



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 06:21 PM UTC

PDB ID : 4V7H / pdb_00004v7h
EMDB ID : EMD-1345
Title : Structure of the 80S rRNA and proteins and P/E tRNA for eukaryotic ribosome based on cryo-EM map of *Thermomyces lanuginosus* ribosome at 8.9Å resolution
Authors : Taylor, D.J.; Devkota, B.; Huang, A.D.; Topf, M.; Narayanan, E.; Sali, A.; Harvey, S.C.; Frank, J.
Deposited on : 2009-09-22
Resolution : 8.90 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:

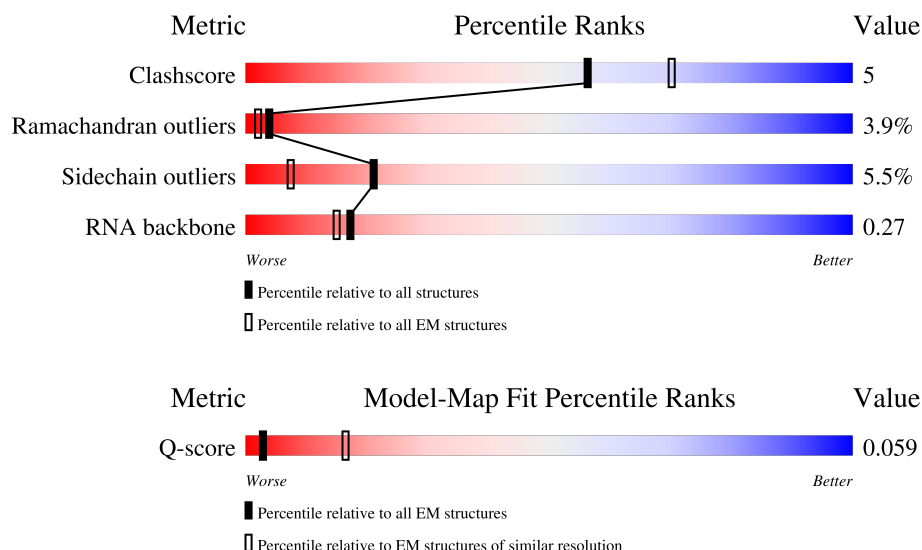
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 8.90 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	258 (8.40 - 9.40)

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	AA	1761	
2	AB	193	
3	AC	188	

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Mol	Chain	Length	Quality of chain
4	AD	158	
5	AE	162	
6	AG	186	
7	AH	125	
8	AI	138	
9	AJ	96	
10	AK	125	
11	AL	118	
12	AM	130	
13	AN	50	
14	AO	84	
15	AQ	80	
16	AS	71	
17	AR	313	
18	AT	141	
19	A7	76	
20	B0	109	
21	B1	48	
22	B2	98	
23	B8	118	
24	B9	72	
25	BA	213	
26	BB	243	
27	BC	362	
28	BD	257	

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Mol	Chain	Length	Quality of chain
29	BE	237	
30	BF	213	
31	BG	113	
32	BH	179	
33	BI	165	
34	BJ	151	
35	BK	138	
36	BL	192	
37	BM	178	
38	BN	150	
39	BO	121	
40	BP	176	
41	BQ	116	
42	BR	131	
43	BS	45	
44	BT	80	
45	BU	116	
46	BV	142	
47	BW	79	
48	BX	86	
49	BY	52	
50	BZ	92	
51	B3	113	
52	B4	157	
53	B5	3170	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 165754 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1761	Total	C	N	O	P	0	3
			37458	16745	6626	12327	1760		

- Molecule 2 is a protein called 40S ribosomal protein S0(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	193	Total	C	N	O	S	0	0
			1500	958	269	271	2		

- Molecule 3 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	188	Total	C	N	O	S	0	0
			1469	929	271	263	6		

- Molecule 4 is a protein called 40S ribosomal protein S9(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	124	Total	C	N	O	S	0	0
			1018	647	189	181	1		

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	162	Total	C	N	O	S	0	0
			1207	765	222	218	2		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	186	Total	C	N	O	S	0	0
			1456	908	277	268	3		

- Molecule 7 is a protein called 40S ribosomal protein S22(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AH	125	Total	C	N	O	S	0	0
			992	634	181	174	3		

- Molecule 8 is a protein called 40S ribosomal protein S16(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	138	Total	C	N	O		0	0
			1087	695	200	192			

- Molecule 9 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	96	Total	C	N	O	S	0	0
			771	487	140	143	1		

- Molecule 10 is a protein called 40S ribosomal protein S14(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	125	Total	C	N	O	S	0	0
			924	566	179	176	3		

- Molecule 11 is a protein called 40S ribosomal protein S23(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AL	118	Total	C	N	O	S	0	0
			906	579	166	159	2		

- Molecule 12 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AM	130	Total	C	N	O	S	0	0
			1077	669	217	189	2		

- Molecule 13 is a protein called 40S ribosomal protein S29(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AN	50	Total	C	N	O	S	0	0
			417	258	87	68	4		

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	84	Total	C	N	O	S	0	0
			694	446	129	118	1		

- Molecule 15 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AQ	80	Total	C	N	O	S	0	0
			643	410	127	104	2		

- Molecule 16 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AS	71	Total	C	N	O	S	0	0
			548	348	101	93	6		

- Molecule 17 is a protein called RACK1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AR	313	Total	C	N	O	S	0	0
			2410	1526	413	463	8		

- Molecule 18 is a protein called s19e protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AT	141	Total	C	N	O	S	0	0
			1102	687	206	207	2		

- Molecule 19 is a RNA chain called P/E tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A7	76	Total	C	N	O	P	0	0
			1648	746	294	533	75		

- Molecule 20 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B0	109	Total	C	N	O	S	0	0
			881	555	176	149	1		

- Molecule 21 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B1	48	Total	C	N	O	S	0	0
			424	263	95	64	2		

- Molecule 22 is a protein called 60S ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B2	98	Total	C	N	O	S	0	0
			752	484	125	142	1		

- Molecule 23 is a protein called 60S ribosomal protein LP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B8	118	Total	C	N	O	S	0	0
			947	609	167	168	3		

- Molecule 24 is a protein called 60S ribosomal protein L43.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B9	72	Total	C	N	O	S	0	0
			539	332	104	98	5		

- Molecule 25 is a protein called 60S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	213	Total	C	N	O	S	0	0
			1683	1074	294	306	9		

- Molecule 26 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	243	Total	C	N	O	S	0	0
			1848	1150	374	323	1		

- Molecule 27 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BC	362	Total	C	N	O	S	0	0
			2887	1833	545	502	7		

- Molecule 28 is a protein called 60S ribosomal protein L4(B).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	257	Total	C	N	O	S	0	0
			1950	1226	375	346	3		

- Molecule 29 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BE	237	Total	C	N	O	S	0	0
			1913	1210	329	372	2		

- Molecule 30 is a protein called 60S ribosomal protein L7(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BF	213	Total	C	N	O	S	0	0
			1561	1010	281	269	1		

- Molecule 31 is a protein called 60S ribosomal protein L8(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BG	113	Total	C	N	O	S	0	0
			844	540	144	158	2		

- Molecule 32 is a protein called 60S ribosomal protein L9(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	179	Total	C	N	O	S	0	0
			1418	896	260	259	3		

- Molecule 33 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BI	165	Total	C	N	O	S	0	0
			1326	834	257	228	7		

- Molecule 34 is a protein called 60S ribosomal protein L11(B).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BJ	151	Total	C	N	O	S	0	0
			1195	744	229	218	4		

- Molecule 35 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BK	138	Total	C	N	O	S	0	0
			1038	651	190	195	2		

- Molecule 36 is a protein called 60S ribosomal protein L15(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BL	192	Total	C	N	O	S	0	0
			1618	1011	340	266	1		

- Molecule 37 is a protein called 60S ribosomal protein L16(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BM	178	Total	C	N	O	S	0	0
			1317	845	254	217	1		

- Molecule 38 is a protein called 60S ribosomal protein L17(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	150	Total	C	N	O		0	0
			1189	742	230	217			

- Molecule 39 is a protein called 60S ribosomal protein L18(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BO	121	Total	C	N	O	S	0	0
			931	598	170	162	1		

- Molecule 40 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	176	Total	C	N	O		0	0
			1317	816	277	224			

- Molecule 41 is a protein called 60S ribosomal protein L21(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BQ	116	Total	C	N	O	S	0	0
			893	564	173	153	3		

- Molecule 42 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BR	131	Total	C	N	O	S	0	0
			977	614	183	173	7		

- Molecule 43 is a protein called 60S ribosomal protein L24(A).

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BS	45	Total	C	N	O	0	0
			371	238	73	60		

- Molecule 44 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BT	80	Total	C	N	O	S	0	0
			642	411	108	121	2		

- Molecule 45 is a protein called 60S ribosomal protein L26(A).

Mol	Chain	Residues	Atoms				AltConf	Trace
45	BU	116	Total	C	N	O	0	0
			916	576	179	161		

- Molecule 46 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	142	Total	C	N	O	S	0	0
			1123	717	218	185	3		

- Molecule 47 is a protein called 60S ribosomal protein L31(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	79	Total	C	N	O	S	0	0
			663	415	135	112	1		

- Molecule 48 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BX	86	Total	C	N	O	S	0	0
			605	379	111	114	1		

- Molecule 49 is a protein called 60S ribosomal protein L37(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	52	Total	C	N	O	S	0	0
			403	245	85	69	4		

- Molecule 50 is a protein called 60S ribosomal protein L42.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BZ	92	Total	C	N	O	S	0	0
			749	472	151	121	5		

- Molecule 51 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B3	113	Total	C	N	O	P	0	0
			2403	1075	429	787	112		

- Molecule 52 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	157	Total	C	N	O	P	0	0
			3329	1490	581	1102	156		

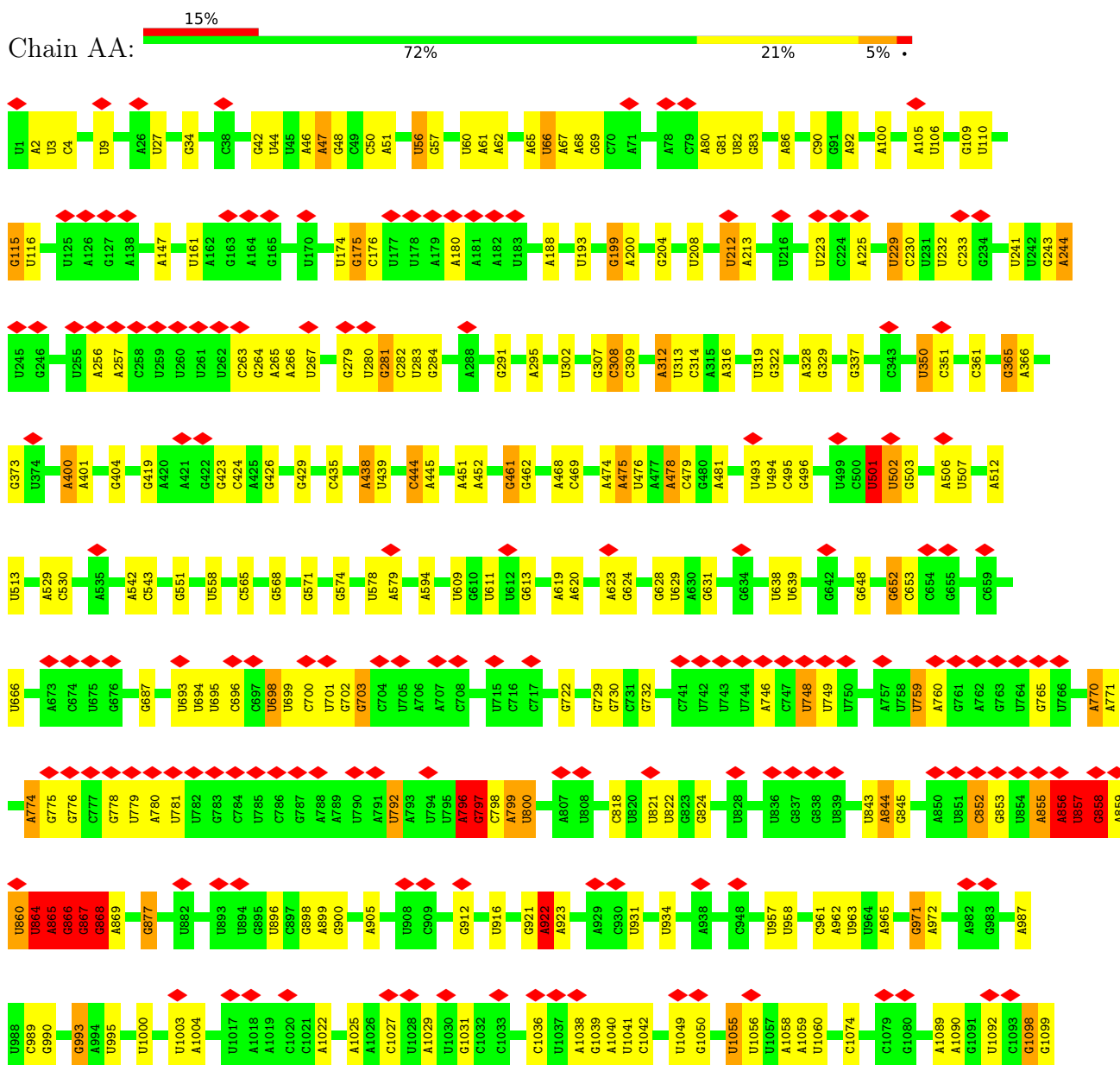
- Molecule 53 is a RNA chain called 26S ribosomal RNA.

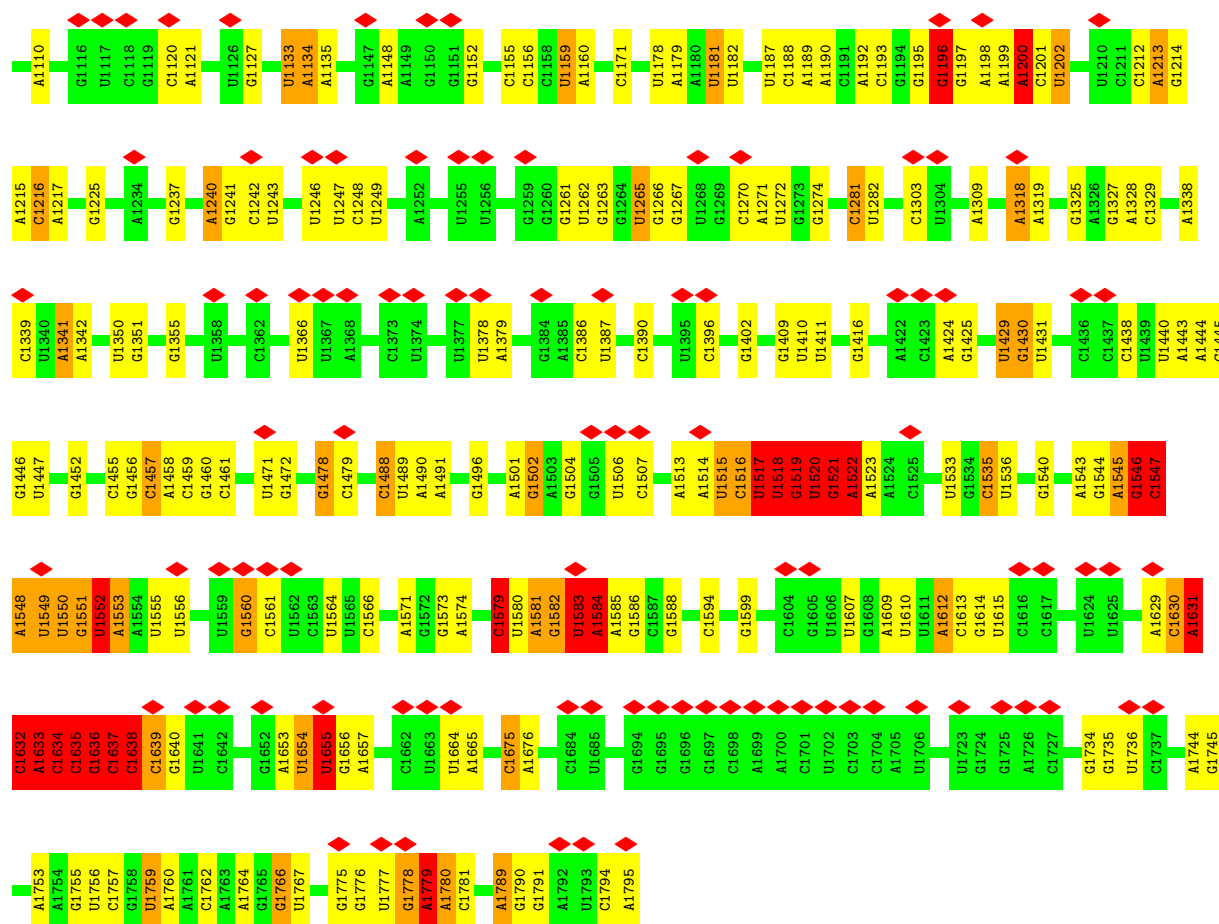
Mol	Chain	Residues	Atoms					AltConf	Trace
53	B5	3170	Total	C	N	O	P	0	0
			67775	30273	12178	22155	3169		

3 Residue-property plots

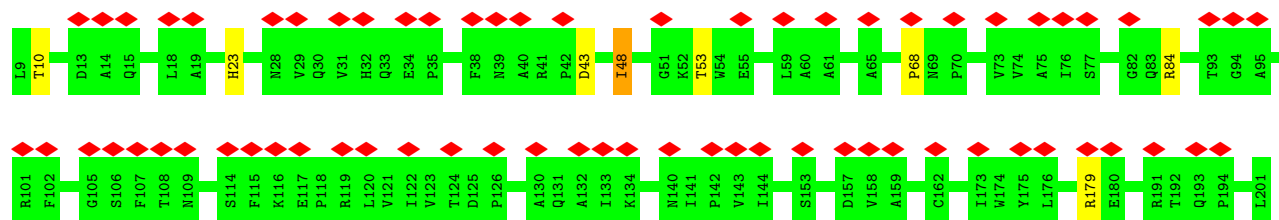
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 18S rRNA

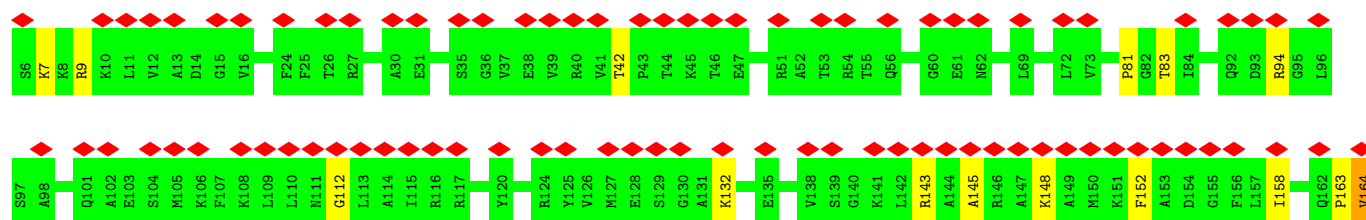
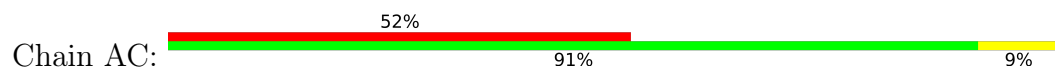


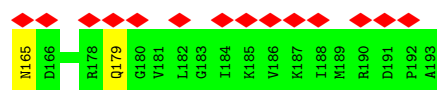


• Molecule 2: 40S ribosomal protein S0(A)

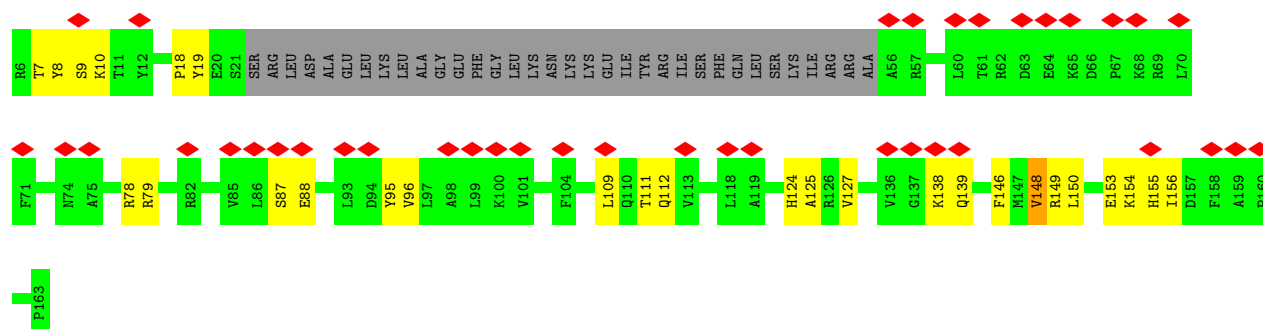


• Molecule 3: 40S ribosomal protein S3

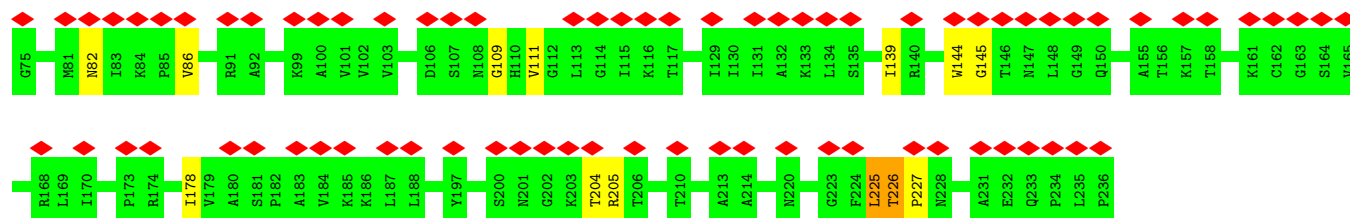




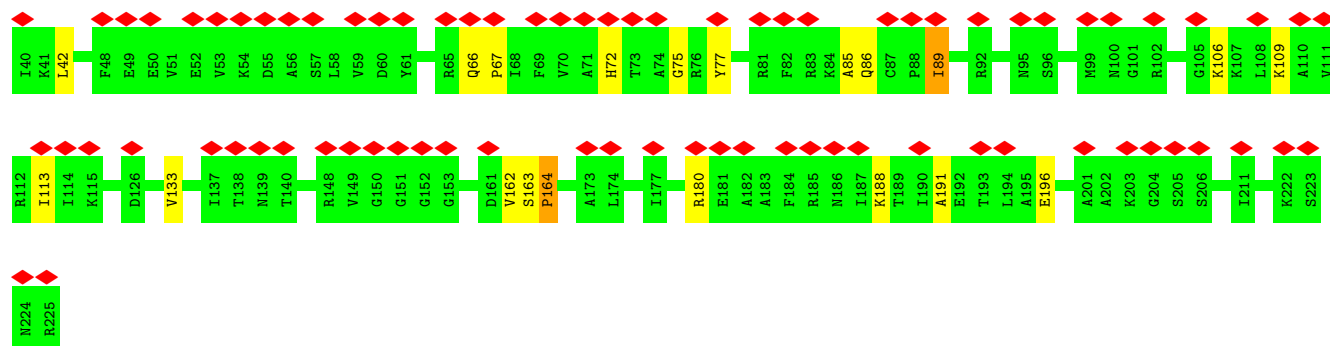
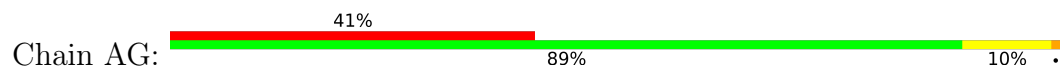
• Molecule 4: 40S ribosomal protein S9(A)



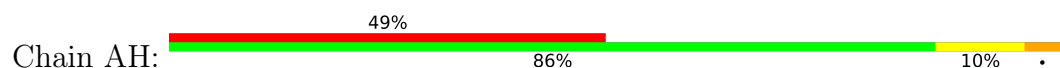
• Molecule 5: 40S ribosomal protein S2

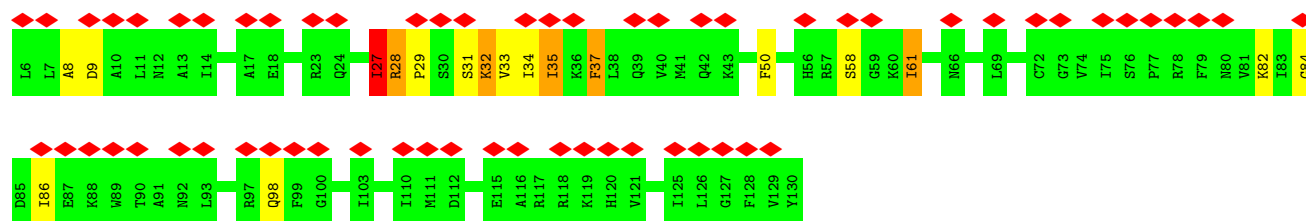


• Molecule 6: 40S ribosomal protein S5

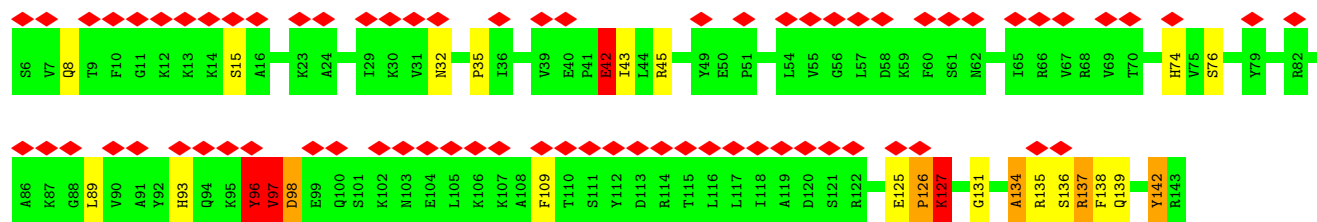
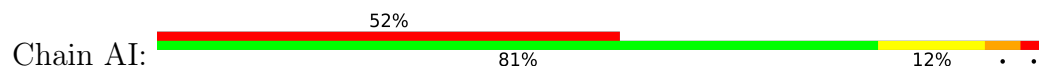


• Molecule 7: 40S ribosomal protein S22(A)

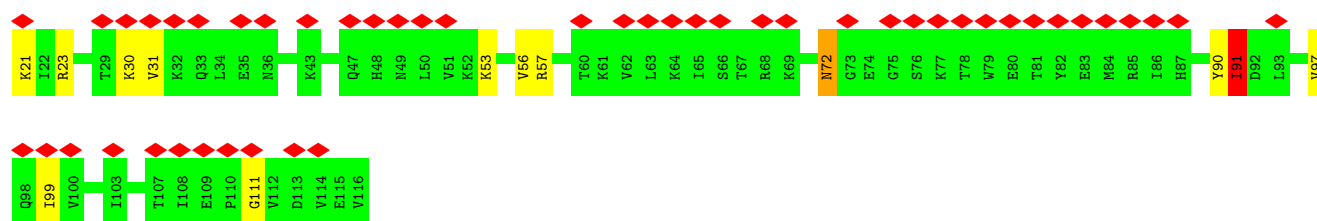
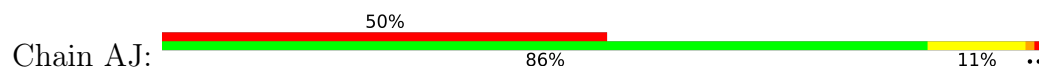




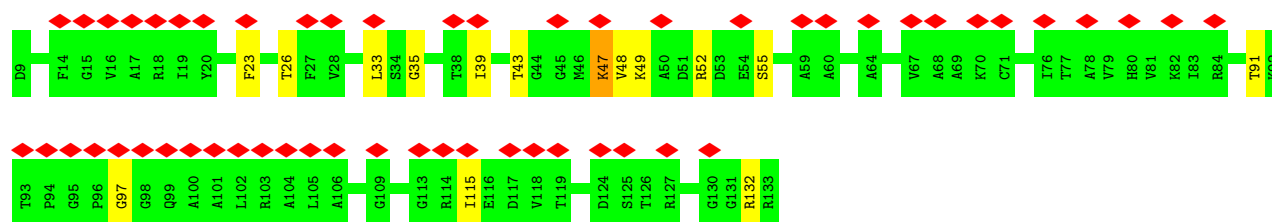
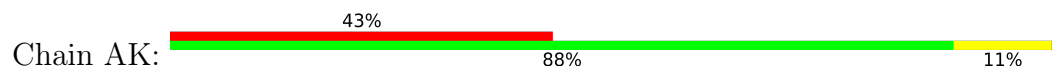
• Molecule 8: 40S ribosomal protein S16(A)



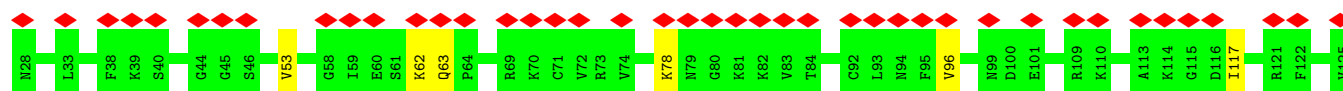
• Molecule 9: 40S ribosomal protein S20

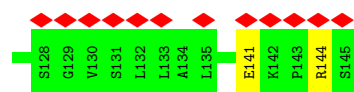


• Molecule 10: 40S ribosomal protein S14(A)

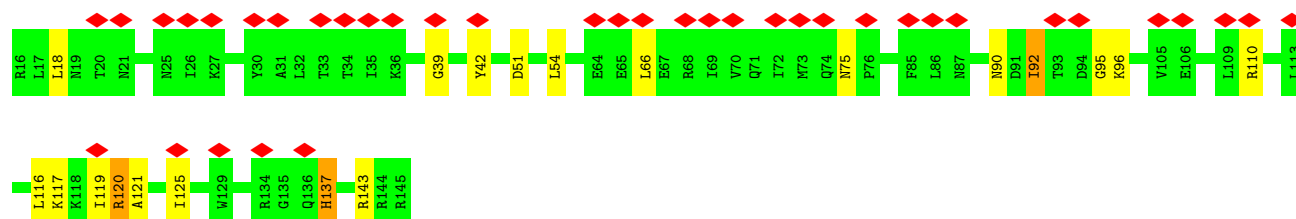
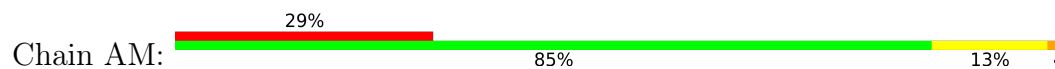


• Molecule 11: 40S ribosomal protein S23(A)

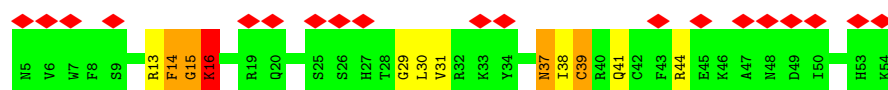
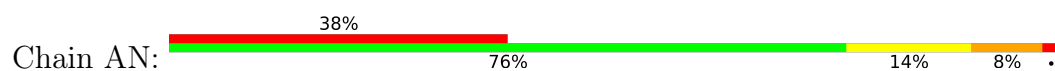




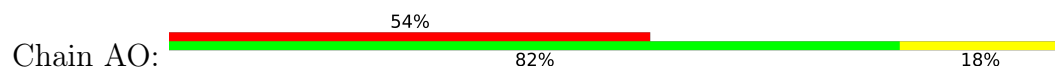
- Molecule 12: 40S ribosomal protein S18



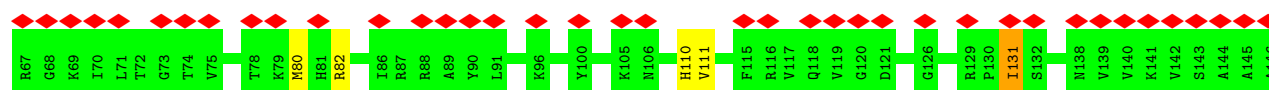
- Molecule 13: 40S ribosomal protein S29(A)



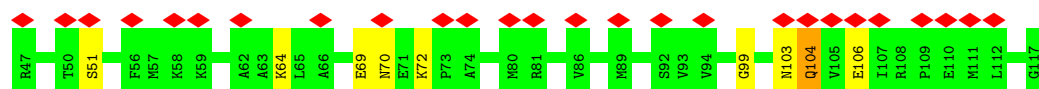
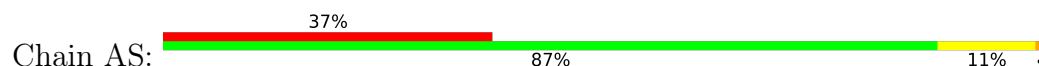
- Molecule 14: 40S ribosomal protein S13



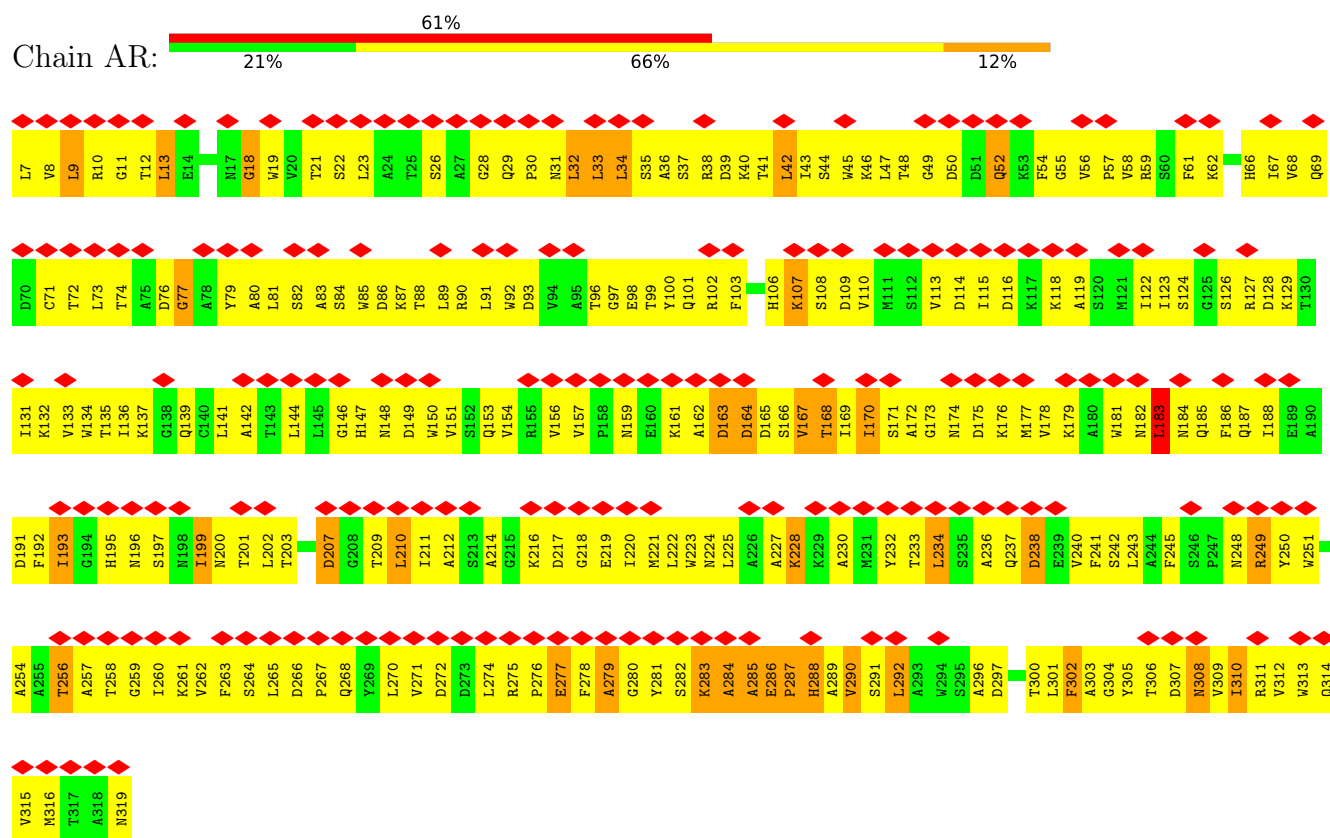
- Molecule 15: 40S ribosomal protein S11



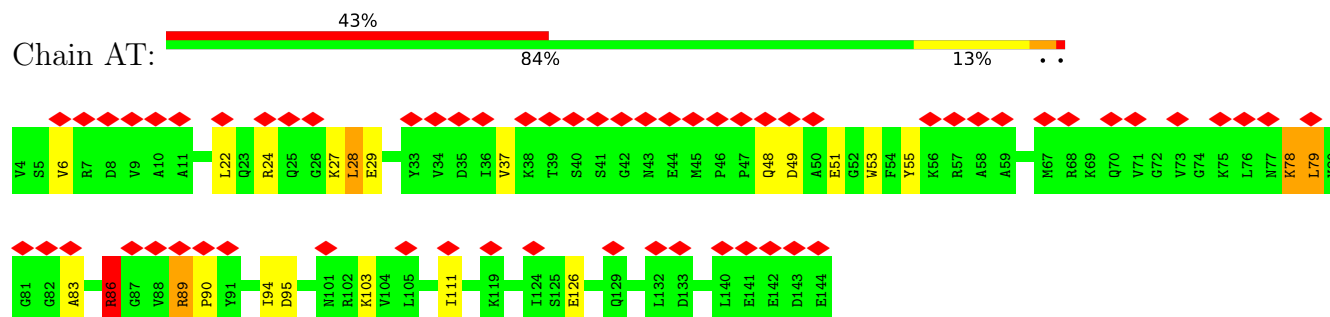
- Molecule 16: 40S ribosomal protein S15



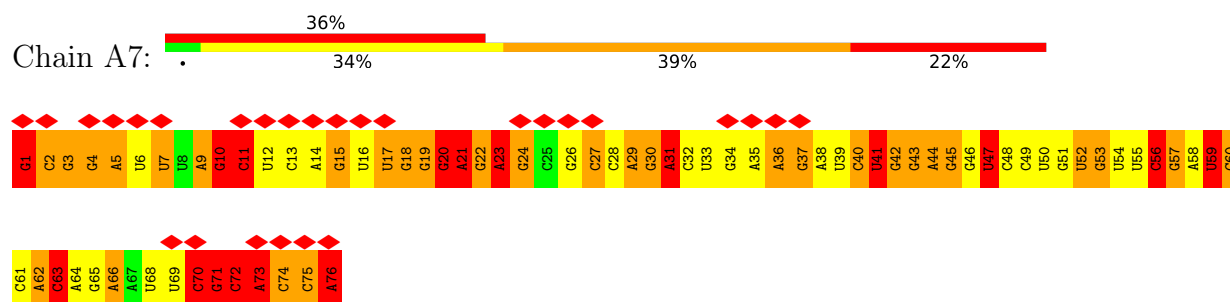
- Molecule 17: RACK1 protein



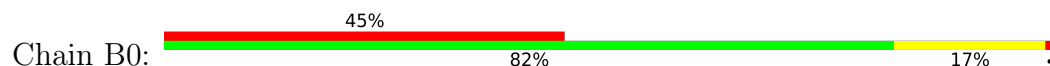
• Molecule 18: s19e protein

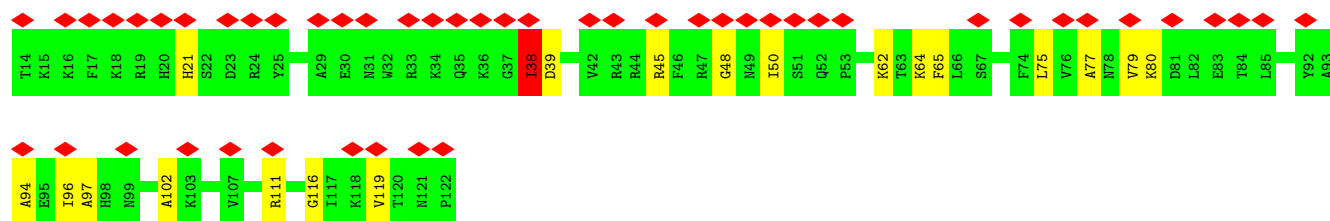


• Molecule 19: P/E tRNA

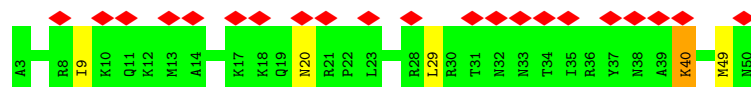
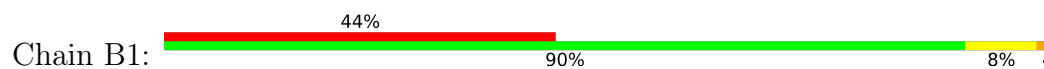


• Molecule 20: 60S ribosomal protein L32

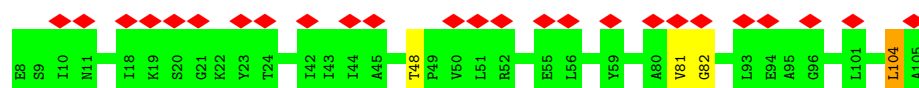




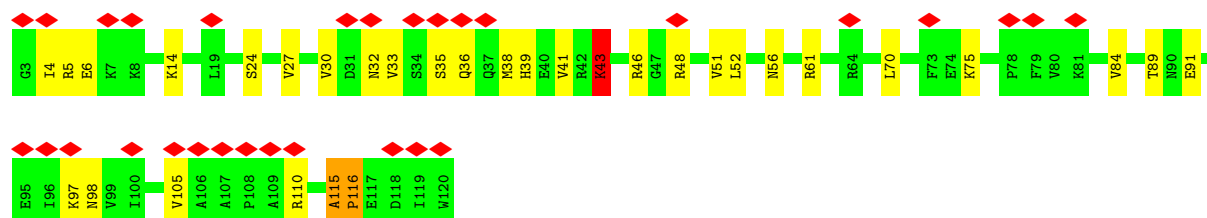
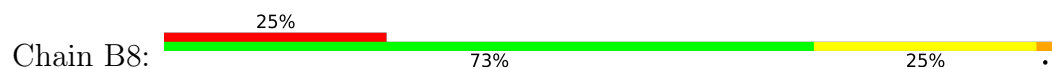
- Molecule 21: 60S ribosomal protein L39



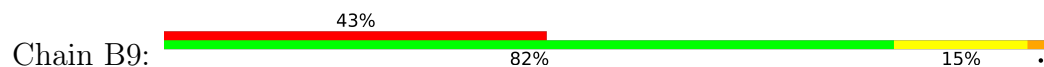
- Molecule 22: 60S ribosomal protein L30e



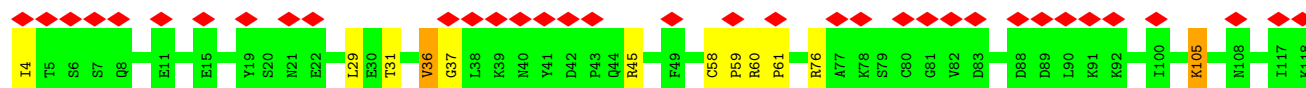
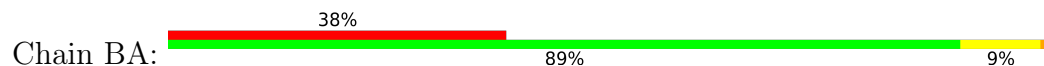
- Molecule 23: 60S ribosomal protein LP0

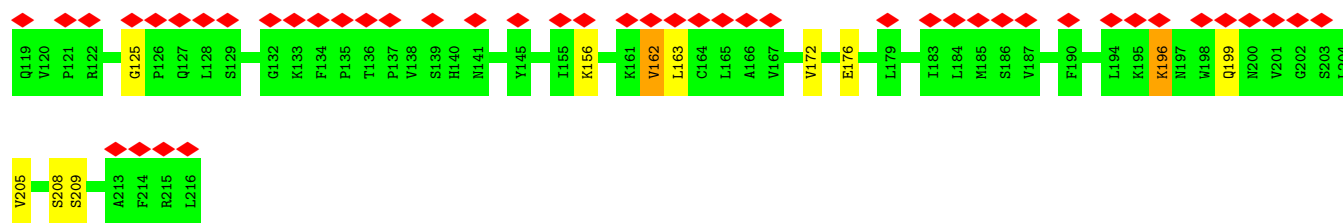


- Molecule 24: 60S ribosomal protein L43

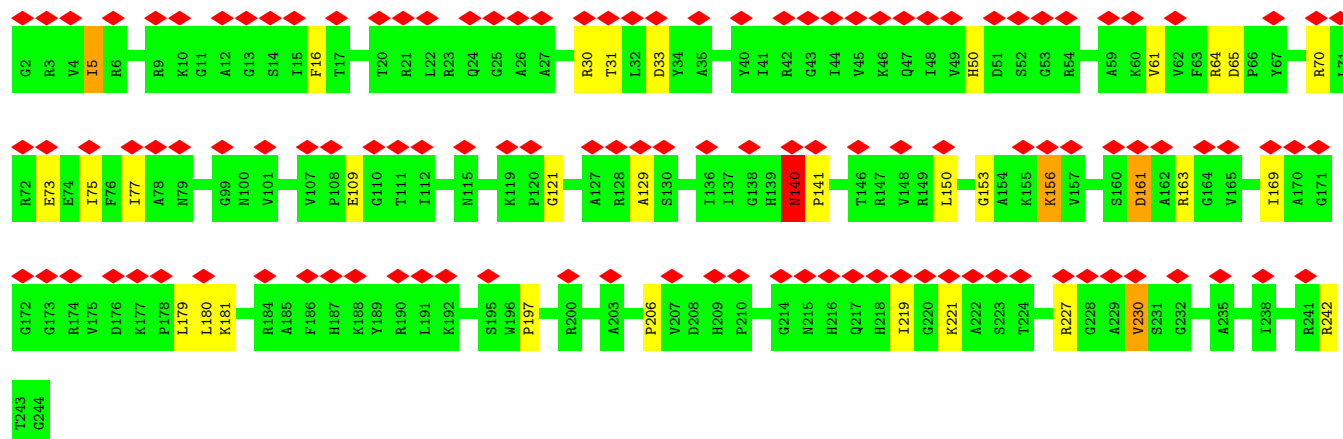
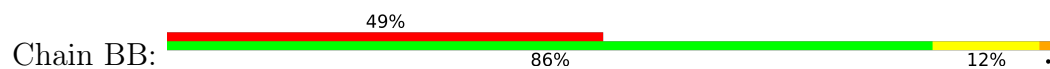


- Molecule 25: 60S ribosomal protein L1

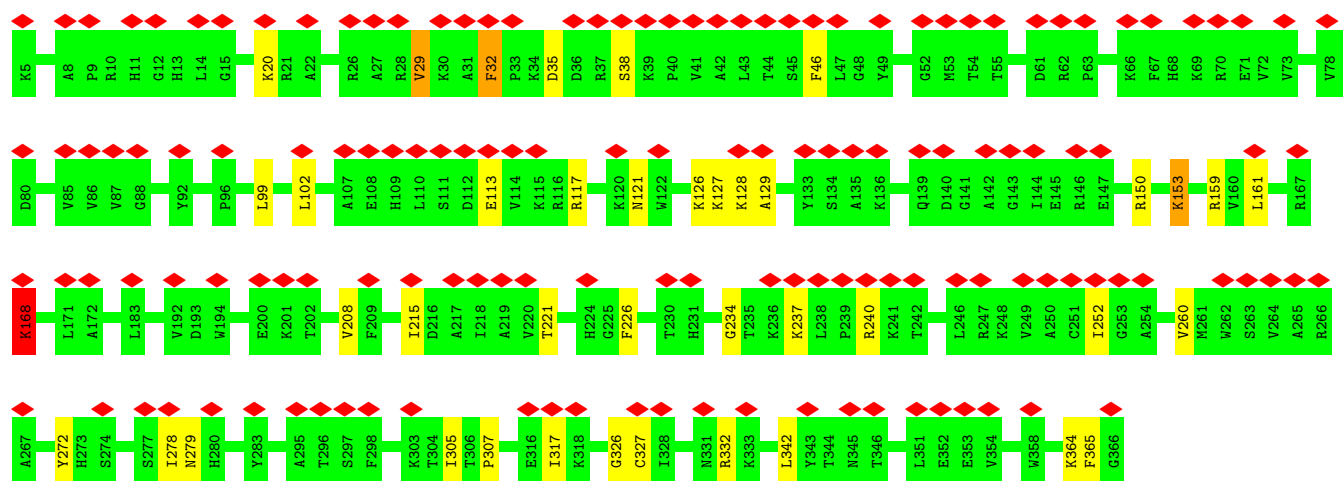
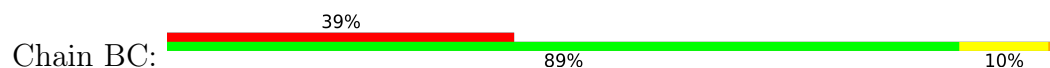




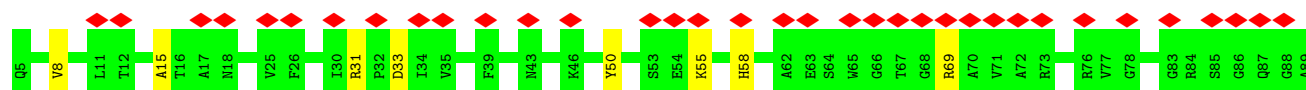
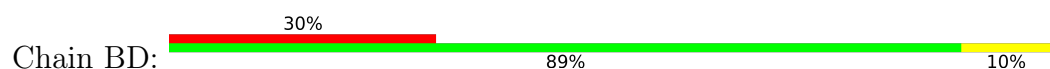
• Molecule 26: 60S ribosomal protein L2

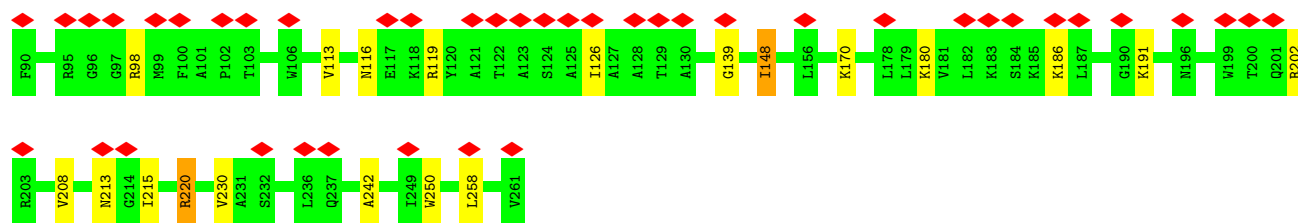


• Molecule 27: 60S ribosomal protein L3

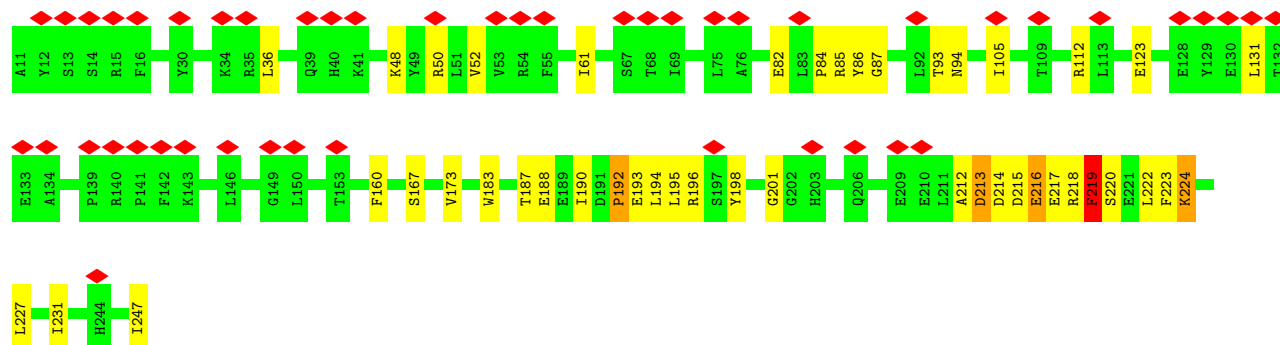
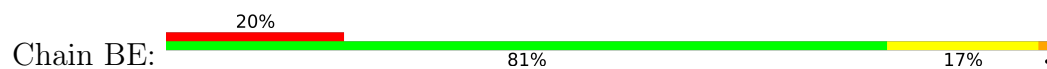


• Molecule 28: 60S ribosomal protein L4(B)

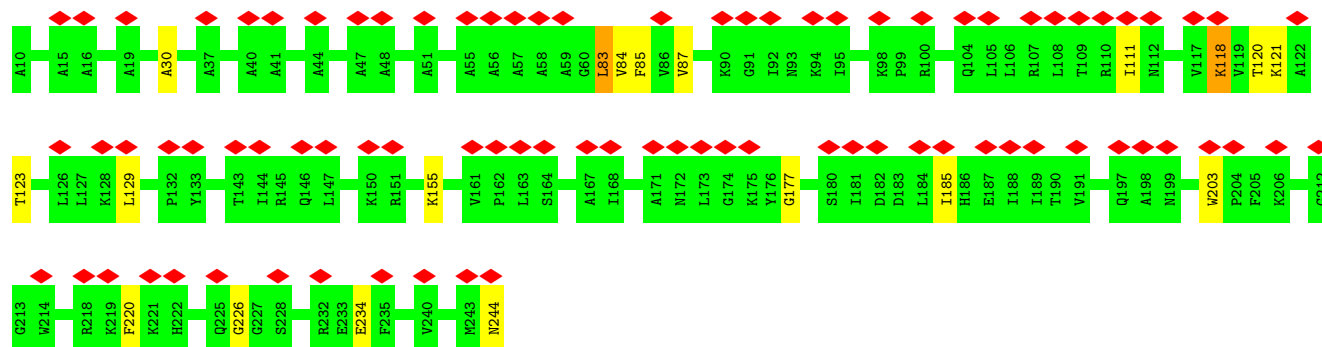
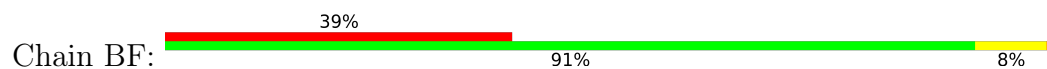




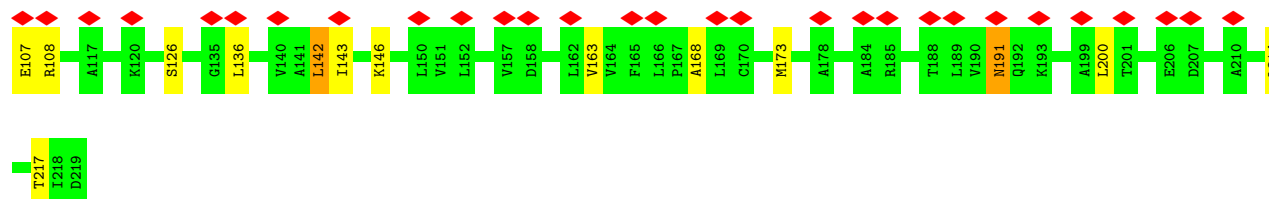
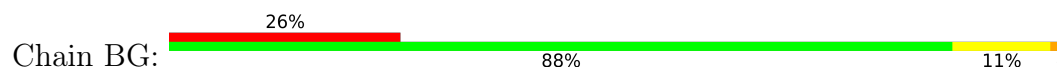
- Molecule 29: 60S ribosomal protein L5



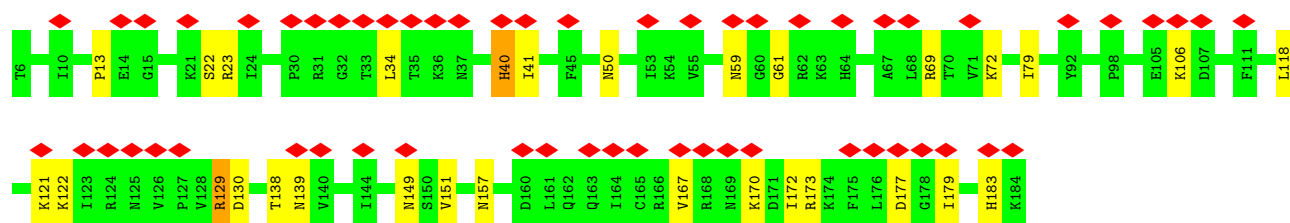
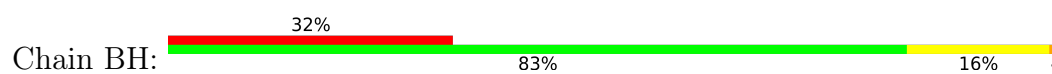
- Molecule 30: 60S ribosomal protein L7(A)



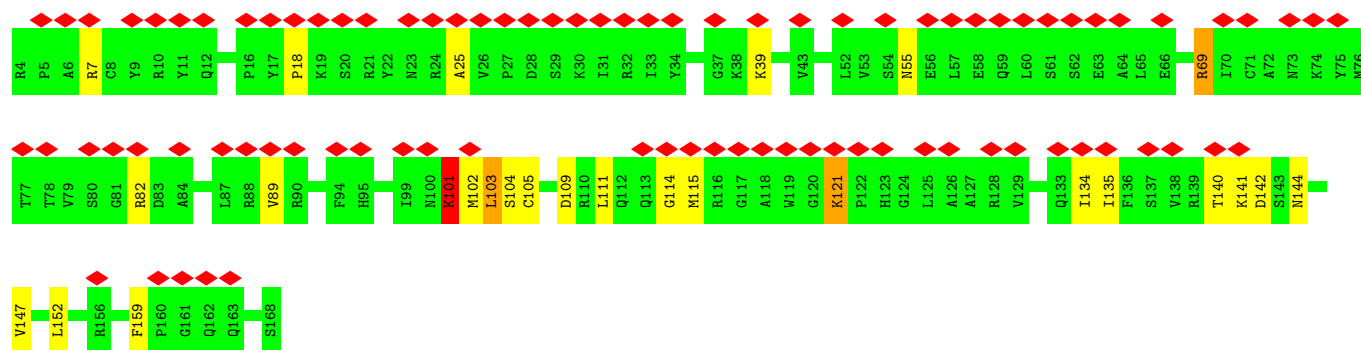
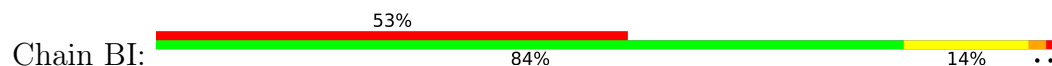
- Molecule 31: 60S ribosomal protein L8(A)



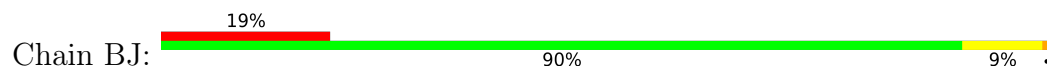
- Molecule 32: 60S ribosomal protein L9(A)



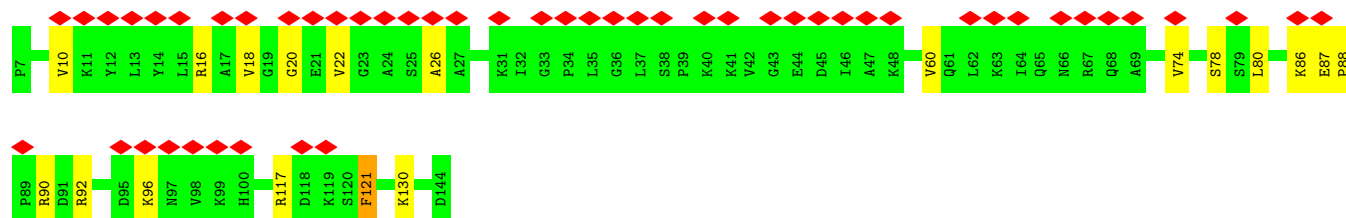
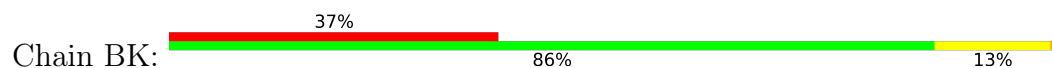
• Molecule 33: 60S ribosomal protein L10



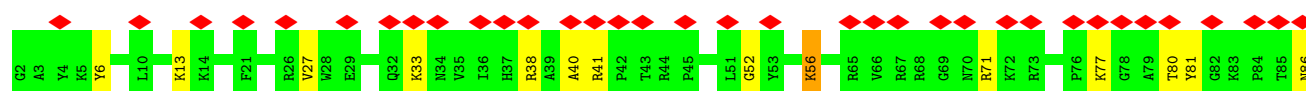
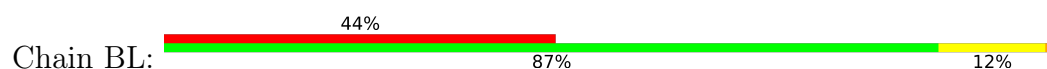
• Molecule 34: 60S ribosomal protein L11(B)

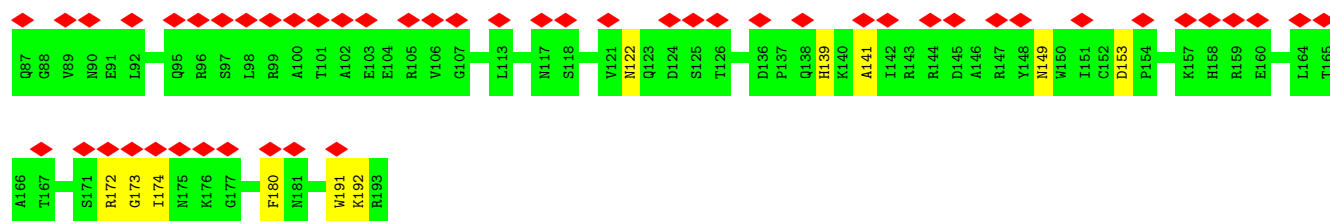


• Molecule 35: 60S ribosomal protein L12

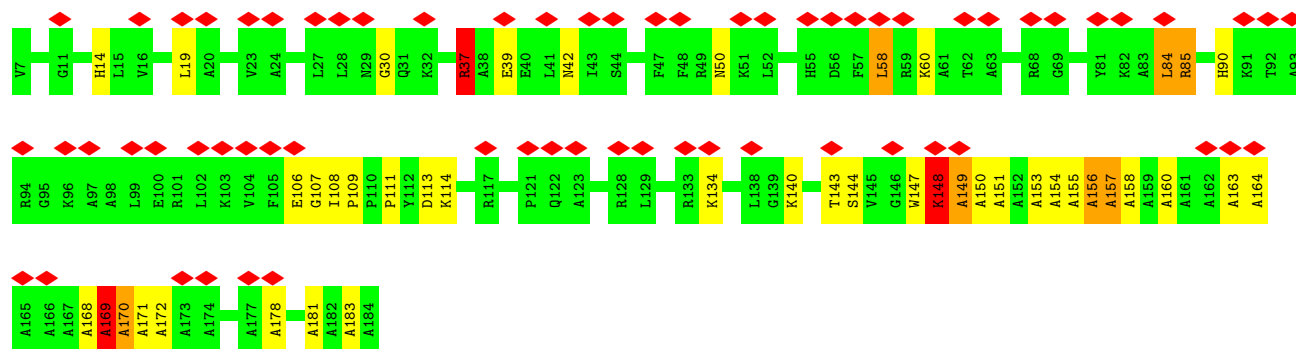
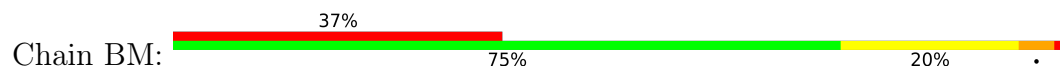


• Molecule 36: 60S ribosomal protein L15(A)

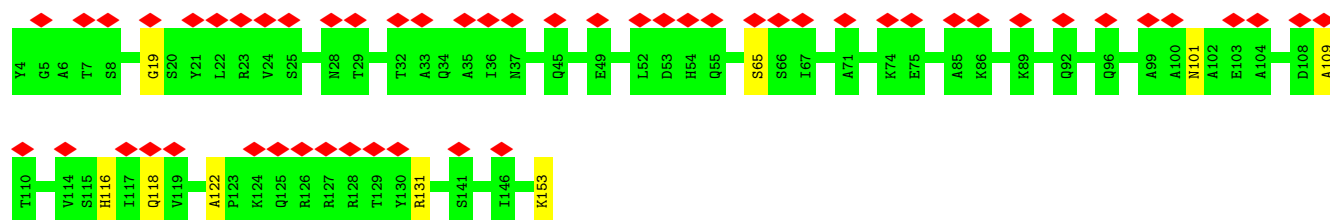




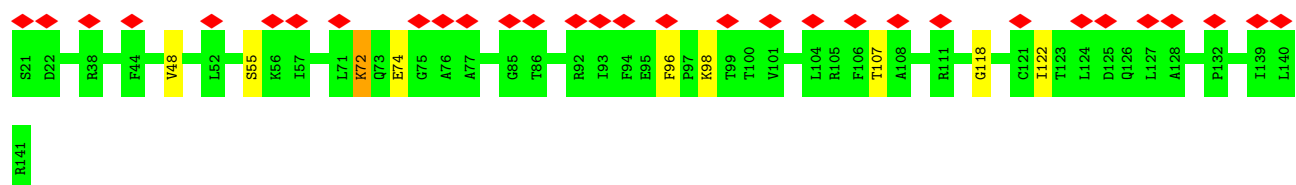
• Molecule 37: 60S ribosomal protein L16(A)



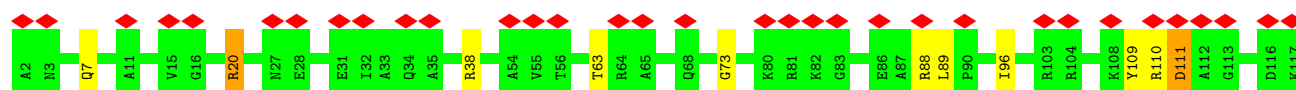
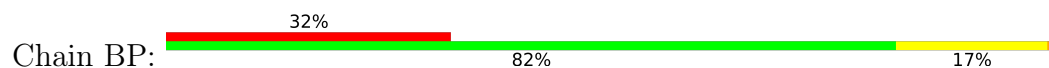
• Molecule 38: 60S ribosomal protein L17(A)

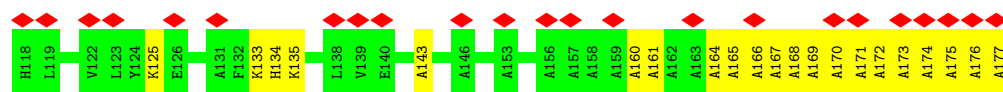


• Molecule 39: 60S ribosomal protein L18(A)

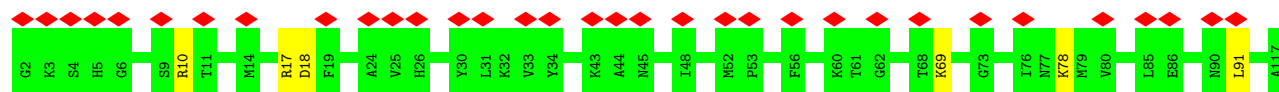


• Molecule 40: 60S ribosomal protein L19

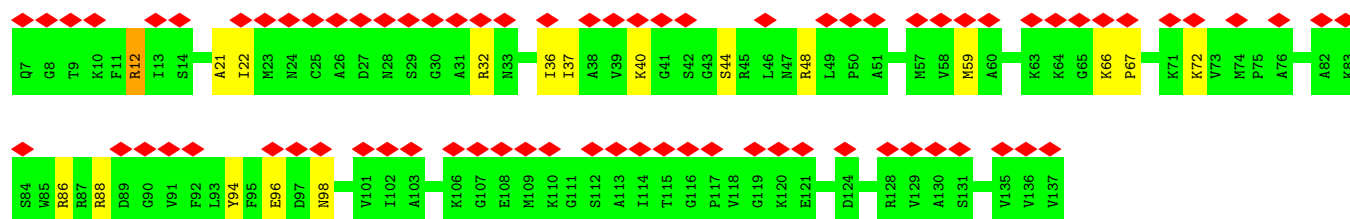
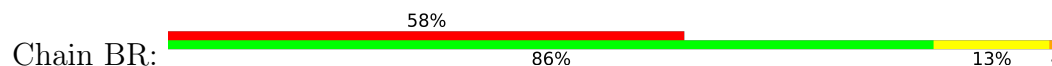




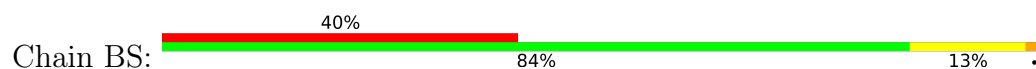
- Molecule 41: 60S ribosomal protein L21(A)



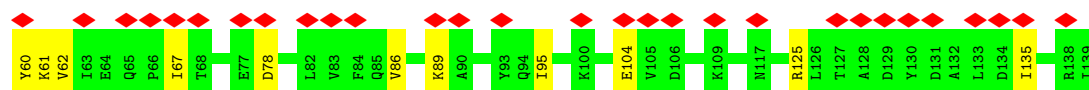
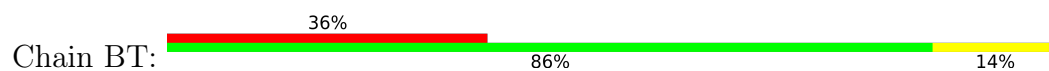
- Molecule 42: 60S ribosomal protein L23



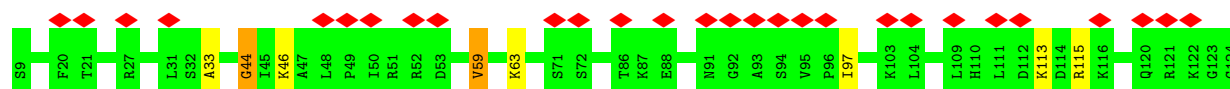
- Molecule 43: 60S ribosomal protein L24(A)



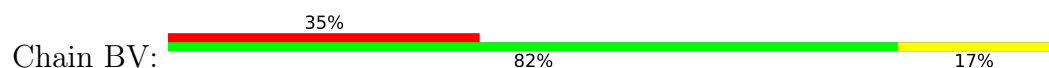
- Molecule 44: 60S ribosomal protein L25

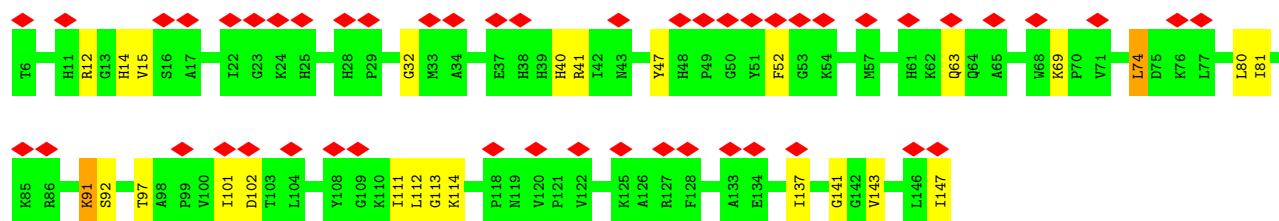


- Molecule 45: 60S ribosomal protein L26(A)

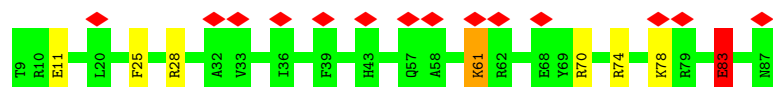
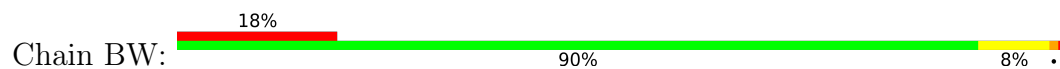


- Molecule 46: 60S ribosomal protein L28

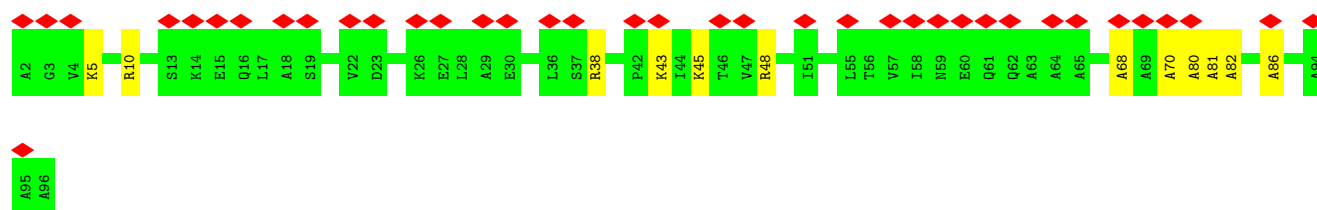
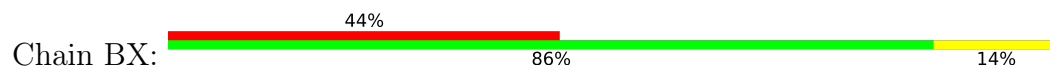




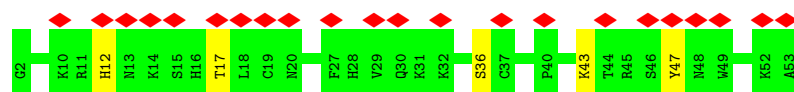
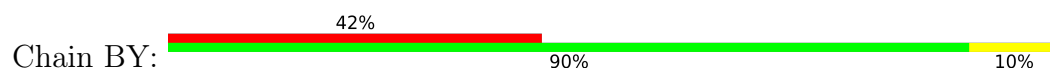
• Molecule 47: 60S ribosomal protein L31(A)



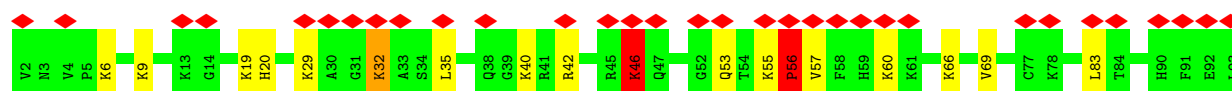
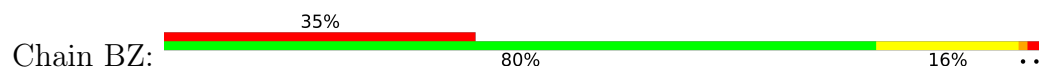
• Molecule 48: 60S ribosomal protein L35



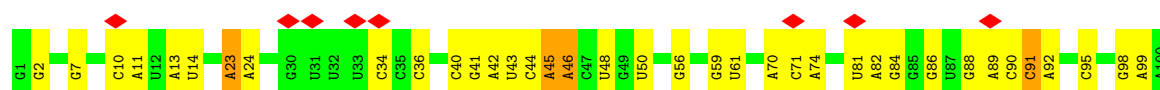
• Molecule 49: 60S ribosomal protein L37(A)

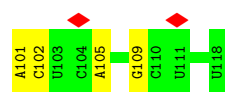


• Molecule 50: 60S ribosomal protein L42

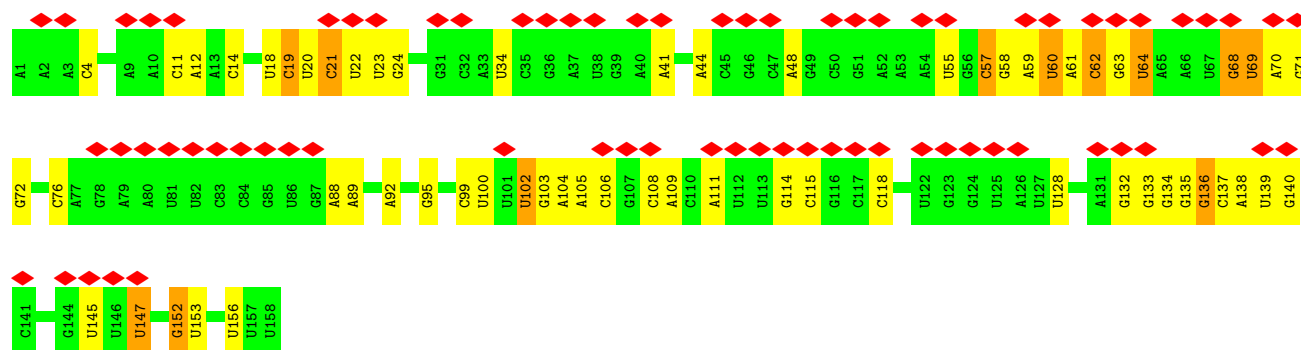


• Molecule 51: 5S ribosomal RNA

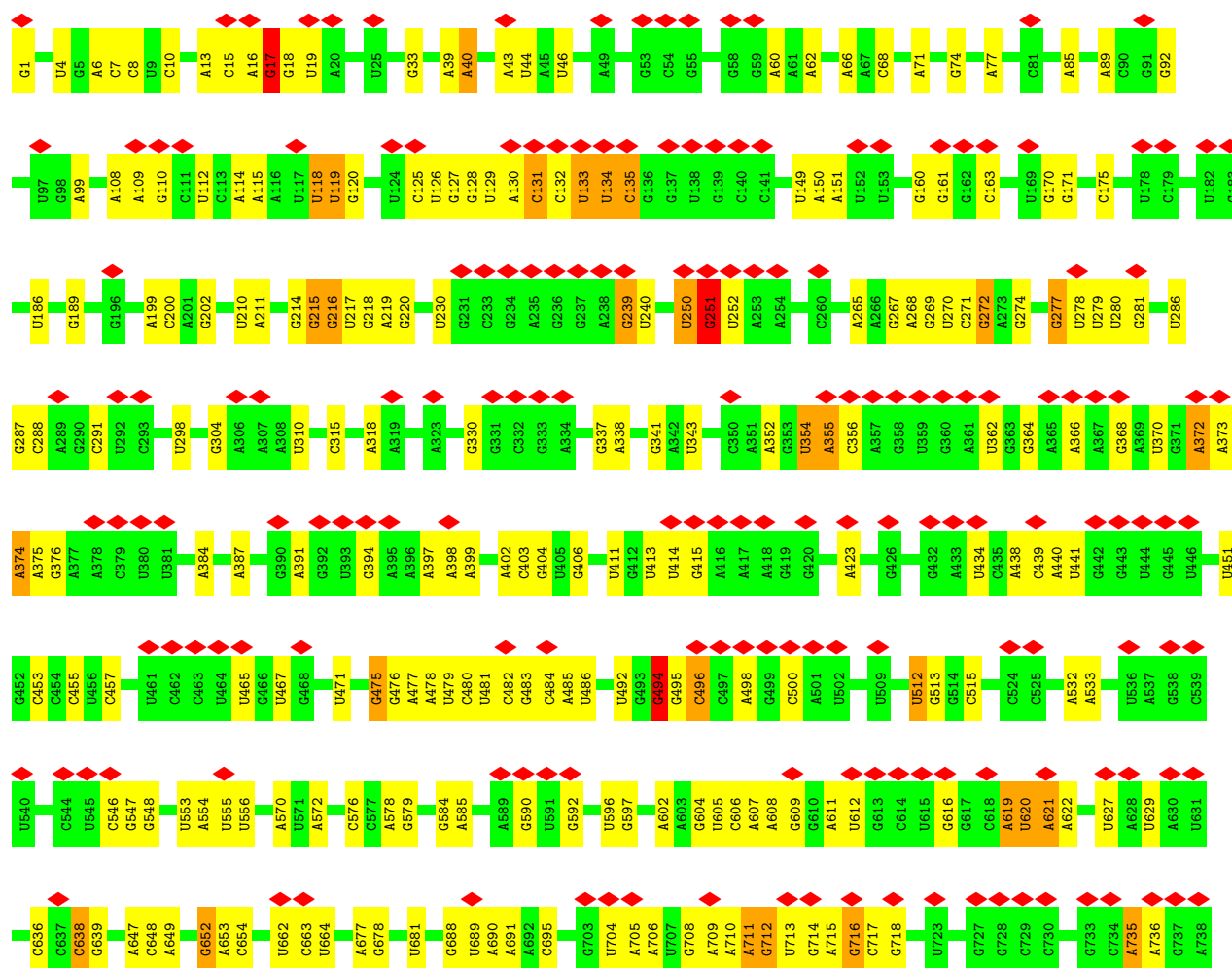




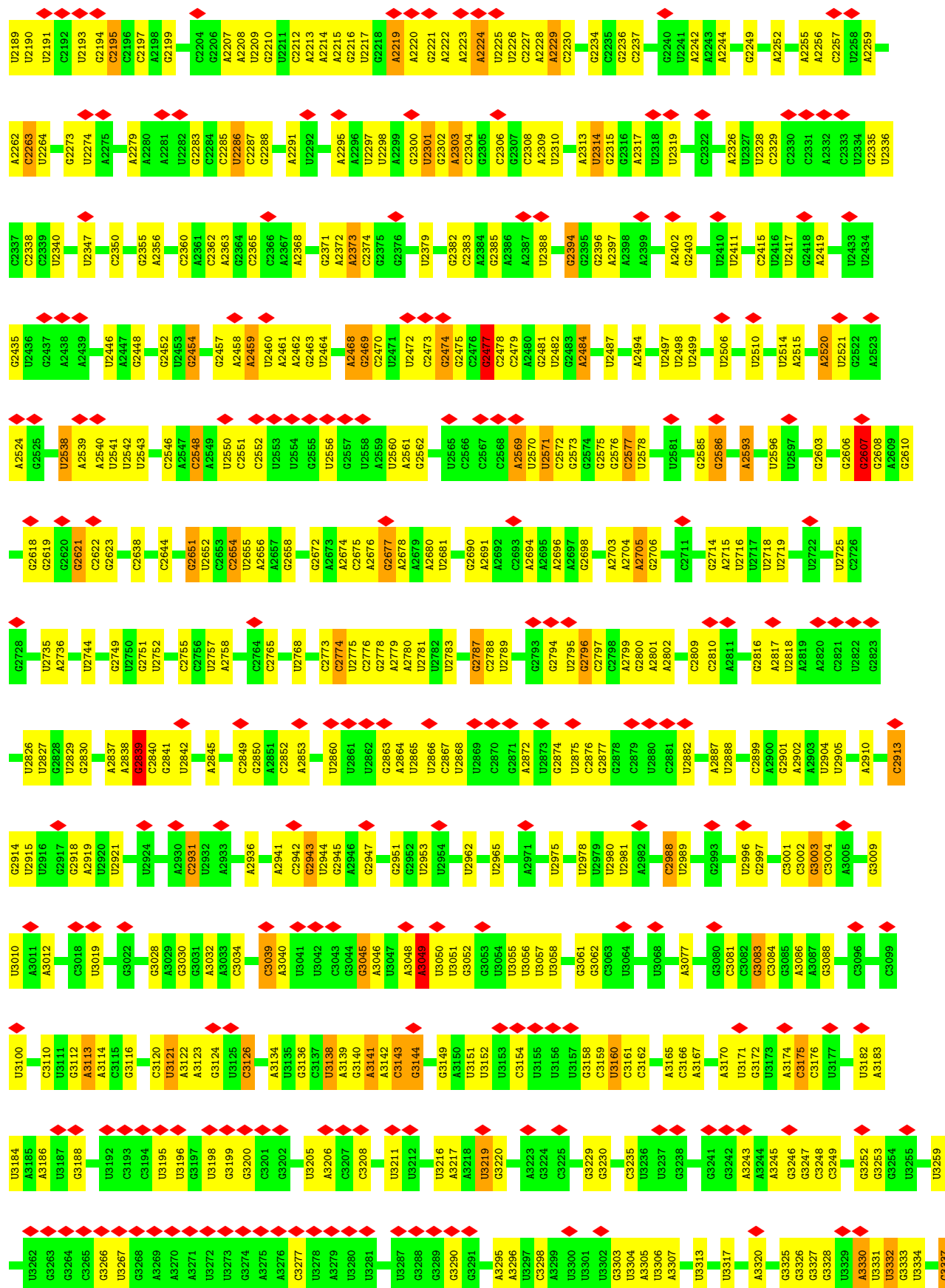
- Molecule 52: 5.8S ribosomal RNA

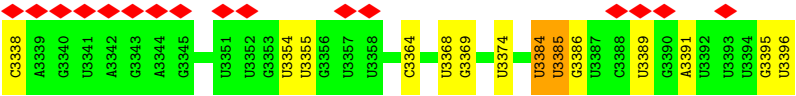


- Molecule 53: 26S ribosomal RNA









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102689	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	280.857	Depositor
Minimum map value	-103.711	Depositor
Average map value	7.703	Depositor
Map value standard deviation	27.906	Depositor
Recommended contour level	70.4	Depositor
Map size ($\text{\AA}$)	381.3, 381.3, 381.3	wwPDB
Map dimensions	205, 205, 205	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	1.86, 1.86, 1.86	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, M2G, 2MG, PSU, 7MG, OMG, 5MC, H2U, YYG, OMC, 5MU

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	AA	1.02	39/41893 (0.1%)	1.16	265/65278 (0.4%)
2	AB	1.11	0/1535	1.33	3/2097 (0.1%)
3	AC	1.16	0/1488	1.32	2/1996 (0.1%)
4	AD	1.16	0/1035	1.52	13/1390 (0.9%)
5	AE	1.11	0/1227	1.32	2/1663 (0.1%)
6	AG	1.14	0/1472	1.40	9/1982 (0.5%)
7	AH	1.27	3/1008 (0.3%)	1.65	11/1351 (0.8%)
8	AI	1.96	7/1106 (0.6%)	1.54	14/1481 (0.9%)
9	AJ	1.12	0/781	1.36	3/1053 (0.3%)
10	AK	1.19	0/935	1.39	2/1257 (0.2%)
11	AL	1.11	0/920	1.25	1/1226 (0.1%)
12	AM	1.19	0/1094	1.45	1/1468 (0.1%)
13	AN	3.93	4/427 (0.9%)	1.93	8/567 (1.4%)
14	AO	1.13	0/707	1.46	5/950 (0.5%)
15	AQ	1.23	0/656	1.30	0/885
16	AS	1.14	0/559	1.30	1/748 (0.1%)
17	AR	1.34	5/2463 (0.2%)	1.77	38/3350 (1.1%)
18	AT	1.20	2/1118 (0.2%)	1.59	9/1498 (0.6%)
19	A7	1.88	16/1483 (1.1%)	2.07	82/2311 (3.5%)
20	B0	1.18	0/898	1.46	4/1201 (0.3%)
21	B1	1.25	0/431	1.42	1/570 (0.2%)
22	B2	1.07	0/760	1.29	1/1020 (0.1%)
23	B8	1.14	0/965	1.48	7/1298 (0.5%)
24	B9	1.16	0/546	1.40	3/729 (0.4%)
25	BA	1.06	0/1709	1.36	3/2295 (0.1%)
26	BB	1.20	0/1882	1.40	5/2528 (0.2%)
27	BC	1.18	0/2953	1.37	8/3974 (0.2%)
28	BD	1.13	0/1987	1.33	1/2690 (0.0%)
29	BE	1.18	0/1956	1.49	25/2646 (0.9%)
30	BF	1.10	1/1593 (0.1%)	1.40	4/2160 (0.2%)
31	BG	1.06	0/853	1.43	9/1153 (0.8%)
32	BH	1.17	0/1437	1.42	11/1935 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BI	1.22	0/1352	1.49	10/1815 (0.6%)
34	BJ	1.19	0/1212	1.35	2/1622 (0.1%)
35	BK	1.64	6/1049 (0.6%)	1.40	5/1408 (0.4%)
36	BL	1.23	0/1652	1.38	10/2211 (0.5%)
37	BM	1.29	2/1341 (0.1%)	1.63	15/1808 (0.8%)
38	BN	1.17	0/1212	1.35	2/1631 (0.1%)
39	BO	1.14	0/943	1.35	4/1274 (0.3%)
40	BP	1.19	0/1334	1.51	4/1791 (0.2%)
41	BQ	1.16	0/909	1.36	0/1216
42	BR	1.15	0/992	1.42	2/1333 (0.2%)
43	BS	1.23	0/380	1.42	6/504 (1.2%)
44	BT	1.08	0/649	1.26	1/873 (0.1%)
45	BU	1.16	0/927	1.33	5/1237 (0.4%)
46	BV	1.16	0/1152	1.49	7/1542 (0.5%)
47	BW	1.24	0/673	1.42	2/894 (0.2%)
48	BX	1.04	0/607	1.39	2/818 (0.2%)
49	BY	1.21	0/413	1.29	0/548
50	BZ	1.19	0/761	1.45	5/1006 (0.5%)
51	B3	0.87	0/2686	1.08	4/4184 (0.1%)
52	B4	0.88	0/3719	1.11	12/5791 (0.2%)
53	B5	0.87	0/75857	1.05	112/118271 (0.1%)
All	All	1.04	85/179697 (0.0%)	1.21	761/268527 (0.3%)

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
1	AA	2	28
2	AB	0	1
4	AD	0	3
5	AE	0	1
7	AH	1	0
8	AI	0	3
9	AJ	0	3
10	AK	0	4
12	AM	0	3
13	AN	0	2
14	AO	0	4
19	A7	0	44
20	B0	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	B8	0	3
24	B9	0	3
26	BB	1	4
27	BC	0	1
28	BD	0	3
29	BE	1	7
30	BF	1	0
31	BG	2	2
32	BH	0	3
33	BI	0	2
34	BJ	0	3
35	BK	0	2
36	BL	1	7
37	BM	0	5
38	BN	0	2
39	BO	0	1
40	BP	0	4
42	BR	0	3
43	BS	0	1
44	BT	0	1
45	BU	0	1
46	BV	0	3
47	BW	0	2
48	BX	2	1
49	BY	0	1
50	BZ	0	5
51	B3	1	0
52	B4	0	6
53	B5	33	112
All	All	45	285

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AN	16	LYS	N-CA	75.73	2.90	1.46
1	AA	501	U	C4-C5	30.64	2.04	1.43
1	AA	856	A	C5-C6	29.28	1.99	1.41
1	AA	856	A	C5-C4	29.21	1.97	1.38
1	AA	856	A	N3-C4	28.45	1.91	1.34
1	AA	501	U	N1-C2	28.19	1.95	1.38
1	AA	501	U	C2-N3	26.61	1.91	1.37
1	AA	856	A	C6-N1	26.17	1.87	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	501	U	N1-C6	25.85	1.89	1.38
1	AA	501	U	N3-C4	25.61	1.89	1.38
1	AA	856	A	C2-N3	25.32	1.84	1.33
8	AI	96	TYR	CG-CD1	24.64	1.91	1.39
8	AI	96	TYR	CG-CD2	24.25	1.90	1.39
1	AA	856	A	N1-C2	24.11	1.82	1.34
1	AA	1200	A	N3-C4	24.03	1.82	1.34
1	AA	1200	A	C5-C4	23.86	1.86	1.38
1	AA	1200	A	C5-C6	23.35	1.87	1.41
1	AA	1200	A	C6-N1	23.29	1.82	1.35
8	AI	96	TYR	CE1-CZ	21.98	1.91	1.38
8	AI	96	TYR	CE2-CZ	21.74	1.90	1.38
1	AA	1200	A	C2-N3	21.10	1.75	1.33
35	BK	121	PHE	CG-CD2	20.57	1.82	1.38
1	AA	1200	A	N1-C2	20.12	1.74	1.34
35	BK	121	PHE	CG-CD1	20.08	1.81	1.38
8	AI	96	TYR	CD1-CE1	16.78	1.89	1.38
8	AI	96	TYR	CD2-CE2	16.63	1.88	1.38
1	AA	501	U	C5-C6	16.50	1.67	1.34
37	BM	148	LYS	C-N	16.48	1.56	1.33
37	BM	169	ALA	C-N	16.47	1.56	1.33
35	BK	121	PHE	CD1-CE1	13.87	1.80	1.38
35	BK	121	PHE	CE2-CZ	13.55	1.79	1.38
35	BK	121	PHE	CE1-CZ	13.14	1.78	1.38
18	AT	78	LYS	CA-C	12.76	1.69	1.52
35	BK	121	PHE	CD2-CE2	12.70	1.76	1.38
7	AH	32	LYS	CA-C	12.20	1.67	1.53
17	AR	167	VAL	CA-CB	-10.96	1.47	1.55
17	AR	163	ASP	CA-C	-9.73	1.40	1.52
1	AA	864	U	C3'-C2'	-9.62	1.38	1.52
17	AR	164	ASP	N-CA	-9.25	1.34	1.46
1	AA	1520	U	C4'-C3'	-9.10	1.38	1.52
13	AN	16	LYS	CA-CB	8.57	1.70	1.53
13	AN	15	GLY	C-N	7.99	1.44	1.33
19	A7	72	C	C5'-C4'	7.86	1.63	1.51
1	AA	864	U	C4'-C3'	7.72	1.64	1.53
19	A7	53	G	C2'-O2'	-7.59	1.31	1.42
19	A7	76	A	C5'-C4'	7.27	1.62	1.51
1	AA	1635	C	C5'-C4'	7.06	1.61	1.51
7	AH	61	ILE	CA-CB	6.96	1.68	1.55
19	A7	74	C	P-O5'	6.83	1.70	1.59
19	A7	34	OMG	O3'-P	-6.72	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	864	U	O3'-P	-6.66	1.51	1.61
1	AA	1547	C	C3'-O3'	-6.58	1.33	1.43
1	AA	1519	G	C3'-O3'	-6.40	1.33	1.43
19	A7	12	U	C4'-O4'	-6.07	1.36	1.45
1	AA	1520	U	C3'-O3'	-6.07	1.33	1.42
1	AA	857	U	C5'-C4'	5.96	1.60	1.51
1	AA	1584	A	C5'-C4'	5.94	1.60	1.51
1	AA	1635	C	O5'-C5'	5.91	1.51	1.42
17	AR	168	THR	CA-C	-5.85	1.45	1.52
19	A7	71	G	C5'-C4'	5.84	1.60	1.51
19	A7	41	U	C2'-O2'	5.79	1.51	1.42
17	AR	162	ALA	CA-C	-5.77	1.46	1.53
19	A7	47	U	C1'-N1	5.75	1.57	1.48
1	AA	858	G	N3-C4	5.74	1.47	1.35
7	AH	61	ILE	CB-CG1	5.69	1.64	1.53
1	AA	864	U	O5'-C5'	5.68	1.51	1.42
1	AA	1547	C	O3'-P	-5.66	1.52	1.61
19	A7	41	U	P-O5'	5.54	1.68	1.59
18	AT	79	LEU	N-CA	5.50	1.56	1.46
19	A7	52	U	P-O5'	5.50	1.68	1.59
1	AA	1583	U	C5'-C4'	5.45	1.59	1.51
19	A7	4	G	C4'-O4'	-5.44	1.37	1.45
1	AA	1521	G	N3-C4	5.42	1.46	1.35
30	BF	85	PHE	C-N	5.40	1.36	1.33
1	AA	1520	U	O3'-P	-5.32	1.53	1.61
19	A7	59	U	O3'-P	-5.31	1.53	1.61
1	AA	1519	G	C4'-C3'	5.25	1.61	1.53
19	A7	69	U	O3'-P	-5.21	1.53	1.61
19	A7	28	C	C2'-O2'	-5.21	1.34	1.42
1	AA	1516	C	P-O5'	-5.14	1.52	1.59
1	AA	1521	G	C5'-C4'	5.14	1.59	1.51
19	A7	69	U	O4'-C1'	5.10	1.49	1.41
1	AA	859	A	O5'-C5'	5.09	1.50	1.42
8	AI	127	LYS	C-N	5.02	1.40	1.33
13	AN	30	LEU	CA-C	-5.02	1.50	1.53

All (761) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	864	U	P-O3'-C3'	-35.57	66.85	120.20
1	AA	1519	G	O3'-P-O5'	30.05	149.08	104.00
1	AA	1520	U	O3'-P-O5'	29.37	148.06	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1545	A	O5'-P-OP1	-25.95	30.14	108.00
1	AA	1520	U	C4'-C3'-O3'	-25.52	74.72	113.00
17	AR	163	ASP	CA-C-N	-25.50	89.69	122.84
17	AR	163	ASP	C-N-CA	-25.50	89.69	122.84
37	BM	148	LYS	O-C-N	-25.00	89.34	122.59
1	AA	1520	U	C2'-C3'-O3'	-23.27	78.80	113.70
18	AT	78	LYS	CA-C-O	-23.00	91.95	119.78
7	AH	32	LYS	CA-C-O	-20.82	95.77	121.58
1	AA	1635	C	C2'-C3'-O3'	18.25	136.87	109.50
37	BM	169	ALA	O-C-N	-18.11	94.02	123.00
1	AA	1520	U	C1'-C2'-O2'	17.39	134.49	108.40
1	AA	858	G	O4'-C4'-C3'	-17.05	86.95	104.00
1	AA	1579	C	P-O3'-C3'	17.00	145.70	120.20
1	AA	1547	C	P-O3'-C3'	-16.70	95.16	120.20
1	AA	1636	G	C2'-C3'-O3'	16.61	138.62	113.70
13	AN	15	GLY	CA-C-N	16.39	151.21	121.70
13	AN	15	GLY	C-N-CA	16.39	151.21	121.70
1	AA	1547	C	C4'-C3'-C2'	16.08	118.68	102.60
1	AA	1212	C	O3'-P-O5'	15.26	126.89	104.00
1	AA	1547	C	C2'-C3'-O3'	-15.06	86.91	109.50
1	AA	865	A	P-O3'-C3'	-14.83	97.95	120.20
1	AA	856	A	P-O3'-C3'	14.59	142.08	120.20
1	AA	1520	U	P-O3'-C3'	-14.27	98.80	120.20
1	AA	858	G	C1'-O4'-C4'	-13.94	95.96	109.90
1	AA	1521	G	O4'-C4'-C3'	-13.45	92.65	106.10
1	AA	1535	C	P-O3'-C3'	13.28	140.12	120.20
1	AA	865	A	O3'-P-O5'	13.21	123.82	104.00
1	AA	852	C	P-O3'-C3'	13.21	140.01	120.20
1	AA	1196	G	P-O3'-C3'	12.85	139.48	120.20
1	AA	1547	C	C1'-C2'-O2'	12.75	130.92	111.80
1	AA	1635	C	P-O3'-C3'	-12.74	101.09	120.20
13	AN	16	LYS	N-CA-CB	12.63	131.97	110.50
1	AA	1546	G	C2'-C3'-O3'	-12.63	94.76	113.70
53	B5	3143	C	P-O3'-C3'	12.61	139.12	120.20
1	AA	748	U	P-O3'-C3'	12.49	138.94	120.20
1	AA	1549	U	C1'-C2'-O2'	12.44	130.46	111.80
1	AA	1543	A	P-O3'-C3'	-12.44	101.54	120.20
53	B5	2787	G	P-O3'-C3'	12.38	138.77	120.20
1	AA	1520	U	C3'-C2'-C1'	-12.31	88.99	101.30
1	AA	1318	A	P-O3'-C3'	12.08	138.33	120.20
1	AA	1521	G	P-O3'-C3'	-11.91	102.33	120.20
1	AA	652	G	P-O3'-C3'	11.91	138.06	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1551	G	C2'-C3'-O3'	-11.76	96.06	113.70
52	B4	152	G	P-O3'-C3'	11.67	137.70	120.20
1	AA	866	G	C1'-C2'-O2'	11.64	125.86	108.40
53	B5	1582	C	P-O3'-C3'	11.46	137.39	120.20
53	B5	475	G	P-O3'-C3'	11.38	137.26	120.20
53	B5	1163	A	P-O3'-C3'	11.32	137.18	120.20
53	B5	1302	A	P-O3'-C3'	11.29	137.13	120.20
52	B4	19	C	P-O3'-C3'	11.28	137.13	120.20
53	B5	638	C	P-O3'-C3'	11.27	137.10	120.20
7	AH	86	ILE	N-CA-C	-11.23	102.80	111.90
1	AA	1516	C	O5'-P-OP2	-11.22	74.33	108.00
1	AA	858	G	C5'-C4'-C3'	11.22	132.83	116.00
53	B5	239	G	P-O3'-C3'	11.21	137.01	120.20
53	B5	712	G	P-O3'-C3'	11.15	136.92	120.20
1	AA	867	G	C2'-C3'-O3'	-11.13	97.01	113.70
1	AA	1629	A	P-O3'-C3'	-11.07	103.59	120.20
1	AA	1560	G	P-O3'-C3'	10.98	136.67	120.20
53	B5	3160	U	P-O3'-C3'	10.97	136.65	120.20
53	B5	1590	G	P-O3'-C3'	10.96	136.63	120.20
53	B5	2571	U	P-O3'-C3'	10.92	136.59	120.20
53	B5	1737	U	P-O3'-C3'	10.90	136.55	120.20
53	B5	1626	U	P-O3'-C3'	10.89	136.54	120.20
1	AA	1098	G	P-O3'-C3'	10.87	136.50	120.20
1	AA	1488	C	P-O3'-C3'	10.83	136.44	120.20
1	AA	1639	C	P-O3'-C3'	10.82	136.42	120.20
1	AA	1055	U	P-O3'-C3'	10.81	136.42	120.20
1	AA	229	U	P-O3'-C3'	10.81	136.41	120.20
51	B3	23	A	P-O3'-C3'	10.81	136.41	120.20
1	AA	1675	C	P-O3'-C3'	10.79	136.39	120.20
1	AA	1429	U	P-O3'-C3'	10.70	136.26	120.20
1	AA	1759	U	P-O3'-C3'	10.66	136.19	120.20
53	B5	3384	U	P-O3'-C3'	10.64	136.17	120.20
1	AA	1478	G	P-O3'-C3'	10.61	136.11	120.20
17	AR	164	ASP	CB-CA-C	10.60	127.74	110.78
1	AA	1518	U	C1'-C2'-O2'	10.60	124.29	108.40
1	AA	1133	U	P-O3'-C3'	10.59	136.09	120.20
53	B5	3083	G	P-O3'-C3'	10.56	136.04	120.20
53	B5	3219	U	P-O3'-C3'	10.55	136.03	120.20
1	AA	759	U	P-O3'-C3'	10.53	136.00	120.20
19	A7	53	G	O4'-C4'-C3'	10.51	114.51	104.00
1	AA	212	U	P-O3'-C3'	10.50	135.95	120.20
1	AA	864	U	N1-C1'-C2'	-10.50	98.25	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	B5	2988	C	P-O3'-C3'	10.48	135.93	120.20
53	B5	1033	U	P-O3'-C3'	10.46	135.90	120.20
53	B5	3049	A	P-O3'-C3'	10.45	135.88	120.20
1	AA	1522	A	C1'-C2'-O2'	10.39	123.99	108.40
1	AA	1281	C	P-O3'-C3'	10.39	135.78	120.20
53	B5	2913	C	P-O3'-C3'	10.37	135.76	120.20
53	B5	801	A	P-O3'-C3'	10.36	135.74	120.20
1	AA	461	G	P-O3'-C3'	10.34	135.71	120.20
53	B5	2459	A	P-O3'-C3'	10.29	135.63	120.20
1	AA	66	U	P-O3'-C3'	10.27	135.61	120.20
1	AA	770	A	P-O3'-C3'	10.23	135.55	120.20
1	AA	922	A	P-O3'-C3'	10.23	135.55	120.20
53	B5	2538	U	P-O3'-C3'	10.23	135.54	120.20
52	B4	102	U	P-O3'-C3'	10.21	135.52	120.20
37	BM	148	LYS	CA-C-N	-10.21	102.05	121.54
37	BM	148	LYS	C-N-CA	-10.21	102.05	121.54
53	B5	1084	A	P-O3'-C3'	10.20	135.50	120.20
1	AA	56	U	P-O3'-C3'	10.17	135.46	120.20
1	AA	199	G	P-O3'-C3'	10.16	135.44	120.20
1	AA	1216	C	P-O3'-C3'	10.16	135.43	120.20
53	B5	3138	U	P-O3'-C3'	10.15	135.43	120.20
1	AA	1520	U	P-O5'-C5'	-10.09	105.76	120.90
53	B5	215	G	P-O3'-C3'	10.04	135.26	120.20
1	AA	867	G	C1'-C2'-O2'	10.03	123.44	108.40
1	AA	365	G	P-O3'-C3'	10.01	135.22	120.20
1	AA	1552	U	C1'-C2'-O2'	10.01	123.42	108.40
53	B5	3141	A	P-O3'-C3'	9.99	135.19	120.20
1	AA	175	G	P-O3'-C3'	9.98	135.17	120.20
1	AA	1549	U	C2'-C3'-O3'	9.94	124.42	109.50
1	AA	1516	C	O5'-P-OP1	9.92	137.77	108.00
1	AA	1583	U	C4'-C3'-C2'	-9.91	92.69	102.60
1	AA	1550	U	C1'-C2'-O2'	9.89	126.64	111.80
51	B3	91	C	P-O3'-C3'	9.88	135.02	120.20
53	B5	1549	U	P-O3'-C3'	9.88	135.02	120.20
1	AA	1789	A	P-O3'-C3'	9.84	134.96	120.20
1	AA	1457	C	P-O3'-C3'	9.83	134.95	120.20
1	AA	1181	U	P-O3'-C3'	9.81	134.91	120.20
1	AA	797	G	P-O5'-C5'	-9.78	106.24	120.90
53	B5	2654	C	P-O3'-C3'	9.74	134.82	120.20
1	AA	438	A	P-O3'-C3'	9.71	134.77	120.20
53	B5	1390	A	P-O3'-C3'	9.68	134.72	120.20
1	AA	1779	A	P-O3'-C3'	9.67	134.71	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AN	16	LYS	CB-CA-C	-9.66	91.74	110.10
1	AA	1518	U	C2'-C3'-O3'	-9.65	99.23	113.70
1	AA	864	U	C4'-C3'-C2'	9.55	112.15	102.60
52	B4	69	U	P-O3'-C3'	9.54	134.51	120.20
1	AA	350	U	P-O3'-C3'	9.52	134.48	120.20
1	AA	866	G	C4'-C3'-C2'	9.47	112.07	102.60
1	AA	1520	U	OP2-P-O3'	-9.46	79.61	108.00
1	AA	865	A	C4'-C3'-O3'	9.44	127.16	113.00
53	B5	372	A	P-O3'-C3'	9.43	134.34	120.20
1	AA	1544	G	C1'-C2'-O2'	9.41	122.51	108.40
53	B5	1643	A	P-O3'-C3'	9.41	134.31	120.20
1	AA	1547	C	C3'-C2'-C1'	-9.40	92.10	101.50
1	AA	858	G	C2'-C3'-O3'	-9.39	99.61	113.70
1	AA	860	U	C1'-C2'-O2'	9.38	125.86	111.80
19	A7	64	A	C4'-C3'-C2'	-9.37	93.23	102.60
19	A7	66	A	C4'-C3'-C2'	-9.36	93.24	102.60
1	AA	1212	C	OP1-P-O3'	-9.35	79.96	108.00
1	AA	1520	U	OP1-P-O3'	-9.31	80.08	108.00
23	B8	43	LYS	CG-CD-CE	9.23	132.52	111.30
1	AA	1516	C	O5'-C5'-C4'	-9.22	97.68	111.50
7	AH	61	ILE	CA-CB-CG1	-9.20	94.77	110.40
17	AR	287	PRO	N-CA-C	-9.20	100.75	113.53
53	B5	134	U	P-O3'-C3'	9.17	133.95	120.20
1	AA	867	G	OP1-P-OP2	-9.16	92.11	119.60
18	AT	78	LYS	N-CA-C	9.16	124.57	113.12
53	B5	2177	G	P-O3'-C3'	9.16	133.94	120.20
53	B5	3330	A	P-O3'-C3'	9.15	133.93	120.20
1	AA	865	A	P-O5'-C5'	-9.14	107.19	120.90
19	A7	44	A	C5'-C4'-C3'	-9.13	102.30	116.00
52	B4	21	C	P-O3'-C3'	9.13	133.90	120.20
53	B5	2314	U	P-O3'-C3'	9.07	133.80	120.20
1	AA	1547	C	O4'-C4'-C3'	-9.06	97.04	106.10
53	B5	2373	A	P-O3'-C3'	9.01	133.72	120.20
1	AA	1212	C	OP2-P-O3'	-9.00	81.00	108.00
1	AA	796	A	C1'-C2'-O2'	9.00	121.89	108.40
1	AA	1265	U	P-O3'-C3'	8.99	133.69	120.20
1	AA	1636	G	C4'-C3'-C2'	-8.98	93.62	102.60
1	AA	860	U	C2'-C3'-O3'	-8.95	96.07	109.50
19	A7	11	C	O3'-P-O5'	8.94	117.41	104.00
53	B5	2474	G	P-O3'-C3'	8.94	133.60	120.20
8	AI	127	LYS	CA-C-O	-8.91	111.04	121.11
1	AA	797	G	C2'-C3'-O3'	-8.89	100.36	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	G	OP1-P-O3'	-8.88	81.38	108.00
1	AA	865	A	C1'-C2'-O2'	8.87	121.70	108.40
53	B5	2520	A	P-O3'-C3'	8.85	133.48	120.20
53	B5	620	U	P-O3'-C3'	8.83	133.44	120.20
17	AR	241	PHE	CA-CB-CG	-8.76	105.04	113.80
1	AA	1520	U	C4'-C3'-C2'	8.76	111.36	102.60
23	B8	43	LYS	CB-CG-CD	8.73	131.38	111.30
1	AA	444	C	P-O3'-C3'	8.68	133.22	120.20
1	AA	1213	A	O5'-P-OP1	-8.66	82.01	108.00
1	AA	1516	C	C1'-C2'-O2'	8.63	121.35	108.40
1	AA	857	U	O5'-C5'-C4'	8.61	124.41	111.50
53	B5	277	G	P-O3'-C3'	8.61	133.11	120.20
53	B5	119	U	P-O3'-C3'	8.53	132.99	120.20
53	B5	1818	U	P-O3'-C3'	8.52	132.97	120.20
53	B5	3385	U	P-O3'-C3'	8.52	132.97	120.20
1	AA	1552	U	C2'-C3'-O3'	-8.51	100.94	113.70
1	AA	867	G	C4'-C3'-C2'	8.47	111.07	102.60
1	AA	1159	U	P-O3'-C3'	8.47	132.90	120.20
1	AA	1213	A	O5'-P-OP2	-8.45	82.65	108.00
1	AA	1654	U	P-O3'-C3'	8.45	132.88	120.20
53	B5	2796	G	P-O3'-C3'	8.38	132.77	120.20
1	AA	1520	U	O4'-C4'-C3'	-8.36	95.64	104.00
19	A7	27	C	C4'-C3'-C2'	-8.35	94.25	102.60
1	AA	792	U	C1'-C2'-O2'	8.32	120.88	108.40
17	AR	77	GLY	N-CA-C	-8.28	103.90	115.32
1	AA	1638	C	P-O5'-C5'	-8.24	108.54	120.90
1	AA	858	G	O4'-C1'-N9	8.24	120.86	108.50
53	B5	1079	A	P-O3'-C3'	8.21	132.51	120.20
19	A7	35	A	C1'-C2'-O2'	-8.17	96.14	108.40
1	AA	860	U	C4'-C3'-C2'	8.12	110.72	102.60
1	AA	859	A	C1'-C2'-O2'	8.11	123.96	111.80
19	A7	44	A	C5'-C4'-O4'	8.08	121.92	109.80
53	B5	3113	A	P-O3'-C3'	8.06	132.29	120.20
1	AA	1519	G	P-O3'-C3'	8.03	132.24	120.20
1	AA	867	G	P-O3'-C3'	-8.00	108.19	120.20
53	B5	3039	C	P-O3'-C3'	7.95	132.13	120.20
1	AA	1134	A	P-O3'-C3'	7.93	132.09	120.20
1	AA	1517	U	C1'-C2'-O2'	7.92	120.29	108.40
53	B5	621	A	P-O3'-C3'	7.90	132.05	120.20
53	B5	2705	A	P-O3'-C3'	7.86	131.99	120.20
19	A7	23	A	C3'-C2'-C1'	7.85	109.15	101.30
53	B5	354	U	P-O3'-C3'	7.85	131.98	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1584	A	O4'-C4'-C3'	-7.84	96.16	104.00
1	AA	1636	G	P-O3'-C3'	7.83	131.94	120.20
1	AA	1518	U	O4'-C4'-C3'	-7.80	96.20	104.00
17	AR	288	HIS	CA-CB-CG	7.79	121.59	113.80
1	AA	856	A	O3'-P-O5'	7.78	115.68	104.00
1	AA	1553	A	C1'-C2'-O2'	7.77	120.05	108.40
1	AA	1631	A	C1'-C2'-O2'	7.76	123.43	111.80
53	B5	1200	A	P-O3'-C3'	7.75	131.83	120.20
17	AR	163	ASP	CA-C-O	7.73	129.82	120.62
1	AA	1548	A	O5'-P-OP1	7.70	133.80	110.70
1	AA	1636	G	O4'-C4'-C3'	7.70	111.70	104.00
1	AA	864	U	O4'-C1'-C2'	7.68	113.48	105.80
1	AA	1521	G	C2'-C3'-O3'	7.68	121.02	109.50
1	AA	1637	C	C1'-C2'-O2'	7.67	119.91	108.40
19	A7	5	A	C4'-C3'-C2'	-7.67	94.93	102.60
27	BC	252	ILE	N-CA-C	-7.66	105.57	111.62
1	AA	916	U	P-O3'-C3'	7.65	131.68	120.20
8	AI	126	PRO	CA-C-N	7.64	134.81	122.81
8	AI	126	PRO	C-N-CA	7.64	134.81	122.81
1	AA	1655	U	P-O3'-C3'	7.64	131.66	120.20
7	AH	37	PHE	CA-CB-CG	7.62	121.42	113.80
1	AA	1546	G	C4'-C3'-C2'	7.62	110.22	102.60
1	AA	1515	U	O3'-P-O5'	-7.60	92.60	104.00
1	AA	1549	U	C3'-C2'-C1'	-7.59	93.91	101.50
37	BM	85	ARG	N-CA-C	-7.59	103.64	113.12
53	B5	742	G	P-O3'-C3'	7.57	131.56	120.20
52	B4	57	C	P-O3'-C3'	7.55	131.53	120.20
29	BE	187	THR	CA-C-N	7.53	135.26	121.70
29	BE	187	THR	C-N-CA	7.53	135.26	121.70
53	B5	1235	U	P-O3'-C3'	7.53	131.50	120.20
17	AR	164	ASP	N-CA-C	-7.52	95.33	108.20
1	AA	1517	U	P-O3'-C3'	-7.51	108.93	120.20
19	A7	24	G	C2'-C3'-O3'	-7.51	102.44	113.70
1	AA	1547	C	O3'-P-O5'	-7.50	92.75	104.00
1	AA	1518	U	P-O3'-C3'	-7.43	109.06	120.20
1	AA	796	A	C2'-C3'-O3'	7.42	124.84	113.70
19	A7	73	A	C4'-C3'-C2'	-7.42	95.18	102.60
1	AA	798	C	C2'-C3'-O3'	7.40	124.80	113.70
17	AR	286	GLU	CB-CA-C	-7.40	97.97	109.22
53	B5	3143	C	C2'-C3'-O3'	7.39	120.59	109.50
53	B5	250	U	P-O3'-C3'	7.39	131.28	120.20
19	A7	43	G	C4'-C3'-C2'	-7.39	95.21	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A7	41	U	C4'-C3'-C2'	-7.38	95.22	102.60
19	A7	12	U	O4'-C4'-C3'	7.36	111.36	104.00
1	AA	1551	G	C1'-C2'-O2'	7.35	119.42	108.40
19	A7	20	G	N9-C1'-C2'	7.34	123.01	112.00
37	BM	183	ALA	N-CA-C	-7.34	103.28	111.28
1	AA	1515	U	P-O3'-C3'	-7.33	109.21	120.20
17	AR	284	ALA	CA-C-N	-7.32	107.56	121.54
17	AR	284	ALA	C-N-CA	-7.32	107.56	121.54
17	AR	285	ALA	CA-C-N	7.30	137.38	123.65
17	AR	285	ALA	C-N-CA	7.30	137.38	123.65
19	A7	5	A	O4'-C4'-C3'	7.30	111.31	104.00
1	AA	1630	C	C1'-C2'-O2'	7.29	119.33	108.40
1	AA	444	C	C2'-C3'-O3'	7.25	120.37	109.50
1	AA	1545	A	C2'-C3'-O3'	7.24	124.56	113.70
53	B5	3045	G	P-O3'-C3'	7.23	131.05	120.20
19	A7	62	A	C5'-C4'-C3'	-7.22	105.17	116.00
17	AR	238	ASP	CA-CB-CG	-7.21	105.39	112.60
45	BU	115	ARG	CA-C-N	7.18	130.22	120.38
45	BU	115	ARG	C-N-CA	7.18	130.22	120.38
53	B5	251	G	P-O3'-C3'	7.17	130.96	120.20
52	B4	68	G	P-O3'-C3'	7.13	130.90	120.20
1	AA	1516	C	C4'-C3'-C2'	7.10	109.70	102.60
1	AA	1213	A	OP1-P-OP2	7.09	140.88	119.60
1	AA	866	G	O5'-C5'-C4'	7.05	122.08	111.50
19	A7	57	G	C3'-C2'-C1'	7.05	108.35	101.30
1	AA	1634	C	P-O3'-C3'	-7.05	109.62	120.20
19	A7	43	G	C2'-C3'-O3'	-7.05	103.12	113.70
53	B5	1648	A	P-O3'-C3'	7.05	130.77	120.20
19	A7	66	A	O4'-C4'-C3'	7.04	111.04	104.00
1	AA	857	U	C5'-C4'-C3'	7.04	126.56	116.00
1	AA	866	G	P-O3'-C3'	-6.99	109.71	120.20
19	A7	47	U	O4'-C1'-N1	6.99	118.99	108.50
19	A7	69	U	O5'-C5'-C4'	6.98	121.98	111.50
1	AA	1553	A	P-O5'-C5'	-6.98	110.43	120.90
18	AT	27	LYS	N-CA-C	-6.97	105.39	114.04
53	B5	711	A	P-O3'-C3'	6.97	130.66	120.20
1	AA	858	G	C1'-C2'-O2'	-6.97	97.95	108.40
7	AH	27	ILE	CB-CA-C	6.94	121.10	110.82
1	AA	1518	U	OP1-P-OP2	-6.93	98.80	119.60
34	BJ	3	THR	N-CA-C	-6.93	102.95	112.03
1	AA	400	A	P-O3'-C3'	6.92	130.57	120.20
19	A7	72	C	O3'-P-O5'	6.90	114.35	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	B5	977	U	P-O3'-C3'	6.89	130.53	120.20
1	AA	1637	C	P-O3'-C3'	-6.88	109.89	120.20
19	A7	13	C	C1'-C2'-O2'	-6.86	98.11	108.40
33	BI	39	LYS	N-CA-C	-6.85	103.56	112.68
23	B8	105	VAL	N-CA-C	-6.85	106.82	113.53
10	AK	91	THR	N-CA-C	-6.84	106.13	114.75
1	AA	400	A	C2'-C3'-O3'	6.83	119.75	109.50
1	AA	867	G	O4'-C4'-C3'	-6.83	97.17	104.00
43	BS	37	ALA	CA-C-N	6.83	129.43	120.28
43	BS	37	ALA	C-N-CA	6.83	129.43	120.28
29	BE	214	ASP	N-CA-C	6.81	120.50	109.40
19	A7	47	U	C1'-O4'-C4'	-6.80	103.10	109.90
1	AA	1518	U	C4'-C3'-C2'	6.78	109.38	102.60
1	AA	1552	U	C4'-C3'-C2'	6.75	109.35	102.60
7	AH	31	SER	N-CA-C	-6.75	100.73	108.49
1	AA	1517	U	O4'-C4'-C3'	-6.75	97.25	104.00
1	AA	1638	C	C1'-C2'-O2'	6.72	118.47	108.40
8	AI	109	PHE	CA-CB-CG	-6.70	107.10	113.80
1	AA	868	G	C1'-C2'-O2'	6.69	118.44	108.40
1	AA	1547	C	C4'-C3'-O3'	-6.69	99.36	109.40
32	BH	40	HIS	CA-CB-CG	6.69	120.49	113.80
29	BE	224	LYS	N-CA-CB	6.68	121.78	110.49
46	BV	80	LEU	CA-C-N	6.66	125.66	120.33
46	BV	80	LEU	C-N-CA	6.66	125.66	120.33
1	AA	866	G	O5'-P-OP2	-6.65	88.05	108.00
53	B5	2651	G	P-O3'-C3'	6.64	130.17	120.20
13	AN	16	LYS	N-CA-C	6.61	129.49	111.00
19	A7	36	A	C4'-C3'-C2'	-6.60	96.00	102.60
19	A7	63	C	C1'-O4'-C4'	-6.59	103.31	109.90
1	AA	312	A	P-O3'-C3'	6.58	130.07	120.20
29	BE	84	PRO	CA-C-N	6.57	129.38	120.38
29	BE	84	PRO	C-N-CA	6.57	129.38	120.38
29	BE	94	ASN	CA-C-N	6.54	129.34	120.44
29	BE	94	ASN	C-N-CA	6.54	129.34	120.44
53	B5	494	G	P-O3'-C3'	6.54	130.01	120.20
1	AA	47	A	P-O3'-C3'	6.53	129.99	120.20
1	AA	864	U	O3'-P-O5'	6.52	113.78	104.00
32	BH	138	THR	N-CA-C	-6.49	103.43	112.12
5	AE	144	TRP	N-CA-C	-6.48	104.06	112.68
8	AI	97	VAL	CB-CA-C	6.46	121.88	111.29
17	AR	279	ALA	N-CA-C	6.44	118.09	111.14
33	BI	135	ILE	N-CA-C	-6.44	105.55	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A7	5	A	O3'-P-O5'	6.44	113.66	104.00
25	BA	209	SER	N-CA-C	-6.43	103.50	112.12
24	B9	35	ALA	N-CA-C	6.41	118.83	110.43
1	AA	797	G	O4'-C4'-C3'	-6.41	97.59	104.00
1	AA	1522	A	C2'-C3'-O3'	-6.41	104.09	113.70
1	AA	865	A	O5'-P-OP2	-6.39	88.82	108.00
19	A7	13	C	C3'-C2'-C1'	6.39	107.69	101.30
1	AA	1635	C	O3'-P-O5'	6.38	113.57	104.00
53	B5	3332	U	P-O3'-C3'	6.37	129.75	120.20
53	B5	133	U	P-O3'-C3'	6.37	129.75	120.20
7	AH	31	SER	N-CA-CB	6.37	116.00	109.51
19	A7	68	U	C4'-C3'-C2'	-6.36	96.24	102.60
26	BB	206	PRO	CA-C-N	6.36	128.48	120.72
26	BB	206	PRO	C-N-CA	6.36	128.48	120.72
53	B5	1947	G	P-O3'-C3'	6.34	129.71	120.20
1	AA	799	A	C1'-C2'-O2'	6.32	117.88	108.40
1	AA	1550	U	C4'-C3'-C2'	6.31	108.91	102.60
23	B8	91	GLU	O-C-N	-6.31	117.67	121.71
53	B5	2477	G	C1'-C2'-O2'	6.30	117.86	108.40
26	BB	156	LYS	N-CA-CB	6.30	121.13	110.49
19	A7	21	A	C5'-C4'-O4'	6.30	119.24	109.80
1	AA	501	U	P-O3'-C3'	6.29	129.64	120.20
1	AA	1545	A	C1'-C2'-O2'	6.29	117.83	108.40
19	A7	18	G	C4'-C3'-C2'	-6.28	96.33	102.60
53	B5	1900	A	P-O3'-C3'	6.28	129.61	120.20
18	AT	95	ASP	CA-C-N	6.27	128.59	120.44
18	AT	95	ASP	C-N-CA	6.27	128.59	120.44
47	BW	25	PHE	CA-CB-CG	-6.27	107.53	113.80
1	AA	1551	G	OP1-P-OP2	-6.27	100.80	119.60
1	AA	1550	U	C3'-C2'-C1'	-6.27	95.23	101.50
19	A7	21	A	O4'-C1'-N9	6.26	117.89	108.50
17	AR	310	ILE	CA-C-N	-6.26	113.86	122.93
17	AR	310	ILE	C-N-CA	-6.26	113.86	122.93
29	BE	218	ARG	N-CA-C	6.25	118.57	109.07
7	AH	8	ALA	CA-C-N	6.25	128.65	120.28
7	AH	8	ALA	C-N-CA	6.25	128.65	120.28
53	B5	2382	G	P-O3'-C3'	6.24	129.56	120.20
19	A7	62	A	C3'-C2'-O2'	6.24	120.06	110.70
36	BL	41	ARG	N-CA-C	-6.24	102.23	110.40
17	AR	207	ASP	CA-CB-CG	-6.24	106.36	112.60
19	A7	28	C	O4'-C1'-N1	6.24	117.85	108.50
19	A7	70	C	O3'-P-O5'	-6.23	94.65	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	307	G	P-O3'-C3'	6.23	129.55	120.20
1	AA	1612	A	P-O5'-C5'	-6.21	111.59	120.90
6	AG	164	PRO	CA-N-CD	-6.21	103.31	112.00
3	AC	42	THR	N-CA-C	-6.20	102.33	110.39
36	BL	141	ALA	CA-C-N	6.19	129.21	120.42
36	BL	141	ALA	C-N-CA	6.19	129.21	120.42
28	BD	220	ARG	N-CA-C	-6.18	105.86	113.41
1	AA	1546	G	C1'-C2'-O2'	6.17	117.66	108.40
42	BR	98	ASN	CA-CB-CG	-6.15	106.45	112.60
4	AD	7	THR	CA-C-N	6.15	132.77	121.70
4	AD	7	THR	C-N-CA	6.15	132.77	121.70
50	BZ	46	LYS	N-CA-CB	6.14	120.88	110.49
1	AA	867	G	C3'-C2'-C1'	-6.14	95.16	101.30
36	BL	6	TYR	N-CA-C	-6.14	105.48	114.39
53	B5	1900	A	C2'-C3'-O3'	6.14	118.70	109.50
1	AA	1551	G	O4'-C4'-C3'	-6.12	97.88	104.00
29	BE	231	ILE	N-CA-C	-6.12	106.94	111.90
8	AI	138	PHE	CA-CB-CG	6.12	119.92	113.80
53	B5	2295	A	P-O5'-C5'	-6.12	111.72	120.90
19	A7	75	C	C4'-C3'-C2'	-6.12	96.48	102.60
19	A7	15	G	O4'-C4'-C3'	6.11	110.11	104.00
32	BH	121	LYS	N-CA-C	-6.11	105.66	113.23
1	AA	866	G	O4'-C4'-C3'	-6.10	97.90	104.00
53	B5	2569	A	P-O3'-C3'	6.10	129.34	120.20
53	B5	131	C	P-O3'-C3'	6.09	129.34	120.20
1	AA	1612	A	O5'-C5'-C4'	6.09	120.63	111.50
1	AA	1549	U	O4'-C4'-C3'	-6.08	100.02	106.10
52	B4	60	U	C5'-C4'-C3'	6.08	125.11	116.00
1	AA	1240	A	C2'-C3'-O3'	6.07	118.61	109.50
1	AA	864	U	C2'-C3'-O3'	-6.07	100.40	109.50
21	B1	29	LEU	N-CA-C	-6.07	106.42	113.88
29	BE	192	PRO	N-CA-C	6.07	120.16	110.21
31	BG	108	ARG	CA-C-N	6.07	128.33	120.44
31	BG	108	ARG	C-N-CA	6.07	128.33	120.44
1	AA	857	U	P-O3'-C3'	-6.06	111.11	120.20
1	AA	867	G	O5'-P-OP1	6.04	126.12	108.00
1	AA	1630	C	P-O3'-C3'	-6.03	111.16	120.20
17	AR	234	LEU	CB-CA-C	-6.02	103.53	111.42
14	AO	129	TYR	CA-C-N	6.02	128.26	120.44
14	AO	129	TYR	C-N-CA	6.02	128.26	120.44
19	A7	32	OMC	O3'-P-O5'	6.01	113.02	104.00
17	AR	183	LEU	N-CA-CB	6.01	120.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	312	A	C2'-C3'-O3'	6.00	118.51	109.50
14	AO	113	PHE	CA-C-N	6.00	128.92	120.28
14	AO	113	PHE	C-N-CA	6.00	128.92	120.28
1	AA	1789	A	C2'-C3'-O3'	6.00	118.50	109.50
1	AA	860	U	C3'-C2'-C1'	-6.00	95.50	101.50
1	AA	1516	C	O4'-C4'-C3'	-6.00	98.00	104.00
17	AR	256	THR	CA-C-N	5.99	128.91	120.28
17	AR	256	THR	C-N-CA	5.99	128.91	120.28
13	AN	41	GLN	N-CA-C	5.99	117.48	111.07
1	AA	1550	U	O4'-C4'-C3'	-5.98	100.12	106.10
53	B5	2826	U	P-O3'-C3'	5.97	129.15	120.20
8	AI	35	PRO	CA-C-N	5.96	128.62	120.46
8	AI	35	PRO	C-N-CA	5.96	128.62	120.46
53	B5	1079	A	C2'-C3'-O3'	5.96	118.43	109.50
19	A7	21	A	N9-C1'-C2'	-5.94	103.08	112.00
19	A7	33	U	O4'-C1'-N1	5.94	117.41	108.50
19	A7	60	C	C3'-C2'-O2'	-5.91	105.74	114.60
9	AJ	91	ILE	CA-CB-CG1	5.89	120.41	110.40
1	AA	864	U	C1'-C2'-O2'	5.88	120.62	111.80
6	AG	164	PRO	N-CA-C	5.88	124.59	112.47
50	BZ	19	LYS	CA-C-N	5.88	129.19	120.90
50	BZ	19	LYS	C-N-CA	5.88	129.19	120.90
8	AI	96	TYR	N-CA-C	-5.87	104.24	111.40
1	AA	1522	A	O4'-C4'-C3'	-5.87	98.13	104.00
39	BO	107	THR	CA-C-N	5.86	128.13	120.28
39	BO	107	THR	C-N-CA	5.86	128.13	120.28
19	A7	13	C	C5'-C4'-O4'	5.85	118.57	109.80
1	AA	1520	U	O4'-C1'-N1	-5.85	99.73	108.50
8	AI	137	ARG	N-CA-C	5.84	118.25	110.53
19	A7	60	C	C4'-C3'-C2'	5.84	108.44	102.60
2	AB	10	THR	N-CA-C	-5.84	102.80	110.39
17	AR	249	ARG	CA-C-N	5.84	131.86	120.99
17	AR	249	ARG	C-N-CA	5.84	131.86	120.99
9	AJ	72	ASN	N-CA-CB	5.84	120.35	110.49
19	A7	11	C	C4'-C3'-C2'	-5.83	96.77	102.60
19	A7	56	C	O4'-C4'-C3'	5.83	109.83	104.00
35	BK	74	VAL	N-CA-C	-5.83	101.08	107.73
1	AA	798	C	C1'-C2'-O2'	5.83	117.14	108.40
19	A7	2	C	C3'-C2'-O2'	5.83	119.44	110.70
17	AR	9	LEU	CA-C-N	5.83	128.09	120.28
17	AR	9	LEU	C-N-CA	5.83	128.09	120.28
40	BP	109	TYR	N-CA-C	-5.82	105.43	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A7	3	G	O5'-C5'-C4'	-5.82	102.77	111.50
31	BG	168	ALA	CA-C-N	5.82	128.00	120.44
31	BG	168	ALA	C-N-CA	5.82	128.00	120.44
29	BE	94	ASN	CA-CB-CG	5.82	118.42	112.60
43	BS	34	SER	CA-C-N	5.81	128.86	120.38
43	BS	34	SER	C-N-CA	5.81	128.86	120.38
1	AA	859	A	C3'-C2'-C1'	-5.80	95.70	101.50
17	AR	302	PHE	CA-CB-CG	-5.80	108.00	113.80
31	BG	214	LEU	N-CA-C	-5.80	105.88	113.12
8	AI	76	SER	CA-C-N	5.79	128.04	120.28
8	AI	76	SER	C-N-CA	5.79	128.04	120.28
1	AA	859	A	O4'-C4'-C3'	-5.79	100.31	106.10
19	A7	45	G	C5'-C4'-C3'	-5.79	107.32	116.00
48	BX	5	LYS	CA-C-N	5.79	128.29	120.65
48	BX	5	LYS	C-N-CA	5.79	128.29	120.65
19	A7	22	G	C5'-C4'-O4'	5.78	118.47	109.80
19	A7	7	U	O4'-C1'-N1	5.77	116.86	108.20
4	AD	150	LEU	CA-C-N	5.76	130.35	121.19
4	AD	150	LEU	C-N-CA	5.76	130.35	121.19
1	AA	1522	A	P-O3'-C3'	-5.75	111.57	120.20
53	B5	2651	G	C2'-C3'-O3'	5.75	118.12	109.50
17	AR	286	GLU	CA-CB-CG	5.75	125.59	114.10
36	BL	180	PHE	N-CA-C	-5.75	106.25	113.72
36	BL	139	HIS	CA-CB-CG	5.74	119.54	113.80
33	BI	159	PHE	CA-CB-CG	5.74	119.54	113.80
53	B5	2918	G	P-O3'-C3'	5.74	128.81	120.20
53	B5	1162	U	P-O5'-C5'	-5.74	112.30	120.90
29	BE	93	THR	N-CA-C	5.73	116.78	107.32
36	BL	149	ASN	CA-C-N	5.73	128.23	120.38
36	BL	149	ASN	C-N-CA	5.73	128.23	120.38
1	AA	1517	U	OP1-P-OP2	-5.73	102.41	119.60
1	AA	1635	C	O5'-C5'-C4'	5.73	120.29	111.70
19	A7	1	G	C3'-C2'-O2'	5.72	119.28	110.70
1	AA	858	G	N9-C1'-C2'	5.72	120.58	112.00
51	B3	46	A	C5'-C4'-C3'	5.72	124.58	116.00
1	AA	1521	G	OP1-P-OP2	-5.71	102.46	119.60
1	AA	1633	A	C1'-O4'-C4'	-5.71	104.19	109.90
34	BJ	120	ILE	N-CA-C	-5.70	106.25	111.67
40	BP	111	ASP	CA-CB-CG	5.70	118.30	112.60
19	A7	20	G	O3'-P-O5'	-5.70	95.45	104.00
8	AI	142	TYR	CA-CB-CG	-5.69	103.66	113.90
19	A7	18	G	O4'-C4'-C3'	5.68	111.78	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	B5	1904	C	O4'-C1'-N1	5.68	117.02	108.50
9	AJ	111	GLY	N-CA-C	-5.68	107.15	113.79
1	AA	1632	C	P-O3'-C3'	-5.67	111.69	120.20
1	AA	47	A	C2'-C3'-O3'	5.67	118.00	109.50
1	AA	1635	C	C4'-C3'-C2'	-5.67	96.93	102.60
53	B5	1721	U	C2'-C3'-O3'	5.67	118.00	109.50
19	A7	1	G	C2'-C3'-O3'	-5.66	105.20	113.70
4	AD	95	TYR	CA-C-N	5.66	132.16	121.97
4	AD	95	TYR	C-N-CA	5.66	132.16	121.97
1	AA	1318	A	C2'-C3'-O3'	5.66	117.99	109.50
1	AA	1583	U	P-O3'-C3'	5.66	128.69	120.20
18	AT	49	ASP	CA-C-N	5.65	128.17	120.54
18	AT	49	ASP	C-N-CA	5.65	128.17	120.54
23	B8	91	GLU	N-CA-C	-5.65	99.74	108.55
19	A7	21	A	C5'-C4'-C3'	-5.64	107.54	116.00
4	AD	125	ALA	CA-C-N	5.63	127.82	120.28
4	AD	125	ALA	C-N-CA	5.63	127.82	120.28
1	AA	1553	A	OP1-P-OP2	-5.62	102.74	119.60
19	A7	31	A	O5'-C5'-C4'	-5.62	103.07	111.50
19	A7	66	A	O3'-P-O5'	-5.62	95.57	104.00
19	A7	18	G	C3'-C2'-C1'	5.61	107.11	101.50
29	BE	214	ASP	CA-C-N	5.61	129.62	121.26
29	BE	214	ASP	C-N-CA	5.61	129.62	121.26
1	AA	1521	G	O4'-C1'-N9	5.60	116.60	108.20
1	AA	1196	G	O4'-C4'-C3'	-5.60	98.40	104.00
20	B0	38	ILE	CB-CA-C	5.60	120.47	111.29
46	BV	81	ILE	O-C-N	-5.59	116.84	120.42
19	A7	70	C	C5'-C4'-O4'	5.59	118.19	109.80
1	AA	1521	G	P-O5'-C5'	-5.59	112.52	120.90
27	BC	326	GLY	N-CA-C	-5.58	105.40	111.21
6	AG	113	ILE	CA-C-N	5.57	127.69	120.56
6	AG	113	ILE	C-N-CA	5.57	127.69	120.56
38	BN	109	ALA	N-CA-C	5.57	117.79	111.11
19	A7	28	C	O3'-P-O5'	-5.56	95.66	104.00
19	A7	69	U	O4'-C1'-C2'	-5.56	102.04	107.60
4	AD	124	HIS	N-CA-C	-5.56	106.63	113.41
1	AA	1520	U	C5'-C4'-C3'	-5.55	107.67	116.00
19	A7	56	C	O4'-C1'-C2'	5.55	113.15	107.60
19	A7	53	G	C4'-C3'-C2'	-5.54	97.06	102.60
43	BS	47	ARG	N-CA-C	-5.54	104.69	112.12
17	AR	200	ASN	CA-CB-CG	-5.53	107.07	112.60
1	AA	1545	A	C4'-C3'-C2'	-5.52	97.08	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	B5	2839	G	P-O3'-C3'	5.52	128.48	120.20
29	BE	216	GLU	N-CA-C	5.52	122.55	110.80
5	AE	225	LEU	N-CA-C	-5.52	101.14	109.85
52	B4	69	U	P-O5'-C5'	-5.51	112.63	120.90
22	B2	48	THR	CA-C-O	-5.50	115.57	120.19
19	A7	35	A	O4'-C4'-C3'	5.50	109.50	104.00
30	BF	155	LYS	N-CA-C	-5.50	102.66	111.02
53	B5	2124	G	P-O3'-C3'	5.50	128.45	120.20
7	AH	32	LYS	N-CA-C	5.50	117.62	107.73
33	BI	101	LYS	CA-C-N	5.49	131.59	121.70
33	BI	101	LYS	C-N-CA	5.49	131.59	121.70
51	B3	45	A	P-O3'-C3'	5.48	128.43	120.20
1	AA	1612	A	C5'-C4'-O4'	5.47	118.01	109.80
19	A7	1	G	C5'-C4'-C3'	5.47	124.21	116.00
37	BM	140	LYS	CA-C-N	5.47	127.93	120.54
37	BM	140	LYS	C-N-CA	5.47	127.93	120.54
1	AA	858	G	O3'-P-O5'	5.47	112.20	104.00
53	B5	546	C	P-O3'-C3'	5.47	128.40	120.20
44	BT	135	ILE	N-CA-C	-5.46	106.48	111.67
45	BU	33	ALA	N-CA-C	-5.46	103.21	108.13
53	B5	439	C	O4'-C1'-N1	5.46	116.69	108.50
33	BI	109	ASP	CA-CB-CG	5.46	118.06	112.60
46	BV	40	HIS	CA-C-N	5.46	131.96	121.54
46	BV	40	HIS	C-N-CA	5.46	131.96	121.54
1	AA	1522	A	C3'-C2'-C1'	-5.45	95.85	101.30
53	B5	374	A	P-O3'-C3'	5.45	128.37	120.20
19	A7	9	A	O4'-C1'-N9	5.45	116.37	108.20
27	BC	278	ILE	CA-C-N	5.45	131.94	121.54
27	BC	278	ILE	C-N-CA	5.45	131.94	121.54
33	BI	147	VAL	N-CA-C	-5.45	108.54	113.71
1	AA	1133	U	C2'-C3'-O3'	5.44	121.86	113.70
53	B5	286	U	P-O3'-C3'	5.44	128.36	120.20
52	B4	136	G	P-O3'-C3'	5.44	128.35	120.20
1	AA	844	A	P-O3'-C3'	5.43	128.35	120.20
35	BK	117	ARG	N-CA-C	-5.43	106.38	114.64
53	B5	1810	A	P-O3'-C3'	5.43	128.34	120.20
19	A7	6	U	C4'-C3'-C2'	-5.43	97.17	102.60
1	AA	858	G	O4'-C1'-C2'	-5.42	102.17	107.60
1	AA	1522	A	C4'-C3'-C2'	5.42	108.02	102.60
1	AA	502	U	C5'-C4'-C3'	5.42	124.13	116.00
19	A7	63	C	C4'-C3'-O3'	5.41	121.12	113.00
37	BM	90	HIS	CA-C-N	5.41	127.80	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BM	90	HIS	C-N-CA	5.41	127.80	120.65
1	AA	1516	C	P-O5'-C5'	-5.41	112.79	120.90
19	A7	45	G	C2'-C3'-O3'	-5.40	105.59	113.70
30	BF	121	LYS	N-CA-C	-5.40	104.81	111.40
1	AA	859	A	O4'-C1'-N9	5.40	116.30	108.20
1	AA	1341	A	C2'-C3'-O3'	5.39	117.58	109.50
4	AD	10	LYS	CA-C-N	5.38	128.27	120.79
4	AD	10	LYS	C-N-CA	5.38	128.27	120.79
19	A7	75	C	C2'-C3'-O3'	5.38	117.57	109.50
1	AA	1552	U	P-O5'-C5'	-5.38	112.83	120.90
42	BR	12	ARG	N-CA-C	-5.37	99.53	108.34
6	AG	67	PRO	O-C-N	-5.37	118.92	122.73
1	AA	859	A	C5'-C4'-C3'	5.37	123.25	115.20
32	BH	130	ASP	CA-C-O	5.36	121.05	117.94
32	BH	139	ASN	N-CA-C	-5.36	102.88	111.02
53	B5	2286	U	P-O3'-C3'	5.36	128.24	120.20
46	BV	92	SER	N-CA-C	-5.36	102.27	110.14
37	BM	164	ALA	N-CA-C	-5.35	104.50	111.02
1	AA	860	U	O4'-C4'-C3'	-5.34	100.76	106.10
1	AA	1636	G	C1'-O4'-C4'	-5.34	104.56	109.90
1	AA	1281	C	C2'-C3'-O3'	5.34	117.51	109.50
16	AS	104	GLN	N-CA-C	5.33	122.16	110.80
29	BE	215	ASP	O-C-N	-5.33	118.59	123.50
39	BO	55	SER	CA-C-N	5.33	128.20	120.79
39	BO	55	SER	C-N-CA	5.33	128.20	120.79
53	B5	3121	U	P-O3'-C3'	5.33	128.19	120.20
53	B5	1410	U	P-O3'-C3'	5.33	128.19	120.20
23	B8	41	VAL	CA-C-N	5.32	127.67	120.38
23	B8	41	VAL	C-N-CA	5.32	127.67	120.38
1	AA	867	G	O5'-P-OP2	5.32	123.95	108.00
31	BG	143	ILE	N-CA-C	5.32	115.98	110.82
19	A7	15	G	C1'-O4'-C4'	-5.31	104.59	109.90
53	B5	2304	C	O4'-C1'-N1	5.31	116.46	108.50
45	BU	44	GLY	CA-C-N	5.31	127.81	120.49
45	BU	44	GLY	C-N-CA	5.31	127.81	120.49
53	B5	712	G	C2'-C3'-O3'	5.30	117.46	109.50
1	AA	1545	A	P-O3'-C3'	5.30	128.15	120.20
50	BZ	53	GLN	N-CA-C	-5.30	104.08	110.44
53	B5	2195	C	O4'-C1'-N1	5.29	116.44	108.50
1	AA	774	A	P-O3'-C3'	-5.29	112.26	120.20
1	AA	281	G	P-O3'-C3'	5.28	128.11	120.20
10	AK	23	PHE	CA-CB-CG	-5.27	108.53	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AT	48	GLN	CA-C-N	5.27	128.32	120.31
18	AT	48	GLN	C-N-CA	5.27	128.32	120.31
1	AA	308	C	P-O5'-C5'	5.27	128.80	120.90
30	BF	203	TRP	N-CA-CB	5.27	115.40	110.39
1	AA	1612	A	O4'-C1'-N9	5.27	116.40	108.50
32	BH	61	GLY	N-CA-C	-5.27	106.76	112.08
1	AA	1518	U	O5'-P-OP1	5.26	123.79	108.00
1	AA	1632	C	C2'-C3'-O3'	5.26	117.39	109.50
4	AD	109	LEU	CA-C-N	5.26	127.64	120.54
4	AD	109	LEU	C-N-CA	5.26	127.64	120.54
20	B0	119	VAL	N-CA-C	-5.25	100.30	108.81
53	B5	546	C	C2'-C3'-O3'	5.25	117.37	109.50
1	AA	857	U	P-O5'-C5'	-5.24	113.04	120.90
1	AA	1134	A	C2'-C3'-O3'	5.24	117.36	109.50
1	AA	799	A	C2'-C3'-O3'	5.24	121.55	113.70
53	B5	2577	C	P-O3'-C3'	5.23	128.05	120.20
1	AA	1523	A	C1'-C2'-O2'	5.23	116.24	108.40
20	B0	102	ALA	CA-C-N	5.23	127.24	120.44
20	B0	102	ALA	C-N-CA	5.23	127.24	120.44
29	BE	82	GLU	N-CA-C	-5.23	106.66	112.57
1	AA	797	G	C1'-C2'-O2'	5.22	116.24	108.40
1	AA	1196	G	O4'-C1'-N9	5.22	116.33	108.50
19	A7	9	A	N9-C1'-C2'	-5.22	106.17	114.00
8	AI	127	LYS	N-CA-CB	-5.22	102.16	111.08
53	B5	2672	G	P-O3'-C3'	5.22	128.03	120.20
13	AN	37	ASN	CA-C-N	5.21	127.13	120.56
13	AN	37	ASN	C-N-CA	5.21	127.13	120.56
36	BL	27	VAL	CA-C-N	5.21	127.27	120.28
36	BL	27	VAL	C-N-CA	5.21	127.27	120.28
35	BK	80	LEU	N-CA-C	-5.21	106.25	113.18
53	B5	1947	G	C1'-C2'-O2'	5.21	116.21	108.40
1	AA	1519	G	P-O5'-C5'	-5.21	113.09	120.90
17	AR	251	TRP	N-CA-C	5.21	117.84	110.50
19	A7	57	G	C2'-C3'-O3'	-5.21	105.89	113.70
32	BH	13	PRO	CA-C-N	5.21	128.03	120.79
32	BH	13	PRO	C-N-CA	5.21	128.03	120.79
52	B4	60	U	O4'-C1'-N1	5.20	116.30	108.50
6	AG	196	GLU	CA-C-N	5.20	127.56	120.54
6	AG	196	GLU	C-N-CA	5.20	127.56	120.54
19	A7	9	A	C4'-C3'-O3'	5.20	117.20	109.40
19	A7	36	A	O4'-C1'-N9	5.20	116.30	108.50
46	BV	111	ILE	N-CA-C	-5.19	101.15	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BK	130	LYS	CA-C-N	5.19	127.55	120.54
35	BK	130	LYS	C-N-CA	5.19	127.55	120.54
53	B5	2716	U	O4'-C1'-N1	5.19	116.29	108.50
17	AR	18	GLY	CA-C-N	5.19	129.66	121.56
17	AR	18	GLY	C-N-CA	5.19	129.66	121.56
31	BG	191	ASN	N-CA-CB	5.19	119.26	110.49
53	B5	2931	C	O4'-C1'-N1	5.19	116.28	108.50
1	AA	860	U	O4'-C1'-N1	5.17	115.96	108.20
26	BB	16	PHE	CA-CB-CG	-5.17	108.63	113.80
31	BG	217	THR	CA-C-N	5.17	127.19	120.88
31	BG	217	THR	C-N-CA	5.17	127.19	120.88
53	B5	512	U	P-O3'-C3'	5.17	127.95	120.20
17	AR	148	ASN	CA-CB-CG	-5.16	107.44	112.60
17	AR	319	ASN	CA-CB-CG	-5.16	107.44	112.60
37	BM	37	ARG	N-CA-CB	5.16	119.21	110.49
37	BM	109	PRO	CA-C-O	-5.16	113.08	120.56
2	AB	53	THR	CA-C-N	5.16	127.14	120.44
2	AB	53	THR	C-N-CA	5.16	127.14	120.44
53	B5	1795	U	P-O3'-C3'	5.16	127.93	120.20
1	AA	798	C	O3'-P-O5'	5.15	111.73	104.00
1	AA	1630	C	C2'-C3'-O3'	-5.15	105.97	113.70
19	A7	59	U	C5'-C4'-C3'	-5.15	108.28	116.00
27	BC	35	ASP	N-CA-C	5.15	116.93	110.24
33	BI	103	LEU	N-CA-C	-5.15	101.47	109.14
37	BM	157	ALA	N-CA-C	-5.14	105.68	111.28
6	AG	109	LYS	CA-C-N	5.14	127.42	120.38
6	AG	109	LYS	C-N-CA	5.14	127.42	120.38
29	BE	220	SER	N-CA-C	5.13	116.87	111.28
1	AA	864	U	O4'-C4'-C3'	-5.12	100.97	106.10
1	AA	1549	U	O4'-C1'-N1	5.12	115.88	108.20
17	AR	28	GLY	N-CA-C	-5.12	108.72	114.40
43	BS	40	PHE	N-CA-C	-5.11	107.71	114.31
50	BZ	20	HIS	CA-CB-CG	5.11	118.91	113.80
1	AA	478	A	C2'-C3'-O3'	5.11	117.16	109.50
30	BF	220	PHE	N-CA-C	5.11	117.51	111.33
3	AC	94	ARG	N-CA-C	-5.11	106.39	113.18
53	B5	2229	A	O5'-C5'-C4'	5.10	119.16	111.50
17	AR	277	GLU	CB-CA-C	-5.10	103.32	111.17
47	BW	83	GLU	N-CA-C	-5.10	99.94	110.80
53	B5	2219	A	P-O3'-C3'	5.10	127.85	120.20
1	AA	1548	A	C1'-C2'-O2'	5.09	118.38	108.20
1	AA	1759	U	C2'-C3'-O3'	5.09	117.13	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A7	21	A	C1'-C2'-O2'	-5.09	100.77	108.40
25	BA	196	LYS	N-CA-CB	5.09	119.08	110.49
53	B5	3126	C	O4'-C1'-N1	5.08	116.12	108.50
53	B5	1581	C	P-O3'-C3'	5.08	127.81	120.20
53	B5	1411	C	P-O3'-C3'	5.08	127.81	120.20
33	BI	89	VAL	N-CA-C	-5.07	101.17	108.48
24	B9	19	GLY	CA-C-N	5.07	127.39	120.54
24	B9	19	GLY	C-N-CA	5.07	127.39	120.54
37	BM	19	LEU	N-CA-C	-5.07	107.16	113.55
17	AR	49	GLY	N-CA-C	-5.07	108.71	115.40
7	AH	27	ILE	CA-CB-CG1	5.07	119.01	110.40
27	BC	226	PHE	N-CA-C	-5.06	106.85	112.57
29	BE	123	GLU	N-CA-C	-5.06	103.80	111.34
40	BP	7	GLN	CA-C-N	5.06	127.02	120.44
40	BP	7	GLN	C-N-CA	5.06	127.02	120.44
19	A7	62	A	O4'-C1'-C2'	5.06	112.66	107.60
53	B5	133	U	C2'-C3'-O3'	5.06	117.09	109.50
32	BH	151	VAL	CA-C-N	5.05	127.32	120.65
32	BH	151	VAL	C-N-CA	5.05	127.32	120.65
1	AA	859	A	C4'-C3'-C2'	5.05	107.65	102.60
33	BI	55	ASN	N-CA-C	-5.05	106.29	112.90
29	BE	160	PHE	CA-CB-CG	-5.05	108.75	113.80
29	BE	61	ILE	N-CA-C	-5.04	102.44	109.45
26	BB	140	ASN	CB-CA-C	5.04	120.10	110.17
29	BE	94	ASN	N-CA-C	5.04	114.89	108.24
19	A7	74	C	C3'-C2'-O2'	-5.04	107.05	114.60
53	B5	3175	C	O4'-C1'-N1	5.03	116.05	108.50
19	A7	60	C	C3'-C2'-C1'	-5.03	96.47	101.50
11	AL	96	VAL	N-CA-C	-5.03	98.88	109.34
1	AA	1631	A	C4'-C3'-C2'	5.03	107.63	102.60
14	AO	84	ILE	N-CA-C	5.03	119.74	108.88
27	BC	153	LYS	N-CA-CB	5.03	118.98	110.49
29	BE	218	ARG	CA-C-N	5.02	131.13	121.54
29	BE	218	ARG	C-N-CA	5.02	131.13	121.54
32	BH	59	ASN	CA-CB-CG	5.02	117.62	112.60
1	AA	1488	C	C2'-C3'-O3'	5.02	117.03	109.50
27	BC	168	LYS	N-CA-C	-5.02	100.11	110.80
52	B4	152	G	C2'-C3'-O3'	5.02	121.23	113.70
12	AM	121	ALA	N-CA-C	-5.01	102.35	110.32
53	B5	1872	C	O4'-C1'-N1	5.01	116.02	108.50
25	BA	163	LEU	N-CA-C	-5.01	107.12	113.43
53	B5	2158	A	P-O3'-C3'	5.01	127.72	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	B5	3039	C	O4'-C1'-N1	5.01	116.02	108.50
38	BN	101	ASN	CA-CB-CG	-5.00	107.60	112.60

All (45) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	109	G	C3'
1	AA	933	C	C2'
7	AH	34	ILE	CB
26	BB	161	ASP	CA
29	BE	216	GLU	CA
30	BF	83	LEU	CA
31	BG	141	ALA	CA
31	BG	142	LEU	CA
36	BL	56	LYS	CA
48	BX	70	ALA	CA
48	BX	80	ALA	CA
51	B3	70	A	C4'
53	B5	114	A	C3'
53	B5	279	U	C3'
53	B5	355	A	C4'
53	B5	477	A	C3'
53	B5	481	U	C3'
53	B5	554	A	C3'
53	B5	596	U	C3'
53	B5	705	A	C3'
53	B5	711	A	C2'
53	B5	735	A	C3',C2'
53	B5	786	A	C3'
53	B5	970	A	C3'
53	B5	1347	U	C3'
53	B5	1583	A	C3',C2'
53	B5	1590	G	C3'
53	B5	1644	C	C2'
53	B5	1737	U	C3'
53	B5	1947	G	C1'
53	B5	2214	A	C3'
53	B5	2224	A	C3'
53	B5	2225	U	C3'
53	B5	2229	A	C3'
53	B5	2469	G	C1',C2'
53	B5	2477	G	C1'

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Mol	Chain	Res	Type	Atom
53	B5	2999	U	C2'
53	B5	3051	U	C4'
53	B5	3142	A	C3'
53	B5	3246	G	C4'
53	B5	3303	G	C2'
53	B5	3304	U	C3'

All (285) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	A7	1	G	Sidechain
19	A7	11	C	Sidechain
19	A7	14	A	Sidechain
19	A7	15	G	Sidechain
19	A7	18	G	Sidechain
19	A7	19	G	Sidechain
19	A7	2	C	Sidechain
19	A7	20	G	Sidechain
19	A7	21	A	Sidechain
19	A7	23	A	Sidechain
19	A7	24	G	Sidechain
19	A7	27	C	Sidechain
19	A7	29	A	Sidechain
19	A7	3	G	Sidechain
19	A7	30	G	Sidechain
19	A7	31	A	Sidechain
19	A7	36	A	Sidechain
19	A7	4	G	Sidechain
19	A7	41	U	Sidechain
19	A7	42	G	Sidechain
19	A7	43	G	Sidechain
19	A7	45	G	Sidechain
19	A7	47	U	Sidechain
19	A7	5	A	Sidechain
19	A7	50	U	Sidechain
19	A7	51	G	Sidechain
19	A7	52	U	Sidechain
19	A7	53	G	Sidechain
19	A7	56	C	Sidechain
19	A7	57	G	Sidechain
19	A7	59	U	Sidechain
19	A7	61	C	Sidechain

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Mol	Chain	Res	Type	Group
19	A7	63	C	Sidechain
19	A7	65	G	Sidechain
19	A7	66	A	Sidechain
19	A7	7	U	Sidechain
19	A7	70	C	Sidechain
19	A7	71	G	Sidechain
19	A7	72	C	Sidechain
19	A7	73	A	Sidechain
19	A7	74	C	Sidechain
19	A7	75	C	Sidechain
19	A7	76	A	Sidechain
19	A7	9	A	Sidechain
1	AA	1089	A	Sidechain
1	AA	1196	G	Sidechain
1	AA	1200	A	Sidechain
1	AA	1202	U	Sidechain
1	AA	1237	G	Sidechain
1	AA	1303	C	Sidechain
1	AA	1309	A	Sidechain
1	AA	1327	G	Sidechain
1	AA	1440	U	Sidechain
1	AA	1502	G	Sidechain
1	AA	1514	A	Sidechain
1	AA	1520	U	Sidechain
1	AA	1551	G	Sidechain
1	AA	1583	U	Sidechain
1	AA	1584	A	Sidechain
1	AA	1586	G	Sidechain
1	AA	1766	G	Sidechain
1	AA	225	A	Sidechain
1	AA	244	A	Sidechain
1	AA	474	A	Sidechain
1	AA	475	A	Sidechain
1	AA	476	U	Sidechain
1	AA	529	A	Sidechain
1	AA	80	A	Sidechain
1	AA	843	U	Sidechain
1	AA	855	A	Sidechain
1	AA	856	A	Sidechain
1	AA	877	G	Sidechain
2	AB	84	ARG	Sidechain
4	AD	149	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	AD	78	ARG	Sidechain
4	AD	79	ARG	Sidechain
5	AE	226	THR	Peptide
8	AI	135	ARG	Sidechain
8	AI	142	TYR	Sidechain
8	AI	96	TYR	Sidechain
9	AJ	23	ARG	Sidechain
9	AJ	53	LYS	Peptide
9	AJ	90	TYR	Sidechain
10	AK	132	ARG	Sidechain,Peptide
10	AK	48	VAL	Peptide
10	AK	52	ARG	Sidechain
12	AM	120	ARG	Peptide
12	AM	137	HIS	Peptide
12	AM	143	ARG	Sidechain
13	AN	13	ARG	Sidechain
13	AN	14	PHE	Sidechain
14	AO	114	ARG	Sidechain
14	AO	121	ARG	Sidechain
14	AO	124	ARG	Sidechain
14	AO	135	LEU	Peptide
20	B0	45	ARG	Sidechain
52	B4	132	G	Sidechain
52	B4	147	U	Sidechain
52	B4	41	A	Sidechain
52	B4	44	A	Sidechain
52	B4	62	C	Sidechain
52	B4	64	U	Sidechain
53	B5	1	G	Sidechain
53	B5	10	C	Sidechain
53	B5	1005	G	Sidechain
53	B5	1026	A	Sidechain
53	B5	1104	G	Sidechain
53	B5	1132	C	Sidechain
53	B5	1169	A	Sidechain
53	B5	118	U	Sidechain
53	B5	1181	U	Sidechain
53	B5	1200	A	Sidechain
53	B5	1236	G	Sidechain
53	B5	1239	C	Sidechain
53	B5	1240	A	Sidechain
53	B5	1257	C	Sidechain

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Mol	Chain	Res	Type	Group
53	B5	1290	A	Sidechain
53	B5	130	A	Sidechain
53	B5	1346	G	Sidechain
53	B5	1347	U	Sidechain
53	B5	135	C	Sidechain
53	B5	1357	G	Sidechain
53	B5	1362	G	Sidechain
53	B5	1368	U	Sidechain
53	B5	1378	U	Sidechain
53	B5	1385	C	Sidechain
53	B5	1417	G	Sidechain
53	B5	1421	G	Sidechain
53	B5	1496	C	Sidechain
53	B5	1510	G	Sidechain
53	B5	1544	G	Sidechain
53	B5	1558	A	Sidechain
53	B5	1622	U	Sidechain
53	B5	1658	G	Sidechain
53	B5	17	G	Sidechain
53	B5	1714	A	Sidechain
53	B5	1734	G	Sidechain
53	B5	1783	U	Sidechain
53	B5	1790	G	Sidechain
53	B5	18	G	Sidechain
53	B5	1811	G	Sidechain
53	B5	1812	G	Sidechain
53	B5	1831	U	Sidechain
53	B5	1874	A	Sidechain
53	B5	1896	A	Sidechain
53	B5	1927	G	Sidechain
53	B5	2112	U	Sidechain
53	B5	2130	G	Sidechain
53	B5	2133	U	Sidechain
53	B5	216	G	Sidechain
53	B5	2167	A	Sidechain
53	B5	2176	U	Sidechain
53	B5	2178	A	Sidechain
53	B5	2180	G	Sidechain
53	B5	2185	G	Sidechain
53	B5	2186	U	Sidechain
53	B5	2224	A	Sidechain
53	B5	2300	G	Sidechain

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Mol	Chain	Res	Type	Group
53	B5	2356	A	Sidechain
53	B5	2394	G	Sidechain
53	B5	2396	G	Sidechain
53	B5	2448	G	Sidechain
53	B5	2468	A	Sidechain
53	B5	2481	G	Sidechain
53	B5	2482	U	Sidechain
53	B5	251	G	Sidechain
53	B5	2548	C	Sidechain
53	B5	2586	G	Sidechain
53	B5	2593	A	Sidechain
53	B5	2607	G	Sidechain
53	B5	2621	G	Sidechain
53	B5	2677	G	Sidechain
53	B5	2681	U	Sidechain
53	B5	2696	A	Sidechain
53	B5	270	U	Sidechain
53	B5	2744	U	Sidechain
53	B5	2751	G	Sidechain
53	B5	2768	U	Sidechain
53	B5	2774	C	Sidechain
53	B5	2789	U	Sidechain
53	B5	2839	G	Sidechain
53	B5	2876	C	Sidechain
53	B5	2901	G	Sidechain
53	B5	2943	G	Sidechain
53	B5	2951	G	Sidechain
53	B5	3003	G	Sidechain
53	B5	3009	G	Sidechain
53	B5	3032	A	Sidechain
53	B5	3049	A	Sidechain
53	B5	3144	G	Sidechain
53	B5	3172	G	Sidechain
53	B5	3303	G	Sidechain
53	B5	3337	G	Sidechain
53	B5	337	G	Sidechain
53	B5	366	A	Sidechain
53	B5	40	A	Sidechain
53	B5	494	G	Sidechain
53	B5	495	G	Sidechain
53	B5	496	C	Sidechain
53	B5	498	A	Sidechain

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Mol	Chain	Res	Type	Group
53	B5	584	G	Sidechain
53	B5	619	A	Sidechain
53	B5	652	G	Sidechain
53	B5	662	U	Sidechain
53	B5	709	A	Sidechain
53	B5	8	C	Sidechain
53	B5	847	A	Sidechain
53	B5	855	U	Sidechain
53	B5	859	G	Sidechain
53	B5	860	G	Sidechain
53	B5	895	A	Sidechain
53	B5	975	G	Sidechain
53	B5	977	U	Sidechain
53	B5	992	G	Sidechain
23	B8	115	ALA	Peptide
23	B8	5	ARG	Sidechain
23	B8	61	ARG	Sidechain
24	B9	18	TYR	Sidechain
24	B9	34	HIS	Peptide
24	B9	43	GLY	Peptide
26	BB	150	LEU	Peptide
26	BB	161	ASP	Peptide
26	BB	163	ARG	Sidechain
26	BB	242	ARG	Sidechain
27	BC	117	ARG	Sidechain
28	BD	202	ARG	Sidechain
28	BD	31	ARG	Sidechain
28	BD	98	ARG	Sidechain
29	BE	112	ARG	Sidechain
29	BE	192	PRO	Peptide
29	BE	198	TYR	Sidechain
29	BE	213	ASP	Peptide
29	BE	219	PHE	Peptide
29	BE	85	ARG	Sidechain
29	BE	86	TYR	Sidechain
31	BG	142	LEU	Peptide
31	BG	173	MET	Peptide
32	BH	173	ARG	Sidechain
32	BH	23	ARG	Sidechain
32	BH	69	ARG	Sidechain
33	BI	69	ARG	Sidechain
33	BI	7	ARG	Sidechain

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Mol	Chain	Res	Type	Group
34	BJ	47	GLN	Peptide
34	BJ	61	ARG	Sidechain
34	BJ	92	ARG	Sidechain
35	BK	16	ARG	Sidechain
35	BK	90	ARG	Sidechain
36	BL	153	ASP	Peptide
36	BL	172	ARG	Sidechain
36	BL	174	ILE	Peptide
36	BL	33	LYS	Peptide
36	BL	38	ARG	Sidechain
36	BL	71	ARG	Sidechain
36	BL	81	TYR	Sidechain
37	BM	148	LYS	Peptide,Mainchain
37	BM	169	ALA	Mainchain
37	BM	84	LEU	Peptide
37	BM	85	ARG	Sidechain
38	BN	116	HIS	Peptide
38	BN	131	ARG	Sidechain
39	BO	72	LYS	Peptide
40	BP	110	ARG	Sidechain
40	BP	20	ARG	Sidechain
40	BP	38	ARG	Sidechain
40	BP	89	LEU	Peptide
42	BR	12	ARG	Sidechain
42	BR	32	ARG	Sidechain
42	BR	86	ARG	Sidechain
43	BS	47	ARG	Sidechain
44	BT	125	ARG	Sidechain
45	BU	63	LYS	Peptide
46	BV	112	LEU	Peptide
46	BV	12	ARG	Sidechain
46	BV	91	LYS	Peptide
47	BW	28	ARG	Sidechain
47	BW	74	ARG	Sidechain
48	BX	10	ARG	Sidechain
49	BY	47	TYR	Sidechain
50	BZ	32	LYS	Peptide
50	BZ	42	ARG	Sidechain
50	BZ	55	LYS	Peptide
50	BZ	56	PRO	Peptide
50	BZ	60	LYS	Peptide

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	AA	37458	0	18828	603	0
2	AB	1500	0	1524	1	0
3	AC	1469	0	1534	1	0
4	AD	1018	0	1067	1	0
5	AE	1207	0	1274	0	0
6	AG	1456	0	1523	2	0
7	AH	992	0	1027	39	0
8	AI	1087	0	1145	19	0
9	AJ	771	0	829	2	0
10	AK	924	0	949	0	0
11	AL	906	0	970	1	0
12	AM	1077	0	1107	19	0
13	AN	417	0	408	23	0
14	AO	694	0	740	13	0
15	AQ	643	0	688	2	0
16	AS	548	0	574	3	0
17	AR	2410	0	2367	555	0
18	AT	1102	0	1112	38	0
19	A7	1648	0	830	55	0
20	B0	881	0	926	1	0
21	B1	424	0	459	1	0
22	B2	752	0	803	1	0
23	B8	947	0	972	19	0
24	B9	539	0	555	1	0
25	BA	1683	0	1772	3	0
26	BB	1848	0	1908	16	0
27	BC	2887	0	2964	3	0
28	BD	1950	0	2019	3	0
29	BE	1913	0	1842	1	0
30	BF	1561	0	1633	1	0
31	BG	844	0	909	0	0
32	BH	1418	0	1483	4	0
33	BI	1326	0	1368	3	0
34	BJ	1195	0	1230	15	0
35	BK	1038	0	1110	23	0
36	BL	1618	0	1673	1	0
37	BM	1317	0	1407	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BN	1189	0	1201	0	0
39	BO	931	0	1010	0	0
40	BP	1317	0	1389	115	0
41	BQ	893	0	924	0	0
42	BR	977	0	1026	14	0
43	BS	371	0	382	1	0
44	BT	642	0	679	0	0
45	BU	916	0	996	0	0
46	BV	1123	0	1160	2	0
47	BW	663	0	700	0	0
48	BX	605	0	661	1	0
49	BY	403	0	398	0	0
50	BZ	749	0	815	0	0
51	B3	2403	0	1219	0	0
52	B4	3329	0	1685	0	0
53	B5	67775	0	34047	225	0
All	All	165754	0	111821	1353	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1353) 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)
35:BK:121:PHE:CZ	35:BK:121:PHE:CE1	1.78	1.71
35:BK:121:PHE:CZ	35:BK:121:PHE:CE2	1.79	1.69
35:BK:121:PHE:CE2	35:BK:121:PHE:CD2	1.76	1.69
35:BK:121:PHE:CE1	35:BK:121:PHE:CD1	1.80	1.69
35:BK:121:PHE:CD2	35:BK:121:PHE:CG	1.82	1.68
35:BK:121:PHE:CD1	35:BK:121:PHE:CG	1.81	1.67
1:AA:1501:A:H1'	1:AA:1546:G:C2	1.33	1.62
1:AA:1756:U:H5'	53:B5:2262:A:C2	1.34	1.62
8:AI:96:TYR:CE1	8:AI:96:TYR:CD1	1.89	1.59
8:AI:96:TYR:CD2	8:AI:96:TYR:CE2	1.88	1.58
8:AI:96:TYR:CD2	8:AI:96:TYR:CG	1.90	1.58
8:AI:96:TYR:CE1	8:AI:96:TYR:CZ	1.91	1.57
8:AI:96:TYR:CD1	8:AI:96:TYR:CG	1.91	1.56
1:AA:1200:A:C6	1:AA:1200:A:C5	1.87	1.56
8:AI:96:TYR:CE2	8:AI:96:TYR:CZ	1.90	1.55
1:AA:1200:A:C2	1:AA:1200:A:N3	1.75	1.54
1:AA:1200:A:C2	1:AA:1200:A:N1	1.74	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BM:111:PRO:HA	37:BM:163:ALA:CB	1.36	1.52
12:AM:110:ARG:NE	34:BJ:116:TYR:CD1	1.76	1.52
1:AA:702:G:C4	40:BP:172:ALA:O	1.64	1.50
1:AA:856:A:C6	1:AA:856:A:C5	1.99	1.50
37:BM:111:PRO:CA	37:BM:163:ALA:HB1	1.04	1.50
1:AA:702:G:C6	40:BP:172:ALA:HB1	0.98	1.49
1:AA:1200:A:C5	1:AA:1200:A:C4	1.86	1.48
1:AA:1630:C:H4'	1:AA:1636:G:N2	1.16	1.48
1:AA:1776:G:C4'	53:B5:2194:G:H5''	1.43	1.48
1:AA:702:G:C6	40:BP:172:ALA:CB	1.93	1.48
1:AA:1200:A:C6	1:AA:1200:A:N1	1.82	1.48
1:AA:699:U:H3'	40:BP:169:ALA:CB	1.42	1.47
1:AA:856:A:N1	1:AA:856:A:C2	1.82	1.47
1:AA:1200:A:N3	1:AA:1200:A:C4	1.82	1.47
37:BM:111:PRO:HB3	37:BM:163:ALA:CA	1.41	1.47
1:AA:1501:A:C6	1:AA:1546:G:C8	2.02	1.46
1:AA:1200:A:C4	13:AN:16:LYS:HA	1.46	1.45
1:AA:701:U:C4	40:BP:169:ALA:O	1.67	1.44
1:AA:856:A:C5	1:AA:856:A:C4	1.97	1.44
1:AA:501:U:C4	1:AA:501:U:C5	2.04	1.43
1:AA:856:A:C2	1:AA:856:A:N3	1.84	1.43
12:AM:110:ARG:NH2	34:BJ:116:TYR:CZ	1.82	1.42
1:AA:1501:A:N7	1:AA:1546:G:H2'	1.29	1.42
1:AA:702:G:C8	40:BP:175:ALA:HB3	1.54	1.40
1:AA:501:U:C6	1:AA:501:U:N1	1.89	1.40
1:AA:856:A:C6	1:AA:856:A:N1	1.87	1.40
1:AA:1756:U:H5'	53:B5:2262:A:N1	1.17	1.39
1:AA:501:U:C4	1:AA:501:U:N3	1.89	1.38
1:AA:856:A:C4	1:AA:856:A:N3	1.91	1.38
37:BM:169:ALA:C	37:BM:171:ALA:N	1.78	1.38
1:AA:501:U:N3	1:AA:501:U:C2	1.91	1.38
1:AA:1776:G:OP1	53:B5:2193:U:C5'	1.71	1.37
1:AA:1755:G:N2	53:B5:2262:A:O2'	1.57	1.36
1:AA:1757:C:O4'	53:B5:2263:C:C5'	1.74	1.35
1:AA:1200:A:C5	13:AN:16:LYS:HA	1.58	1.35
1:AA:1501:A:C6	1:AA:1546:G:N7	1.93	1.35
1:AA:501:U:N1	1:AA:501:U:C2	1.94	1.34
1:AA:1756:U:C5'	53:B5:2262:A:C2	2.09	1.33
1:AA:702:G:O6	40:BP:172:ALA:CB	1.68	1.33
1:AA:1501:A:H1'	1:AA:1546:G:N2	1.43	1.33
12:AM:110:ARG:NE	34:BJ:116:TYR:CE1	1.74	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AO:149:LEU:HD12	53:B5:847:A:OP1	1.22	1.33
1:AA:1521:G:H5''	1:AA:1522:A:P	1.68	1.32
1:AA:1630:C:C4'	1:AA:1636:G:N2	1.90	1.32
1:AA:702:G:N3	40:BP:176:ALA:HB3	1.44	1.32
1:AA:1665:A:OP1	53:B5:1936:A:C5'	1.78	1.32
1:AA:699:U:C3'	40:BP:169:ALA:HB3	1.60	1.31
1:AA:1501:A:N1	1:AA:1546:G:N7	1.77	1.31
1:AA:1756:U:O3'	53:B5:2263:C:C4'	1.64	1.31
1:AA:1502:G:C5	1:AA:1547:C:C4	2.17	1.30
1:AA:1501:A:C1'	1:AA:1546:G:C2	2.11	1.30
1:AA:1655:U:C4	53:B5:2329:C:H1'	1.50	1.30
1:AA:972:A:H5'	53:B5:848:A:C2	1.64	1.29
37:BM:108:ILE:HG23	37:BM:160:ALA:CB	1.60	1.28
1:AA:1755:G:O2'	53:B5:2262:A:C2	1.84	1.27
1:AA:972:A:H5'	53:B5:848:A:N3	1.48	1.27
1:AA:1521:G:C2	18:AT:78:LYS:CG	2.16	1.27
1:AA:858:G:C2	7:AH:61:ILE:CB	2.16	1.27
1:AA:858:G:C6	7:AH:61:ILE:CB	2.18	1.27
1:AA:1735:G:H4'	53:B5:1933:A:O2'	1.31	1.27
37:BM:108:ILE:CG2	37:BM:160:ALA:CB	2.11	1.27
1:AA:858:G:N1	7:AH:61:ILE:CB	1.99	1.26
1:AA:1501:A:C8	1:AA:1546:G:H2'	1.70	1.26
1:AA:1630:C:C4'	1:AA:1636:G:H21	1.46	1.26
1:AA:1501:A:C4	1:AA:1546:G:C4	2.16	1.26
1:AA:1521:G:C2	18:AT:78:LYS:HG3	1.68	1.25
1:AA:1776:G:OP1	53:B5:2193:U:H5''	1.14	1.25
1:AA:698:U:N1	40:BP:164:ALA:O	1.58	1.25
1:AA:698:U:C2	40:BP:164:ALA:O	1.90	1.24
37:BM:111:PRO:CA	37:BM:163:ALA:CB	2.01	1.24
1:AA:699:U:C3'	40:BP:169:ALA:CB	2.13	1.24
12:AM:110:ARG:NH2	34:BJ:116:TYR:CE2	2.04	1.23
14:AO:123:HIS:ND1	53:B5:846:A:N3	1.84	1.23
1:AA:1502:G:N7	1:AA:1547:C:C2	2.07	1.23
1:AA:1776:G:H5''	53:B5:2194:G:C5'	1.69	1.22
1:AA:702:G:C5	40:BP:172:ALA:HB1	1.75	1.22
1:AA:698:U:C6	40:BP:164:ALA:O	1.91	1.22
1:AA:1574:A:N3	19:A7:41:U:O4'	1.70	1.21
1:AA:971:G:H21	53:B5:846:A:N6	1.37	1.21
1:AA:1574:A:N3	19:A7:41:U:C4'	1.84	1.21
1:AA:1653:A:C6	53:B5:2302:G:C5'	2.16	1.20
1:AA:1657:A:H5''	42:BR:67:PRO:CD	1.72	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:702:G:O6	40:BP:172:ALA:HB1	1.02	1.19
1:AA:1776:G:O3'	53:B5:2194:G:C4'	1.90	1.19
37:BM:111:PRO:CB	37:BM:163:ALA:HB1	1.72	1.19
1:AA:799:A:N3	40:BP:161:ALA:CB	1.99	1.19
1:AA:1756:U:C1'	53:B5:2262:A:H2'	1.72	1.19
1:AA:1756:U:C3'	53:B5:2263:C:H4'	1.52	1.18
1:AA:1635:C:C4'	1:AA:1636:G:OP2	1.84	1.18
1:AA:1461:C:OP1	19:A7:30:G:H1'	1.40	1.17
1:AA:1757:C:O4'	53:B5:2263:C:H5'	1.31	1.17
1:AA:1776:G:O3'	53:B5:2194:G:H4'	0.99	1.17
1:AA:1630:C:C5'	1:AA:1636:G:H21	1.56	1.16
1:AA:921:G:H4'	26:BB:141:PRO:HD3	1.28	1.15
1:AA:1756:U:H1'	53:B5:2262:A:C2'	1.75	1.15
1:AA:1776:G:H4'	53:B5:2194:G:C5'	1.76	1.15
17:AR:34:LEU:HD21	17:AR:42:LEU:HD21	1.27	1.15
1:AA:1521:G:N1	18:AT:78:LYS:CG	2.01	1.15
1:AA:1635:C:H4'	1:AA:1636:G:OP2	1.43	1.15
17:AR:34:LEU:HG	17:AR:42:LEU:HD11	1.24	1.15
1:AA:1655:U:C4	53:B5:2329:C:C1'	2.26	1.15
1:AA:1121:A:C1'	53:B5:2191:U:C5'	2.24	1.14
1:AA:1776:G:C5'	53:B5:2194:G:C5'	2.23	1.14
17:AR:38:ARG:HA	17:AR:67:ILE:HG23	1.29	1.14
1:AA:1121:A:H1'	53:B5:2191:U:H5''	1.16	1.14
1:AA:1521:G:H1'	18:AT:86:ARG:NH2	1.63	1.14
37:BM:111:PRO:CB	37:BM:163:ALA:CA	2.26	1.14
37:BM:169:ALA:O	37:BM:170:ALA:C	1.79	1.14
1:AA:1502:G:C5	1:AA:1547:C:N3	2.14	1.13
1:AA:1653:A:H1'	53:B5:2302:G:OP2	1.45	1.13
1:AA:1502:G:C8	1:AA:1547:C:N3	2.17	1.13
1:AA:1521:G:N2	18:AT:78:LYS:CD	2.10	1.13
1:AA:1521:G:O2'	18:AT:83:ALA:HA	1.48	1.13
1:AA:1502:G:C6	1:AA:1547:C:C4	2.35	1.13
37:BM:108:ILE:CG2	37:BM:160:ALA:HB1	1.72	1.13
1:AA:1521:G:N1	18:AT:78:LYS:HG3	1.28	1.13
1:AA:1200:A:C5	13:AN:16:LYS:CA	2.32	1.12
1:AA:1521:G:C5	18:AT:79:LEU:N	2.17	1.12
1:AA:1200:A:C4	13:AN:16:LYS:CA	2.32	1.12
1:AA:1502:G:N7	1:AA:1547:C:N3	1.97	1.12
1:AA:1200:A:C2	13:AN:16:LYS:CA	2.33	1.12
1:AA:1501:A:C5	1:AA:1546:G:C4	2.36	1.12
1:AA:1630:C:H4'	1:AA:1636:G:C2	1.83	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1757:C:O4'	53:B5:2263:C:H5''	1.50	1.12
1:AA:1776:G:C5'	53:B5:2194:G:H5'	1.78	1.12
17:AR:209:THR:HG23	17:AR:210:LEU:HD22	1.16	1.12
37:BM:108:ILE:CG2	37:BM:160:ALA:HB2	1.76	1.12
1:AA:1756:U:C5'	53:B5:2262:A:N1	2.07	1.12
1:AA:1665:A:OP1	53:B5:1936:A:H5'	0.94	1.12
1:AA:1776:G:C4'	53:B5:2194:G:C5'	2.26	1.12
1:AA:1778:G:OP1	53:B5:2274:U:H5'	1.44	1.11
1:AA:858:G:C5	7:AH:61:ILE:CB	2.31	1.11
1:AA:856:A:C4	7:AH:32:LYS:C	2.29	1.11
37:BM:151:ALA:O	37:BM:155:ALA:CB	1.98	1.11
1:AA:1653:A:C1'	53:B5:2302:G:OP2	1.96	1.10
14:AO:149:LEU:CD1	53:B5:847:A:OP1	1.98	1.10
14:AO:149:LEU:HD13	53:B5:847:A:H5'	1.21	1.10
1:AA:1521:G:H5''	1:AA:1522:A:OP2	1.47	1.10
1:AA:1657:A:C5'	42:BR:67:PRO:HG2	1.81	1.09
1:AA:1665:A:O4'	53:B5:1935:G:H5'	1.52	1.09
1:AA:856:A:C5	7:AH:32:LYS:C	2.30	1.09
1:AA:1574:A:H2'	19:A7:40:5MC:O2'	1.41	1.09
1:AA:699:U:O2	40:BP:170:ALA:HB3	1.35	1.09
1:AA:1501:A:N7	1:AA:1546:G:C2'	2.15	1.08
1:AA:1664:U:O3'	53:B5:1935:G:O2'	1.71	1.08
1:AA:1756:U:C3'	53:B5:2263:C:C4'	2.16	1.08
17:AR:211:ILE:HD11	17:AR:225:LEU:HD13	1.16	1.08
1:AA:1574:A:C2	19:A7:41:U:O4'	2.05	1.08
1:AA:856:A:C5	7:AH:33:VAL:N	2.22	1.08
1:AA:1200:A:C6	13:AN:16:LYS:CA	2.37	1.08
1:AA:1632:C:H4'	1:AA:1633:A:OP2	1.50	1.08
1:AA:856:A:C2	7:AH:32:LYS:C	2.32	1.07
1:AA:1776:G:H5'	53:B5:2194:G:OP1	1.54	1.07
1:AA:1521:G:C5'	1:AA:1522:A:OP2	2.03	1.07
1:AA:1521:G:C2	18:AT:78:LYS:CB	2.38	1.07
1:AA:972:A:C5'	53:B5:848:A:N3	2.16	1.07
1:AA:1521:G:C5'	1:AA:1522:A:P	2.33	1.06
17:AR:164:ASP:HB2	17:AR:168:THR:HA	1.09	1.06
1:AA:1501:A:C5	1:AA:1546:G:C8	2.44	1.06
37:BM:108:ILE:HG23	37:BM:160:ALA:HB1	1.32	1.06
14:AO:149:LEU:HD12	53:B5:847:A:P	1.95	1.06
37:BM:111:PRO:CB	37:BM:163:ALA:CB	2.28	1.06
1:AA:702:G:N7	40:BP:172:ALA:HA	1.71	1.05
1:AA:1757:C:C4'	53:B5:2263:C:H5''	1.78	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:699:U:O2	40:BP:170:ALA:CB	1.77	1.05
1:AA:699:U:C1'	40:BP:169:ALA:HB3	1.77	1.05
1:AA:800:U:OP1	40:BP:160:ALA:HB1	1.56	1.05
1:AA:858:G:C4	7:AH:61:ILE:CB	2.39	1.05
17:AR:260:ILE:HG13	17:AR:284:ALA:HB1	1.38	1.05
1:AA:1657:A:H5'	42:BR:67:PRO:HG2	1.33	1.05
17:AR:164:ASP:HB2	17:AR:168:THR:CA	1.87	1.05
17:AR:258:THR:HG21	17:AR:261:LYS:HE2	1.39	1.05
1:AA:856:A:C6	7:AH:32:LYS:C	2.35	1.05
1:AA:856:A:C4	7:AH:33:VAL:N	2.24	1.05
1:AA:1744:A:C2	53:B5:2302:G:O5'	2.09	1.05
1:AA:1200:A:C5	13:AN:16:LYS:N	2.25	1.04
1:AA:1734:G:H21	53:B5:1934:G:H4'	1.19	1.04
12:AM:110:ARG:CZ	34:BJ:116:TYR:CE1	2.40	1.04
23:B8:43:LYS:NZ	35:BK:121:PHE:CE1	2.25	1.04
1:AA:856:A:C6	7:AH:33:VAL:N	2.26	1.04
14:AO:149:LEU:HD13	53:B5:847:A:C5'	1.87	1.04
37:BM:111:PRO:CB	37:BM:163:ALA:HA	1.86	1.04
1:AA:702:G:C5	40:BP:172:ALA:O	2.10	1.03
1:AA:799:A:C4'	40:BP:161:ALA:O	2.04	1.03
1:AA:856:A:C2	7:AH:33:VAL:N	2.26	1.03
1:AA:1200:A:C4	13:AN:16:LYS:N	2.25	1.03
8:AI:93:HIS:CE1	17:AR:59:ARG:HH22	1.76	1.03
17:AR:83:ALA:HB2	17:AR:113:VAL:HG13	1.41	1.03
17:AR:257:ALA:HA	17:AR:283:LYS:HD2	1.07	1.03
1:AA:699:U:O4'	40:BP:166:ALA:HA	1.56	1.03
1:AA:922:A:H5'	26:BB:109:GLU:OE1	1.57	1.03
1:AA:1501:A:N6	1:AA:1546:G:C8	2.26	1.03
1:AA:1744:A:H4'	53:B5:2291:A:H1'	1.37	1.03
1:AA:1630:C:C5'	1:AA:1636:G:N2	2.18	1.03
17:AR:93:ASP:HB3	17:AR:96:THR:HG22	1.41	1.03
37:BM:111:PRO:HB3	37:BM:163:ALA:HA	1.07	1.03
1:AA:1200:A:C2	13:AN:16:LYS:N	2.27	1.02
1:AA:699:U:C2'	40:BP:169:ALA:HB3	1.89	1.02
1:AA:699:U:H3'	40:BP:169:ALA:HB1	1.04	1.02
1:AA:701:U:C5	40:BP:169:ALA:O	2.11	1.02
1:AA:702:G:C8	40:BP:175:ALA:CB	2.41	1.02
1:AA:1521:G:N2	18:AT:78:LYS:HD2	1.73	1.02
19:A7:71:G:H5'	53:B5:2236:G:H4'	1.42	1.02
1:AA:702:G:C5	40:BP:172:ALA:CA	2.43	1.02
1:AA:1121:A:H1'	53:B5:2191:U:C5'	1.85	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:286:GLU:HG2	17:AR:289:ALA:HA	1.41	1.02
1:AA:799:A:N3	40:BP:161:ALA:HB2	1.43	1.01
1:AA:1000:U:OP1	19:A7:38:A:H5'	1.58	1.01
1:AA:1520:U:H5''	1:AA:1522:A:OP2	1.59	1.01
1:AA:1653:A:C6	53:B5:2302:G:H5''	1.88	1.01
17:AR:210:LEU:HD12	17:AR:222:LEU:HD21	1.40	1.01
1:AA:699:U:O4'	40:BP:166:ALA:CA	2.07	1.01
1:AA:799:A:O4'	40:BP:161:ALA:O	1.71	1.01
1:AA:1574:A:C2	19:A7:41:U:C4'	2.42	1.01
37:BM:169:ALA:C	37:BM:171:ALA:H	1.68	1.01
1:AA:1755:G:O2'	53:B5:2262:A:H2	1.25	1.00
1:AA:1200:A:C6	13:AN:16:LYS:N	2.29	1.00
1:AA:1756:U:H1'	53:B5:2262:A:H2'	1.01	1.00
1:AA:1657:A:C5'	42:BR:67:PRO:CG	2.39	1.00
1:AA:1501:A:C5	1:AA:1546:G:C5	2.44	1.00
1:AA:1756:U:O4'	53:B5:2262:A:N3	1.93	1.00
1:AA:699:U:C2	40:BP:167:ALA:C	2.39	1.00
1:AA:1777:U:P	53:B5:2194:G:H4'	2.02	1.00
37:BM:111:PRO:HB3	37:BM:163:ALA:C	1.86	1.00
1:AA:912:G:O6	53:B5:2207:A:O5'	1.71	0.99
1:AA:1121:A:C4'	53:B5:2191:U:H5'	1.92	0.99
1:AA:1744:A:C4'	53:B5:2291:A:H1'	1.92	0.99
17:AR:12:THR:HG22	17:AR:311:ARG:HG2	1.40	0.99
1:AA:1574:A:C2'	19:A7:40:5MC:O2'	2.11	0.99
1:AA:1635:C:C5'	1:AA:1636:G:OP2	2.10	0.99
1:AA:702:G:H1'	40:BP:175:ALA:CB	1.78	0.99
1:AA:1501:A:C1'	1:AA:1546:G:N2	2.15	0.99
17:AR:259:GLY:HA2	17:AR:284:ALA:HA	1.41	0.99
1:AA:1756:U:C4'	53:B5:2262:A:C2	2.46	0.98
1:AA:1502:G:C6	1:AA:1547:C:C5	2.52	0.98
1:AA:1502:G:C8	1:AA:1547:C:C2	2.50	0.98
1:AA:1657:A:H5'	42:BR:67:PRO:CG	1.93	0.98
1:AA:1121:A:C1'	53:B5:2191:U:H5'	1.91	0.98
1:AA:993:G:H5''	53:B5:2195:C:OP2	1.64	0.98
1:AA:1460:G:H4'	19:A7:30:G:H5'	1.46	0.97
1:AA:1521:G:N2	18:AT:78:LYS:NZ	2.11	0.97
1:AA:1756:U:O3'	53:B5:2263:C:C1'	1.98	0.97
1:AA:1756:U:C2'	53:B5:2263:C:OP1	2.12	0.97
1:AA:1756:U:O2'	53:B5:2263:C:O5'	1.80	0.97
1:AA:971:G:N2	53:B5:846:A:N6	2.12	0.96
12:AM:110:ARG:CZ	34:BJ:116:TYR:CZ	2.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:972:A:C5'	53:B5:848:A:C2	2.49	0.96
1:AA:1655:U:O2	53:B5:2124:G:N2	1.99	0.96
1:AA:701:U:O4	40:BP:169:ALA:O	1.80	0.96
1:AA:699:U:C2	40:BP:167:ALA:O	2.20	0.95
17:AR:40:LYS:HE2	17:AR:66:HIS:HA	1.48	0.95
37:BM:108:ILE:HG22	37:BM:160:ALA:HB2	1.46	0.95
1:AA:1502:G:C4	1:AA:1547:C:N4	2.35	0.94
17:AR:34:LEU:CG	17:AR:42:LEU:HD11	1.97	0.94
17:AR:286:GLU:HG3	17:AR:305:TYR:CG	2.02	0.94
17:AR:164:ASP:CB	17:AR:168:THR:HA	1.97	0.94
37:BM:151:ALA:O	37:BM:155:ALA:HB3	1.66	0.94
17:AR:257:ALA:CA	17:AR:283:LYS:HD2	1.97	0.93
1:AA:1735:G:C4'	53:B5:1933:A:O2'	2.16	0.93
1:AA:1776:G:C5'	53:B5:2194:G:H5''	1.92	0.93
19:A7:63:C:H5''	25:BA:45:ARG:HD2	1.49	0.93
1:AA:1520:U:H4'	1:AA:1522:A:C8	2.03	0.93
1:AA:865:A:OP1	1:AA:865:A:H8	1.51	0.93
1:AA:1657:A:H5''	42:BR:67:PRO:HD2	1.48	0.93
1:AA:1735:G:H4'	53:B5:1933:A:HO2'	1.31	0.93
1:AA:1776:G:H5''	53:B5:2194:G:H5'	0.94	0.93
1:AA:1521:G:C2	18:AT:78:LYS:HB2	2.02	0.93
17:AR:46:LYS:HB2	17:AR:58:VAL:CG1	1.98	0.93
1:AA:1653:A:H2	53:B5:2301:U:HO2'	1.09	0.93
17:AR:164:ASP:HB3	17:AR:183:LEU:H	1.33	0.92
37:BM:155:ALA:O	37:BM:158:ALA:N	2.01	0.92
1:AA:702:G:C5	40:BP:172:ALA:C	2.47	0.92
17:AR:36:ALA:HB1	17:AR:68:VAL:HG13	1.46	0.92
1:AA:993:G:C5'	53:B5:2195:C:OP2	2.17	0.92
1:AA:702:G:N9	40:BP:175:ALA:HB3	1.84	0.92
1:AA:1501:A:C5	1:AA:1546:G:N9	2.37	0.92
1:AA:702:G:N3	40:BP:176:ALA:CB	2.30	0.92
12:AM:110:ARG:CD	34:BJ:116:TYR:CD1	2.53	0.92
17:AR:156:VAL:HB	17:AR:167:VAL:CG2	2.00	0.92
1:AA:1655:U:C5	53:B5:2329:C:H1'	2.05	0.92
17:AR:83:ALA:HB2	17:AR:113:VAL:CG1	1.99	0.92
1:AA:1501:A:C6	1:AA:1546:G:C5	2.57	0.92
1:AA:1756:U:C1'	53:B5:2263:C:OP1	2.18	0.92
23:B8:43:LYS:NZ	35:BK:121:PHE:CD1	2.38	0.92
1:AA:1755:G:C2'	53:B5:2262:A:H2	1.83	0.91
1:AA:1501:A:C2	1:AA:1546:G:N7	2.25	0.91
1:AA:1657:A:C5'	42:BR:67:PRO:CD	2.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1744:A:C5	53:B5:2303:A:OP2	2.24	0.91
1:AA:1460:G:O3'	19:A7:30:G:O4'	1.87	0.91
17:AR:258:THR:CG2	17:AR:261:LYS:HE2	2.00	0.91
17:AR:286:GLU:HB3	17:AR:288:HIS:H	1.36	0.91
19:A7:56:C:C5	53:B5:2484:A:H1'	2.06	0.91
1:AA:1521:G:H22	18:AT:78:LYS:NZ	1.69	0.90
1:AA:1756:U:O3'	53:B5:2263:C:H4'	1.42	0.90
17:AR:259:GLY:HA2	17:AR:284:ALA:CA	2.00	0.90
8:AI:93:HIS:CE1	17:AR:59:ARG:NH2	2.40	0.90
14:AO:149:LEU:CD1	53:B5:847:A:P	2.58	0.90
1:AA:1460:G:C4'	19:A7:30:G:H5'	2.02	0.90
23:B8:43:LYS:CE	35:BK:121:PHE:CD1	2.55	0.90
1:AA:1744:A:N7	53:B5:2303:A:OP2	1.89	0.90
1:AA:1756:U:O3'	53:B5:2263:C:O4'	1.89	0.89
17:AR:283:LYS:HD3	17:AR:288:HIS:HA	1.54	0.89
17:AR:61:PHE:CE2	17:AR:97:GLY:HA2	2.06	0.89
8:AI:93:HIS:HE1	17:AR:59:ARG:HH22	1.09	0.89
17:AR:266:ASP:HB3	17:AR:267:PRO:HD3	1.52	0.89
1:AA:1521:G:H1	18:AT:78:LYS:HG3	1.07	0.89
1:AA:800:U:OP1	40:BP:160:ALA:CB	2.21	0.89
1:AA:701:U:O2	40:BP:174:ALA:N	2.04	0.88
17:AR:93:ASP:HB3	17:AR:96:THR:CG2	2.03	0.88
1:AA:972:A:O4'	53:B5:847:A:H2	1.56	0.88
1:AA:972:A:O4'	53:B5:847:A:C2	2.25	0.88
1:AA:1520:U:H4'	1:AA:1522:A:N7	1.86	0.88
1:AA:1757:C:OP1	53:B5:2264:U:C5'	2.21	0.88
1:AA:1632:C:C4'	1:AA:1633:A:OP2	2.21	0.88
17:AR:257:ALA:HA	17:AR:283:LYS:CD	2.01	0.88
1:AA:922:A:C5'	26:BB:109:GLU:OE1	2.21	0.88
1:AA:1200:A:N1	13:AN:16:LYS:CA	2.37	0.88
1:AA:1502:G:C4	1:AA:1547:C:C4	2.62	0.88
1:AA:1121:A:O4'	53:B5:2191:U:H5'	1.73	0.88
1:AA:1756:U:H2'	53:B5:2263:C:C5'	2.02	0.88
37:BM:151:ALA:O	37:BM:155:ALA:HB2	1.73	0.88
1:AA:1521:G:H1'	18:AT:86:ARG:HH22	1.35	0.88
17:AR:164:ASP:CG	17:AR:182:ASN:HA	1.98	0.88
1:AA:1521:G:H22	18:AT:78:LYS:HZ2	1.18	0.88
1:AA:1777:U:OP1	53:B5:2194:G:H1'	1.72	0.88
17:AR:283:LYS:HD3	17:AR:288:HIS:CA	2.04	0.88
17:AR:286:GLU:HG2	17:AR:289:ALA:CA	2.04	0.88
17:AR:38:ARG:HA	17:AR:67:ILE:CG2	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B8:43:LYS:HB2	35:BK:121:PHE:CD1	2.10	0.87
1:AA:1121:A:C1'	53:B5:2191:U:H5''	1.77	0.87
1:AA:1501:A:N9	1:AA:1546:G:N3	2.23	0.87
17:AR:260:ILE:HG13	17:AR:284:ALA:CB	2.03	0.87
17:AR:197:SER:CB	17:AR:216:LYS:HB3	2.04	0.87
1:AA:1521:G:N2	18:AT:78:LYS:CG	2.34	0.87
17:AR:89:LEU:HD21	17:AR:124:SER:HB3	1.53	0.87
1:AA:856:A:C5	7:AH:32:LYS:HA	2.08	0.87
1:AA:1521:G:N2	18:AT:78:LYS:HG3	1.90	0.87
37:BM:108:ILE:HG23	37:BM:160:ALA:HB2	1.42	0.87
1:AA:1756:U:H2'	53:B5:2263:C:H5'	1.57	0.86
23:B8:43:LYS:HE3	35:BK:121:PHE:HD1	1.40	0.86
17:AR:283:LYS:CB	17:AR:288:HIS:HA	2.05	0.86
23:B8:43:LYS:CG	35:BK:121:PHE:CE1	2.58	0.86
1:AA:1757:C:OP1	53:B5:2264:U:H5'	1.76	0.86
17:AR:52:GLN:HE21	17:AR:52:GLN:HA	1.41	0.86
1:AA:702:G:C5	40:BP:172:ALA:CB	2.41	0.86
1:AA:865:A:OP1	1:AA:865:A:C8	2.28	0.86
1:AA:922:A:OP1	26:BB:109:GLU:OE2	1.93	0.86
1:AA:1516:C:OP2	1:AA:1516:C:H6	1.57	0.86
1:AA:1744:A:N3	53:B5:2302:G:O5'	2.04	0.86
37:BM:111:PRO:HB3	37:BM:163:ALA:CB	1.99	0.86
1:AA:1776:G:OP1	53:B5:2193:U:H5'	1.72	0.85
17:AR:164:ASP:O	17:AR:183:LEU:HB2	1.75	0.85
1:AA:699:U:H3	40:BP:171:ALA:H	1.24	0.85
1:AA:701:U:C2'	40:BP:176:ALA:O	2.23	0.85
1:AA:1574:A:C2	19:A7:41:U:H4'	2.08	0.85
1:AA:699:U:H2'	40:BP:169:ALA:C	2.00	0.85
12:AM:110:ARG:CZ	34:BJ:116:TYR:CD1	2.57	0.85
17:AR:164:ASP:CG	17:AR:168:THR:HG22	2.02	0.85
17:AR:165:ASP:HB2	17:AR:183:LEU:O	1.77	0.85
17:AR:281:TYR:O	17:AR:287:PRO:HA	1.76	0.85
17:AR:283:LYS:CG	17:AR:288:HIS:HA	2.06	0.85
1:AA:1000:U:OP1	19:A7:38:A:C5'	2.24	0.85
1:AA:1501:A:N9	1:AA:1546:G:C2	2.45	0.85
1:AA:1653:A:C5	53:B5:2302:G:H5''	2.08	0.85
17:AR:164:ASP:HB3	17:AR:183:LEU:N	1.91	0.84
1:AA:1777:U:OP1	53:B5:2194:G:C1'	2.24	0.84
1:AA:799:A:C4'	40:BP:161:ALA:C	2.47	0.84
17:AR:209:THR:HG23	17:AR:210:LEU:CD2	2.05	0.84
17:AR:29:GLN:HB2	17:AR:296:ALA:HB3	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1734:G:N2	53:B5:1934:G:H4'	1.91	0.84
17:AR:164:ASP:CB	17:AR:183:LEU:H	1.90	0.84
17:AR:193:ILE:HD13	17:AR:193:ILE:H	1.42	0.84
1:AA:856:A:N1	7:AH:32:LYS:C	2.36	0.84
37:BM:150:ALA:O	37:BM:154:ALA:N	2.10	0.83
1:AA:702:G:H8	40:BP:175:ALA:HB3	1.36	0.83
17:AR:288:HIS:HB3	17:AR:306:THR:CG2	2.09	0.83
17:AR:33:LEU:CD2	17:AR:45:TRP:HB2	2.08	0.83
17:AR:197:SER:HB3	17:AR:216:LYS:HB3	1.59	0.83
1:AA:858:G:N3	7:AH:61:ILE:CB	2.41	0.83
17:AR:169:ILE:HG13	17:AR:183:LEU:HD21	1.60	0.83
37:BM:168:ALA:C	37:BM:171:ALA:HB3	2.04	0.83
1:AA:699:U:C4'	40:BP:169:ALA:HB3	2.09	0.83
19:A7:71:G:H5'	53:B5:2236:G:C4'	2.08	0.83
1:AA:1200:A:N3	13:AN:16:LYS:CA	2.42	0.82
1:AA:1653:A:H2	53:B5:2301:U:O2'	1.61	0.82
17:AR:262:VAL:HG23	17:AR:271:VAL:HG12	1.61	0.82
17:AR:133:VAL:HG13	17:AR:141:LEU:HB2	1.60	0.82
1:AA:1339:C:H5'	17:AR:102:ARG:NH2	1.94	0.82
1:AA:699:U:N3	40:BP:167:ALA:O	2.13	0.82
1:AA:921:G:H1'	26:BB:141:PRO:HG3	1.59	0.82
17:AR:21:THR:HG21	17:AR:68:VAL:O	1.79	0.82
23:B8:43:LYS:HE3	35:BK:121:PHE:CD1	2.14	0.82
17:AR:163:ASP:HB2	17:AR:165:ASP:O	1.80	0.82
17:AR:203:THR:HG22	17:AR:212:ALA:HB3	1.62	0.82
17:AR:276:PRO:N	17:AR:285:ALA:HA	1.95	0.82
12:AM:110:ARG:HE	34:BJ:116:TYR:HE1	1.18	0.81
17:AR:305:TYR:CZ	17:AR:311:ARG:HB2	2.15	0.81
1:AA:1665:A:O4'	53:B5:1935:G:C5'	2.28	0.81
17:AR:177:MET:SD	17:AR:191:ASP:HB2	2.20	0.81
17:AR:34:LEU:CD2	17:AR:42:LEU:HD21	2.10	0.81
1:AA:1573:G:N1	19:A7:41:U:O2'	1.93	0.81
1:AA:856:A:N3	7:AH:32:LYS:C	2.39	0.81
1:AA:702:G:C1'	40:BP:175:ALA:CB	2.58	0.81
17:AR:38:ARG:HG2	17:AR:67:ILE:HG21	1.62	0.81
1:AA:699:U:H2'	40:BP:170:ALA:N	1.95	0.80
37:BM:148:LYS:HB2	37:BM:149:ALA:CB	2.11	0.80
1:AA:702:G:N9	40:BP:172:ALA:O	2.14	0.80
1:AA:1501:A:C8	1:AA:1546:G:C2'	2.62	0.80
17:AR:164:ASP:HB3	17:AR:182:ASN:HA	1.62	0.80
1:AA:702:G:N7	40:BP:172:ALA:CA	2.42	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1501:A:H1'	1:AA:1546:G:N1	1.95	0.80
1:AA:1521:G:N3	18:AT:78:LYS:HB2	1.90	0.80
17:AR:283:LYS:CD	17:AR:288:HIS:HA	2.10	0.80
19:A7:56:C:C6	53:B5:2484:A:H1'	2.17	0.80
1:AA:1665:A:P	53:B5:1935:G:O2'	2.39	0.80
1:AA:1776:G:C5'	53:B5:2194:G:OP1	2.30	0.80
1:AA:700:C:C6	40:BP:173:ALA:HB3	2.17	0.80
17:AR:283:LYS:HD3	17:AR:288:HIS:CG	2.16	0.80
1:AA:1655:U:O4	53:B5:2328:U:O2	1.99	0.80
17:AR:96:THR:HG23	17:AR:98:GLU:H	1.45	0.80
1:AA:1653:A:C2'	53:B5:2302:G:OP2	2.29	0.79
17:AR:164:ASP:CB	17:AR:182:ASN:HA	2.11	0.79
1:AA:699:U:C2'	40:BP:169:ALA:CB	2.56	0.79
1:AA:856:A:N1	7:AH:33:VAL:N	2.31	0.79
1:AA:1521:G:O2'	18:AT:83:ALA:CA	2.30	0.79
17:AR:285:ALA:HB3	17:AR:313:TRP:CZ2	2.17	0.79
1:AA:921:G:C4'	26:BB:141:PRO:HD3	2.09	0.79
23:B8:43:LYS:CD	35:BK:121:PHE:CE1	2.66	0.79
1:AA:1657:A:H5''	42:BR:67:PRO:HD3	1.64	0.79
17:AR:115:ILE:CG2	17:AR:119:ALA:HA	2.13	0.78
1:AA:1573:G:H1	19:A7:41:U:HO2'	0.80	0.78
1:AA:1775:G:O3'	53:B5:2193:U:OP1	2.00	0.78
1:AA:1776:G:P	53:B5:2193:U:H5''	2.23	0.78
17:AR:83:ALA:HB1	17:AR:110:VAL:CG1	2.12	0.78
1:AA:1516:C:OP2	1:AA:1516:C:C6	2.36	0.78
1:AA:1521:G:N2	18:AT:78:LYS:CE	2.46	0.78
1:AA:856:A:C5	7:AH:32:LYS:CA	2.66	0.78
17:AR:211:ILE:HD11	17:AR:225:LEU:CD1	2.09	0.78
1:AA:699:U:C3'	40:BP:169:ALA:HB1	1.94	0.77
17:AR:13:LEU:HD11	17:AR:54:PHE:HB3	1.64	0.77
1:AA:1200:A:C6	13:AN:16:LYS:C	2.62	0.77
17:AR:40:LYS:HG2	17:AR:66:HIS:C	2.08	0.77
1:AA:1744:A:H4'	53:B5:2291:A:C1'	2.13	0.77
1:AA:1200:A:N3	13:AN:16:LYS:N	2.33	0.77
1:AA:1756:U:O2'	53:B5:2263:C:P	2.42	0.77
8:AI:97:VAL:HG21	17:AR:59:ARG:CZ	2.14	0.77
1:AA:1745:G:O3'	53:B5:2303:A:H3'	1.81	0.77
19:A7:63:C:H5''	25:BA:45:ARG:CD	2.14	0.77
37:BM:108:ILE:HG22	37:BM:160:ALA:CB	2.03	0.77
1:AA:856:A:N3	7:AH:33:VAL:N	2.33	0.77
1:AA:1521:G:H5''	1:AA:1522:A:OP1	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1736:U:H5'	53:B5:1932:A:H61	1.48	0.77
1:AA:700:C:C5	40:BP:169:ALA:O	2.36	0.77
1:AA:1502:G:C2	1:AA:1547:C:N4	2.54	0.76
1:AA:1521:G:N2	18:AT:78:LYS:HZ2	1.78	0.76
1:AA:1573:G:C4	19:A7:42:G:OP1	2.34	0.76
17:AR:286:GLU:HA	17:AR:305:TYR:CD2	2.19	0.76
37:BM:111:PRO:HA	37:BM:163:ALA:HB3	1.60	0.76
17:AR:286:GLU:HG3	17:AR:305:TYR:CD2	2.20	0.76
1:AA:698:U:C2	40:BP:164:ALA:C	2.57	0.76
1:AA:1501:A:N9	1:AA:1546:G:C4	2.53	0.76
17:AR:165:ASP:HB2	17:AR:183:LEU:C	2.10	0.76
1:AA:702:G:C1'	40:BP:175:ALA:HB3	2.16	0.76
17:AR:173:GLY:H	17:AR:199:ILE:CG2	1.99	0.76
17:AR:275:ARG:C	17:AR:285:ALA:HA	2.11	0.76
17:AR:286:GLU:HB3	17:AR:288:HIS:N	2.00	0.76
1:AA:702:G:N3	40:BP:172:ALA:O	2.18	0.76
17:AR:170:ILE:HG22	17:AR:202:LEU:HD13	1.68	0.76
1:AA:1200:A:N1	13:AN:16:LYS:N	2.33	0.76
1:AA:1338:A:O3'	17:AR:102:ARG:CZ	2.33	0.76
8:AI:97:VAL:HG21	17:AR:59:ARG:NH2	1.99	0.75
17:AR:164:ASP:CA	17:AR:183:LEU:H	1.98	0.75
17:AR:19:TRP:CB	17:AR:38:ARG:HD2	2.16	0.75
1:AA:1502:G:C4	1:AA:1547:C:N3	2.54	0.75
1:AA:1000:U:H5'	19:A7:38:A:OP1	1.86	0.75
1:AA:1521:G:H1'	18:AT:86:ARG:HH21	1.52	0.75
17:AR:172:ALA:CB	17:AR:199:ILE:HD12	2.16	0.75
1:AA:1520:U:C4'	1:AA:1522:A:N7	2.49	0.75
17:AR:164:ASP:HB3	17:AR:182:ASN:CA	2.16	0.75
17:AR:288:HIS:HB3	17:AR:306:THR:HG23	1.69	0.75
17:AR:305:TYR:OH	17:AR:311:ARG:HB2	1.86	0.75
17:AR:13:LEU:CD1	17:AR:54:PHE:HB3	2.16	0.75
17:AR:33:LEU:HD23	17:AR:45:TRP:HB2	1.66	0.75
1:AA:701:U:O4	40:BP:172:ALA:CB	2.26	0.75
1:AA:1776:G:H4'	53:B5:2194:G:H5''	0.79	0.75
17:AR:86:ASP:OD1	17:AR:88:THR:HG22	1.87	0.75
1:AA:1519:G:H4'	1:AA:1520:U:OP1	1.87	0.75
1:AA:1635:C:H5'	1:AA:1636:G:OP2	1.87	0.75
1:AA:1657:A:C4'	42:BR:67:PRO:HG2	2.17	0.75
1:AA:1756:U:C4'	53:B5:2262:A:N3	2.49	0.75
1:AA:701:U:O4	40:BP:169:ALA:HA	1.87	0.74
1:AA:1502:G:C5	1:AA:1547:C:N4	2.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1521:G:C2	18:AT:78:LYS:CD	2.66	0.74
17:AR:114:ASP:OD1	17:AR:123:ILE:HG13	1.87	0.74
17:AR:126:SER:HB3	17:AR:128:ASP:OD1	1.87	0.74
8:AI:93:HIS:HE1	17:AR:59:ARG:NH2	1.82	0.74
17:AR:173:GLY:O	17:AR:199:ILE:HG22	1.87	0.74
17:AR:46:LYS:HB2	17:AR:58:VAL:HG13	1.69	0.74
1:AA:1757:C:OP1	53:B5:2264:U:O5'	2.05	0.74
1:AA:1501:A:C4	1:AA:1546:G:C2	2.74	0.74
17:AR:41:THR:HG23	17:AR:61:PHE:O	1.88	0.74
1:AA:1665:A:P	53:B5:1936:A:H5'	2.27	0.74
1:AA:1756:U:H2'	53:B5:2263:C:OP1	1.87	0.74
17:AR:19:TRP:HB3	17:AR:38:ARG:HD2	1.70	0.74
1:AA:701:U:O4	40:BP:172:ALA:HB3	1.33	0.74
17:AR:44:SER:O	17:AR:58:VAL:HG22	1.87	0.74
17:AR:219:GLU:OE2	17:AR:221:MET:HE3	1.87	0.74
14:AO:123:HIS:CE1	53:B5:846:A:N3	2.56	0.73
37:BM:147:TRP:CZ2	37:BM:153:ALA:CB	2.70	0.73
1:AA:1521:G:C4	18:AT:79:LEU:N	2.55	0.73
1:AA:1521:G:H4'	1:AA:1522:A:OP1	1.88	0.73
17:AR:36:ALA:HB1	17:AR:68:VAL:CG1	2.18	0.73
17:AR:42:LEU:HD13	17:AR:43:ILE:N	2.03	0.73
1:AA:702:G:O6	40:BP:172:ALA:HB2	1.82	0.73
1:AA:1521:G:C5'	1:AA:1522:A:OP1	2.34	0.73
17:AR:203:THR:HG23	17:AR:245:PHE:HE1	1.54	0.73
1:AA:799:A:N3	40:BP:161:ALA:HB3	1.99	0.73
37:BM:147:TRP:HZ2	37:BM:153:ALA:CB	2.02	0.73
1:AA:699:U:C2'	40:BP:170:ALA:N	2.50	0.72
1:AA:972:A:C1'	53:B5:847:A:H2	2.01	0.72
17:AR:262:VAL:HG22	17:AR:272:ASP:O	1.89	0.72
1:AA:700:C:H5	40:BP:169:ALA:O	1.55	0.72
17:AR:199:ILE:HD11	17:AR:201:THR:O	1.90	0.72
17:AR:222:LEU:HD13	17:AR:232:TYR:OH	1.89	0.72
1:AA:1501:A:C4	1:AA:1546:G:N3	2.57	0.72
1:AA:799:A:H4'	40:BP:161:ALA:O	1.87	0.72
1:AA:1653:A:H2	53:B5:2301:U:C2'	1.96	0.72
23:B8:43:LYS:CE	35:BK:121:PHE:CE1	2.73	0.72
23:B8:43:LYS:CB	35:BK:121:PHE:CE1	2.73	0.72
17:AR:172:ALA:HB2	17:AR:202:LEU:HG	1.70	0.71
17:AR:34:LEU:CD2	17:AR:42:LEU:HD11	2.19	0.71
17:AR:34:LEU:HD11	17:AR:80:ALA:HB1	1.71	0.71
17:AR:172:ALA:HB1	17:AR:199:ILE:HD12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AM:110:ARG:NH2	34:BJ:116:TYR:CE1	2.50	0.71
17:AR:164:ASP:OD2	17:AR:168:THR:HG22	1.90	0.71
17:AR:283:LYS:HB3	17:AR:288:HIS:HA	1.73	0.71
17:AR:115:ILE:HG22	17:AR:116:ASP:O	1.90	0.71
1:AA:698:U:C6	40:BP:164:ALA:C	2.62	0.71
17:AR:207:ASP:HB3	17:AR:209:THR:HG22	1.72	0.71
1:AA:1461:C:P	19:A7:30:G:H1'	2.31	0.71
1:AA:1633:A:O3'	1:AA:1634:C:H4'	1.91	0.71
1:AA:1657:A:H4'	42:BR:67:PRO:HG2	1.73	0.71
12:AM:110:ARG:CZ	34:BJ:116:TYR:CE2	2.71	0.71
17:AR:66:HIS:CE1	17:AR:67:ILE:HD13	2.26	0.71
1:AA:1756:U:O4'	53:B5:2262:A:C2	2.42	0.71
1:AA:1776:G:O3'	53:B5:2194:G:C5'	2.38	0.70
1:AA:702:G:H8	40:BP:175:ALA:CB	1.93	0.70
1:AA:698:U:C5	40:BP:164:ALA:O	2.43	0.70
1:AA:1573:G:N3	19:A7:41:U:H5''	2.06	0.70
1:AA:1501:A:C1'	1:AA:1546:G:N3	2.53	0.70
17:AR:286:GLU:CD	17:AR:289:ALA:HB2	2.15	0.70
37:BM:108:ILE:HG21	37:BM:160:ALA:HB1	1.73	0.70
1:AA:1121:A:H4'	53:B5:2191:U:H5'	1.74	0.70
17:AR:96:THR:HG23	17:AR:98:GLU:N	2.05	0.70
17:AR:283:LYS:HD3	17:AR:288:HIS:CB	2.22	0.70
17:AR:285:ALA:HB3	17:AR:313:TRP:HZ2	1.54	0.70
1:AA:1461:C:OP1	19:A7:30:G:C1'	2.32	0.70
1:AA:702:G:OP1	40:BP:177:ALA:HA	1.91	0.70
1:AA:857:U:H2'	1:AA:858:G:O5'	1.91	0.70
1:AA:1502:G:O6	1:AA:1547:C:C5	2.45	0.70
17:AR:34:LEU:HG	17:AR:42:LEU:CD1	2.14	0.70
17:AR:263:PHE:CE1	17:AR:270:LEU:HG	2.26	0.70
1:AA:699:U:N3	40:BP:167:ALA:C	2.50	0.69
1:AA:1502:G:C8	1:AA:1547:C:O2	2.45	0.69
1:AA:799:A:H4'	40:BP:161:ALA:C	2.16	0.69
1:AA:856:A:C2	7:AH:32:LYS:O	2.45	0.69
17:AR:275:ARG:HB3	17:AR:276:PRO:HD2	1.75	0.69
1:AA:1521:G:H22	18:AT:78:LYS:CE	2.04	0.69
1:AA:1756:U:H4'	53:B5:2262:A:C4	2.28	0.69
17:AR:26:SER:HB2	17:AR:30:PRO:HD2	1.75	0.69
17:AR:34:LEU:HD12	17:AR:73:LEU:HD21	1.75	0.69
17:AR:26:SER:CB	17:AR:30:PRO:HD2	2.23	0.69
17:AR:170:ILE:CG2	17:AR:202:LEU:HD13	2.23	0.69
1:AA:1390:C:OP2	17:AR:281:TYR:OH	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:135:THR:HG23	17:AR:137:LYS:H	1.58	0.69
17:AR:164:ASP:H	17:AR:168:THR:N	1.91	0.68
17:AR:203:THR:HG23	17:AR:245:PHE:CE1	2.28	0.68
23:B8:43:LYS:NZ	35:BK:121:PHE:HE1	1.88	0.68
17:AR:173:GLY:H	17:AR:199:ILE:HG23	1.57	0.68
1:AA:702:G:H1'	40:BP:175:ALA:HB1	1.70	0.68
14:AO:149:LEU:CD1	53:B5:846:A:O3'	2.42	0.68
1:AA:1630:C:H5''	1:AA:1636:G:H21	1.51	0.68
17:AR:283:LYS:HE2	17:AR:289:ALA:N	2.09	0.68
32:BH:40:HIS:CG	32:BH:41:ILE:H	2.11	0.68
1:AA:1521:G:C2	18:AT:78:LYS:HD2	2.29	0.68
17:AR:211:ILE:CD1	17:AR:225:LEU:HD13	2.09	0.68
1:AA:701:U:O4	40:BP:169:ALA:C	2.35	0.68
17:AR:314:GLN:HG2	17:AR:315:VAL:N	2.09	0.68
1:AA:699:U:O4'	40:BP:169:ALA:HB3	1.93	0.68
17:AR:87:LYS:HD2	17:AR:106:HIS:O	1.93	0.68
17:AR:240:VAL:HG22	17:AR:256:THR:HG22	1.75	0.68
17:AR:276:PRO:CA	17:AR:285:ALA:HA	2.24	0.68
17:AR:164:ASP:C	17:AR:183:LEU:HB2	2.19	0.67
17:AR:170:ILE:HG22	17:AR:202:LEU:CD1	2.24	0.67
17:AR:34:LEU:HD21	17:AR:71:CYS:SG	2.33	0.67
17:AR:169:ILE:CG1	17:AR:183:LEU:HD21	2.25	0.67
17:AR:257:ALA:O	17:AR:283:LYS:HA	1.95	0.67
1:AA:1521:G:C4'	1:AA:1522:A:OP1	2.37	0.67
17:AR:33:LEU:HD23	17:AR:33:LEU:H	1.59	0.67
37:BM:107:GLY:HA3	37:BM:156:ALA:HB1	1.77	0.67
1:AA:1516:C:C2'	1:AA:1517:U:O5'	2.42	0.67
1:AA:1390:C:P	17:AR:281:TYR:OH	2.50	0.67
17:AR:259:GLY:HA2	17:AR:284:ALA:N	2.08	0.67
37:BM:168:ALA:O	37:BM:172:ALA:N	2.28	0.67
17:AR:199:ILE:HD11	17:AR:202:LEU:HD23	1.77	0.67
17:AR:259:GLY:CA	17:AR:284:ALA:HA	2.22	0.66
17:AR:10:ARG:HG2	17:AR:54:PHE:CE1	2.30	0.66
17:AR:32:LEU:HD22	17:AR:32:LEU:O	1.95	0.66
17:AR:86:ASP:CG	17:AR:88:THR:HG22	2.19	0.66
37:BM:150:ALA:O	37:BM:154:ALA:HB3	1.96	0.66
17:AR:21:THR:HA	17:AR:290:VAL:HG11	1.78	0.66
17:AR:285:ALA:O	17:AR:305:TYR:HE2	1.78	0.66
17:AR:12:THR:HG22	17:AR:311:ARG:CG	2.23	0.66
17:AR:203:THR:CG2	17:AR:212:ALA:HB3	2.25	0.66
17:AR:238:ASP:CG	17:AR:258:THR:HB	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1502:G:N3	1:AA:1547:C:N4	2.44	0.66
1:AA:1756:U:H4'	53:B5:2263:C:H1'	1.77	0.66
17:AR:67:ILE:O	17:AR:84:SER:HB2	1.95	0.65
17:AR:83:ALA:HB1	17:AR:110:VAL:HG12	1.75	0.65
1:AA:921:G:C1'	26:BB:141:PRO:HG3	2.26	0.65
17:AR:93:ASP:CB	17:AR:96:THR:HG22	2.23	0.65
12:AM:110:ARG:NE	34:BJ:116:TYR:CG	2.60	0.65
17:AR:11:GLY:N	17:AR:312:VAL:HG23	2.11	0.65
17:AR:32:LEU:HD13	17:AR:32:LEU:N	2.11	0.65
17:AR:46:LYS:HB2	17:AR:58:VAL:HG11	1.76	0.65
17:AR:81:LEU:HD13	17:AR:91:LEU:HD23	1.78	0.65
1:AA:629:U:H5'	53:B5:846:A:H1'	1.78	0.65
23:B8:43:LYS:CE	35:BK:121:PHE:HD1	2.01	0.65
17:AR:260:ILE:CG1	17:AR:284:ALA:HB1	2.23	0.65
1:AA:1521:G:N7	18:AT:79:LEU:N	2.44	0.65
17:AR:209:THR:CG2	17:AR:210:LEU:HD22	2.10	0.65
17:AR:35:SER:O	17:AR:42:LEU:HD22	1.97	0.65
17:AR:196:ASN:HD21	17:AR:217:ASP:HB2	1.61	0.65
17:AR:38:ARG:O	17:AR:67:ILE:HG13	1.96	0.65
17:AR:283:LYS:HG2	17:AR:284:ALA:H	1.61	0.65
12:AM:110:ARG:CZ	34:BJ:116:TYR:CG	2.80	0.65
17:AR:33:LEU:HD22	17:AR:47:LEU:HD21	1.78	0.64
19:A7:19:G:N7	53:B5:2454:G:C8	2.65	0.64
1:AA:702:G:P	40:BP:177:ALA:HA	2.38	0.64
1:AA:1756:U:H1'	53:B5:2263:C:OP1	1.96	0.64
17:AR:164:ASP:H	17:AR:167:VAL:C	2.05	0.64
17:AR:34:LEU:HD21	17:AR:42:LEU:CD2	2.16	0.64
17:AR:74:THR:HG22	17:AR:79:TYR:H	1.61	0.64
1:AA:1502:G:C6	1:AA:1547:C:N4	2.65	0.64
1:AA:1736:U:C5'	53:B5:1932:A:H61	2.11	0.64
17:AR:7:LEU:HA	17:AR:315:VAL:CG2	2.28	0.64
17:AR:7:LEU:HA	17:AR:315:VAL:HG22	1.78	0.64
1:AA:1460:G:H4'	19:A7:30:G:C5'	2.26	0.64
1:AA:921:G:H5''	26:BB:140:ASN:HD21	1.62	0.64
17:AR:22:SER:O	17:AR:23:LEU:HD23	1.98	0.64
17:AR:90:ARG:NH1	17:AR:99:THR:HG21	2.12	0.64
17:AR:256:THR:O	17:AR:283:LYS:HE3	1.97	0.64
1:AA:1756:U:C2'	53:B5:2263:C:C5'	2.43	0.64
17:AR:34:LEU:HD11	17:AR:80:ALA:CB	2.28	0.64
1:AA:1755:G:HO2'	53:B5:2262:A:H2	0.65	0.63
17:AR:262:VAL:HG23	17:AR:272:ASP:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1630:C:H5'	1:AA:1636:G:N2	2.08	0.63
17:AR:274:LEU:HD13	17:AR:313:TRP:CD2	2.33	0.63
17:AR:286:GLU:HA	17:AR:305:TYR:HD2	1.63	0.63
1:AA:1501:A:O4'	1:AA:1546:G:N2	2.31	0.63
1:AA:1636:G:O6	1:AA:1762:C:O2	2.16	0.63
17:AR:13:LEU:N	17:AR:13:LEU:HD22	2.13	0.63
17:AR:40:LYS:HG2	17:AR:66:HIS:O	1.96	0.63
17:AR:274:LEU:O	17:AR:284:ALA:HA	1.99	0.63
1:AA:1756:U:C4'	53:B5:2262:A:C4	2.81	0.63
17:AR:214:ALA:HB1	17:AR:240:VAL:HB	1.81	0.63
1:AA:972:A:H5'	53:B5:848:A:H2	1.57	0.63
1:AA:1516:C:H2'	1:AA:1517:U:O5'	1.99	0.63
37:BM:168:ALA:O	37:BM:172:ALA:HB2	1.99	0.63
1:AA:1736:U:H5'	53:B5:1932:A:N6	2.13	0.63
1:AA:1776:G:C3'	53:B5:2194:G:H5''	2.26	0.62
17:AR:86:ASP:O	17:AR:87:LYS:HG2	1.99	0.62
17:AR:181:TRP:CZ3	17:AR:188:ILE:HB	2.34	0.62
1:AA:699:U:O2	40:BP:167:ALA:O	2.17	0.62
17:AR:21:THR:HG22	17:AR:36:ALA:C	2.23	0.62
1:AA:701:U:O4	40:BP:169:ALA:CA	2.47	0.62
17:AR:19:TRP:CZ3	17:AR:306:THR:HG22	2.34	0.62
17:AR:170:ILE:HD12	17:AR:170:ILE:N	2.14	0.62
1:AA:1120:C:O2'	53:B5:2190:U:H5''	1.99	0.62
1:AA:972:A:C4'	53:B5:847:A:C2	2.83	0.62
17:AR:238:ASP:OD2	17:AR:258:THR:HB	2.00	0.62
37:BM:168:ALA:CA	37:BM:171:ALA:HB3	2.29	0.62
1:AA:1460:G:O3'	19:A7:30:G:C4'	2.47	0.62
17:AR:178:VAL:HB	17:AR:192:PHE:HB2	1.81	0.62
1:AA:858:G:H3'	7:AH:27:ILE:HB	1.79	0.61
17:AR:175:ASP:O	17:AR:176:LYS:HG2	2.00	0.61
1:AA:921:G:H5''	26:BB:140:ASN:ND2	2.15	0.61
1:AA:1574:A:C2	19:A7:41:U:C1'	2.83	0.61
17:AR:286:GLU:HG2	17:AR:289:ALA:N	2.15	0.61
1:AA:1519:G:C4'	1:AA:1520:U:OP1	2.44	0.61
17:AR:283:LYS:HZ3	17:AR:288:HIS:CD2	2.18	0.61
17:AR:131:ILE:CD1	17:AR:151:VAL:HG11	2.31	0.61
17:AR:100:TYR:CD2	17:AR:101:GLN:HG3	2.36	0.61
17:AR:242:SER:OG	17:AR:292:LEU:HD22	2.01	0.61
17:AR:259:GLY:HA2	17:AR:283:LYS:C	2.25	0.61
1:AA:1653:A:C2	53:B5:2301:U:C2'	2.82	0.61
17:AR:256:THR:O	17:AR:283:LYS:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:288:HIS:HB3	17:AR:306:THR:HG21	1.82	0.61
1:AA:1121:A:H1'	53:B5:2191:U:OP1	2.01	0.61
17:AR:9:LEU:HD21	17:AR:311:ARG:HB3	1.83	0.61
17:AR:220:ILE:HD12	17:AR:220:ILE:N	2.16	0.61
17:AR:287:PRO:HG3	17:AR:307:ASP:HB3	1.83	0.61
1:AA:699:U:C4'	40:BP:166:ALA:HA	2.31	0.61
17:AR:276:PRO:HB2	17:AR:278:PHE:CE1	2.35	0.61
37:BM:111:PRO:HA	37:BM:163:ALA:HB1	0.62	0.61
37:BM:111:PRO:N	37:BM:163:ALA:HB1	2.04	0.61
1:AA:1665:A:OP1	53:B5:1935:G:O2'	2.19	0.61
17:AR:224:ASN:CG	17:AR:227:ALA:HB3	2.26	0.61
23:B8:43:LYS:CD	35:BK:121:PHE:HE1	2.12	0.61
17:AR:8:VAL:HG12	17:AR:9:LEU:N	2.16	0.60
17:AR:164:ASP:HB2	17:AR:168:THR:N	2.16	0.60
7:AH:32:LYS:C	7:AH:33:VAL:N	2.59	0.60
14:AO:149:LEU:CD1	53:B5:847:A:H5'	2.14	0.60
17:AR:144:LEU:N	17:AR:144:LEU:HD12	2.16	0.60
17:AR:30:PRO:HB2	17:AR:32:LEU:HD11	1.82	0.60
17:AR:222:LEU:HD23	17:AR:223:TRP:N	2.16	0.60
17:AR:223:TRP:CZ3	17:AR:230:ALA:HB2	2.37	0.60
17:AR:156:VAL:HB	17:AR:167:VAL:HG21	1.80	0.60
1:AA:701:U:H2'	40:BP:176:ALA:O	2.02	0.60
1:AA:1200:A:C2	13:AN:16:LYS:CB	2.84	0.60
17:AR:262:VAL:CG2	17:AR:271:VAL:HG12	2.31	0.60
17:AR:169:ILE:C	17:AR:169:ILE:HD12	2.27	0.60
17:AR:34:LEU:C	17:AR:34:LEU:HD23	2.27	0.59
17:AR:266:ASP:CB	17:AR:267:PRO:HD3	2.26	0.59
37:BM:111:PRO:HB3	37:BM:163:ALA:O	2.01	0.59
1:AA:1501:A:C8	1:AA:1546:G:C4	2.90	0.59
17:AR:41:THR:HG22	17:AR:42:LEU:N	2.17	0.59
17:AR:193:ILE:H	17:AR:193:ILE:CD1	2.12	0.59
1:AA:1579:C:H3'	8:AI:131:GLY:H	1.67	0.59
12:AM:110:ARG:CZ	34:BJ:116:TYR:CD2	2.86	0.59
17:AR:264:SER:HB3	17:AR:267:PRO:HD2	1.83	0.59
1:AA:1778:G:O5'	53:B5:2274:U:C5'	2.47	0.59
17:AR:11:GLY:O	17:AR:312:VAL:HG22	2.01	0.59
17:AR:33:LEU:HD23	17:AR:33:LEU:N	2.17	0.59
1:AA:699:U:C5'	40:BP:166:ALA:HA	2.32	0.59
1:AA:703:G:OP2	40:BP:176:ALA:HB1	2.01	0.59
1:AA:1521:G:H21	18:AT:78:LYS:NZ	2.00	0.59
17:AR:199:ILE:HD13	17:AR:199:ILE:C	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BM:111:PRO:CG	37:BM:163:ALA:HA	2.33	0.59
17:AR:222:LEU:HD23	17:AR:222:LEU:C	2.27	0.59
1:AA:864:U:H5''	1:AA:865:A:H5'	1.85	0.59
1:AA:995:U:OP1	53:B5:2197:C:OP2	2.21	0.59
17:AR:42:LEU:HD13	17:AR:43:ILE:H	1.68	0.59
17:AR:201:THR:O	17:AR:202:LEU:HD23	2.02	0.59
37:BM:111:PRO:CB	37:BM:163:ALA:C	2.68	0.59
1:AA:699:U:C2'	40:BP:169:ALA:C	2.72	0.59
53:B5:1018:G:H1	53:B5:1034:U:H3	1.51	0.59
17:AR:199:ILE:HD11	17:AR:202:LEU:CD2	2.32	0.59
17:AR:284:ALA:HB3	17:AR:286:GLU:OE1	2.01	0.59
1:AA:971:G:H21	53:B5:846:A:H62	1.43	0.59
1:AA:856:A:C6	7:AH:32:LYS:CA	2.85	0.58
1:AA:1200:A:C6	13:AN:16:LYS:HA	2.37	0.58
17:AR:31:ASN:C	17:AR:32:LEU:HD13	2.28	0.58
1:AA:1573:G:N2	19:A7:42:G:P	2.57	0.58
1:AA:1574:A:C5	19:A7:41:U:H4'	2.23	0.58
1:AA:1775:G:H5''	53:B5:2193:U:OP1	2.03	0.58
1:AA:1746:G:P	53:B5:2303:A:H3'	2.43	0.58
1:AA:1777:U:P	53:B5:2194:G:C4'	2.82	0.58
1:AA:1502:G:N9	1:AA:1547:C:N3	2.51	0.58
1:AA:1637:C:C2'	1:AA:1638:C:O5'	2.49	0.58
1:AA:1744:A:C2	53:B5:2302:G:H8	2.21	0.58
17:AR:72:THR:HG22	17:AR:73:LEU:N	2.18	0.58
17:AR:197:SER:HB2	17:AR:216:LYS:HB3	1.83	0.58
37:BM:148:LYS:HB2	37:BM:149:ALA:HB3	1.85	0.58
1:AA:1777:U:OP1	53:B5:2194:G:O2'	2.22	0.58
17:AR:42:LEU:HD21	17:AR:71:CYS:CB	2.34	0.58
1:AA:701:U:O2	40:BP:171:ALA:C	2.45	0.58
1:AA:972:A:P	53:B5:848:A:H2	2.27	0.58
1:AA:1637:C:H2'	1:AA:1638:C:O5'	2.04	0.58
17:AR:106:HIS:CE1	17:AR:132:LYS:HD2	2.39	0.58
17:AR:114:ASP:OD1	17:AR:154:VAL:HG23	2.03	0.58
17:AR:224:ASN:ND2	17:AR:227:ALA:HB3	2.19	0.58
1:AA:698:U:N3	40:BP:164:ALA:O	2.35	0.57
17:AR:33:LEU:HD21	17:AR:45:TRP:HB2	1.86	0.57
1:AA:1573:G:N2	19:A7:41:U:O5'	2.37	0.57
17:AR:135:THR:HG23	17:AR:137:LYS:N	2.18	0.57
17:AR:283:LYS:HG2	17:AR:289:ALA:H	1.69	0.57
1:AA:1390:C:P	17:AR:281:TYR:HH	2.28	0.57
17:AR:166:SER:O	17:AR:167:VAL:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:169:ILE:HD11	17:AR:181:TRP:CD1	2.40	0.57
1:AA:1501:A:N6	1:AA:1546:G:H8	1.97	0.57
17:AR:284:ALA:C	17:AR:286:GLU:H	2.13	0.57
17:AR:301:LEU:HB3	17:AR:313:TRP:HB2	1.85	0.57
1:AA:702:G:C4	40:BP:176:ALA:HB3	2.32	0.57
17:AR:22:SER:HA	17:AR:291:SER:OG	2.04	0.57
17:AR:164:ASP:H	17:AR:167:VAL:CA	2.17	0.57
17:AR:283:LYS:HE2	17:AR:289:ALA:O	2.04	0.57
27:BC:99:LEU:HD21	27:BC:159:ARG:HH22	1.68	0.57
1:AA:702:G:C4	40:BP:176:ALA:CB	2.88	0.57
1:AA:1521:G:O5'	1:AA:1522:A:OP2	2.23	0.57
17:AR:21:THR:HG22	17:AR:36:ALA:O	2.05	0.57
17:AR:262:VAL:HG23	17:AR:271:VAL:CG1	2.34	0.57
17:AR:34:LEU:HD11	17:AR:71:CYS:SG	2.45	0.57
37:BM:148:LYS:HB2	37:BM:149:ALA:HB2	1.84	0.57
37:BM:150:ALA:O	37:BM:154:ALA:CB	2.53	0.57
1:AA:701:U:O2	40:BP:171:ALA:O	2.22	0.57
17:AR:286:GLU:CG	17:AR:305:TYR:CD2	2.87	0.57
17:AR:31:ASN:HA	17:AR:47:LEU:HD12	1.87	0.56
1:AA:1756:U:C2'	53:B5:2263:C:P	2.94	0.56
17:AR:106:HIS:HA	17:AR:132:LYS:HE3	1.87	0.56
1:AA:702:G:C4	40:BP:172:ALA:C	2.62	0.56
1:AA:799:A:H5'	40:BP:165:ALA:N	2.20	0.56
17:AR:10:ARG:HB3	17:AR:312:VAL:HG23	1.88	0.56
17:AR:34:LEU:HD23	17:AR:35:SER:N	2.20	0.56
17:AR:83:ALA:CB	17:AR:113:VAL:HG13	2.25	0.56
17:AR:156:VAL:HB	17:AR:167:VAL:HG23	1.85	0.56
17:AR:141:LEU:HD12	17:AR:141:LEU:N	2.21	0.56
1:AA:972:A:C4'	53:B5:847:A:H2	2.18	0.56
17:AR:9:LEU:C	17:AR:9:LEU:HD13	2.29	0.56
20:B0:38:ILE:HG23	20:B0:39:ASP:H	1.69	0.56
17:AR:163:ASP:HA	17:AR:167:VAL:HA	1.87	0.56
17:AR:284:ALA:HB3	17:AR:289:ALA:HB2	1.86	0.56
1:AA:858:G:O4'	1:AA:858:G:OP2	2.24	0.56
17:AR:237:GLN:O	17:AR:237:GLN:HG2	2.06	0.56
1:AA:1777:U:H5''	53:B5:2194:G:O2'	2.05	0.56
1:AA:1756:U:H4'	53:B5:2262:A:C5	2.41	0.56
1:AA:1776:G:C3'	53:B5:2194:G:C5'	2.82	0.56
26:BB:50:HIS:H	53:B5:1796:G:H5''	1.71	0.56
1:AA:867:G:H5''	1:AA:868:G:OP2	2.06	0.56
1:AA:1777:U:C5'	53:B5:2194:G:O2'	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:275:ARG:HB3	17:AR:276:PRO:CD	2.35	0.56
17:AR:305:TYR:HB2	17:AR:309:VAL:O	2.06	0.56
37:BM:106:GLU:OE1	37:BM:153:ALA:O	2.24	0.56
1:AA:1461:C:P	19:A7:30:G:C1'	2.94	0.55
1:AA:1518:U:H5''	1:AA:1519:G:OP2	2.06	0.55
14:AO:149:LEU:HD12	53:B5:846:A:O3'	2.04	0.55
17:AR:179:LYS:HD3	17:AR:181:TRP:CZ2	2.41	0.55
17:AR:9:LEU:CD2	17:AR:311:ARG:HB3	2.36	0.55
17:AR:34:LEU:HD12	17:AR:73:LEU:CD2	2.35	0.55
1:AA:1631:A:OP1	1:AA:1636:G:O2'	2.13	0.55
17:AR:302:PHE:CD2	17:AR:312:VAL:HG12	2.42	0.55
1:AA:858:G:C4	7:AH:61:ILE:CG1	2.88	0.55
6:AG:72:HIS:CD2	6:AG:89:ILE:H	2.24	0.55
1:AA:972:A:H5''	53:B5:848:A:N3	2.14	0.55
17:AR:276:PRO:HB2	17:AR:278:PHE:CD1	2.40	0.55
18:AT:28:LEU:HD21	18:AT:111:ILE:HD11	1.88	0.55
1:AA:1734:G:H21	53:B5:1934:G:C4'	2.06	0.55
17:AR:210:LEU:HD12	17:AR:222:LEU:CD2	2.26	0.55
17:AR:283:LYS:CG	17:AR:284:ALA:H	2.19	0.55
1:AA:1756:U:H1'	53:B5:2262:A:O2'	2.05	0.55
17:AR:264:SER:CB	17:AR:267:PRO:HD2	2.37	0.55
23:B8:43:LYS:HB2	35:BK:121:PHE:CE1	2.41	0.55
17:AR:19:TRP:CG	17:AR:38:ARG:HD2	2.42	0.55
1:AA:1521:G:N2	18:AT:78:LYS:HZ3	2.03	0.54
17:AR:164:ASP:HB3	17:AR:182:ASN:C	2.31	0.54
17:AR:250:TYR:O	17:AR:265:LEU:HG	2.06	0.54
17:AR:256:THR:C	17:AR:283:LYS:HE3	2.32	0.54
19:A7:56:C:N4	53:B5:2484:A:N3	2.55	0.54
37:BM:155:ALA:O	37:BM:157:ALA:N	2.41	0.54
1:AA:1756:U:C5'	53:B5:2262:A:C6	2.88	0.54
17:AR:150:TRP:HB2	17:AR:174:ASN:ND2	2.22	0.54
1:AA:702:G:C5	40:BP:172:ALA:HA	2.23	0.54
1:AA:1501:A:C8	1:AA:1546:G:N3	2.76	0.54
1:AA:1521:G:C8	18:AT:79:LEU:N	2.75	0.54
17:AR:21:THR:HG23	17:AR:36:ALA:HB3	1.90	0.54
17:AR:188:ILE:HG23	17:AR:188:ILE:O	2.07	0.54
17:AR:315:VAL:HG12	17:AR:316:MET:N	2.22	0.54
1:AA:1200:A:C2	13:AN:16:LYS:HB2	2.42	0.54
1:AA:1735:G:C5'	53:B5:1933:A:O2'	2.56	0.54
17:AR:276:PRO:HA	17:AR:285:ALA:CA	2.38	0.54
1:AA:799:A:O3'	40:BP:164:ALA:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:262:VAL:HG23	17:AR:272:ASP:N	2.23	0.54
17:AR:199:ILE:HG23	17:AR:199:ILE:O	2.08	0.53
17:AR:248:ASN:ND2	17:AR:249:ARG:HG2	2.22	0.53
1:AA:858:G:C3'	7:AH:27:ILE:HB	2.38	0.53
1:AA:864:U:C5'	1:AA:865:A:H5'	2.37	0.53
17:AR:13:LEU:HB2	17:AR:310:ILE:HB	1.89	0.53
1:AA:1664:U:H1'	53:B5:1934:G:O2'	2.09	0.53
17:AR:270:LEU:N	17:AR:270:LEU:HD12	2.24	0.53
1:AA:1521:G:H21	18:AT:78:LYS:HZ3	1.56	0.53
37:BM:111:PRO:CG	37:BM:163:ALA:CB	2.87	0.53
1:AA:701:U:C4'	40:BP:173:ALA:HB1	2.05	0.53
17:AR:263:PHE:HE1	17:AR:270:LEU:CD1	2.22	0.53
17:AR:136:ILE:HG23	17:AR:137:LYS:N	2.23	0.53
17:AR:193:ILE:O	17:AR:223:TRP:HH2	1.91	0.53
17:AR:220:ILE:HB	17:AR:234:LEU:HB2	1.90	0.53
17:AR:170:ILE:HG22	17:AR:171:SER:N	2.24	0.53
19:A7:19:G:N1	53:B5:2454:G:C6	2.69	0.53
1:AA:1339:C:H5'	17:AR:102:ARG:HH21	1.68	0.53
17:AR:98:GLU:HG2	17:AR:99:THR:N	2.24	0.53
17:AR:164:ASP:H	17:AR:167:VAL:HA	1.74	0.53
17:AR:178:VAL:HG13	17:AR:202:LEU:HD11	1.91	0.53
17:AR:276:PRO:HB3	17:AR:286:GLU:N	2.23	0.53
21:B1:40:LYS:H	53:B5:355:A:H4'	1.74	0.53
1:AA:858:G:C2	7:AH:61:ILE:CA	2.92	0.52
1:AA:1744:A:N3	53:B5:2302:G:C8	2.77	0.52
17:AR:286:GLU:HG2	17:AR:288:HIS:C	2.34	0.52
19:A7:56:C:N4	53:B5:2484:A:C2	2.77	0.52
17:AR:172:ALA:HB1	17:AR:199:ILE:CD1	2.40	0.52
40:BP:134:HIS:CG	40:BP:135:LYS:H	2.27	0.52
1:AA:1735:G:H4'	53:B5:1933:A:C2'	2.33	0.52
1:AA:1755:G:C2'	53:B5:2262:A:C2	2.70	0.52
17:AR:146:GLY:C	17:AR:179:LYS:HE2	2.33	0.52
17:AR:170:ILE:HG12	17:AR:211:ILE:HD13	1.90	0.52
17:AR:287:PRO:HG2	17:AR:306:THR:OG1	2.09	0.52
17:AR:85:TRP:HB3	17:AR:109:ASP:OD1	2.10	0.52
17:AR:263:PHE:HE1	17:AR:270:LEU:HD11	1.75	0.52
1:AA:1120:C:O2'	53:B5:2190:U:H4'	2.09	0.52
1:AA:1502:G:N1	1:AA:1547:C:N4	2.57	0.52
19:A7:59:U:C5	19:A7:60:C:C4	2.98	0.52
26:BB:5:ILE:HD13	26:BB:5:ILE:H	1.75	0.52
1:AA:722:G:H22	1:AA:732:G:H1	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:48:THR:HG22	17:AR:50:ASP:CG	2.35	0.52
17:AR:74:THR:HG23	17:AR:77:GLY:H	1.75	0.52
17:AR:270:LEU:HD12	17:AR:270:LEU:H	1.75	0.52
17:AR:256:THR:OG1	17:AR:258:THR:HG22	2.10	0.52
19:A7:56:C:O4'	53:B5:2484:A:H4'	2.10	0.52
1:AA:1460:G:H5'	19:A7:29:A:O2'	2.10	0.52
17:AR:69:GLN:HG2	17:AR:85:TRP:CD1	2.45	0.52
17:AR:149:ASP:HB3	17:AR:174:ASN:HB2	1.92	0.52
1:AA:1657:A:C5'	42:BR:67:PRO:HD2	2.28	0.51
17:AR:285:ALA:CB	17:AR:313:TRP:CH2	2.93	0.51
17:AR:118:LYS:HD2	17:AR:118:LYS:N	2.25	0.51
17:AR:283:LYS:HD3	17:AR:288:HIS:CD2	2.44	0.51
1:AA:922:A:H5''	26:BB:109:GLU:OE1	2.06	0.51
17:AR:19:TRP:HE1	17:AR:290:VAL:HG21	1.76	0.51
17:AR:93:ASP:O	17:AR:96:THR:HG22	2.10	0.51
1:AA:701:U:O2	40:BP:173:ALA:C	2.49	0.51
17:AR:26:SER:HB3	17:AR:30:PRO:HD2	1.92	0.51
17:AR:66:HIS:ND1	17:AR:67:ILE:HD13	2.25	0.51
37:BM:168:ALA:O	37:BM:172:ALA:CB	2.58	0.51
1:AA:1521:G:C6	18:AT:79:LEU:N	2.76	0.51
1:AA:1744:A:N3	53:B5:2302:G:H8	2.08	0.51
17:AR:89:LEU:HB2	17:AR:103:PHE:HB2	1.93	0.51
1:AA:1636:G:H2'	1:AA:1637:C:O4'	2.11	0.51
17:AR:30:PRO:HB2	17:AR:32:LEU:CD1	2.41	0.51
17:AR:292:LEU:HD23	17:AR:292:LEU:O	2.11	0.51
1:AA:699:U:C2	40:BP:168:ALA:N	2.79	0.50
1:AA:799:A:H4'	40:BP:164:ALA:H	1.76	0.50
1:AA:857:U:C2'	1:AA:858:G:O5'	2.59	0.50
1:AA:1501:A:N7	1:AA:1546:G:N9	2.59	0.50
17:AR:157:VAL:O	17:AR:167:VAL:HG21	2.11	0.50
23:B8:43:LYS:HG2	35:BK:121:PHE:CE1	2.45	0.50
15:AQ:131:ILE:HD13	15:AQ:131:ILE:H	1.74	0.50
17:AR:173:GLY:N	17:AR:199:ILE:HG23	2.26	0.50
17:AR:276:PRO:HA	17:AR:285:ALA:HA	1.93	0.50
17:AR:305:TYR:HD2	17:AR:311:ARG:HH21	1.56	0.50
1:AA:1460:G:C4'	19:A7:30:G:C5'	2.84	0.50
17:AR:81:LEU:HD21	17:AR:122:ILE:CG2	2.41	0.50
17:AR:114:ASP:OD2	17:AR:156:VAL:HG13	2.11	0.50
1:AA:972:A:C1'	53:B5:847:A:C2	2.87	0.50
1:AA:1776:G:OP1	53:B5:2193:U:C4'	2.53	0.50
17:AR:19:TRP:CZ3	17:AR:306:THR:CG2	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:99:THR:O	17:AR:99:THR:HG23	2.11	0.50
17:AR:176:LYS:HD3	17:AR:195:HIS:O	2.11	0.50
17:AR:285:ALA:HB3	17:AR:313:TRP:CH2	2.47	0.50
17:AR:314:GLN:HG2	17:AR:315:VAL:H	1.76	0.50
1:AA:701:U:C4	40:BP:169:ALA:C	2.71	0.50
1:AA:971:G:N2	53:B5:846:A:H61	2.05	0.50
17:AR:7:LEU:HD12	17:AR:7:LEU:N	2.27	0.50
17:AR:89:LEU:HD21	17:AR:124:SER:CB	2.34	0.50
17:AR:169:ILE:CD1	17:AR:181:TRP:CD1	2.95	0.50
17:AR:305:TYR:N	17:AR:305:TYR:CD1	2.80	0.50
33:BI:121:LYS:H	33:BI:121:LYS:HD2	1.76	0.50
37:BM:147:TRP:HZ2	37:BM:153:ALA:HB1	1.73	0.50
37:BM:155:ALA:O	37:BM:156:ALA:C	2.54	0.50
17:AR:96:THR:CG2	17:AR:98:GLU:H	2.20	0.50
1:AA:701:U:C5'	40:BP:173:ALA:HB1	2.41	0.49
17:AR:81:LEU:HD21	17:AR:122:ILE:HG21	1.93	0.49
17:AR:115:ILE:HG22	17:AR:119:ALA:HA	1.93	0.49
17:AR:290:VAL:O	17:AR:290:VAL:HG13	2.06	0.49
1:AA:699:U:C6	40:BP:165:ALA:O	2.66	0.49
1:AA:1744:A:C2	53:B5:2302:G:C5'	2.77	0.49
17:AR:44:SER:OG	17:AR:58:VAL:HG23	2.11	0.49
17:AR:277:GLU:O	17:AR:278:PHE:HB3	2.12	0.49
1:AA:1338:A:O3'	17:AR:102:ARG:NH2	2.44	0.49
17:AR:13:LEU:HD23	17:AR:310:ILE:CG2	2.43	0.49
1:AA:1665:A:OP1	53:B5:1936:A:O5'	2.28	0.49
17:AR:263:PHE:CE1	17:AR:270:LEU:CD1	2.95	0.49
1:AA:700:C:C5	40:BP:173:ALA:HB3	2.47	0.49
17:AR:69:GLN:CG	17:AR:85:TRP:HE1	2.26	0.49
17:AR:29:GLN:OE1	17:AR:297:ASP:HB3	2.12	0.49
17:AR:131:ILE:HD11	17:AR:151:VAL:HG11	1.94	0.49
17:AR:185:GLN:O	17:AR:186:PHE:HB2	2.12	0.49
53:B5:512:U:H3	53:B5:579:G:H1	1.61	0.49
1:AA:972:A:O4'	53:B5:847:A:N1	2.43	0.49
17:AR:52:GLN:HA	17:AR:52:GLN:NE2	2.20	0.49
17:AR:159:ASN:O	17:AR:167:VAL:HG12	2.13	0.49
17:AR:187:GLN:OE1	17:AR:187:GLN:HA	2.13	0.49
17:AR:8:VAL:HG12	17:AR:9:LEU:H	1.77	0.49
17:AR:34:LEU:CD2	17:AR:71:CYS:HB3	2.43	0.49
17:AR:123:ILE:HG22	17:AR:133:VAL:HA	1.95	0.49
17:AR:131:ILE:HD13	17:AR:151:VAL:HG11	1.95	0.49
17:AR:258:THR:HG23	17:AR:261:LYS:HE2	1.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:286:GLU:CA	17:AR:305:TYR:CD2	2.93	0.49
17:AR:9:LEU:HD13	17:AR:11:GLY:N	2.27	0.49
37:BM:147:TRP:CZ2	37:BM:153:ALA:HB2	2.48	0.49
16:AS:69:GLU:HG3	16:AS:70:ASN:H	1.78	0.48
17:AR:29:GLN:O	17:AR:29:GLN:HG2	2.13	0.48
17:AR:286:GLU:OE2	17:AR:289:ALA:HB2	2.12	0.48
17:AR:123:ILE:HD13	17:AR:169:ILE:HG21	1.95	0.48
17:AR:178:VAL:HG13	17:AR:202:LEU:CD1	2.43	0.48
1:AA:1460:G:O3'	19:A7:30:G:C1'	2.60	0.48
1:AA:1520:U:C2'	1:AA:1521:G:OP1	2.58	0.48
1:AA:1552:U:OP1	13:AN:14:PHE:CG	2.67	0.48
17:AR:54:PHE:CD1	17:AR:312:VAL:HG21	2.49	0.48
17:AR:87:LYS:HD3	17:AR:107:LYS:O	2.13	0.48
17:AR:33:LEU:HD13	17:AR:302:PHE:CD2	2.48	0.48
17:AR:286:GLU:CD	17:AR:305:TYR:CZ	2.91	0.48
32:BH:40:HIS:CG	32:BH:41:ILE:N	2.78	0.48
1:AA:698:U:C4	40:BP:164:ALA:O	2.67	0.48
17:AR:183:LEU:N	17:AR:183:LEU:HD22	2.28	0.48
14:AO:149:LEU:HB2	53:B5:847:A:OP1	2.14	0.48
17:AR:41:THR:HG22	17:AR:42:LEU:O	2.13	0.48
17:AR:154:VAL:HG23	17:AR:154:VAL:O	2.12	0.48
17:AR:169:ILE:HG23	17:AR:183:LEU:CD2	2.43	0.48
17:AR:218:GLY:O	17:AR:236:ALA:HB3	2.14	0.48
17:AR:309:VAL:HG12	17:AR:310:ILE:N	2.29	0.48
1:AA:1779:A:H2'	1:AA:1780:A:C8	2.49	0.48
17:AR:100:TYR:CE2	17:AR:101:GLN:HG3	2.49	0.48
1:AA:698:U:C6	1:AA:799:A:OP2	2.67	0.47
1:AA:1520:U:O4'	1:AA:1522:A:N7	2.47	0.47
1:AA:1756:U:H4'	53:B5:2263:C:C1'	2.44	0.47
1:AA:1775:G:C4'	53:B5:2193:U:OP1	2.62	0.47
17:AR:83:ALA:HB2	17:AR:113:VAL:HG11	1.93	0.47
17:AR:109:ASP:HB2	17:AR:127:ARG:HD2	1.95	0.47
22:B2:104:LEU:HD13	22:B2:104:LEU:H	1.79	0.47
1:AA:858:G:N1	7:AH:61:ILE:CA	2.77	0.47
19:A7:62:A:H2'	19:A7:63:C:C6	2.50	0.47
1:AA:1200:A:C6	13:AN:15:GLY:HA2	2.48	0.47
17:AR:210:LEU:CD1	17:AR:222:LEU:HD21	2.28	0.47
1:AA:702:G:C8	40:BP:172:ALA:HA	2.42	0.47
17:AR:81:LEU:HD13	17:AR:91:LEU:CD2	2.45	0.47
17:AR:134:TRP:C	17:AR:141:LEU:HD13	2.39	0.47
17:AR:221:MET:SD	17:AR:223:TRP:CZ2	3.07	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:629:U:H5'	53:B5:846:A:C1'	2.44	0.47
17:AR:284:ALA:HB3	17:AR:286:GLU:CD	2.39	0.47
37:BM:155:ALA:C	37:BM:157:ALA:N	2.72	0.47
1:AA:698:U:C6	40:BP:165:ALA:O	2.61	0.47
1:AA:856:A:C4	7:AH:33:VAL:CA	2.96	0.47
1:AA:1582:G:H21	8:AI:134:ALA:HB1	1.79	0.47
17:AR:10:ARG:NE	17:AR:54:PHE:HE1	2.13	0.47
17:AR:11:GLY:H	17:AR:312:VAL:HG23	1.79	0.47
17:AR:165:ASP:CB	17:AR:183:LEU:CB	2.93	0.47
17:AR:222:LEU:HD13	17:AR:232:TYR:CZ	2.49	0.47
17:AR:276:PRO:HB3	17:AR:286:GLU:O	2.15	0.47
37:BM:148:LYS:HB3	37:BM:149:ALA:H	1.28	0.47
37:BM:151:ALA:O	37:BM:155:ALA:N	2.46	0.47
17:AR:13:LEU:HD13	17:AR:54:PHE:HB3	1.94	0.47
17:AR:227:ALA:O	17:AR:228:LYS:HG3	2.15	0.47
17:AR:285:ALA:C	17:AR:305:TYR:HE2	2.22	0.47
1:AA:1120:C:O2'	53:B5:2190:U:C5'	2.62	0.47
1:AA:1520:U:C3'	1:AA:1520:U:C6	2.97	0.47
17:AR:34:LEU:HD21	17:AR:71:CYS:CB	2.45	0.47
17:AR:66:HIS:CE1	17:AR:85:TRP:CE3	3.03	0.47
17:AR:164:ASP:C	17:AR:183:LEU:H	2.21	0.47
28:BD:148:ILE:HD13	28:BD:148:ILE:H	1.79	0.47
17:AR:67:ILE:N	17:AR:67:ILE:HD12	2.30	0.46
17:AR:278:PHE:CD2	17:AR:279:ALA:N	2.83	0.46
17:AR:278:PHE:HZ	17:AR:287:PRO:CA	2.27	0.46
8:AI:42:GLU:HB3	8:AI:74:HIS:CE1	2.49	0.46
1:AA:1778:G:O5'	53:B5:2274:U:H5''	2.14	0.46
17:AR:164:ASP:OD2	17:AR:182:ASN:HA	2.15	0.46
17:AR:185:GLN:HB3	17:AR:187:GLN:HG2	1.96	0.46
17:AR:262:VAL:HG23	17:AR:262:VAL:O	2.16	0.46
17:AR:281:TYR:H	17:AR:281:TYR:HD1	1.61	0.46
17:AR:283:LYS:CD	17:AR:288:HIS:CA	2.81	0.46
17:AR:87:LYS:HA	17:AR:110:VAL:HG23	1.97	0.46
17:AR:93:ASP:HB3	17:AR:96:THR:HG21	1.95	0.46
19:A7:37:YYG:H31	19:A7:37:YYG:H1'	1.95	0.46
1:AA:1200:A:C2	1:AA:1200:A:C4	3.03	0.46
17:AR:283:LYS:CD	17:AR:288:HIS:CD2	2.98	0.46
17:AR:283:LYS:HB3	17:AR:288:HIS:CA	2.43	0.46
1:AA:1521:G:H22	18:AT:78:LYS:HG3	1.76	0.46
1:AA:1746:G:OP2	53:B5:2303:A:H3'	2.16	0.46
17:AR:19:TRP:HB3	17:AR:38:ARG:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:274:LEU:HD13	17:AR:313:TRP:CE3	2.50	0.46
17:AR:285:ALA:CB	17:AR:313:TRP:CZ2	2.95	0.46
1:AA:866:G:OP1	1:AA:866:G:H8	1.98	0.46
12:AM:110:ARG:CD	34:BJ:116:TYR:HD1	2.23	0.46
19:A7:72:C:H5''	53:B5:2234:G:O6	2.16	0.46
24:B9:51:ALA:HB3	24:B9:54:ILE:HB	1.97	0.46
1:AA:702:G:C8	40:BP:172:ALA:O	2.69	0.46
1:AA:1547:C:H6	1:AA:1547:C:H2'	1.60	0.46
1:AA:1744:A:H3'	53:B5:2303:A:OP1	2.16	0.46
17:AR:48:THR:HG22	17:AR:50:ASP:H	1.81	0.46
17:AR:96:THR:HG23	17:AR:97:GLY:N	2.30	0.46
17:AR:157:VAL:HG12	17:AR:167:VAL:HB	1.97	0.46
17:AR:218:GLY:HA2	17:AR:238:ASP:O	2.16	0.46
19:A7:1:G:C6	19:A7:73:A:C2	3.04	0.46
1:AA:1521:G:HO2'	18:AT:83:ALA:HA	1.70	0.46
17:AR:10:ARG:HE	17:AR:54:PHE:HE1	1.60	0.46
1:AA:506:A:H3'	1:AA:507:U:C5'	2.46	0.46
1:AA:858:G:H1'	7:AH:34:ILE:HG21	1.97	0.46
1:AA:1460:G:H4'	19:A7:29:A:O2'	2.16	0.46
17:AR:134:TRP:CA	17:AR:141:LEU:HD13	2.46	0.46
17:AR:153:GLN:HG3	17:AR:154:VAL:N	2.31	0.46
1:AA:700:C:OP2	40:BP:169:ALA:HB1	2.15	0.45
1:AA:858:G:O3'	7:AH:29:PRO:HD2	2.17	0.45
17:AR:108:SER:OG	17:AR:127:ARG:HB2	2.16	0.45
1:AA:701:U:O2'	40:BP:176:ALA:O	2.34	0.45
1:AA:1121:A:C1'	53:B5:2191:U:OP1	2.64	0.45
15:AQ:82:ARG:HB3	15:AQ:110:HIS:CE1	2.51	0.45
17:AR:69:GLN:CG	17:AR:85:TRP:NE1	2.80	0.45
17:AR:156:VAL:HG12	17:AR:169:ILE:HG22	1.97	0.45
17:AR:276:PRO:CA	17:AR:285:ALA:CA	2.94	0.45
17:AR:276:PRO:HG3	17:AR:282:SER:HA	1.97	0.45
17:AR:286:GLU:HG3	17:AR:305:TYR:HA	1.97	0.45
23:B8:43:LYS:CB	35:BK:121:PHE:CD1	2.93	0.45
37:BM:150:ALA:C	37:BM:154:ALA:HB3	2.41	0.45
1:AA:1756:U:O2'	53:B5:2262:A:H3'	2.17	0.45
12:AM:119:ILE:HG22	16:AS:106:GLU:H	1.81	0.45
12:AM:120:ARG:HD3	16:AS:103:ASN:H	1.80	0.45
17:AR:283:LYS:CG	17:AR:284:ALA:N	2.78	0.45
17:AR:284:ALA:CB	17:AR:289:ALA:HB2	2.46	0.45
46:BV:113:GLY:HA3	53:B5:716:G:C4	2.51	0.45
1:AA:856:A:C6	7:AH:32:LYS:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1630:C:H5'	1:AA:1636:G:H22	1.82	0.45
17:AR:10:ARG:CG	17:AR:54:PHE:CE1	2.97	0.45
17:AR:31:ASN:HB3	17:AR:47:LEU:HB2	1.99	0.45
17:AR:286:GLU:CD	17:AR:305:TYR:CE2	2.95	0.45
53:B5:1003:A:H61	53:B5:1046:A:H61	1.64	0.45
1:AA:1200:A:N3	13:AN:16:LYS:CB	2.79	0.45
1:AA:1584:A:C8	8:AI:127:LYS:HB2	2.52	0.45
17:AR:169:ILE:HD12	17:AR:169:ILE:O	2.17	0.45
17:AR:262:VAL:CG2	17:AR:271:VAL:CG1	2.94	0.45
26:BB:30:ARG:HG2	26:BB:31:THR:H	1.81	0.45
37:BM:37:ARG:NH2	37:BM:157:ALA:HA	2.32	0.45
1:AA:701:U:C2	40:BP:171:ALA:C	2.91	0.45
17:AR:164:ASP:N	17:AR:167:VAL:HA	2.32	0.45
26:BB:77:ILE:HD11	26:BB:169:ILE:HD11	1.98	0.45
37:BM:111:PRO:CB	37:BM:163:ALA:O	2.65	0.45
1:AA:856:A:C2	7:AH:33:VAL:HB	2.52	0.45
1:AA:856:A:N3	7:AH:33:VAL:CA	2.79	0.45
1:AA:1521:G:H21	18:AT:78:LYS:HD2	1.69	0.45
3:AC:164:VAL:HG13	3:AC:165:ASN:H	1.82	0.44
17:AR:34:LEU:CD1	17:AR:80:ALA:HB2	2.47	0.44
17:AR:34:LEU:CD1	17:AR:73:LEU:CD2	2.95	0.44
1:AA:1777:U:OP1	53:B5:2194:G:C2'	2.65	0.44
17:AR:106:HIS:ND1	17:AR:126:SER:HB2	2.32	0.44
1:AA:972:A:H4'	53:B5:847:A:C2	2.52	0.44
17:AR:123:ILE:HA	17:AR:132:LYS:O	2.18	0.44
19:A7:73:A:OP1	53:B5:2603:G:OP1	2.36	0.44
30:BF:118:LYS:H	30:BF:118:LYS:HD3	1.82	0.44
1:AA:1756:U:C3'	53:B5:2263:C:C1'	2.89	0.44
17:AR:91:LEU:HG	17:AR:103:PHE:CE1	2.52	0.44
17:AR:133:VAL:CG1	17:AR:141:LEU:HB2	2.40	0.44
17:AR:259:GLY:HA2	17:AR:283:LYS:O	2.18	0.44
17:AR:278:PHE:CE2	17:AR:280:GLY:N	2.85	0.44
18:AT:22:LEU:HD12	18:AT:55:TYR:HA	2.00	0.44
35:BK:121:PHE:CD2	35:BK:121:PHE:CB	2.86	0.44
17:AR:172:ALA:HB1	17:AR:199:ILE:O	2.18	0.44
17:AR:8:VAL:CG1	17:AR:9:LEU:N	2.80	0.44
17:AR:68:VAL:HA	17:AR:84:SER:HB3	2.00	0.44
17:AR:115:ILE:HG22	17:AR:116:ASP:N	2.32	0.44
19:A7:70:C:O2'	53:B5:2236:G:H4'	2.18	0.44
32:BH:129:ARG:H	32:BH:157:ASN:HD21	1.66	0.44
37:BM:108:ILE:HG23	37:BM:160:ALA:CA	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1778:G:OP1	53:B5:2274:U:C5'	2.34	0.44
17:AR:34:LEU:CD1	17:AR:80:ALA:CB	2.94	0.44
17:AR:38:ARG:CA	17:AR:67:ILE:HG23	2.22	0.44
17:AR:56:VAL:HB	17:AR:57:PRO:HD2	1.99	0.44
1:AA:1516:C:H6	1:AA:1516:C:O5'	2.01	0.44
17:AR:42:LEU:HD21	17:AR:71:CYS:SG	2.58	0.44
17:AR:91:LEU:HG	17:AR:103:PHE:HE1	1.83	0.44
1:AA:856:A:N3	7:AH:32:LYS:O	2.50	0.43
1:AA:1501:A:C4'	1:AA:1546:G:N2	2.81	0.43
17:AR:54:PHE:CE2	17:AR:302:PHE:CE2	3.06	0.43
1:AA:1776:G:P	53:B5:2193:U:C5'	2.94	0.43
17:AR:68:VAL:HG23	17:AR:84:SER:HB3	2.00	0.43
1:AA:1520:U:H1'	1:AA:1522:A:H62	1.82	0.43
1:AA:1581:A:C8	8:AI:137:ARG:HA	2.54	0.43
17:AR:47:LEU:HD22	17:AR:54:PHE:CE2	2.53	0.43
17:AR:161:LYS:HA	17:AR:161:LYS:HE2	2.00	0.43
17:AR:171:SER:C	17:AR:202:LEU:HD11	2.43	0.43
17:AR:262:VAL:CG2	17:AR:272:ASP:N	2.81	0.43
27:BC:342:LEU:HD23	27:BC:342:LEU:H	1.83	0.43
17:AR:116:ASP:OD2	17:AR:166:SER:HB2	2.19	0.43
17:AR:193:ILE:HD13	17:AR:193:ILE:N	2.20	0.43
17:AR:196:ASN:OD1	17:AR:217:ASP:HB3	2.19	0.43
17:AR:41:THR:OG1	17:AR:62:LYS:HG2	2.18	0.43
42:BR:22:ILE:H	53:B5:1899:G:H5''	1.83	0.43
1:AA:699:U:N3	40:BP:171:ALA:N	2.57	0.43
1:AA:857:U:C6	7:AH:33:VAL:O	2.71	0.43
17:AR:48:THR:H	17:AR:55:GLY:HA2	1.84	0.43
17:AR:74:THR:HG23	17:AR:76:ASP:N	2.34	0.43
1:AA:858:G:C4	7:AH:61:ILE:HG12	2.53	0.43
17:AR:13:LEU:CD1	17:AR:55:GLY:N	2.82	0.43
17:AR:285:ALA:CB	17:AR:313:TRP:HH2	2.32	0.43
17:AR:300:THR:HG23	17:AR:313:TRP:O	2.19	0.43
1:AA:700:C:C6	40:BP:173:ALA:CB	2.98	0.43
1:AA:1777:U:OP1	53:B5:2194:G:C4'	2.66	0.43
33:BI:140:THR:HG22	33:BI:141:LYS:H	1.83	0.43
1:AA:1520:U:H4'	1:AA:1522:A:H8	1.75	0.43
17:AR:19:TRP:NE1	17:AR:290:VAL:HG21	2.34	0.43
17:AR:54:PHE:CE2	17:AR:302:PHE:HE2	2.36	0.43
37:BM:106:GLU:OE1	37:BM:156:ALA:CB	2.67	0.43
1:AA:796:A:C2'	1:AA:797:G:O5'	2.67	0.43
1:AA:1734:G:C2	53:B5:1934:G:H4'	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:34:LEU:CD2	17:AR:34:LEU:C	2.92	0.43
17:AR:133:VAL:HG12	17:AR:142:ALA:N	2.33	0.43
17:AR:240:VAL:HG22	17:AR:256:THR:CG2	2.46	0.43
1:AA:1755:G:H2'	53:B5:2262:A:H2	1.77	0.42
12:AM:39:GLY:H	12:AM:42:TYR:HB2	1.85	0.42
17:AR:10:ARG:HG2	17:AR:54:PHE:HE1	1.81	0.42
17:AR:71:CYS:SG	17:AR:80:ALA:HB1	2.59	0.42
17:AR:83:ALA:HB1	17:AR:110:VAL:HG11	1.95	0.42
17:AR:89:LEU:HD12	17:AR:89:LEU:N	2.33	0.42
17:AR:172:ALA:HB2	17:AR:199:ILE:HD12	1.96	0.42
17:AR:185:GLN:NE2	17:AR:187:GLN:HG3	2.34	0.42
17:AR:262:VAL:HG21	17:AR:272:ASP:HB3	2.01	0.42
17:AR:292:LEU:N	17:AR:292:LEU:CD2	2.82	0.42
1:AA:701:U:O5'	40:BP:173:ALA:HB1	2.18	0.42
1:AA:1664:U:O3'	53:B5:1935:G:C2'	2.62	0.42
17:AR:35:SER:CB	17:AR:45:TRP:HE1	2.33	0.42
17:AR:41:THR:CG2	17:AR:42:LEU:N	2.81	0.42
17:AR:263:PHE:CE1	17:AR:270:LEU:CG	2.99	0.42
17:AR:33:LEU:CD2	17:AR:33:LEU:N	2.82	0.42
1:AA:1461:C:H4'	19:A7:31:A:O5'	2.20	0.42
1:AA:1573:G:N2	19:A7:41:U:C5'	2.39	0.42
17:AR:133:VAL:CG1	17:AR:142:ALA:N	2.82	0.42
23:B8:4:ILE:HG12	23:B8:6:GLU:H	1.84	0.42
53:B5:271:C:C5	53:B5:272:G:H1'	2.55	0.42
17:AR:106:HIS:NE2	17:AR:132:LYS:HD2	2.35	0.42
17:AR:118:LYS:O	17:AR:119:ALA:HB3	2.20	0.42
32:BH:40:HIS:CD2	32:BH:41:ILE:H	2.37	0.42
48:BX:81:ALA:HA	53:B5:17:G:C4	2.54	0.42
17:AR:147:HIS:CD2	17:AR:151:VAL:HG22	2.55	0.42
17:AR:288:HIS:O	17:AR:306:THR:HG23	2.19	0.42
27:BC:32:PHE:CD1	53:B5:3003:G:H4'	2.53	0.42
28:BD:208:VAL:HG11	28:BD:250:TRP:CZ3	2.55	0.42
29:BE:193:GLU:H	29:BE:213:ASP:H	1.68	0.42
53:B5:126:U:H2'	53:B5:127:G:C8	2.55	0.42
1:AA:115:G:H1	1:AA:302:U:H1'	1.85	0.42
17:AR:29:GLN:N	17:AR:30:PRO:CD	2.83	0.42
17:AR:129:LYS:HG2	17:AR:149:ASP:C	2.45	0.42
17:AR:96:THR:CG2	17:AR:97:GLY:N	2.82	0.42
17:AR:257:ALA:C	17:AR:283:LYS:HG3	2.45	0.42
1:AA:1574:A:C6	19:A7:41:U:H4'	2.54	0.42
17:AR:116:ASP:CG	17:AR:166:SER:CB	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:116:ASP:CG	17:AR:166:SER:HB2	2.45	0.42
17:AR:284:ALA:C	17:AR:286:GLU:N	2.77	0.42
17:AR:33:LEU:HD21	17:AR:45:TRP:CB	2.50	0.42
17:AR:135:THR:N	17:AR:141:LEU:CD1	2.83	0.42
17:AR:165:ASP:CB	17:AR:183:LEU:HB3	2.50	0.42
17:AR:165:ASP:N	17:AR:184:ASN:N	2.68	0.42
17:AR:203:THR:CG2	17:AR:245:PHE:CE1	3.01	0.42
17:AR:260:ILE:HG13	17:AR:284:ALA:HB2	1.98	0.42
17:AR:313:TRP:O	17:AR:314:GLN:HB2	2.20	0.42
1:AA:865:A:H2'	1:AA:866:G:OP2	2.19	0.41
1:AA:1520:U:C5'	1:AA:1521:G:P	3.05	0.41
1:AA:1657:A:H4'	42:BR:67:PRO:CG	2.47	0.41
17:AR:32:LEU:HD22	17:AR:32:LEU:C	2.44	0.41
17:AR:139:GLN:OE1	17:AR:139:GLN:HA	2.20	0.41
17:AR:172:ALA:CB	17:AR:199:ILE:CD1	2.94	0.41
1:AA:703:G:H4'	40:BP:176:ALA:HB2	2.02	0.41
17:AR:18:GLY:C	17:AR:308:ASN:HB3	2.45	0.41
17:AR:245:PHE:HE2	17:AR:265:LEU:HD11	1.84	0.41
37:BM:178:ALA:O	37:BM:181:ALA:HB3	2.21	0.41
1:AA:1502:G:O6	1:AA:1547:C:C6	2.72	0.41
1:AA:1520:U:C6	1:AA:1520:U:H3'	2.55	0.41
1:AA:1755:G:H2'	53:B5:2262:A:C2	2.54	0.41
17:AR:135:THR:N	17:AR:141:LEU:HD11	2.34	0.41
17:AR:157:VAL:O	17:AR:157:VAL:HG13	2.20	0.41
17:AR:224:ASN:OD1	17:AR:227:ALA:HB3	2.20	0.41
17:AR:262:VAL:CG2	17:AR:272:ASP:HB3	2.49	0.41
42:BR:48:ARG:HA	53:B5:2338:C:H4'	2.01	0.41
1:AA:1120:C:O2'	53:B5:2190:U:C4'	2.68	0.41
1:AA:1200:A:C6	13:AN:15:GLY:C	2.95	0.41
17:AR:79:TYR:HD2	17:AR:92:TRP:O	2.03	0.41
33:BI:101:LYS:HA	33:BI:102:MET:C	2.45	0.41
1:AA:1775:G:C5'	53:B5:2193:U:OP1	2.68	0.41
17:AR:13:LEU:N	17:AR:13:LEU:CD2	2.83	0.41
17:AR:243:LEU:HD23	17:AR:254:ALA:HA	2.01	0.41
53:B5:2621:G:C8	53:B5:2622:C:C5	3.09	0.41
1:AA:223:U:H3	1:AA:244:A:H61	1.68	0.41
1:AA:501:U:C6	1:AA:501:U:C1'	2.93	0.41
9:AJ:56:VAL:HG22	9:AJ:57:ARG:N	2.36	0.41
12:AM:92:ILE:H	12:AM:92:ILE:HD13	1.84	0.41
14:AO:149:LEU:HD13	53:B5:847:A:P	2.46	0.41
17:AR:131:ILE:HD12	17:AR:154:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:233:THR:O	17:AR:234:LEU:HD23	2.21	0.41
17:AR:278:PHE:CZ	17:AR:281:TYR:O	2.73	0.41
53:B5:1384:U:H1'	53:B5:1385:C:C2	2.55	0.41
1:AA:628:G:H4'	53:B5:846:A:N3	2.36	0.41
2:AB:23:HIS:HA	2:AB:48:ILE:HG22	2.03	0.41
17:AR:41:THR:HG23	17:AR:61:PHE:C	2.44	0.41
17:AR:136:ILE:CG2	17:AR:137:LYS:N	2.83	0.41
17:AR:157:VAL:CG1	17:AR:167:VAL:HB	2.51	0.41
17:AR:256:THR:O	17:AR:283:LYS:CG	2.66	0.41
17:AR:267:PRO:O	17:AR:268:GLN:HB2	2.20	0.41
17:AR:305:TYR:CE2	17:AR:311:ARG:NE	2.85	0.41
17:AR:315:VAL:CG1	17:AR:316:MET:N	2.83	0.41
1:AA:799:A:O3'	40:BP:160:ALA:O	2.39	0.41
1:AA:921:G:O2'	26:BB:141:PRO:HG3	2.20	0.41
4:AD:155:HIS:CG	4:AD:156:ILE:H	2.39	0.41
6:AG:77:TYR:H	6:AG:191:ALA:HB2	1.85	0.41
8:AI:93:HIS:CE1	17:AR:59:ARG:CZ	3.03	0.41
8:AI:97:VAL:HG12	8:AI:98:ASP:N	2.36	0.41
17:AR:170:ILE:N	17:AR:170:ILE:CD1	2.82	0.41
19:A7:21:A:C6	19:A7:48:C:C6	3.09	0.41
1:AA:921:G:O3'	26:BB:140:ASN:ND2	2.54	0.41
1:AA:1573:G:N3	19:A7:41:U:C5'	2.67	0.41
17:AR:72:THR:CG2	17:AR:73:LEU:N	2.82	0.41
17:AR:219:GLU:HG2	17:AR:220:ILE:N	2.36	0.41
17:AR:276:PRO:N	17:AR:284:ALA:O	2.54	0.41
17:AR:304:GLY:C	17:AR:305:TYR:CD1	2.99	0.41
43:BS:49:ILE:H	43:BS:49:ILE:HD12	1.86	0.41
19:A7:10:2MG:HM23	19:A7:11:C:H1'	2.03	0.41
1:AA:856:A:C2	7:AH:33:VAL:CA	3.04	0.40
1:AA:1430:G:H1'	13:AN:38:ILE:HD11	2.03	0.40
28:BD:55:LYS:HA	28:BD:58:HIS:CD2	2.56	0.40
36:BL:80:THR:HG23	53:B5:2607:G:H22	1.86	0.40
17:AR:13:LEU:HD23	17:AR:310:ILE:HG22	2.03	0.40
17:AR:37:SER:HB3	17:AR:39:ASP:OD1	2.21	0.40
17:AR:61:PHE:HE2	17:AR:97:GLY:HA2	1.73	0.40
17:AR:286:GLU:OE2	17:AR:305:TYR:CE1	2.74	0.40
17:AR:303:ALA:O	17:AR:305:TYR:CE1	2.74	0.40
25:BA:105:LYS:HE2	53:B5:2477:G:C5	2.57	0.40
46:BV:74:LEU:HD13	46:BV:74:LEU:H	1.86	0.40
17:AR:171:SER:C	17:AR:202:LEU:CD1	2.94	0.40
17:AR:172:ALA:HB1	17:AR:199:ILE:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:174:ASN:C	17:AR:176:LYS:H	2.28	0.40
17:AR:183:LEU:HD13	17:AR:183:LEU:HA	1.98	0.40
17:AR:285:ALA:HB2	17:AR:313:TRP:CH2	2.57	0.40
17:AR:300:THR:HG22	17:AR:301:LEU:N	2.36	0.40
1:AA:1744:A:C5'	53:B5:2291:A:H1'	2.47	0.40
9:AJ:30:LYS:HG3	9:AJ:31:VAL:H	1.85	0.40
11:AL:62:LYS:HG2	11:AL:63:GLN:H	1.86	0.40
17:AR:34:LEU:CD1	17:AR:73:LEU:HD21	2.48	0.40
17:AR:42:LEU:CD2	17:AR:71:CYS:HB2	2.52	0.40
17:AR:68:VAL:HG21	17:AR:82:SER:HB2	2.04	0.40
17:AR:79:TYR:CD2	17:AR:93:ASP:HA	2.55	0.40
17:AR:127:ARG:C	17:AR:129:LYS:H	2.30	0.40
17:AR:133:VAL:HG12	17:AR:142:ALA:H	1.87	0.40
17:AR:199:ILE:CD1	17:AR:202:LEU:CD2	2.97	0.40
17:AR:234:LEU:HD13	17:AR:263:PHE:CD2	2.57	0.40
17:AR:256:THR:C	17:AR:283:LYS:CE	2.94	0.40
17:AR:285:ALA:HB2	17:AR:313:TRP:HH2	1.86	0.40
37:BM:143:THR:HG23	37:BM:144:SER:H	1.86	0.40
1:AA:858:G:H2'	7:AH:28:ARG:N	2.37	0.40
17:AR:106:HIS:CD2	17:AR:132:LYS:HD2	2.56	0.40
17:AR:199:ILE:C	17:AR:199:ILE:CD1	2.95	0.40
17:AR:262:VAL:CG2	17:AR:272:ASP:H	2.30	0.40
23:B8:24:SER:HA	23:B8:115:ALA:H	1.86	0.40
23:B8:84:VAL:HG23	23:B8:110:ARG:HE	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	191/193 (99%)	173 (91%)	16 (8%)	2 (1%)	12 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	186/188 (99%)	148 (80%)	28 (15%)	10 (5%)	1	15
4	AD	120/158 (76%)	97 (81%)	16 (13%)	7 (6%)	1	14
5	AE	160/162 (99%)	141 (88%)	13 (8%)	6 (4%)	2	19
6	AG	184/186 (99%)	156 (85%)	20 (11%)	8 (4%)	2	17
7	AH	121/125 (97%)	105 (87%)	11 (9%)	5 (4%)	2	18
8	AI	136/138 (99%)	106 (78%)	21 (15%)	9 (7%)	1	12
9	AJ	94/96 (98%)	77 (82%)	14 (15%)	3 (3%)	3	21
10	AK	123/125 (98%)	99 (80%)	20 (16%)	4 (3%)	3	21
11	AL	116/118 (98%)	89 (77%)	25 (22%)	2 (2%)	7	36
12	AM	128/130 (98%)	103 (80%)	20 (16%)	5 (4%)	2	19
13	AN	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	0	9
14	AO	82/84 (98%)	68 (83%)	11 (13%)	3 (4%)	2	20
15	AQ	78/80 (98%)	66 (85%)	11 (14%)	1 (1%)	9	42
16	AS	69/71 (97%)	54 (78%)	12 (17%)	3 (4%)	2	17
17	AR	311/313 (99%)	282 (91%)	28 (9%)	1 (0%)	36	72
18	AT	137/141 (97%)	110 (80%)	21 (15%)	6 (4%)	2	17
20	B0	107/109 (98%)	75 (70%)	20 (19%)	12 (11%)	0	5
21	B1	46/48 (96%)	36 (78%)	9 (20%)	1 (2%)	5	29
22	B2	96/98 (98%)	87 (91%)	7 (7%)	2 (2%)	5	30
23	B8	116/118 (98%)	85 (73%)	25 (22%)	6 (5%)	1	15
24	B9	70/72 (97%)	48 (69%)	16 (23%)	6 (9%)	0	9
25	BA	211/213 (99%)	172 (82%)	30 (14%)	9 (4%)	2	17
26	BB	241/243 (99%)	174 (72%)	53 (22%)	14 (6%)	1	14
27	BC	360/362 (99%)	279 (78%)	68 (19%)	13 (4%)	2	20
28	BD	255/257 (99%)	208 (82%)	41 (16%)	6 (2%)	4	27
29	BE	235/237 (99%)	175 (74%)	47 (20%)	13 (6%)	1	15
30	BF	211/213 (99%)	150 (71%)	55 (26%)	6 (3%)	4	24
31	BG	111/113 (98%)	88 (79%)	20 (18%)	3 (3%)	4	25
32	BH	177/179 (99%)	146 (82%)	25 (14%)	6 (3%)	3	21
33	BI	163/165 (99%)	123 (76%)	31 (19%)	9 (6%)	1	15
34	BJ	149/151 (99%)	112 (75%)	33 (22%)	4 (3%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BK	136/138 (99%)	107 (79%)	22 (16%)	7 (5%)	1	15
36	BL	190/192 (99%)	156 (82%)	29 (15%)	5 (3%)	4	25
37	BM	176/178 (99%)	134 (76%)	34 (19%)	8 (4%)	2	17
38	BN	148/150 (99%)	122 (82%)	23 (16%)	3 (2%)	6	31
39	BO	119/121 (98%)	92 (77%)	23 (19%)	4 (3%)	3	21
40	BP	174/176 (99%)	155 (89%)	15 (9%)	4 (2%)	5	28
41	BQ	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	3	20
42	BR	129/131 (98%)	96 (74%)	28 (22%)	5 (4%)	2	19
43	BS	43/45 (96%)	33 (77%)	10 (23%)	0	100	100
44	BT	78/80 (98%)	59 (76%)	16 (20%)	3 (4%)	2	19
45	BU	114/116 (98%)	95 (83%)	15 (13%)	4 (4%)	3	20
46	BV	140/142 (99%)	98 (70%)	31 (22%)	11 (8%)	1	10
47	BW	77/79 (98%)	58 (75%)	16 (21%)	3 (4%)	2	19
48	BX	84/86 (98%)	63 (75%)	14 (17%)	7 (8%)	0	9
49	BY	50/52 (96%)	39 (78%)	10 (20%)	1 (2%)	6	31
50	BZ	90/92 (98%)	68 (76%)	18 (20%)	4 (4%)	2	17
All	All	6694/6830 (98%)	5337 (80%)	1095 (16%)	262 (4%)	4	19

All (262) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	81	PRO
3	AC	179	GLN
4	AD	96	VAL
5	AE	86	VAL
5	AE	226	THR
5	AE	227	PRO
6	AG	89	ILE
6	AG	164	PRO
7	AH	35	ILE
8	AI	97	VAL
8	AI	134	ALA
8	AI	136	SER
9	AJ	72	ASN
11	AL	53	VAL
12	AM	51	ASP

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Mol	Chain	Res	Type
13	AN	16	LYS
14	AO	108	ASP
16	AS	104	GLN
18	AT	51	GLU
20	B0	38	ILE
20	B0	50	ILE
20	B0	64	LYS
24	B9	14	TYR
24	B9	34	HIS
25	BA	60	ARG
26	BB	140	ASN
26	BB	161	ASP
26	BB	197	PRO
27	BC	168	LYS
27	BC	279	ASN
29	BE	188	GLU
29	BE	212	ALA
29	BE	216	GLU
30	BF	83	LEU
30	BF	123	THR
33	BI	18	PRO
33	BI	104	SER
35	BK	78	SER
35	BK	92	ARG
36	BL	56	LYS
37	BM	149	ALA
37	BM	170	ALA
46	BV	41	ARG
48	BX	68	ALA
48	BX	70	ALA
48	BX	80	ALA
50	BZ	46	LYS
50	BZ	57	VAL
2	AB	43	ASP
2	AB	68	PRO
3	AC	163	PRO
3	AC	164	VAL
4	AD	18	PRO
4	AD	148	VAL
5	AE	205	ARG
7	AH	58	SER
7	AH	98	GLN

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Mol	Chain	Res	Type
8	AI	15	SER
11	AL	144	ARG
12	AM	137	HIS
14	AO	128	TYR
18	AT	37	VAL
20	B0	77	ALA
20	B0	116	GLY
23	B8	35	SER
25	BA	36	VAL
25	BA	105	LYS
25	BA	162	VAL
26	BB	156	LYS
27	BC	128	LYS
27	BC	129	ALA
28	BD	180	LYS
29	BE	167	SER
29	BE	183	TRP
29	BE	224	LYS
31	BG	142	LEU
33	BI	142	ASP
35	BK	10	VAL
36	BL	40	ALA
37	BM	60	LYS
37	BM	156	ALA
40	BP	88	ARG
40	BP	143	ALA
42	BR	37	ILE
46	BV	52	PHE
46	BV	101	ILE
47	BW	61	LYS
48	BX	86	ALA
3	AC	83	THR
3	AC	112	GLY
3	AC	145	ALA
3	AC	148	LYS
4	AD	9	SER
4	AD	87	SER
4	AD	88	GLU
6	AG	66	GLN
6	AG	75	GLY
6	AG	85	ALA
6	AG	163	SER

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Mol	Chain	Res	Type
7	AH	28	ARG
7	AH	84	GLY
8	AI	42	GLU
8	AI	139	GLN
17	AR	283	LYS
18	AT	53	TRP
18	AT	86	ARG
20	B0	48	GLY
20	B0	62	LYS
20	B0	65	PHE
21	B1	40	LYS
23	B8	89	THR
24	B9	59	CYS
24	B9	66	GLY
26	BB	70	ARG
27	BC	38	SER
27	BC	46	PHE
27	BC	365	PHE
29	BE	36	LEU
29	BE	194	LEU
29	BE	219	PHE
30	BF	120	THR
31	BG	191	ASN
32	BH	22	SER
33	BI	105	CYS
33	BI	144	ASN
34	BJ	147	THR
35	BK	20	GLY
35	BK	88	PRO
37	BM	169	ALA
38	BN	122	ALA
39	BO	118	GLY
39	BO	122	ILE
40	BP	73	GLY
40	BP	133	LYS
41	BQ	10	ARG
44	BT	62	VAL
46	BV	14	HIS
47	BW	78	LYS
48	BX	48	ARG
50	BZ	35	LEU
3	AC	9	ARG

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Mol	Chain	Res	Type
4	AD	19	TYR
8	AI	125	GLU
10	AK	97	GLY
12	AM	90	ASN
13	AN	39	CYS
14	AO	147	SER
20	B0	94	ALA
22	B2	82	GLY
23	B8	116	PRO
24	B9	61	LYS
25	BA	58	CYS
25	BA	196	LYS
25	BA	208	SER
26	BB	73	GLU
26	BB	129	ALA
26	BB	153	GLY
26	BB	179	LEU
26	BB	221	LYS
26	BB	230	VAL
27	BC	102	LEU
27	BC	234	GLY
27	BC	272	TYR
28	BD	186	LYS
28	BD	213	ASN
28	BD	242	ALA
29	BE	227	LEU
30	BF	30	ALA
30	BF	177	GLY
30	BF	226	GLY
31	BG	126	SER
32	BH	129	ARG
33	BI	25	ALA
34	BJ	4	LYS
35	BK	26	ALA
37	BM	37	ARG
39	BO	74	GLU
41	BQ	18	ASP
41	BQ	69	LYS
42	BR	72	LYS
42	BR	96	GLU
44	BT	104	GLU
45	BU	59	VAL

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Mol	Chain	Res	Type
46	BV	63	GLN
46	BV	114	LYS
47	BW	83	GLU
48	BX	38	ARG
48	BX	82	ALA
3	AC	152	PHE
6	AG	86	GLN
8	AI	32	ASN
9	AJ	97	VAL
10	AK	47	LYS
10	AK	55	SER
13	AN	37	ASN
16	AS	51	SER
18	AT	89	ARG
23	B8	32	ASN
23	B8	46	ARG
26	BB	33	ASP
26	BB	180	LEU
28	BD	15	ALA
32	BH	50	ASN
32	BH	118	LEU
32	BH	122	LYS
33	BI	101	LYS
33	BI	111	LEU
41	BQ	17	ARG
42	BR	21	ALA
45	BU	46	LYS
46	BV	32	GLY
46	BV	102	ASP
46	BV	141	GLY
49	BY	36	SER
8	AI	126	PRO
18	AT	90	PRO
20	B0	97	ALA
25	BA	125	GLY
27	BC	29	VAL
29	BE	87	GLY
29	BE	201	GLY
29	BE	223	PHE
32	BH	106	LYS
34	BJ	12	LEU
35	BK	86	LYS

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Mol	Chain	Res	Type
36	BL	173	GLY
36	BL	191	TRP
37	BM	58	LEU
38	BN	65	SER
42	BR	44	SER
45	BU	113	LYS
5	AE	145	GLY
12	AM	75	ASN
15	AQ	111	VAL
16	AS	99	GLY
20	B0	96	ILE
24	B9	43	GLY
25	BA	37	GLY
34	BJ	58	GLY
39	BO	96	PHE
44	BT	86	VAL
46	BV	143	VAL
50	BZ	56	PRO
6	AG	162	VAL
9	AJ	91	ILE
22	B2	81	VAL
27	BC	260	VAL
37	BM	30	GLY
5	AE	109	GLY
12	AM	95	GLY
28	BD	139	GLY
38	BN	19	GLY
45	BU	44	GLY
46	BV	15	VAL
10	AK	35	GLY
13	AN	29	GLY
23	B8	70	LEU
26	BB	121	GLY
33	BI	114	GLY
36	BL	52	GLY
20	B0	79	VAL
27	BC	307	PRO

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	161/161 (100%)	159 (99%)	2 (1%)	63	75
3	AC	152/152 (100%)	148 (97%)	4 (3%)	40	62
4	AD	113/142 (80%)	103 (91%)	10 (9%)	9	28
5	AE	127/127 (100%)	121 (95%)	6 (5%)	23	45
6	AG	155/155 (100%)	150 (97%)	5 (3%)	34	56
7	AH	106/106 (100%)	100 (94%)	6 (6%)	18	40
8	AI	115/115 (100%)	108 (94%)	7 (6%)	17	38
9	AJ	90/90 (100%)	87 (97%)	3 (3%)	33	55
10	AK	95/95 (100%)	88 (93%)	7 (7%)	13	33
11	AL	98/98 (100%)	95 (97%)	3 (3%)	35	56
12	AM	115/115 (100%)	107 (93%)	8 (7%)	14	35
13	AN	45/45 (100%)	42 (93%)	3 (7%)	15	36
14	AO	74/74 (100%)	71 (96%)	3 (4%)	27	49
15	AQ	71/71 (100%)	69 (97%)	2 (3%)	38	60
16	AS	57/57 (100%)	55 (96%)	2 (4%)	32	53
17	AR	257/257 (100%)	241 (94%)	16 (6%)	16	38
18	AT	114/114 (100%)	105 (92%)	9 (8%)	11	32
20	B0	94/94 (100%)	89 (95%)	5 (5%)	20	41
21	B1	44/44 (100%)	41 (93%)	3 (7%)	14	36
22	B2	82/82 (100%)	81 (99%)	1 (1%)	63	75
23	B8	100/100 (100%)	84 (84%)	16 (16%)	2	11
24	B9	55/55 (100%)	53 (96%)	2 (4%)	31	52
25	BA	194/194 (100%)	181 (93%)	13 (7%)	15	36
26	BB	186/186 (100%)	177 (95%)	9 (5%)	23	44
27	BC	302/302 (100%)	281 (93%)	21 (7%)	14	35
28	BD	199/199 (100%)	184 (92%)	15 (8%)	12	33
29	BE	199/199 (100%)	186 (94%)	13 (6%)	15	37
30	BF	143/143 (100%)	134 (94%)	9 (6%)	16	37
31	BG	89/89 (100%)	84 (94%)	5 (6%)	19	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	BH	160/160 (100%)	150 (94%)	10 (6%)	16	37
33	BI	141/141 (100%)	134 (95%)	7 (5%)	22	43
34	BJ	129/129 (100%)	123 (95%)	6 (5%)	23	45
35	BK	112/112 (100%)	107 (96%)	5 (4%)	24	46
36	BL	164/164 (100%)	158 (96%)	6 (4%)	30	51
37	BM	119/119 (100%)	110 (92%)	9 (8%)	12	33
38	BN	122/122 (100%)	120 (98%)	2 (2%)	55	70
39	BO	99/99 (100%)	96 (97%)	3 (3%)	36	57
40	BP	118/118 (100%)	113 (96%)	5 (4%)	26	48
41	BQ	87/87 (100%)	85 (98%)	2 (2%)	44	64
42	BR	102/102 (100%)	96 (94%)	6 (6%)	18	39
43	BS	38/38 (100%)	36 (95%)	2 (5%)	20	41
44	BT	71/71 (100%)	65 (92%)	6 (8%)	10	29
45	BU	100/100 (100%)	98 (98%)	2 (2%)	48	66
46	BV	113/113 (100%)	106 (94%)	7 (6%)	16	38
47	BW	69/69 (100%)	65 (94%)	4 (6%)	18	40
48	BX	55/55 (100%)	53 (96%)	2 (4%)	31	52
49	BY	42/42 (100%)	39 (93%)	3 (7%)	13	35
50	BZ	81/81 (100%)	71 (88%)	10 (12%)	4	17
All	All	5554/5583 (100%)	5249 (94%)	305 (6%)	21	41

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	48	ILE
2	AB	179	ARG
3	AC	7	LYS
3	AC	132	LYS
3	AC	143	ARG
3	AC	158	ILE
4	AD	8	TYR
4	AD	111	THR
4	AD	112	GLN
4	AD	127	VAL
4	AD	138	LYS

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Mol	Chain	Res	Type
4	AD	139	GLN
4	AD	146	PHE
4	AD	148	VAL
4	AD	153	GLU
4	AD	154	LYS
5	AE	82	ASN
5	AE	111	VAL
5	AE	139	ILE
5	AE	178	ILE
5	AE	204	THR
5	AE	225	LEU
6	AG	42	LEU
6	AG	106	LYS
6	AG	133	VAL
6	AG	180	ARG
6	AG	188	LYS
7	AH	9	ASP
7	AH	27	ILE
7	AH	35	ILE
7	AH	37	PHE
7	AH	50	PHE
7	AH	82	LYS
8	AI	8	GLN
8	AI	42	GLU
8	AI	43	ILE
8	AI	45	ARG
8	AI	89	LEU
8	AI	98	ASP
8	AI	127	LYS
9	AJ	21	LYS
9	AJ	91	ILE
9	AJ	99	ILE
10	AK	26	THR
10	AK	33	LEU
10	AK	39	ILE
10	AK	43	THR
10	AK	47	LYS
10	AK	49	LYS
10	AK	115	ILE
11	AL	78	LYS
11	AL	117	ILE
11	AL	141	GLU

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Mol	Chain	Res	Type
12	AM	18	LEU
12	AM	54	LEU
12	AM	66	LEU
12	AM	92	ILE
12	AM	96	LYS
12	AM	116	LEU
12	AM	117	LYS
12	AM	125	ILE
13	AN	31	VAL
13	AN	39	CYS
13	AN	44	ARG
14	AO	78	ASN
14	AO	125	LEU
14	AO	134	VAL
15	AQ	80	MET
15	AQ	131	ILE
16	AS	64	LYS
16	AS	72	LYS
17	AR	13	LEU
17	AR	32	LEU
17	AR	33	LEU
17	AR	34	LEU
17	AR	42	LEU
17	AR	52	GLN
17	AR	107	LYS
17	AR	170	ILE
17	AR	183	LEU
17	AR	193	ILE
17	AR	199	ILE
17	AR	210	LEU
17	AR	228	LYS
17	AR	290	VAL
17	AR	292	LEU
17	AR	308	ASN
18	AT	6	VAL
18	AT	24	ARG
18	AT	28	LEU
18	AT	29	GLU
18	AT	86	ARG
18	AT	89	ARG
18	AT	94	ILE
18	AT	103	LYS

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Mol	Chain	Res	Type
18	AT	126	GLU
20	B0	21	HIS
20	B0	38	ILE
20	B0	75	LEU
20	B0	80	LYS
20	B0	111	ARG
21	B1	9	ILE
21	B1	20	ASN
21	B1	49	MET
22	B2	104	LEU
23	B8	14	LYS
23	B8	27	VAL
23	B8	30	VAL
23	B8	33	VAL
23	B8	36	GLN
23	B8	38	MET
23	B8	39	HIS
23	B8	43	LYS
23	B8	48	ARG
23	B8	51	VAL
23	B8	52	LEU
23	B8	56	ASN
23	B8	75	LYS
23	B8	97	LYS
23	B8	98	ASN
23	B8	116	PRO
24	B9	22	LEU
24	B9	45	LYS
25	BA	4	ILE
25	BA	29	LEU
25	BA	31	THR
25	BA	36	VAL
25	BA	59	PRO
25	BA	61	PRO
25	BA	76	ARG
25	BA	156	LYS
25	BA	162	VAL
25	BA	172	VAL
25	BA	176	GLU
25	BA	199	GLN
25	BA	205	VAL
26	BB	5	ILE

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Mol	Chain	Res	Type
26	BB	61	VAL
26	BB	64	ARG
26	BB	65	ASP
26	BB	75	ILE
26	BB	181	LYS
26	BB	219	ILE
26	BB	227	ARG
26	BB	230	VAL
27	BC	20	LYS
27	BC	29	VAL
27	BC	32	PHE
27	BC	113	GLU
27	BC	121	ASN
27	BC	126	LYS
27	BC	127	LYS
27	BC	150	ARG
27	BC	153	LYS
27	BC	161	LEU
27	BC	168	LYS
27	BC	208	VAL
27	BC	215	ILE
27	BC	221	THR
27	BC	237	LYS
27	BC	240	ARG
27	BC	305	ILE
27	BC	317	ILE
27	BC	327	CYS
27	BC	332	ARG
27	BC	364	LYS
28	BD	8	VAL
28	BD	33	ASP
28	BD	50	TYR
28	BD	69	ARG
28	BD	113	VAL
28	BD	116	ASN
28	BD	119	ARG
28	BD	126	ILE
28	BD	148	ILE
28	BD	170	LYS
28	BD	191	LYS
28	BD	215	ILE
28	BD	220	ARG

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Mol	Chain	Res	Type
28	BD	230	VAL
28	BD	258	LEU
29	BE	48	LYS
29	BE	50	ARG
29	BE	52	VAL
29	BE	105	ILE
29	BE	131	LEU
29	BE	173	VAL
29	BE	190	ILE
29	BE	195	LEU
29	BE	196	ARG
29	BE	217	GLU
29	BE	219	PHE
29	BE	222	LEU
29	BE	247	ILE
30	BF	83	LEU
30	BF	84	VAL
30	BF	87	VAL
30	BF	111	ILE
30	BF	118	LYS
30	BF	129	LEU
30	BF	185	ILE
30	BF	234	GLU
30	BF	244	ASN
31	BG	107	GLU
31	BG	136	LEU
31	BG	146	LYS
31	BG	163	VAL
31	BG	200	LEU
32	BH	34	LEU
32	BH	72	LYS
32	BH	79	ILE
32	BH	149	ASN
32	BH	167	VAL
32	BH	170	LYS
32	BH	172	ILE
32	BH	177	ASP
32	BH	179	ILE
32	BH	183	HIS
33	BI	69	ARG
33	BI	82	ARG
33	BI	103	LEU

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Mol	Chain	Res	Type
33	BI	115	MET
33	BI	121	LYS
33	BI	134	ILE
33	BI	152	LEU
34	BJ	44	THR
34	BJ	47	GLN
34	BJ	75	LYS
34	BJ	78	GLU
34	BJ	123	PHE
34	BJ	131	MET
35	BK	18	VAL
35	BK	22	VAL
35	BK	60	VAL
35	BK	87	GLU
35	BK	96	LYS
36	BL	13	LYS
36	BL	56	LYS
36	BL	77	LYS
36	BL	86	ASN
36	BL	122	ASN
36	BL	192	LYS
37	BM	14	HIS
37	BM	39	GLU
37	BM	42	ASN
37	BM	50	ASN
37	BM	58	LEU
37	BM	84	LEU
37	BM	113	ASP
37	BM	114	LYS
37	BM	134	LYS
38	BN	118	GLN
38	BN	153	LYS
39	BO	48	VAL
39	BO	72	LYS
39	BO	98	LYS
40	BP	20	ARG
40	BP	63	THR
40	BP	96	ILE
40	BP	111	ASP
40	BP	125	LYS
41	BQ	78	LYS
41	BQ	91	LEU

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Mol	Chain	Res	Type
42	BR	36	ILE
42	BR	40	LYS
42	BR	59	MET
42	BR	66	LYS
42	BR	88	ARG
42	BR	94	TYR
43	BS	14	TYR
43	BS	28	ILE
44	BT	60	TYR
44	BT	61	LYS
44	BT	67	ILE
44	BT	78	ASP
44	BT	89	LYS
44	BT	95	ILE
45	BU	59	VAL
45	BU	97	ILE
46	BV	47	TYR
46	BV	69	LYS
46	BV	74	LEU
46	BV	91	LYS
46	BV	97	THR
46	BV	137	ILE
46	BV	147	ILE
47	BW	11	GLU
47	BW	61	LYS
47	BW	70	ARG
47	BW	83	GLU
48	BX	43	LYS
48	BX	45	LYS
49	BY	12	HIS
49	BY	17	THR
49	BY	43	LYS
50	BZ	6	LYS
50	BZ	9	LYS
50	BZ	29	LYS
50	BZ	32	LYS
50	BZ	40	LYS
50	BZ	46	LYS
50	BZ	56	PRO
50	BZ	66	LYS
50	BZ	69	VAL
50	BZ	83	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	39	ASN
2	AB	46	HIS
2	AB	69	ASN
2	AB	109	ASN
2	AB	193	GLN
3	AC	111	ASN
3	AC	159	HIS
3	AC	174	HIS
3	AC	179	GLN
4	AD	124	HIS
4	AD	142	ASN
5	AE	147	ASN
5	AE	220	ASN
5	AE	228	ASN
6	AG	66	GLN
6	AG	72	HIS
6	AG	116	HIS
6	AG	170	GLN
7	AH	66	ASN
7	AH	120	HIS
8	AI	74	HIS
8	AI	93	HIS
9	AJ	40	ASN
9	AJ	48	HIS
9	AJ	87	HIS
10	AK	10	ASN
10	AK	24	ASN
11	AL	89	ASN
12	AM	78	HIS
12	AM	89	GLN
12	AM	122	HIS
12	AM	127	HIS
15	AQ	110	HIS
16	AS	79	HIS
16	AS	98	ASN
16	AS	104	GLN
17	AR	31	ASN
17	AR	52	GLN
17	AR	69	GLN
17	AR	101	GLN
17	AR	185	GLN

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Mol	Chain	Res	Type
17	AR	196	ASN
17	AR	198	ASN
17	AR	308	ASN
20	B0	21	HIS
20	B0	60	ASN
21	B1	43	ASN
21	B1	50	ASN
23	B8	103	ASN
24	B9	25	GLN
25	BA	8	GLN
25	BA	21	ASN
25	BA	35	GLN
25	BA	40	ASN
25	BA	119	GLN
26	BB	38	HIS
26	BB	50	HIS
26	BB	140	ASN
26	BB	187	HIS
26	BB	211	HIS
27	BC	13	HIS
27	BC	109	HIS
27	BC	139	GLN
27	BC	173	GLN
27	BC	177	HIS
27	BC	256	HIS
27	BC	269	GLN
28	BD	58	HIS
28	BD	92	ASN
28	BD	110	ASN
28	BD	140	HIS
28	BD	175	HIS
28	BD	243	HIS
29	BE	32	GLN
29	BE	90	HIS
30	BF	172	ASN
30	BF	194	HIS
30	BF	200	ASN
30	BF	225	GLN
30	BF	231	ASN
32	BH	40	HIS
32	BH	59	ASN
32	BH	100	ASN

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Mol	Chain	Res	Type
32	BH	116	ASN
32	BH	157	ASN
32	BH	162	GLN
32	BH	169	ASN
33	BI	12	GLN
33	BI	92	HIS
33	BI	95	HIS
33	BI	163	GLN
34	BJ	20	ASN
34	BJ	68	HIS
34	BJ	109	HIS
35	BK	65	GLN
35	BK	66	ASN
35	BK	68	GLN
35	BK	137	GLN
36	BL	23	GLN
36	BL	32	GLN
36	BL	90	ASN
36	BL	123	GLN
36	BL	149	ASN
36	BL	156	HIS
37	BM	14	HIS
37	BM	72	HIS
37	BM	90	HIS
38	BN	45	GLN
38	BN	101	ASN
38	BN	133	HIS
38	BN	145	HIS
39	BO	135	GLN
40	BP	36	ASN
40	BP	58	HIS
41	BQ	22	HIS
41	BQ	26	HIS
41	BQ	45	ASN
41	BQ	82	ASN
41	BQ	95	HIS
41	BQ	98	HIS
44	BT	65	GLN
44	BT	117	ASN
45	BU	100	HIS
46	BV	14	HIS
46	BV	48	HIS

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Mol	Chain	Res	Type
46	BV	61	HIS
47	BW	21	HIS
47	BW	43	HIS
48	BX	61	GLN
49	BY	16	HIS
50	BZ	23	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1757/1761 (99%)	382 (21%)	79 (4%)
19	A7	75/76 (98%)	9 (12%)	3 (4%)
51	B3	112/113 (99%)	40 (35%)	4 (3%)
52	B4	156/157 (99%)	55 (35%)	10 (6%)
53	B5	3169/3170 (99%)	949 (29%)	139 (4%)
All	All	5269/5277 (99%)	1435 (27%)	235 (4%)

All (1435) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	3	U
1	AA	4	C
1	AA	9	U
1	AA	27	U
1	AA	34	G
1	AA	42	G
1	AA	44	U
1	AA	46	A
1	AA	47	A
1	AA	48	G
1	AA	50	C
1	AA	51	A
1	AA	57	G
1	AA	60	U
1	AA	61	A
1	AA	62	A
1	AA	65	A
1	AA	67	A
1	AA	68	A
1	AA	69	G

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Mol	Chain	Res	Type
1	AA	81	G
1	AA	82	U
1	AA	83	G
1	AA	86	A
1	AA	90	C
1	AA	92	A
1	AA	100	A
1	AA	105	A
1	AA	106	U
1	AA	109	G
1	AA	110	U
1	AA	115	G
1	AA	116	U
1	AA	147	A
1	AA	161	U
1	AA	174	U
1	AA	176	C
1	AA	180	A
1	AA	188	A
1	AA	193	U
1	AA	200	A
1	AA	204	G
1	AA	208	U
1	AA	213	A
1	AA	230	C
1	AA	232	U
1	AA	233	C
1	AA	241	U
1	AA	243	G
1	AA	256	A
1	AA	257	A
1	AA	263	C
1	AA	264	G
1	AA	265	A
1	AA	266	A
1	AA	267	U
1	AA	279	G
1	AA	280	U
1	AA	281	G
1	AA	282	C
1	AA	283	U
1	AA	284	G

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Mol	Chain	Res	Type
1	AA	291	G
1	AA	295	A
1	AA	308	C
1	AA	309	C
1	AA	312	A
1	AA	313	U
1	AA	314	C
1	AA	316	A
1	AA	319	U
1	AA	322	G
1	AA	328	A
1	AA	329	G
1	AA	337	G
1	AA	351	C
1	AA	361	C
1	AA	365	G
1	AA	366	A
1	AA	373	G
1	AA	400	A
1	AA	401	A
1	AA	404	G
1	AA	419	G
1	AA	423	G
1	AA	424	C
1	AA	426	G
1	AA	429	G
1	AA	435	C
1	AA	439	U
1	AA	445	A
1	AA	451	A
1	AA	452	A
1	AA	462	G
1	AA	468	A
1	AA	469	C
1	AA	475	A
1	AA	478	A
1	AA	479	C
1	AA	481	A
1	AA	493	U
1	AA	494	U
1	AA	495	C
1	AA	496	G

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Mol	Chain	Res	Type
1	AA	501	U
1	AA	503	G
1	AA	512	A
1	AA	513	U
1	AA	530	C
1	AA	542	A
1	AA	543	C
1	AA	551	G
1	AA	558	U
1	AA	565	C
1	AA	568	G
1	AA	571	G
1	AA	574	G
1	AA	578	U
1	AA	579	A
1	AA	594	A
1	AA	609	U
1	AA	611	U
1	AA	613	G
1	AA	619	A
1	AA	620	A
1	AA	623	A
1	AA	624	G
1	AA	631	G
1	AA	638	U
1	AA	639	U
1	AA	648	G
1	AA	653	C
1	AA	666	U
1	AA	687	G
1	AA	693	U
1	AA	694	U
1	AA	695	U
1	AA	696	C
1	AA	698	U
1	AA	703	G
1	AA	729	G
1	AA	730	G
1	AA	746	A
1	AA	749	U
1	AA	760	A
1	AA	765	G

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Mol	Chain	Res	Type
1	AA	771	A
1	AA	774	A
1	AA	775	G
1	AA	776	G
1	AA	778	G
1	AA	779	U
1	AA	780	A
1	AA	781	U
1	AA	792	U
1	AA	797	G
1	AA	800	U
1	AA	818	C
1	AA	821	U
1	AA	822	U
1	AA	824	G
1	AA	844	A
1	AA	845	G
1	AA	853	G
1	AA	855	A
1	AA	856	A
1	AA	857	U
1	AA	858	G
1	AA	860	U
1	AA	864	U
1	AA	865	A
1	AA	866	G
1	AA	867	G
1	AA	868	G
1	AA	869	A
1	AA	877	G
1	AA	896	U
1	AA	898	G
1	AA	899	A
1	AA	900	G
1	AA	905	A
1	AA	923	A
1	AA	931	U
1	AA	934	U
1	AA	957	U
1	AA	958	U
1	AA	961	C
1	AA	962	A

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Mol	Chain	Res	Type
1	AA	963	U
1	AA	965	A
1	AA	971	G
1	AA	987	A
1	AA	989	C
1	AA	990	G
1	AA	993	G
1	AA	1003	U
1	AA	1004	A
1	AA	1022	A
1	AA	1025	A
1	AA	1027	C
1	AA	1029	A
1	AA	1031	G
1	AA	1036	C
1	AA	1038	A
1	AA	1039	G
1	AA	1040	A
1	AA	1041	U
1	AA	1042	C
1	AA	1049	U
1	AA	1050	G
1	AA	1056	U
1	AA	1058	A
1	AA	1059	A
1	AA	1060	U
1	AA	1074	C
1	AA	1090	A
1	AA	1092	U
1	AA	1098	G
1	AA	1099	G
1	AA	1110	A
1	AA	1127	G
1	AA	1134	A
1	AA	1135	A
1	AA	1148	A
1	AA	1152	G
1	AA	1155	C
1	AA	1156	C
1	AA	1160	A
1	AA	1171	C
1	AA	1178	U

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Mol	Chain	Res	Type
1	AA	1179	A
1	AA	1181	U
1	AA	1182	U
1	AA	1187	U
1	AA	1188	C
1	AA	1189	A
1	AA	1190	A
1	AA	1192	A
1	AA	1193	C
1	AA	1195	G
1	AA	1196	G
1	AA	1197	G
1	AA	1198	A
1	AA	1199	A
1	AA	1201	C
1	AA	1202	U
1	AA	1213	A
1	AA	1214	G
1	AA	1215	A
1	AA	1216	C
1	AA	1217	A
1	AA	1225	G
1	AA	1241	G
1	AA	1242	C
1	AA	1243	U
1	AA	1246	U
1	AA	1247	U
1	AA	1248	C
1	AA	1249	U
1	AA	1261	G
1	AA	1262	U
1	AA	1263	G
1	AA	1265	U
1	AA	1266	G
1	AA	1267	G
1	AA	1270	C
1	AA	1271	A
1	AA	1272	U
1	AA	1274	G
1	AA	1281	C
1	AA	1282	U
1	AA	1318	A

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Mol	Chain	Res	Type
1	AA	1319	A
1	AA	1325	G
1	AA	1329	C
1	AA	1341	A
1	AA	1342	A
1	AA	1350	U
1	AA	1351	G
1	AA	1355	G
1	AA	1366	U
1	AA	1378	U
1	AA	1379	A
1	AA	1386	C
1	AA	1387	U
1	AA	1396	C
1	AA	1402	G
1	AA	1409	G
1	AA	1410	U
1	AA	1411	U
1	AA	1416	G
1	AA	1424	A
1	AA	1425	G
1	AA	1429	U
1	AA	1430	G
1	AA	1431	U
1	AA	1438	C
1	AA	1443	A
1	AA	1444	A
1	AA	1445	C
1	AA	1446	G
1	AA	1447	U
1	AA	1452	G
1	AA	1455	C
1	AA	1456	G
1	AA	1457	C
1	AA	1458	A
1	AA	1459	C
1	AA	1471	U
1	AA	1472	G
1	AA	1479	C
1	AA	1489	U
1	AA	1490	A
1	AA	1491	A

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Mol	Chain	Res	Type
1	AA	1496	G
1	AA	1504	G
1	AA	1506	U
1	AA	1507	C
1	AA	1513	A
1	AA	1515	U
1	AA	1517	U
1	AA	1518	U
1	AA	1519	G
1	AA	1520	U
1	AA	1521	G
1	AA	1522	A
1	AA	1533	U
1	AA	1536	U
1	AA	1540	G
1	AA	1546	G
1	AA	1547	C
1	AA	1548	A
1	AA	1549	U
1	AA	1550	U
1	AA	1552	U
1	AA	1553	A
1	AA	1555	U
1	AA	1556	U
1	AA	1561	C
1	AA	1564	U
1	AA	1571	A
1	AA	1580	U
1	AA	1581	A
1	AA	1582	G
1	AA	1583	U
1	AA	1584	A
1	AA	1585	A
1	AA	1588	G
1	AA	1594	C
1	AA	1599	G
1	AA	1607	U
1	AA	1609	A
1	AA	1610	U
1	AA	1612	A
1	AA	1613	C
1	AA	1614	G

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Mol	Chain	Res	Type
1	AA	1615	U
1	AA	1631	A
1	AA	1633	A
1	AA	1634	C
1	AA	1635	C
1	AA	1636	G
1	AA	1637	C
1	AA	1638	C
1	AA	1640	G
1	AA	1655	U
1	AA	1656	G
1	AA	1676	A
1	AA	1753	A
1	AA	1760	A
1	AA	1764	A
1	AA	1766	G
1	AA	1767	U
1	AA	1778	G
1	AA	1779	A
1	AA	1780	A
1	AA	1781	C
1	AA	1790	G
1	AA	1791	G
1	AA	1794	C
1	AA	1795	A
19	A7	10	2MG
19	A7	11	C
19	A7	17	H2U
19	A7	20	G
19	A7	22	G
19	A7	23	A
19	A7	44	A
19	A7	47	U
19	A7	76	A
51	B3	2	G
51	B3	7	G
51	B3	10	C
51	B3	11	A
51	B3	13	A
51	B3	14	U
51	B3	24	A
51	B3	34	C

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Mol	Chain	Res	Type
51	B3	36	C
51	B3	40	C
51	B3	41	G
51	B3	42	A
51	B3	43	U
51	B3	44	C
51	B3	45	A
51	B3	46	A
51	B3	48	U
51	B3	50	U
51	B3	56	G
51	B3	59	G
51	B3	61	U
51	B3	70	A
51	B3	71	C
51	B3	74	A
51	B3	81	U
51	B3	82	A
51	B3	84	G
51	B3	86	G
51	B3	88	G
51	B3	89	A
51	B3	90	C
51	B3	91	C
51	B3	92	A
51	B3	95	C
51	B3	98	G
51	B3	99	A
51	B3	101	A
51	B3	102	C
51	B3	105	A
51	B3	109	G
52	B4	4	C
52	B4	11	C
52	B4	12	A
52	B4	14	C
52	B4	18	U
52	B4	20	U
52	B4	22	U
52	B4	23	U
52	B4	24	G
52	B4	34	U

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Mol	Chain	Res	Type
52	B4	48	A
52	B4	55	U
52	B4	58	G
52	B4	59	A
52	B4	60	U
52	B4	61	A
52	B4	62	C
52	B4	63	G
52	B4	64	U
52	B4	68	G
52	B4	69	U
52	B4	70	A
52	B4	71	G
52	B4	72	G
52	B4	76	C
52	B4	88	A
52	B4	89	A
52	B4	92	A
52	B4	95	G
52	B4	99	C
52	B4	100	U
52	B4	102	U
52	B4	103	G
52	B4	104	A
52	B4	105	A
52	B4	106	C
52	B4	108	C
52	B4	109	A
52	B4	111	A
52	B4	114	G
52	B4	115	C
52	B4	118	C
52	B4	128	U
52	B4	133	G
52	B4	134	G
52	B4	135	G
52	B4	136	G
52	B4	137	C
52	B4	138	A
52	B4	139	U
52	B4	140	G
52	B4	145	U

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Mol	Chain	Res	Type
52	B4	147	U
52	B4	153	U
52	B4	156	U
53	B5	4	U
53	B5	6	A
53	B5	7	C
53	B5	13	A
53	B5	15	C
53	B5	16	A
53	B5	17	G
53	B5	19	U
53	B5	33	G
53	B5	39	A
53	B5	40	A
53	B5	43	A
53	B5	44	U
53	B5	46	U
53	B5	60	A
53	B5	62	A
53	B5	66	A
53	B5	68	C
53	B5	71	A
53	B5	74	G
53	B5	77	A
53	B5	85	A
53	B5	89	A
53	B5	92	G
53	B5	99	A
53	B5	108	A
53	B5	109	A
53	B5	110	G
53	B5	112	U
53	B5	114	A
53	B5	115	A
53	B5	118	U
53	B5	120	G
53	B5	125	C
53	B5	128	G
53	B5	129	U
53	B5	131	C
53	B5	132	C
53	B5	133	U

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Mol	Chain	Res	Type
53	B5	134	U
53	B5	135	C
53	B5	149	U
53	B5	150	A
53	B5	151	A
53	B5	160	G
53	B5	161	G
53	B5	163	C
53	B5	170	G
53	B5	171	G
53	B5	175	C
53	B5	186	U
53	B5	189	G
53	B5	199	A
53	B5	200	C
53	B5	202	G
53	B5	210	U
53	B5	211	A
53	B5	214	G
53	B5	216	G
53	B5	217	U
53	B5	218	G
53	B5	219	A
53	B5	220	G
53	B5	230	U
53	B5	240	U
53	B5	250	U
53	B5	251	G
53	B5	252	U
53	B5	265	A
53	B5	268	A
53	B5	269	G
53	B5	272	G
53	B5	274	G
53	B5	278	U
53	B5	279	U
53	B5	280	U
53	B5	281	G
53	B5	287	G
53	B5	288	C
53	B5	291	C
53	B5	298	U

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Mol	Chain	Res	Type
53	B5	304	G
53	B5	310	U
53	B5	315	C
53	B5	318	A
53	B5	330	G
53	B5	338	A
53	B5	341	G
53	B5	343	U
53	B5	352	A
53	B5	354	U
53	B5	355	A
53	B5	356	C
53	B5	362	U
53	B5	364	G
53	B5	368	G
53	B5	370	U
53	B5	372	A
53	B5	373	A
53	B5	375	A
53	B5	376	G
53	B5	384	A
53	B5	387	A
53	B5	391	A
53	B5	394	G
53	B5	398	A
53	B5	399	A
53	B5	402	A
53	B5	403	C
53	B5	404	G
53	B5	406	G
53	B5	411	U
53	B5	413	U
53	B5	414	U
53	B5	415	G
53	B5	423	A
53	B5	434	U
53	B5	438	A
53	B5	440	A
53	B5	441	U
53	B5	451	U
53	B5	453	C
53	B5	455	C

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Mol	Chain	Res	Type
53	B5	457	C
53	B5	465	U
53	B5	467	U
53	B5	471	U
53	B5	476	G
53	B5	477	A
53	B5	478	A
53	B5	479	U
53	B5	480	C
53	B5	481	U
53	B5	482	C
53	B5	483	G
53	B5	484	C
53	B5	485	A
53	B5	486	U
53	B5	492	U
53	B5	494	G
53	B5	496	C
53	B5	500	C
53	B5	513	G
53	B5	515	C
53	B5	532	A
53	B5	533	A
53	B5	547	G
53	B5	548	G
53	B5	553	U
53	B5	554	A
53	B5	555	U
53	B5	556	U
53	B5	570	A
53	B5	572	A
53	B5	576	C
53	B5	578	A
53	B5	585	A
53	B5	590	G
53	B5	592	G
53	B5	596	U
53	B5	597	G
53	B5	602	A
53	B5	604	G
53	B5	605	U
53	B5	606	C

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Mol	Chain	Res	Type
53	B5	607	A
53	B5	608	A
53	B5	609	G
53	B5	611	A
53	B5	612	U
53	B5	616	G
53	B5	619	A
53	B5	620	U
53	B5	621	A
53	B5	622	A
53	B5	627	U
53	B5	629	U
53	B5	636	C
53	B5	638	C
53	B5	639	G
53	B5	647	A
53	B5	648	C
53	B5	649	A
53	B5	652	G
53	B5	653	A
53	B5	654	C
53	B5	663	C
53	B5	664	U
53	B5	677	A
53	B5	678	G
53	B5	681	U
53	B5	688	G
53	B5	689	U
53	B5	690	A
53	B5	691	A
53	B5	695	C
53	B5	704	U
53	B5	705	A
53	B5	706	A
53	B5	708	G
53	B5	710	A
53	B5	711	A
53	B5	712	G
53	B5	713	U
53	B5	714	G
53	B5	715	A
53	B5	716	G

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Mol	Chain	Res	Type
53	B5	717	C
53	B5	718	G
53	B5	735	A
53	B5	736	A
53	B5	742	G
53	B5	743	C
53	B5	744	A
53	B5	748	U
53	B5	766	U
53	B5	767	U
53	B5	783	A
53	B5	784	A
53	B5	785	G
53	B5	786	A
53	B5	787	G
53	B5	800	G
53	B5	801	A
53	B5	802	C
53	B5	808	A
53	B5	817	A
53	B5	819	U
53	B5	820	A
53	B5	833	G
53	B5	837	A
53	B5	844	G
53	B5	846	A
53	B5	848	A
53	B5	851	C
53	B5	856	G
53	B5	858	A
53	B5	860	G
53	B5	861	C
53	B5	879	U
53	B5	880	G
53	B5	882	A
53	B5	884	A
53	B5	894	G
53	B5	896	A
53	B5	907	G
53	B5	913	A
53	B5	914	A
53	B5	915	A

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Mol	Chain	Res	Type
53	B5	916	G
53	B5	917	A
53	B5	921	A
53	B5	923	C
53	B5	925	A
53	B5	932	U
53	B5	933	A
53	B5	934	G
53	B5	937	G
53	B5	944	C
53	B5	951	A
53	B5	959	C
53	B5	962	A
53	B5	963	G
53	B5	965	A
53	B5	970	A
53	B5	971	C
53	B5	972	G
53	B5	973	A
53	B5	978	C
53	B5	979	G
53	B5	987	U
53	B5	990	A
53	B5	994	G
53	B5	1009	A
53	B5	1011	A
53	B5	1017	C
53	B5	1024	G
53	B5	1025	A
53	B5	1027	A
53	B5	1029	G
53	B5	1030	A
53	B5	1033	U
53	B5	1034	U
53	B5	1035	G
53	B5	1036	A
53	B5	1041	U
53	B5	1047	A
53	B5	1054	A
53	B5	1056	U
53	B5	1065	A
53	B5	1066	G

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Mol	Chain	Res	Type
53	B5	1078	U
53	B5	1079	A
53	B5	1080	A
53	B5	1085	A
53	B5	1088	U
53	B5	1093	A
53	B5	1099	A
53	B5	1101	G
53	B5	1104	G
53	B5	1105	A
53	B5	1110	U
53	B5	1111	U
53	B5	1112	A
53	B5	1116	G
53	B5	1117	G
53	B5	1126	G
53	B5	1127	G
53	B5	1128	U
53	B5	1129	A
53	B5	1133	A
53	B5	1135	A
53	B5	1142	G
53	B5	1144	U
53	B5	1150	A
53	B5	1153	A
53	B5	1160	C
53	B5	1162	U
53	B5	1164	G
53	B5	1166	G
53	B5	1173	U
53	B5	1174	G
53	B5	1175	C
53	B5	1177	G
53	B5	1181	U
53	B5	1182	A
53	B5	1191	U
53	B5	1200	A
53	B5	1201	C
53	B5	1208	U
53	B5	1219	C
53	B5	1227	C
53	B5	1228	C

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Mol	Chain	Res	Type
53	B5	1229	G
53	B5	1231	A
53	B5	1232	C
53	B5	1235	U
53	B5	1236	G
53	B5	1237	G
53	B5	1238	C
53	B5	1244	A
53	B5	1245	A
53	B5	1248	C
53	B5	1250	G
53	B5	1251	A
53	B5	1253	U
53	B5	1254	C
53	B5	1257	C
53	B5	1258	U
53	B5	1259	A
53	B5	1263	A
53	B5	1264	G
53	B5	1268	G
53	B5	1273	A
53	B5	1274	A
53	B5	1279	C
53	B5	1282	G
53	B5	1287	A
53	B5	1291	A
53	B5	1298	C
53	B5	1303	A
53	B5	1304	A
53	B5	1305	U
53	B5	1306	G
53	B5	1307	G
53	B5	1308	A
53	B5	1309	U
53	B5	1311	G
53	B5	1313	G
53	B5	1318	A
53	B5	1319	G
53	B5	1347	U
53	B5	1357	G
53	B5	1358	C
53	B5	1359	C

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Mol	Chain	Res	Type
53	B5	1360	C
53	B5	1361	U
53	B5	1363	A
53	B5	1370	G
53	B5	1384	U
53	B5	1385	C
53	B5	1391	C
53	B5	1392	G
53	B5	1402	C
53	B5	1404	G
53	B5	1406	A
53	B5	1407	A
53	B5	1408	G
53	B5	1412	G
53	B5	1418	A
53	B5	1421	G
53	B5	1422	G
53	B5	1423	C
53	B5	1425	U
53	B5	1426	C
53	B5	1429	G
53	B5	1431	G
53	B5	1434	G
53	B5	1439	U
53	B5	1442	U
53	B5	1447	G
53	B5	1452	A
53	B5	1453	A
53	B5	1455	U
53	B5	1456	A
53	B5	1457	U
53	B5	1481	A
53	B5	1482	A
53	B5	1507	G
53	B5	1510	G
53	B5	1515	A
53	B5	1526	U
53	B5	1529	A
53	B5	1530	U
53	B5	1532	C
53	B5	1533	U
53	B5	1548	C

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Mol	Chain	Res	Type
53	B5	1550	C
53	B5	1554	U
53	B5	1555	U
53	B5	1571	A
53	B5	1572	U
53	B5	1580	A
53	B5	1582	C
53	B5	1583	A
53	B5	1584	U
53	B5	1588	A
53	B5	1590	G
53	B5	1591	G
53	B5	1592	G
53	B5	1593	A
53	B5	1598	G
53	B5	1602	A
53	B5	1607	U
53	B5	1617	G
53	B5	1622	U
53	B5	1623	G
53	B5	1624	G
53	B5	1627	U
53	B5	1628	C
53	B5	1637	A
53	B5	1639	C
53	B5	1640	G
53	B5	1642	A
53	B5	1644	C
53	B5	1647	A
53	B5	1648	A
53	B5	1649	U
53	B5	1650	G
53	B5	1657	C
53	B5	1658	G
53	B5	1666	G
53	B5	1668	G
53	B5	1669	C
53	B5	1670	C
53	B5	1671	C
53	B5	1672	U
53	B5	1681	U
53	B5	1682	U

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Mol	Chain	Res	Type
53	B5	1683	A
53	B5	1688	U
53	B5	1689	U
53	B5	1697	A
53	B5	1698	C
53	B5	1701	C
53	B5	1702	U
53	B5	1703	U
53	B5	1704	A
53	B5	1709	C
53	B5	1710	C
53	B5	1712	G
53	B5	1715	A
53	B5	1718	G
53	B5	1719	G
53	B5	1720	U
53	B5	1721	U
53	B5	1722	U
53	B5	1727	G
53	B5	1729	A
53	B5	1733	G
53	B5	1735	G
53	B5	1736	G
53	B5	1737	U
53	B5	1738	C
53	B5	1744	G
53	B5	1745	C
53	B5	1746	U
53	B5	1750	A
53	B5	1751	G
53	B5	1759	C
53	B5	1762	C
53	B5	1764	U
53	B5	1765	U
53	B5	1768	U
53	B5	1769	G
53	B5	1774	C
53	B5	1775	G
53	B5	1777	U
53	B5	1784	G
53	B5	1797	A
53	B5	1805	C

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Mol	Chain	Res	Type
53	B5	1806	A
53	B5	1813	A
53	B5	1814	A
53	B5	1817	G
53	B5	1819	U
53	B5	1824	U
53	B5	1826	C
53	B5	1830	G
53	B5	1832	C
53	B5	1840	U
53	B5	1841	A
53	B5	1842	A
53	B5	1849	C
53	B5	1853	U
53	B5	1855	U
53	B5	1859	A
53	B5	1864	A
53	B5	1866	C
53	B5	1867	A
53	B5	1880	U
53	B5	1886	A
53	B5	1889	G
53	B5	1890	U
53	B5	1892	G
53	B5	1895	A
53	B5	1900	A
53	B5	1901	A
53	B5	1902	G
53	B5	1906	G
53	B5	1909	A
53	B5	1918	C
53	B5	1919	G
53	B5	1925	U
53	B5	1926	C
53	B5	1927	G
53	B5	1932	A
53	B5	1933	A
53	B5	1934	G
53	B5	1935	G
53	B5	1946	A
53	B5	2102	U
53	B5	2103	U

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Mol	Chain	Res	Type
53	B5	2104	A
53	B5	2114	C
53	B5	2115	G
53	B5	2116	G
53	B5	2120	A
53	B5	2122	G
53	B5	2125	A
53	B5	2126	A
53	B5	2131	A
53	B5	2134	G
53	B5	2138	A
53	B5	2139	A
53	B5	2140	U
53	B5	2142	A
53	B5	2159	U
53	B5	2160	G
53	B5	2161	G
53	B5	2167	A
53	B5	2170	U
53	B5	2173	U
53	B5	2174	G
53	B5	2175	U
53	B5	2178	A
53	B5	2189	U
53	B5	2199	G
53	B5	2208	A
53	B5	2209	U
53	B5	2210	G
53	B5	2212	C
53	B5	2213	A
53	B5	2214	A
53	B5	2215	A
53	B5	2216	G
53	B5	2217	U
53	B5	2219	A
53	B5	2220	A
53	B5	2221	G
53	B5	2222	A
53	B5	2223	A
53	B5	2224	A
53	B5	2225	U
53	B5	2226	U

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Mol	Chain	Res	Type
53	B5	2227	C
53	B5	2228	A
53	B5	2229	A
53	B5	2230	C
53	B5	2237	C
53	B5	2242	A
53	B5	2244	A
53	B5	2249	G
53	B5	2252	A
53	B5	2255	A
53	B5	2256	A
53	B5	2257	C
53	B5	2259	A
53	B5	2263	C
53	B5	2273	G
53	B5	2279	A
53	B5	2285	C
53	B5	2286	U
53	B5	2287	C
53	B5	2288	G
53	B5	2297	U
53	B5	2298	U
53	B5	2301	U
53	B5	2303	A
53	B5	2306	C
53	B5	2308	C
53	B5	2309	A
53	B5	2310	U
53	B5	2313	A
53	B5	2314	U
53	B5	2315	G
53	B5	2317	A
53	B5	2319	U
53	B5	2326	A
53	B5	2335	G
53	B5	2336	U
53	B5	2340	U
53	B5	2347	U
53	B5	2350	C
53	B5	2355	G
53	B5	2360	C
53	B5	2362	C

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Mol	Chain	Res	Type
53	B5	2363	A
53	B5	2365	C
53	B5	2368	A
53	B5	2371	G
53	B5	2372	A
53	B5	2373	A
53	B5	2374	C
53	B5	2379	U
53	B5	2383	C
53	B5	2385	G
53	B5	2388	U
53	B5	2394	G
53	B5	2397	A
53	B5	2402	A
53	B5	2403	G
53	B5	2411	U
53	B5	2415	C
53	B5	2417	U
53	B5	2419	A
53	B5	2435	G
53	B5	2446	U
53	B5	2452	G
53	B5	2454	G
53	B5	2457	G
53	B5	2458	A
53	B5	2460	U
53	B5	2461	A
53	B5	2462	A
53	B5	2463	G
53	B5	2464	U
53	B5	2468	A
53	B5	2469	G
53	B5	2470	C
53	B5	2472	U
53	B5	2473	C
53	B5	2474	G
53	B5	2475	G
53	B5	2477	G
53	B5	2478	C
53	B5	2479	C
53	B5	2484	A
53	B5	2487	U

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Mol	Chain	Res	Type
53	B5	2494	A
53	B5	2497	U
53	B5	2498	U
53	B5	2499	U
53	B5	2506	U
53	B5	2510	U
53	B5	2514	U
53	B5	2515	A
53	B5	2521	U
53	B5	2524	A
53	B5	2539	A
53	B5	2540	A
53	B5	2541	U
53	B5	2542	U
53	B5	2543	U
53	B5	2546	C
53	B5	2548	C
53	B5	2550	U
53	B5	2551	C
53	B5	2552	C
53	B5	2556	U
53	B5	2560	U
53	B5	2561	A
53	B5	2562	G
53	B5	2570	U
53	B5	2572	C
53	B5	2573	G
53	B5	2575	G
53	B5	2576	G
53	B5	2577	C
53	B5	2578	U
53	B5	2585	G
53	B5	2586	G
53	B5	2593	A
53	B5	2596	U
53	B5	2606	G
53	B5	2607	G
53	B5	2608	G
53	B5	2610	G
53	B5	2618	G
53	B5	2619	G
53	B5	2623	G

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Mol	Chain	Res	Type
53	B5	2638	C
53	B5	2652	U
53	B5	2655	U
53	B5	2656	A
53	B5	2658	G
53	B5	2674	A
53	B5	2675	C
53	B5	2676	A
53	B5	2677	G
53	B5	2678	A
53	B5	2680	A
53	B5	2690	G
53	B5	2691	A
53	B5	2694	A
53	B5	2698	G
53	B5	2703	A
53	B5	2704	A
53	B5	2706	G
53	B5	2714	G
53	B5	2715	A
53	B5	2718	U
53	B5	2719	U
53	B5	2725	U
53	B5	2735	U
53	B5	2736	A
53	B5	2749	G
53	B5	2752	U
53	B5	2755	C
53	B5	2757	U
53	B5	2758	A
53	B5	2765	C
53	B5	2773	C
53	B5	2774	C
53	B5	2775	U
53	B5	2776	C
53	B5	2778	G
53	B5	2779	A
53	B5	2780	A
53	B5	2781	U
53	B5	2783	U
53	B5	2788	C
53	B5	2794	G

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Mol	Chain	Res	Type
53	B5	2795	U
53	B5	2796	G
53	B5	2797	C
53	B5	2799	A
53	B5	2800	G
53	B5	2801	A
53	B5	2802	A
53	B5	2809	C
53	B5	2810	C
53	B5	2816	G
53	B5	2817	A
53	B5	2818	U
53	B5	2827	U
53	B5	2829	U
53	B5	2830	G
53	B5	2837	A
53	B5	2838	A
53	B5	2839	G
53	B5	2840	C
53	B5	2841	G
53	B5	2842	U
53	B5	2845	A
53	B5	2849	C
53	B5	2850	G
53	B5	2852	C
53	B5	2853	A
53	B5	2860	U
53	B5	2863	G
53	B5	2864	A
53	B5	2865	U
53	B5	2866	U
53	B5	2867	C
53	B5	2868	U
53	B5	2872	A
53	B5	2874	G
53	B5	2875	U
53	B5	2877	G
53	B5	2882	U
53	B5	2887	A
53	B5	2888	U
53	B5	2899	C
53	B5	2902	A

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Mol	Chain	Res	Type
53	B5	2904	U
53	B5	2905	U
53	B5	2910	A
53	B5	2914	G
53	B5	2915	U
53	B5	2919	A
53	B5	2921	U
53	B5	2931	C
53	B5	2936	A
53	B5	2941	A
53	B5	2942	C
53	B5	2943	G
53	B5	2944	U
53	B5	2945	G
53	B5	2947	G
53	B5	2953	U
53	B5	2962	U
53	B5	2965	U
53	B5	2975	U
53	B5	2978	U
53	B5	2980	U
53	B5	2981	U
53	B5	2988	C
53	B5	2989	U
53	B5	2996	U
53	B5	2997	G
53	B5	3001	C
53	B5	3002	C
53	B5	3004	C
53	B5	3010	U
53	B5	3012	A
53	B5	3019	U
53	B5	3028	G
53	B5	3030	G
53	B5	3034	C
53	B5	3040	A
53	B5	3046	A
53	B5	3048	A
53	B5	3049	A
53	B5	3050	U
53	B5	3051	U
53	B5	3052	G

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Mol	Chain	Res	Type
53	B5	3055	U
53	B5	3056	U
53	B5	3057	U
53	B5	3058	U
53	B5	3061	G
53	B5	3062	G
53	B5	3081	C
53	B5	3083	G
53	B5	3084	C
53	B5	3086	A
53	B5	3088	G
53	B5	3100	U
53	B5	3112	G
53	B5	3113	A
53	B5	3114	A
53	B5	3116	G
53	B5	3120	C
53	B5	3121	U
53	B5	3122	A
53	B5	3123	A
53	B5	3124	G
53	B5	3126	C
53	B5	3134	A
53	B5	3136	G
53	B5	3139	A
53	B5	3140	G
53	B5	3141	A
53	B5	3142	A
53	B5	3143	C
53	B5	3144	G
53	B5	3149	G
53	B5	3151	U
53	B5	3152	U
53	B5	3154	C
53	B5	3158	G
53	B5	3159	C
53	B5	3160	U
53	B5	3161	C
53	B5	3162	C
53	B5	3165	A
53	B5	3166	C
53	B5	3167	A

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Mol	Chain	Res	Type
53	B5	3170	A
53	B5	3171	U
53	B5	3174	A
53	B5	3175	C
53	B5	3176	C
53	B5	3182	U
53	B5	3183	A
53	B5	3184	U
53	B5	3186	A
53	B5	3188	G
53	B5	3195	U
53	B5	3196	U
53	B5	3198	U
53	B5	3199	G
53	B5	3200	G
53	B5	3205	U
53	B5	3206	A
53	B5	3208	C
53	B5	3211	U
53	B5	3216	U
53	B5	3217	A
53	B5	3220	G
53	B5	3229	G
53	B5	3230	G
53	B5	3235	C
53	B5	3243	A
53	B5	3245	A
53	B5	3246	G
53	B5	3247	G
53	B5	3248	C
53	B5	3249	C
53	B5	3252	G
53	B5	3253	G
53	B5	3259	U
53	B5	3266	G
53	B5	3267	U
53	B5	3277	C
53	B5	3290	G
53	B5	3295	A
53	B5	3296	A
53	B5	3298	C
53	B5	3304	U

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Mol	Chain	Res	Type
53	B5	3305	A
53	B5	3306	U
53	B5	3307	A
53	B5	3317	U
53	B5	3320	A
53	B5	3325	G
53	B5	3326	G
53	B5	3327	G
53	B5	3328	G
53	B5	3330	A
53	B5	3331	U
53	B5	3332	U
53	B5	3333	G
53	B5	3334	U
53	B5	3337	G
53	B5	3338	C
53	B5	3354	U
53	B5	3355	U
53	B5	3364	C
53	B5	3368	U
53	B5	3369	G
53	B5	3374	U
53	B5	3385	U
53	B5	3386	G
53	B5	3389	U
53	B5	3391	A
53	B5	3395	G
53	B5	3396	U

All (235) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	42	G
1	AA	47	A
1	AA	56	U
1	AA	60	U
1	AA	66	U
1	AA	109	G
1	AA	175	G
1	AA	199	G
1	AA	212	U

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Mol	Chain	Res	Type
1	AA	229	U
1	AA	312	A
1	AA	350	U
1	AA	365	G
1	AA	400	A
1	AA	438	A
1	AA	444	C
1	AA	461	G
1	AA	478	A
1	AA	502	U
1	AA	578	U
1	AA	652	G
1	AA	748	U
1	AA	759	U
1	AA	770	A
1	AA	796	A
1	AA	852	C
1	AA	857	U
1	AA	864	U
1	AA	922	A
1	AA	1049	U
1	AA	1055	U
1	AA	1090	A
1	AA	1098	G
1	AA	1133	U
1	AA	1134	A
1	AA	1159	U
1	AA	1181	U
1	AA	1192	A
1	AA	1196	G
1	AA	1199	A
1	AA	1216	C
1	AA	1240	A
1	AA	1241	G
1	AA	1265	U
1	AA	1281	C
1	AA	1318	A
1	AA	1328	A
1	AA	1341	A
1	AA	1378	U
1	AA	1429	U
1	AA	1457	C

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Mol	Chain	Res	Type
1	AA	1478	G
1	AA	1488	C
1	AA	1520	U
1	AA	1521	G
1	AA	1535	C
1	AA	1545	A
1	AA	1546	G
1	AA	1547	C
1	AA	1560	G
1	AA	1566	C
1	AA	1579	C
1	AA	1583	U
1	AA	1584	A
1	AA	1612	A
1	AA	1632	C
1	AA	1634	C
1	AA	1635	C
1	AA	1636	G
1	AA	1639	C
1	AA	1654	U
1	AA	1655	U
1	AA	1675	C
1	AA	1759	U
1	AA	1766	G
1	AA	1779	A
1	AA	1789	A
1	AA	1790	G
19	A7	10	2MG
19	A7	22	G
19	A7	41	U
51	B3	23	A
51	B3	70	A
51	B3	89	A
51	B3	91	C
52	B4	19	C
52	B4	21	C
52	B4	57	C
52	B4	60	U
52	B4	61	A
52	B4	69	U
52	B4	71	G
52	B4	102	U

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Mol	Chain	Res	Type
52	B4	106	C
52	B4	152	G
53	B5	114	A
53	B5	119	U
53	B5	133	U
53	B5	134	U
53	B5	210	U
53	B5	215	G
53	B5	239	G
53	B5	250	U
53	B5	251	G
53	B5	267	G
53	B5	277	G
53	B5	279	U
53	B5	355	A
53	B5	372	A
53	B5	374	A
53	B5	397	A
53	B5	475	G
53	B5	477	A
53	B5	481	U
53	B5	554	A
53	B5	596	U
53	B5	620	U
53	B5	621	A
53	B5	638	C
53	B5	677	A
53	B5	705	A
53	B5	711	A
53	B5	712	G
53	B5	714	G
53	B5	715	A
53	B5	735	A
53	B5	742	G
53	B5	786	A
53	B5	801	A
53	B5	860	G
53	B5	914	A
53	B5	932	U
53	B5	970	A
53	B5	977	U
53	B5	979	G

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Mol	Chain	Res	Type
53	B5	1033	U
53	B5	1079	A
53	B5	1084	A
53	B5	1163	A
53	B5	1181	U
53	B5	1200	A
53	B5	1235	U
53	B5	1240	A
53	B5	1244	A
53	B5	1258	U
53	B5	1263	A
53	B5	1302	A
53	B5	1303	A
53	B5	1318	A
53	B5	1331	U
53	B5	1347	U
53	B5	1390	A
53	B5	1514	G
53	B5	1549	U
53	B5	1553	U
53	B5	1582	C
53	B5	1583	A
53	B5	1590	G
53	B5	1623	G
53	B5	1626	U
53	B5	1643	A
53	B5	1648	A
53	B5	1654	A
53	B5	1666	G
53	B5	1720	U
53	B5	1721	U
53	B5	1737	U
53	B5	1776	G
53	B5	1818	U
53	B5	1842	A
53	B5	1900	A
53	B5	1925	U
53	B5	1947	G
53	B5	2138	A
53	B5	2174	G
53	B5	2177	G
53	B5	2214	A

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Mol	Chain	Res	Type
53	B5	2219	A
53	B5	2224	A
53	B5	2225	U
53	B5	2229	A
53	B5	2283	G
53	B5	2286	U
53	B5	2297	U
53	B5	2314	U
53	B5	2360	C
53	B5	2373	A
53	B5	2459	A
53	B5	2468	A
53	B5	2469	G
53	B5	2474	G
53	B5	2477	G
53	B5	2520	A
53	B5	2538	U
53	B5	2569	A
53	B5	2571	U
53	B5	2618	G
53	B5	2644	C
53	B5	2651	G
53	B5	2654	C
53	B5	2677	G
53	B5	2705	A
53	B5	2714	G
53	B5	2778	G
53	B5	2787	G
53	B5	2796	G
53	B5	2830	G
53	B5	2837	A
53	B5	2875	U
53	B5	2913	C
53	B5	2941	A
53	B5	2988	C
53	B5	3039	C
53	B5	3045	G
53	B5	3049	A
53	B5	3051	U
53	B5	3077	A
53	B5	3083	G
53	B5	3110	C

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Mol	Chain	Res	Type
53	B5	3113	A
53	B5	3121	U
53	B5	3138	U
53	B5	3141	A
53	B5	3142	A
53	B5	3143	C
53	B5	3160	U
53	B5	3195	U
53	B5	3219	U
53	B5	3246	G
53	B5	3304	U
53	B5	3313	U
53	B5	3330	A
53	B5	3384	U
53	B5	3385	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	5MC	A7	40	19	19,22,23	1.87	5 (26%)	26,32,35	2.38	12 (46%)
19	H2U	A7	16	19	18,21,22	1.94	3 (16%)	19,30,33	1.96	6 (31%)
19	PSU	A7	55	19	18,21,22	1.74	4 (22%)	21,30,33	1.43	2 (9%)
19	M2G	A7	26	19	24,27,28	1.34	4 (16%)	33,40,43	1.49	6 (18%)
19	H2U	A7	17	19	18,21,22	2.59	7 (38%)	19,30,33	2.70	4 (21%)
19	YYG	A7	37	19	38,42,43	1.69	6 (15%)	45,62,65	2.92	15 (33%)
19	PSU	A7	39	19	18,21,22	1.64	6 (33%)	21,30,33	1.89	6 (28%)
19	5MC	A7	49	19	19,22,23	1.59	2 (10%)	26,32,35	2.17	11 (42%)
19	2MG	A7	10	19	23,26,27	1.35	4 (17%)	33,38,41	1.62	5 (15%)
19	OMG	A7	34	19	23,26,27	1.27	2 (8%)	32,38,41	1.23	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	OMC	A7	32	19	19,22,23	1.37	2 (10%)	25,31,34	2.01	8 (32%)
19	5MU	A7	54	19	19,22,23	1.37	2 (10%)	27,32,35	2.53	11 (40%)
19	1MA	A7	58	19	21,25,26	1.31	3 (14%)	30,37,40	1.73	9 (30%)
19	7MG	A7	46	19	23,26,27	1.79	2 (8%)	27,39,42	2.52	9 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	5MC	A7	40	19	-	2/7/25/26	0/2/2/2
19	H2U	A7	16	19	-	0/7/38/39	0/2/2/2
19	PSU	A7	55	19	-	1/7/25/26	0/2/2/2
19	M2G	A7	26	19	-	0/11/29/30	0/3/3/3
19	H2U	A7	17	19	-	0/7/38/39	0/2/2/2
19	YYG	A7	37	19	-	7/24/42/43	0/4/4/4
19	PSU	A7	39	19	-	3/7/25/26	0/2/2/2
19	5MC	A7	49	19	-	0/7/25/26	0/2/2/2
19	2MG	A7	10	19	-	0/9/27/28	0/3/3/3
19	OMG	A7	34	19	-	0/9/27/28	0/3/3/3
19	OMC	A7	32	19	-	0/9/27/28	0/2/2/2
19	5MU	A7	54	19	-	0/7/25/26	0/2/2/2
19	1MA	A7	58	19	-	0/7/25/26	0/3/3/3
19	7MG	A7	46	19	-	2/7/37/38	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A7	46	7MG	C8-N9	-6.58	1.41	1.45
19	A7	17	H2U	C2-N3	-6.33	1.26	1.38
19	A7	37	YYG	C2-N1	-6.00	1.29	1.38
19	A7	17	H2U	C4-N3	-5.75	1.28	1.37
19	A7	49	5MC	C5-C4	5.30	1.48	1.44
19	A7	16	H2U	C2-N1	4.76	1.42	1.35
19	A7	40	5MC	C5-C4	4.27	1.47	1.44
19	A7	16	H2U	C2-N3	-3.90	1.31	1.38
19	A7	34	OMG	C3'-C2'	3.90	1.61	1.53
19	A7	54	5MU	C6-N1	3.64	1.44	1.38
19	A7	17	H2U	C1'-N1	3.61	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A7	55	PSU	C4-N3	-3.53	1.32	1.38
19	A7	58	1MA	C5-N7	3.50	1.46	1.39
19	A7	39	PSU	C6-N1	-3.48	1.30	1.36
19	A7	16	H2U	C4-N3	-3.48	1.31	1.37
19	A7	40	5MC	C6-C5	3.47	1.40	1.34
19	A7	40	5MC	C4-N3	-3.38	1.28	1.34
19	A7	32	OMC	O2'-C2'	-3.27	1.34	1.42
19	A7	37	YYG	C2-N2	3.26	1.38	1.33
19	A7	58	1MA	CM1-N1	3.17	1.53	1.46
19	A7	55	PSU	C6-N1	-3.04	1.31	1.36
19	A7	49	5MC	CM5-C5	3.04	1.58	1.50
19	A7	55	PSU	C6-C5	-2.87	1.32	1.35
19	A7	39	PSU	O2'-C2'	-2.79	1.36	1.43
19	A7	10	2MG	O2'-C2'	-2.74	1.36	1.43
19	A7	17	H2U	C2-N1	2.72	1.39	1.35
19	A7	46	7MG	C5-N7	2.69	1.39	1.35
19	A7	17	H2U	C6-N1	2.69	1.51	1.47
19	A7	39	PSU	O4'-C1'	-2.67	1.40	1.43
19	A7	10	2MG	C2'-C3'	2.63	1.60	1.53
19	A7	17	H2U	O4'-C4'	-2.59	1.39	1.45
19	A7	26	M2G	C5'-C4'	2.58	1.59	1.51
19	A7	26	M2G	O4'-C1'	-2.54	1.36	1.42
19	A7	54	5MU	C6-C5	2.44	1.38	1.34
19	A7	37	YYG	C14-C15	2.40	1.59	1.53
19	A7	39	PSU	O4'-C4'	-2.38	1.39	1.45
19	A7	34	OMG	O4'-C1'	-2.31	1.36	1.42
19	A7	40	5MC	O4'-C1'	2.29	1.47	1.42
19	A7	37	YYG	C5-C4	2.25	1.43	1.38
19	A7	58	1MA	C6-N6	2.23	1.33	1.28
19	A7	10	2MG	C2-N1	-2.18	1.33	1.36
19	A7	26	M2G	O5'-C5'	2.17	1.50	1.44
19	A7	40	5MC	C2'-C1'	-2.16	1.46	1.53
19	A7	26	M2G	C4-N9	-2.16	1.32	1.38
19	A7	10	2MG	C5-N7	-2.14	1.34	1.39
19	A7	17	H2U	C2'-C1'	-2.11	1.46	1.53
19	A7	37	YYG	C8-N9	-2.11	1.32	1.37
19	A7	55	PSU	C2-N1	2.07	1.39	1.36
19	A7	37	YYG	C4-N9	2.07	1.44	1.38
19	A7	32	OMC	O4'-C1'	2.06	1.46	1.42
19	A7	39	PSU	C2-N1	-2.04	1.34	1.36
19	A7	39	PSU	C4-N3	-2.02	1.35	1.38

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A7	17	H2U	N3-C2-N1	9.33	126.03	116.65
19	A7	37	YYG	C11-C12-N1	-9.29	98.76	105.31
19	A7	54	5MU	C6-C5-C4	6.82	123.64	118.02
19	A7	37	YYG	C24-O23-C21	6.81	123.52	115.63
19	A7	37	YYG	C5-C4-N3	-6.59	118.64	123.99
19	A7	40	5MC	C5-C6-N1	-6.32	116.45	123.31
19	A7	46	7MG	N9-C8-N7	6.15	112.07	103.37
19	A7	54	5MU	C5-C6-N1	-6.00	116.79	123.31
19	A7	46	7MG	C4-C5-N7	5.65	112.06	105.38
19	A7	46	7MG	N1-C2-N3	5.35	133.12	123.32
19	A7	16	H2U	N3-C2-N1	5.31	121.98	116.65
19	A7	37	YYG	N1-C2-N2	-4.98	106.89	114.03
19	A7	37	YYG	C15-N20-C21	4.91	133.14	120.93
19	A7	10	2MG	C2-N3-C4	4.73	117.92	112.00
19	A7	32	OMC	O2-C2-N3	-4.60	115.08	122.33
19	A7	55	PSU	O2'-C2'-C1'	-4.44	100.66	111.21
19	A7	37	YYG	C14-C15-C16	4.34	122.53	110.38
19	A7	49	5MC	C5-C6-N1	-4.24	118.70	123.31
19	A7	17	H2U	O2-C2-N1	-4.23	118.01	123.10
19	A7	37	YYG	O23-C21-N20	4.22	117.88	110.77
19	A7	37	YYG	C2-N1-C12	4.21	117.51	109.94
19	A7	46	7MG	C6-C5-N7	-4.20	125.42	131.93
19	A7	39	PSU	C4-N3-C2	-4.18	120.61	126.37
19	A7	49	5MC	C3'-C2'-C1'	4.17	109.34	101.46
19	A7	46	7MG	C2-N1-C6	-4.00	117.85	125.11
19	A7	54	5MU	O2-C2-N3	-3.97	114.16	121.49
19	A7	40	5MC	N4-C4-N3	-3.91	111.44	118.51
19	A7	37	YYG	O23-C21-O22	-3.87	118.99	124.62
19	A7	39	PSU	N1-C2-N3	3.78	119.15	115.17
19	A7	37	YYG	C8-N9-C4	-3.68	102.99	106.54
19	A7	54	5MU	O2-C2-N1	3.53	127.39	122.80
19	A7	58	1MA	C5-C4-N3	-3.48	122.14	127.27
19	A7	40	5MC	C4-N3-C2	-3.43	116.04	120.81
19	A7	40	5MC	CM5-C5-C6	-3.34	118.33	122.85
19	A7	32	OMC	N4-C4-N3	-3.29	112.02	117.91
19	A7	49	5MC	C2'-C3'-C4'	-3.28	96.27	102.61
19	A7	49	5MC	O4'-C1'-C2'	-3.26	99.64	106.62
19	A7	32	OMC	C4-N3-C2	-3.26	115.14	120.26
19	A7	49	5MC	C4'-O4'-C1'	3.22	116.58	109.47
19	A7	26	M2G	C3'-C2'-C1'	-3.22	95.38	101.46
19	A7	46	7MG	N2-C2-N3	-3.21	113.41	119.67
19	A7	32	OMC	C1'-N1-C6	3.20	127.61	120.78
19	A7	39	PSU	O4'-C1'-C2'	3.16	109.52	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A7	32	OMC	N1-C2-N3	3.14	124.26	118.80
19	A7	58	1MA	C1'-N9-C8	3.13	135.63	126.73
19	A7	17	H2U	O2-C2-N3	-3.11	115.75	121.49
19	A7	37	YYG	C19-O18-C16	3.08	122.90	115.92
19	A7	40	5MC	C1'-N1-C6	-3.06	116.11	121.15
19	A7	40	5MC	O2-C2-N3	-3.06	117.51	122.33
19	A7	10	2MG	C6-C5-C4	-3.02	114.29	118.83
19	A7	39	PSU	C6-C5-C4	2.98	120.19	118.17
19	A7	16	H2U	O2'-C2'-C1'	-2.93	100.00	110.10
19	A7	26	M2G	C8-N7-C5	-2.93	99.04	104.26
19	A7	10	2MG	CM2-N2-C2	2.92	129.93	123.65
19	A7	49	5MC	CM5-C5-C6	-2.91	118.91	122.85
19	A7	54	5MU	C5M-C5-C4	-2.91	115.68	118.78
19	A7	54	5MU	C4'-O4'-C1'	-2.88	103.10	109.47
19	A7	40	5MC	C4'-O4'-C1'	-2.80	103.28	109.47
19	A7	58	1MA	C1'-N9-C4	-2.77	118.31	126.49
19	A7	49	5MC	O2'-C2'-C1'	-2.76	100.61	110.10
19	A7	58	1MA	O2'-C2'-C1'	2.76	119.59	110.10
19	A7	49	5MC	O3'-C3'-C4'	2.73	118.93	111.08
19	A7	58	1MA	C4-C5-N7	-2.69	106.41	110.67
19	A7	49	5MC	O2-C2-N3	-2.66	118.14	122.33
19	A7	40	5MC	N1-C2-N3	2.63	123.38	118.80
19	A7	26	M2G	CM2-N2-C2	2.63	125.99	120.61
19	A7	49	5MC	C5-C4-N4	2.63	125.09	121.39
19	A7	54	5MU	N3-C2-N1	2.62	118.31	114.89
19	A7	58	1MA	CM1-N1-C6	-2.62	116.09	120.15
19	A7	46	7MG	O4'-C1'-N9	2.62	112.86	109.30
19	A7	16	H2U	C5-C4-N3	2.62	119.47	116.69
19	A7	32	OMC	C6-N1-C2	-2.55	116.15	120.46
19	A7	10	2MG	C2-N1-C6	-2.53	121.49	124.55
19	A7	58	1MA	CM1-N1-C2	2.52	125.66	120.50
19	A7	34	OMG	C2'-C3'-C4'	-2.51	96.59	101.99
19	A7	39	PSU	O4-C4-N3	-2.51	115.39	120.11
19	A7	54	5MU	O4'-C4'-C5'	2.51	117.38	109.33
19	A7	54	5MU	O4'-C4'-C3'	2.49	110.10	105.15
19	A7	49	5MC	N4-C4-N3	-2.45	114.06	118.51
19	A7	17	H2U	C3'-C2'-C1'	-2.45	96.82	101.46
19	A7	40	5MC	C2'-C3'-C4'	-2.43	97.91	102.61
19	A7	55	PSU	C2'-C3'-C4'	-2.43	97.92	102.61
19	A7	54	5MU	O4'-C1'-C2'	2.40	111.76	106.62
19	A7	40	5MC	O3'-C3'-C2'	-2.38	104.18	111.82
19	A7	40	5MC	C1'-N1-C2	2.37	123.68	118.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A7	37	YYG	N9-C4-N3	2.36	133.27	129.45
19	A7	26	M2G	O3'-C3'-C4'	-2.32	104.41	111.08
19	A7	58	1MA	O4'-C1'-N9	2.32	113.62	108.36
19	A7	39	PSU	C5-C6-N1	-2.29	118.96	122.14
19	A7	32	OMC	CM2-O2'-C2'	-2.29	108.59	114.47
19	A7	16	H2U	O4'-C4'-C3'	2.28	109.67	105.15
19	A7	34	OMG	N2-C2-N3	-2.27	115.25	119.67
19	A7	54	5MU	C4-N3-C2	-2.20	124.45	127.34
19	A7	37	YYG	C14-C15-N20	-2.19	106.58	110.91
19	A7	10	2MG	C5'-C4'-C3'	-2.17	107.39	115.21
19	A7	16	H2U	O2-C2-N3	-2.17	117.49	121.49
19	A7	16	H2U	O2-C2-N1	-2.16	120.51	123.10
19	A7	37	YYG	O3'-C3'-C4'	2.15	117.27	111.08
19	A7	46	7MG	C5-C4-N9	2.10	109.03	106.33
19	A7	26	M2G	C4-C5-N7	2.08	113.96	110.67
19	A7	46	7MG	C5-C4-N3	-2.08	124.23	128.13
19	A7	40	5MC	C5-C4-N3	2.07	123.88	121.75
19	A7	58	1MA	C5-C4-N9	2.06	109.33	105.66
19	A7	32	OMC	O4'-C4'-C5'	2.04	115.87	109.33
19	A7	37	YYG	O4'-C4'-C5'	2.04	115.86	109.33
19	A7	26	M2G	CM2-N2-CM1	-2.00	109.48	115.87

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A7	39	PSU	O4'-C1'-C5-C4
19	A7	39	PSU	O4'-C1'-C5-C6
19	A7	40	5MC	O4'-C4'-C5'-O5'
19	A7	37	YYG	N20-C15-C16-O18
19	A7	37	YYG	N20-C15-C16-O17
19	A7	55	PSU	O4'-C1'-C5-C4
19	A7	37	YYG	O4'-C4'-C5'-O5'
19	A7	39	PSU	O4'-C4'-C5'-O5'
19	A7	40	5MC	C3'-C4'-C5'-O5'
19	A7	37	YYG	O23-C21-N20-C15
19	A7	37	YYG	C14-C15-C16-O18
19	A7	37	YYG	O22-C21-N20-C15
19	A7	37	YYG	C14-C15-C16-O17
19	A7	46	7MG	C2'-C1'-N9-C8
19	A7	46	7MG	O4'-C1'-N9-C8

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A7	40	5MC	2	0
19	A7	37	YYG	1	0
19	A7	10	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	AH	1
18	AT	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AH	32:LYS	C	33:VAL	N	2.59
1	AT	78:LYS	C	79:LEU	N	2.49

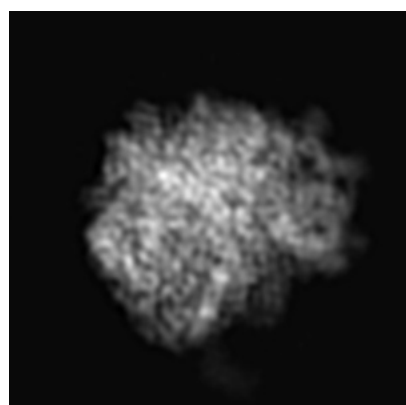
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1345. These allow visual inspection of the internal detail of the map and identification of artifacts.

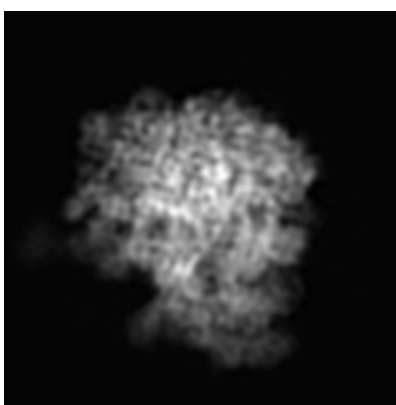
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

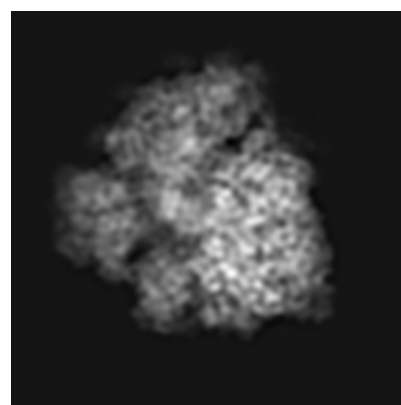
6.1.1 Primary map



X



Y

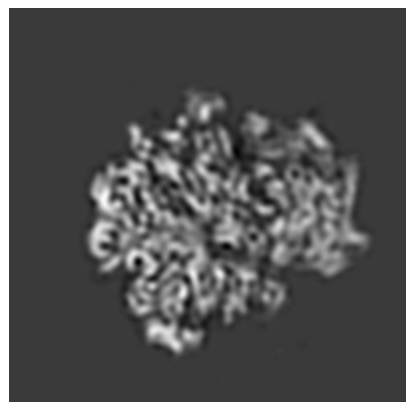


Z

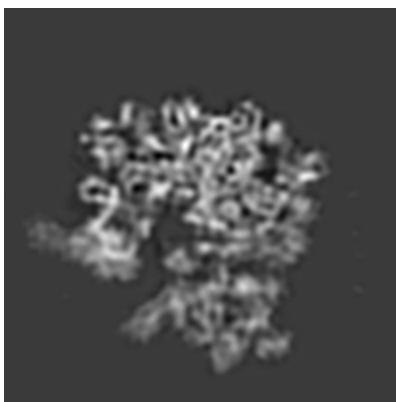
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

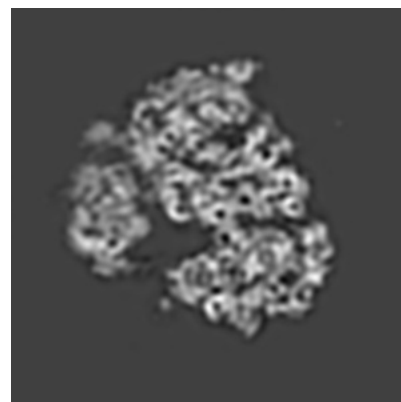
6.2.1 Primary map



X Index: 102



Y Index: 102

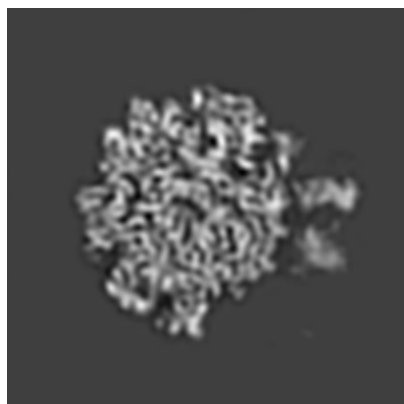


Z Index: 102

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

6.3 Largest variance slices [i](#)

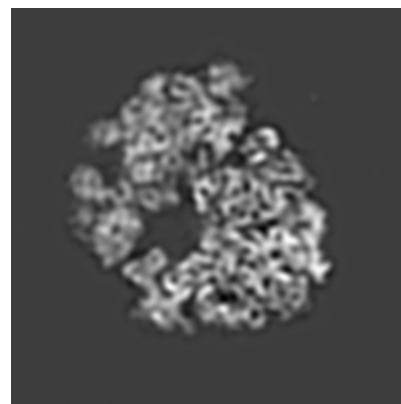
6.3.1 Primary map



X Index: 123



Y Index: 72

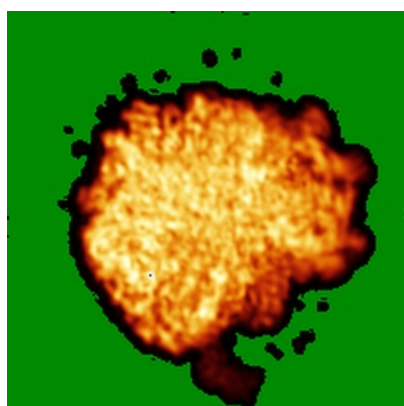


Z Index: 95

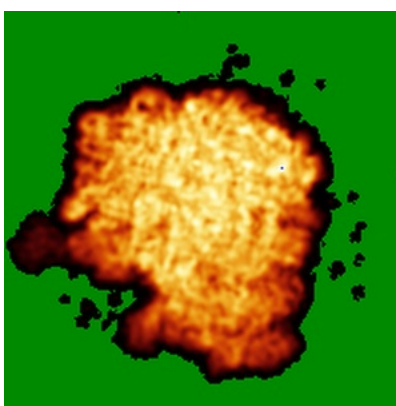
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

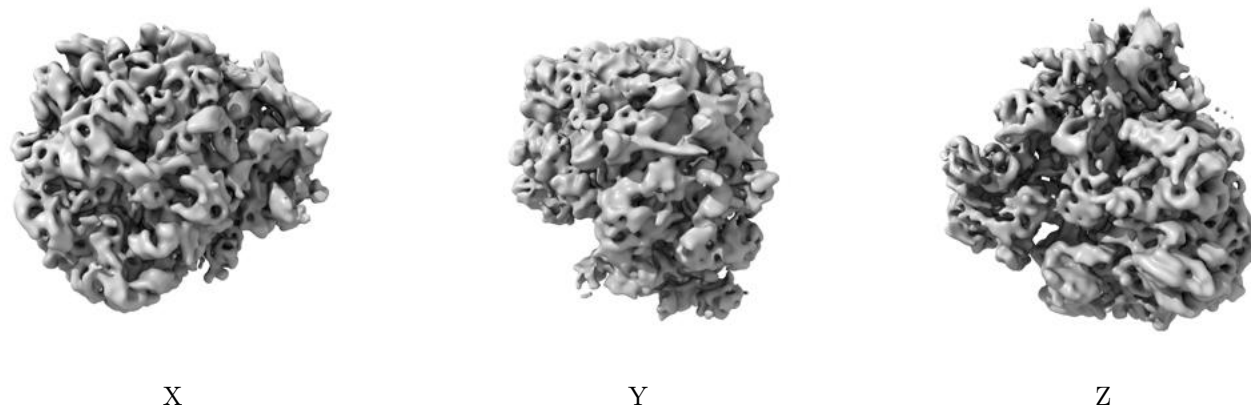


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 70.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

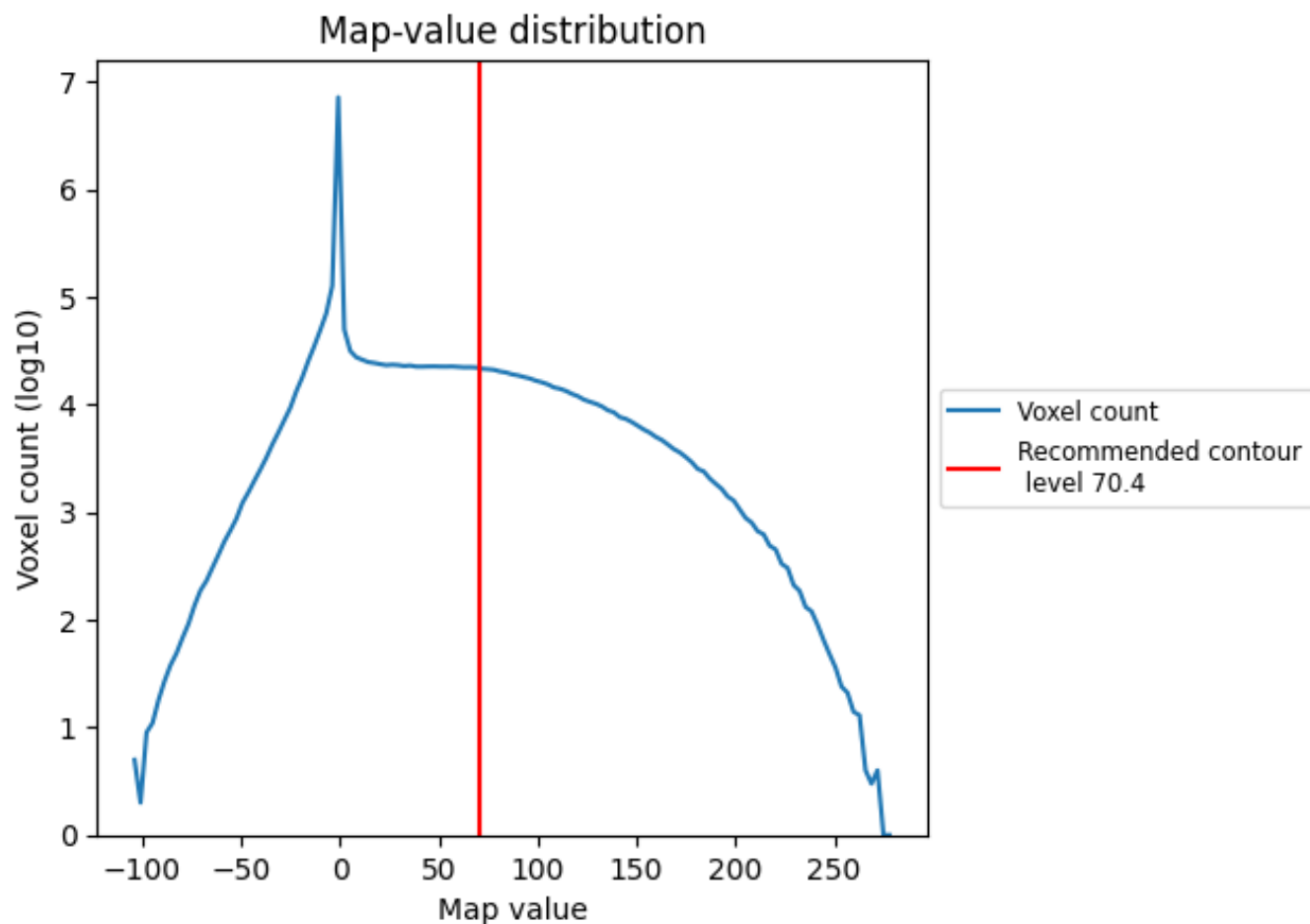
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

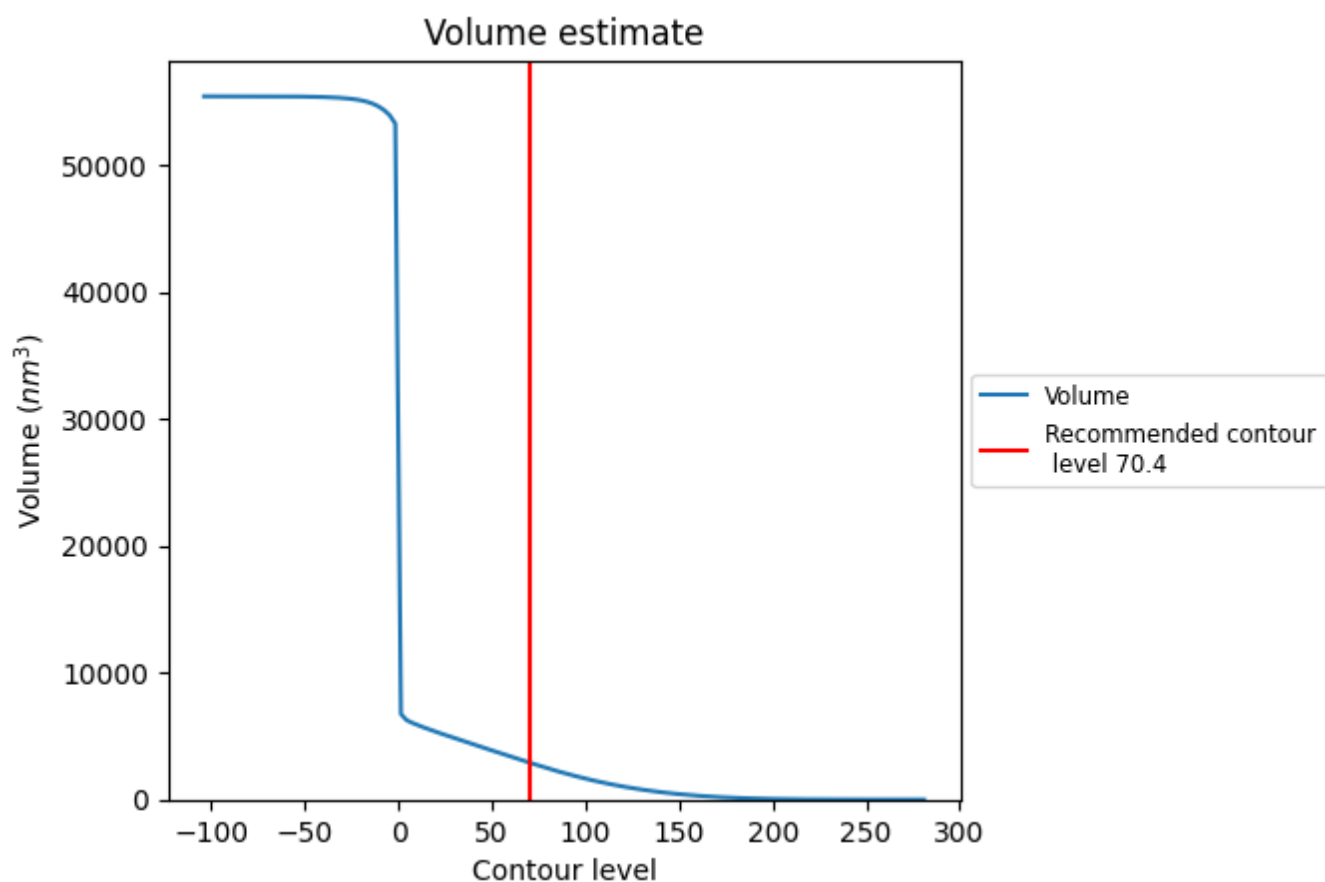
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

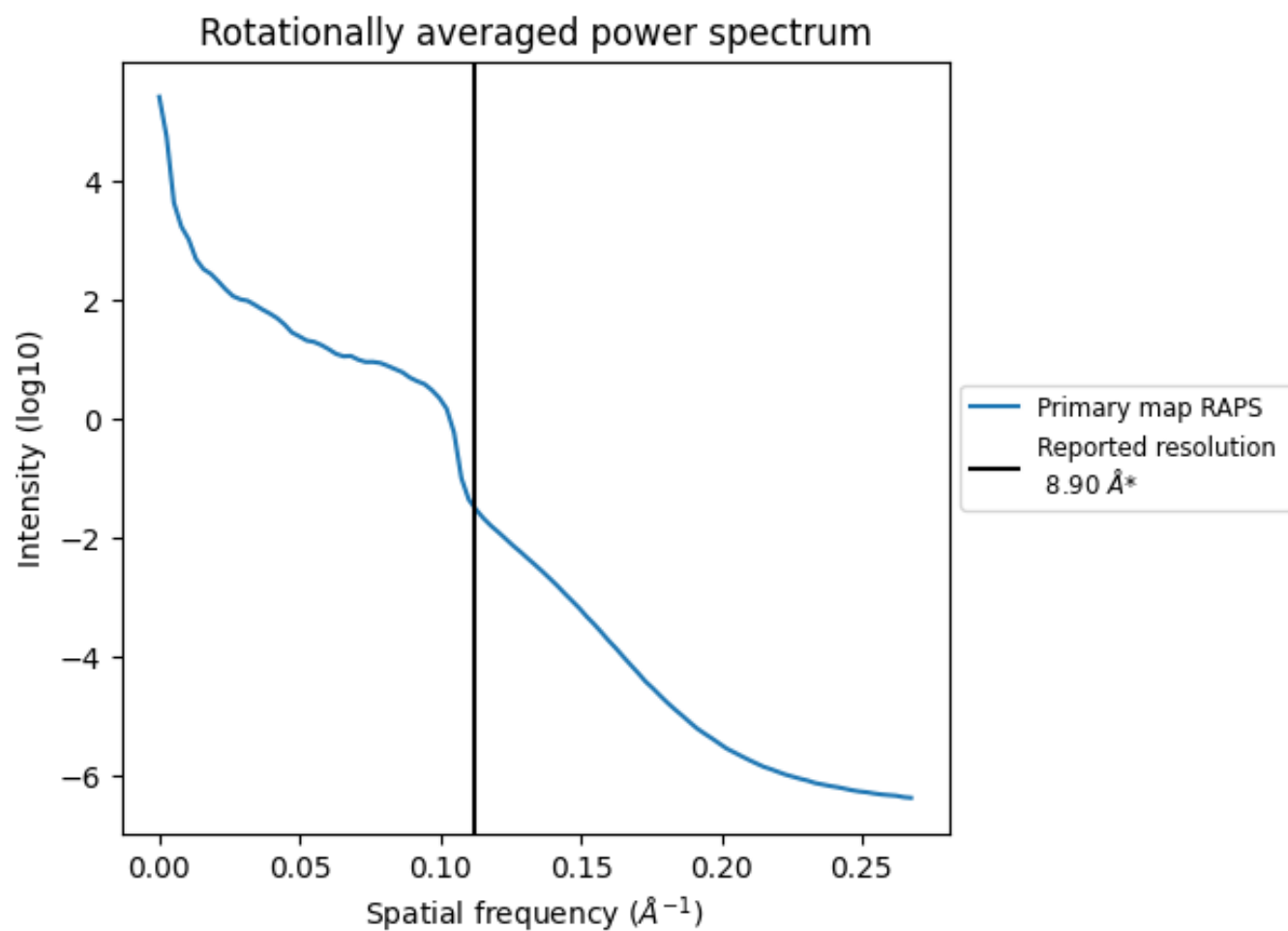
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2899 nm³; this corresponds to an approximate mass of 2619 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 0.112 Å⁻¹

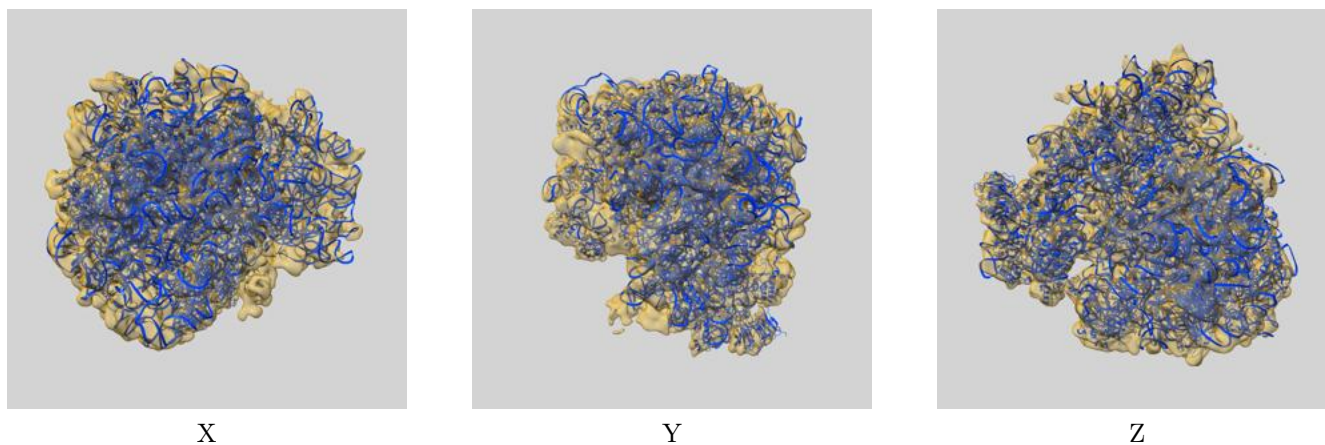
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

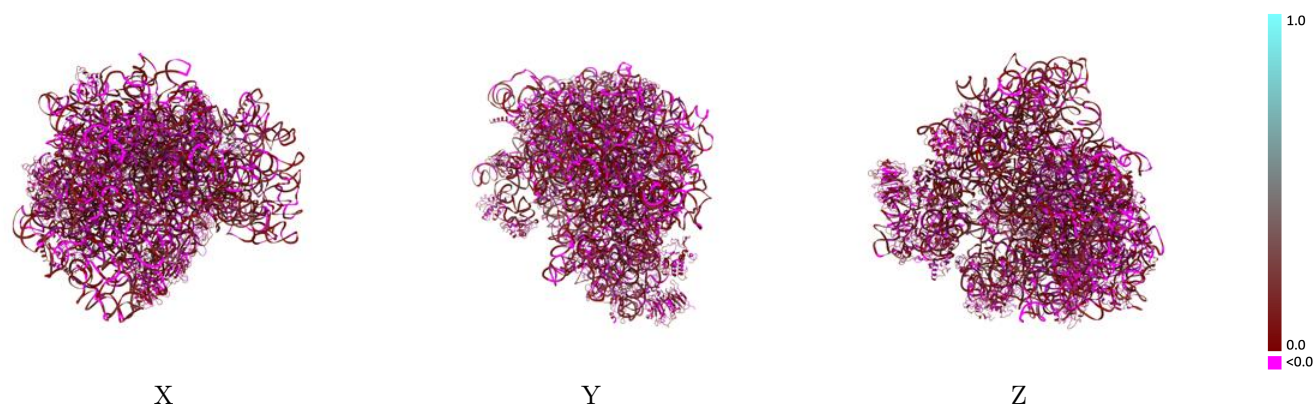
This section contains information regarding the fit between EMDB map EMD-1345 and PDB model 4V7H. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



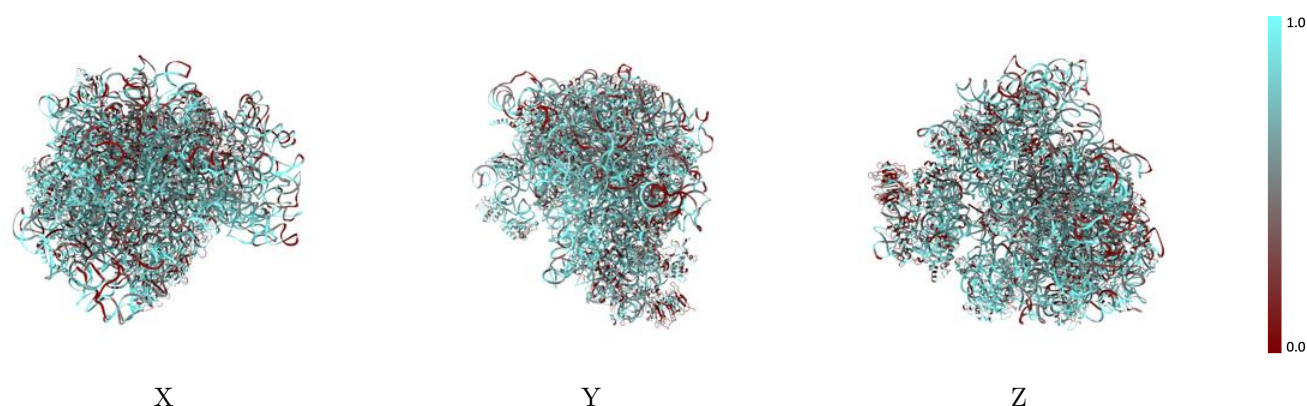
The images above show the 3D surface view of the map at the recommended contour level 70.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



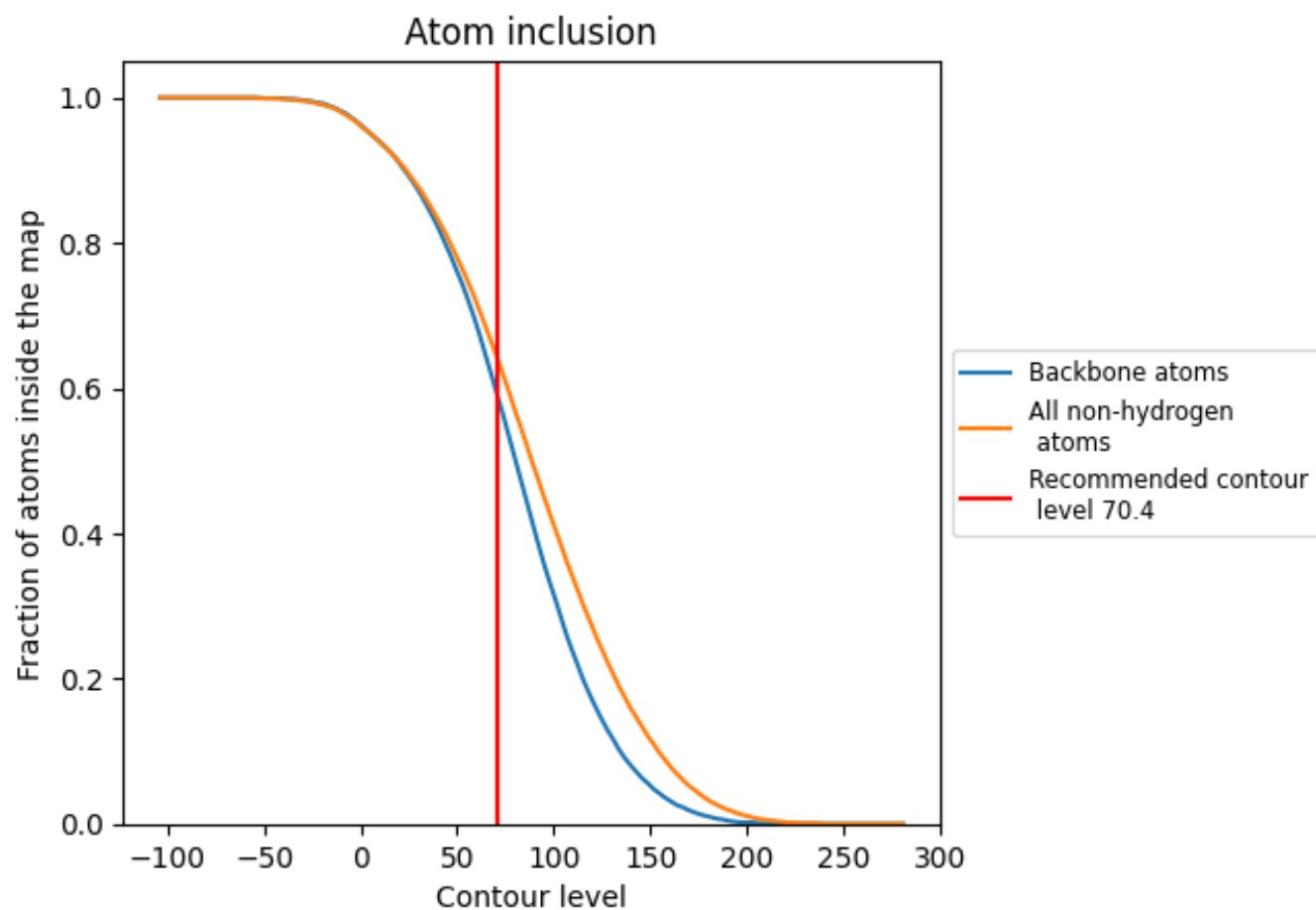
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (70.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 64% 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 (70.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6440	 0.0590
A7	 0.6250	 0.0690
AA	 0.7150	 0.0810
AB	 0.5860	 0.0440
AC	 0.4370	 0.0790
AD	 0.6270	 0.0740
AE	 0.4930	 0.0380
AG	 0.5130	 0.0470
AH	 0.4520	 0.0510
AI	 0.4310	 0.0380
AJ	 0.4360	 0.0600
AK	 0.5070	 0.0250
AL	 0.4450	 0.0330
AM	 0.6320	 0.0330
AN	 0.5590	 0.0070
AO	 0.3760	 0.0450
AQ	 0.4540	 0.0400
AR	 0.3520	 0.0550
AS	 0.5710	 0.0410
AT	 0.4880	 0.0450
B0	 0.4680	 0.0460
B1	 0.5210	 0.0470
B2	 0.6660	 0.0540
B3	 0.7910	 0.0860
B4	 0.5150	 0.0090
B5	 0.6860	 0.0610
B8	 0.6470	 0.0680
B9	 0.4460	 0.0210
BA	 0.5860	 0.0200
BB	 0.4580	 0.0210
BC	 0.5450	 0.0230
BD	 0.6210	 0.0550
BE	 0.7260	 0.0290
BF	 0.5320	 0.0470
BG	 0.6530	 0.0250



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Chain	Atom inclusion	Q-score
BH	 0.5830	 0.0570
BI	 0.4170	 0.0070
BJ	 0.7080	 0.0700
BK	 0.5710	 0.0460
BL	 0.5070	 0.0290
BM	 0.5470	 0.0580
BN	 0.5850	 0.0310
BO	 0.6280	 0.0600
BP	 0.6030	 0.0800
BQ	 0.5990	 0.0300
BR	 0.3650	 0.0500
BS	 0.5490	 0.0290
BT	 0.5170	 0.0780
BU	 0.6370	 0.0850
BV	 0.5750	 0.0340
BW	 0.7120	 0.0670
BX	 0.5120	 0.0720
BY	 0.5080	 -0.0070
BZ	 0.5470	 0.0380