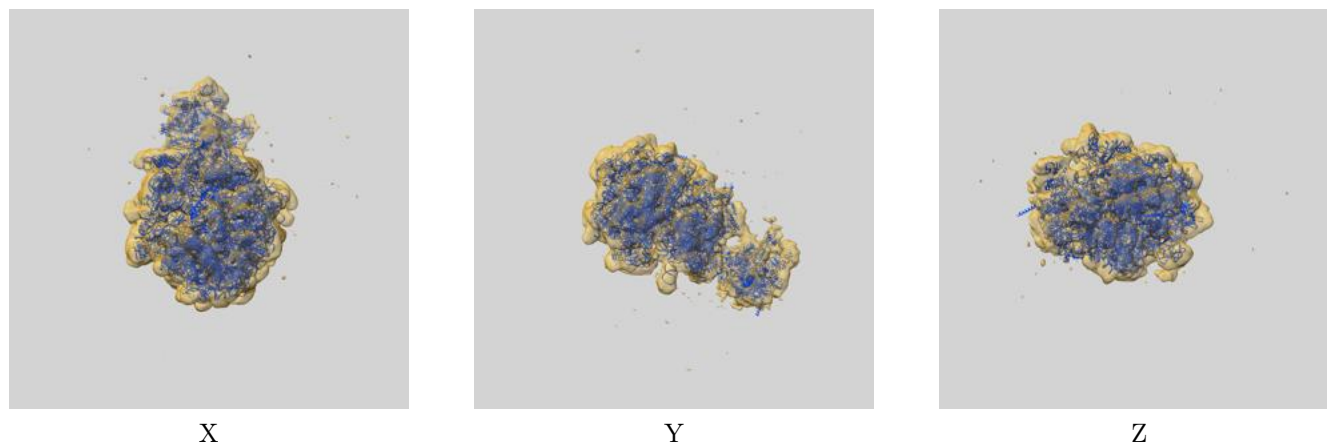
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

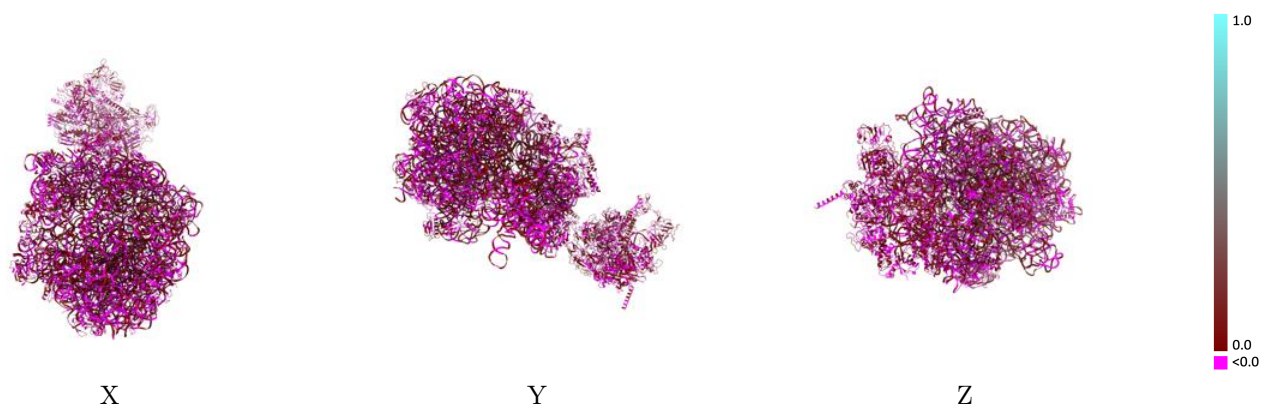
This section contains information regarding the fit between EMDB map EMD-21477 and PDB model 6VYZ. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



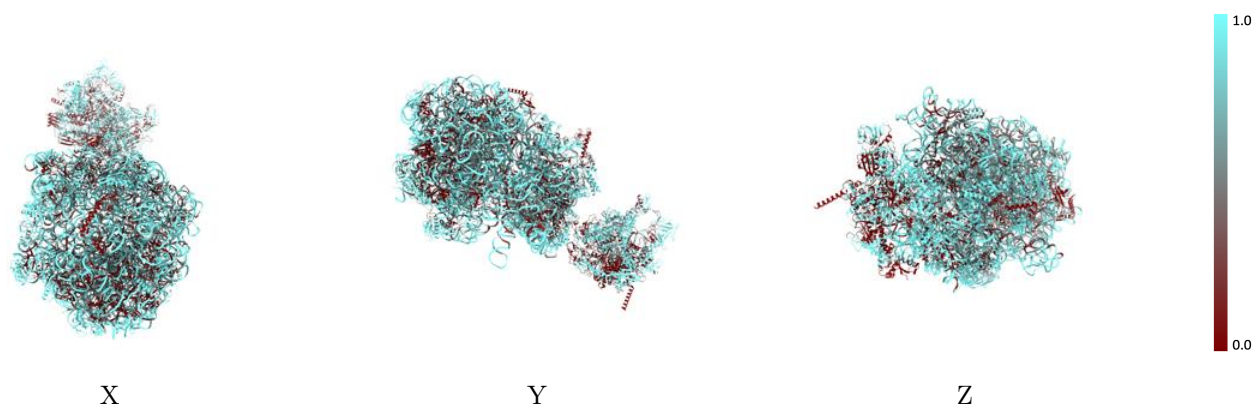
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



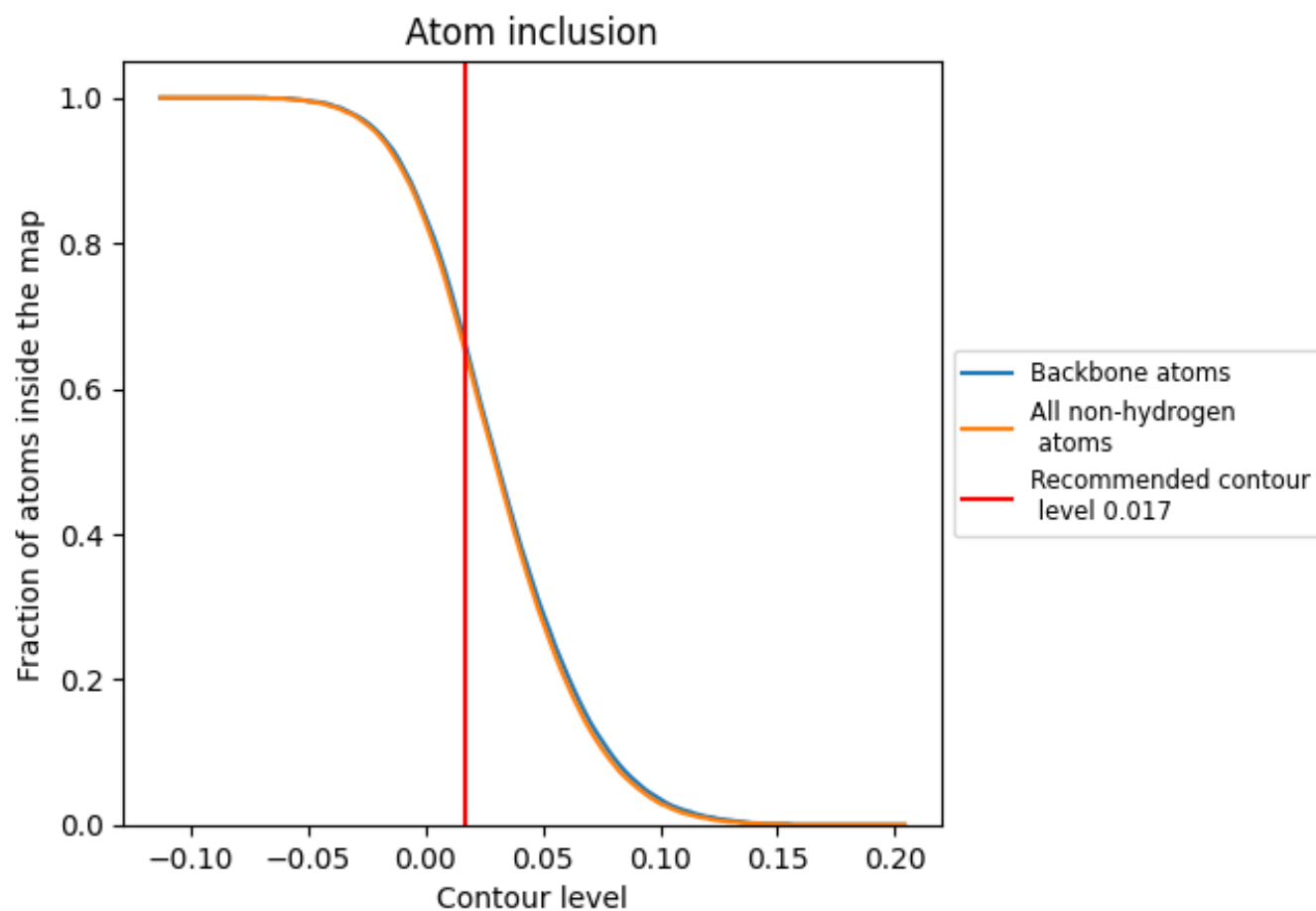
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 65% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6520	 0.0330
0	 0.6930	 0.0040
1	 0.2950	 0.0070
2	 0.5230	 -0.0190
3	 0.7370	 0.0080
4	 0.6980	 0.0180
5	 0.6550	 0.0520
6	 0.6090	 0.0390
7	 0.3720	 0.0540
A	 0.6970	 0.0770
AA	 0.5960	 0.0400
AB	 0.3460	 -0.0030
AC	 0.4790	 0.0480
AD	 0.5020	 0.0210
AE	 0.5280	 0.0260
AF	 0.2690	 -0.0030
B	 0.7480	 0.0610
C	 0.7970	 -0.0040
D	 0.7690	 0.0490
E	 0.4750	 0.0030
F	 0.2360	 0.0230
G	 0.7550	 0.0120
H	 0.3460	 0.0070
I	 0.6000	 0.0040
J	 0.5180	 -0.0110
K	 0.5650	 0.0240
L	 0.8100	 0.0340
M	 0.6460	 0.0070
N	 0.5600	 -0.0260
O	 0.6060	 -0.0190
P	 0.5670	 0.0110
Q	 0.7940	 0.0410
R	 0.6540	 0.0560
S	 0.5140	 -0.0230
T	 0.7900	 0.0220



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
U	 0.4160	 -0.0230
V	 0.5270	 0.0380
W	 0.7730	 0.0060
X	 0.6840	 -0.0070
Y	 0.0000	 -0.0390
a	 0.7160	 0.0460
b	 0.3980	 -0.0290
c	 0.4480	 0.0050
d	 0.6220	 0.0180
e	 0.6810	 -0.0050
f	 0.3370	 -0.0200
g	 0.8380	 0.0410
h	 0.5170	 0.0280
i	 0.4700	 -0.0100
j	 0.5120	 -0.0170
k	 0.6750	 0.0190
l	 0.5950	 0.0100
m	 0.3660	 0.0140
n	 0.7810	 0.0190
o	 0.1490	 -0.0240
p	 0.7920	 0.0230
q	 0.5480	 0.0050
r	 0.1740	 -0.0310
s	 0.3830	 -0.0210
t	 0.5360	 0.0210
u	 0.5610	 0.0090
v	 0.5620	 0.0340
w	 0.3910	 -0.0290
x	 0.6860	 -0.0030
y	 0.4310	 -0.0270
z	 0.5250	 -0.0280