



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 02:28 AM EDT

PDB ID : 6ORE / pdb_00006ore
EMDB ID : EMD-20173
Title : Release complex 70S
Authors : Fu, Z.
Deposited on : 2019-04-30
Resolution : 2.90 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:

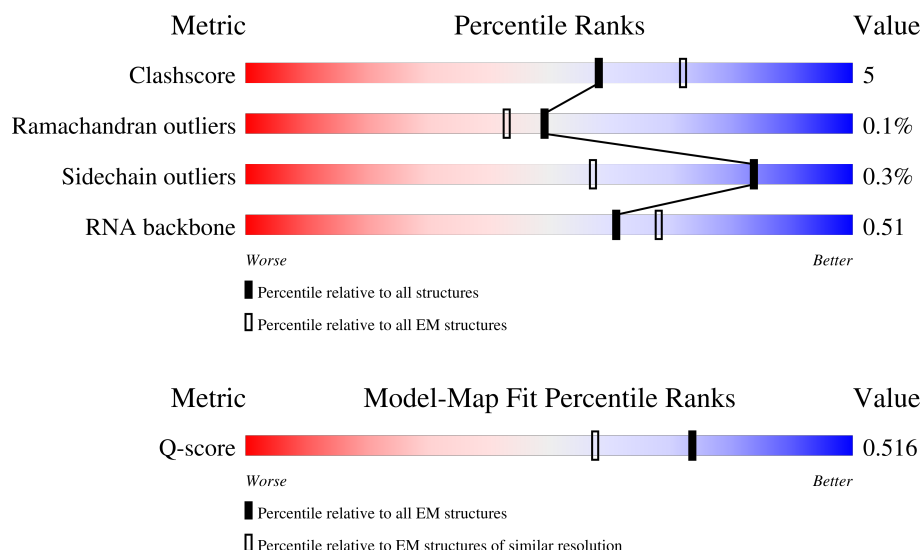
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
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 2.90 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	13054 (2.40 - 3.40)

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	1	2903	
2	2	1534	
3	3	120	

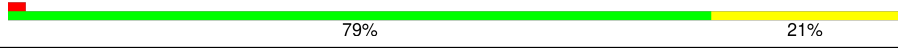
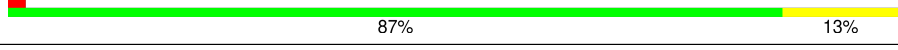
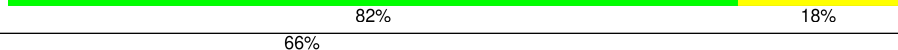
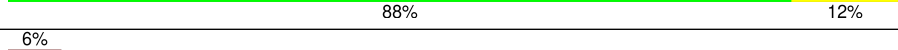
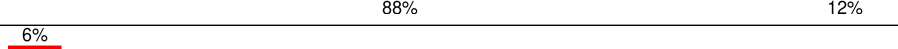
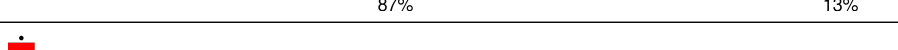
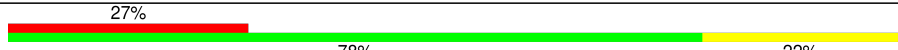
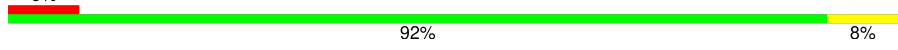
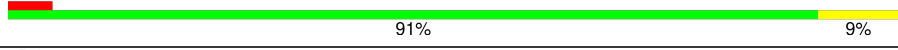
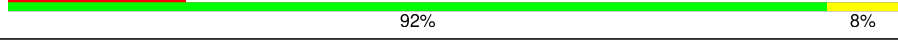
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Mol	Chain	Length	Quality of chain
4	4	9	
5	5	76	
6	A	3	
7	B	271	
8	C	209	
9	D	201	
10	E	177	
11	F	175	
12	G	149	
13	J	142	
14	K	123	
15	L	144	
16	M	136	
17	N	119	
18	O	116	
19	P	114	
20	Q	117	
21	R	103	
22	S	110	
23	T	94	
24	U	103	
25	V	94	
26	W	76	
27	X	77	
28	Y	62	

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Mol	Chain	Length	Quality of chain
29	Z	58	
30	a	66	
31	b	56	
32	c	52	
33	d	46	
34	e	64	
35	f	38	
36	g	225	
37	h	208	
38	i	205	
39	j	156	
40	k	104	
41	l	151	
42	m	129	
43	n	127	
44	o	99	
45	p	117	
46	q	123	
47	r	116	
48	s	100	
49	t	88	
50	u	82	
51	v	80	
52	w	66	
53	x	83	

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Mol	Chain	Length	Quality of chain
54	y	86	6% 94% 6%
55	z	70	40% 86% 14%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 144774 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a RNA chain called RNA (5'-R(P*UP*UP*CP*UP*UP*CP*UP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	9	Total	C	N	O	P	0	0
			184	83	26	66	9		

- Molecule 5 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	5	76	Total	C	N	O	P	S	0	0
			1627	727	296	527	76	1		

- Molecule 6 is a protein called FME-PHE-PHE.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	3	Total	C	N	O	S	0	0
			32	24	3	4	1		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 9 is a protein called 50S ribosomal protein L4.

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

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	103	Total	C	N	O		0	0
			788	498	148	142			

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

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

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

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

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

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

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

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

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	1	290	Total 290	Mg 290	0
56	2	126	Total 126	Mg 126	0
56	3	8	Total 8	Mg 8	0
56	5	4	Total 4	Mg 4	0
56	B	1	Total 1	Mg 1	0
56	C	1	Total 1	Mg 1	0
56	Q	1	Total 1	Mg 1	0
56	b	2	Total 2	Mg 2	0
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56	i	1	Total 1	Mg 1	0
56	r	1	Total 1	Mg 1	0

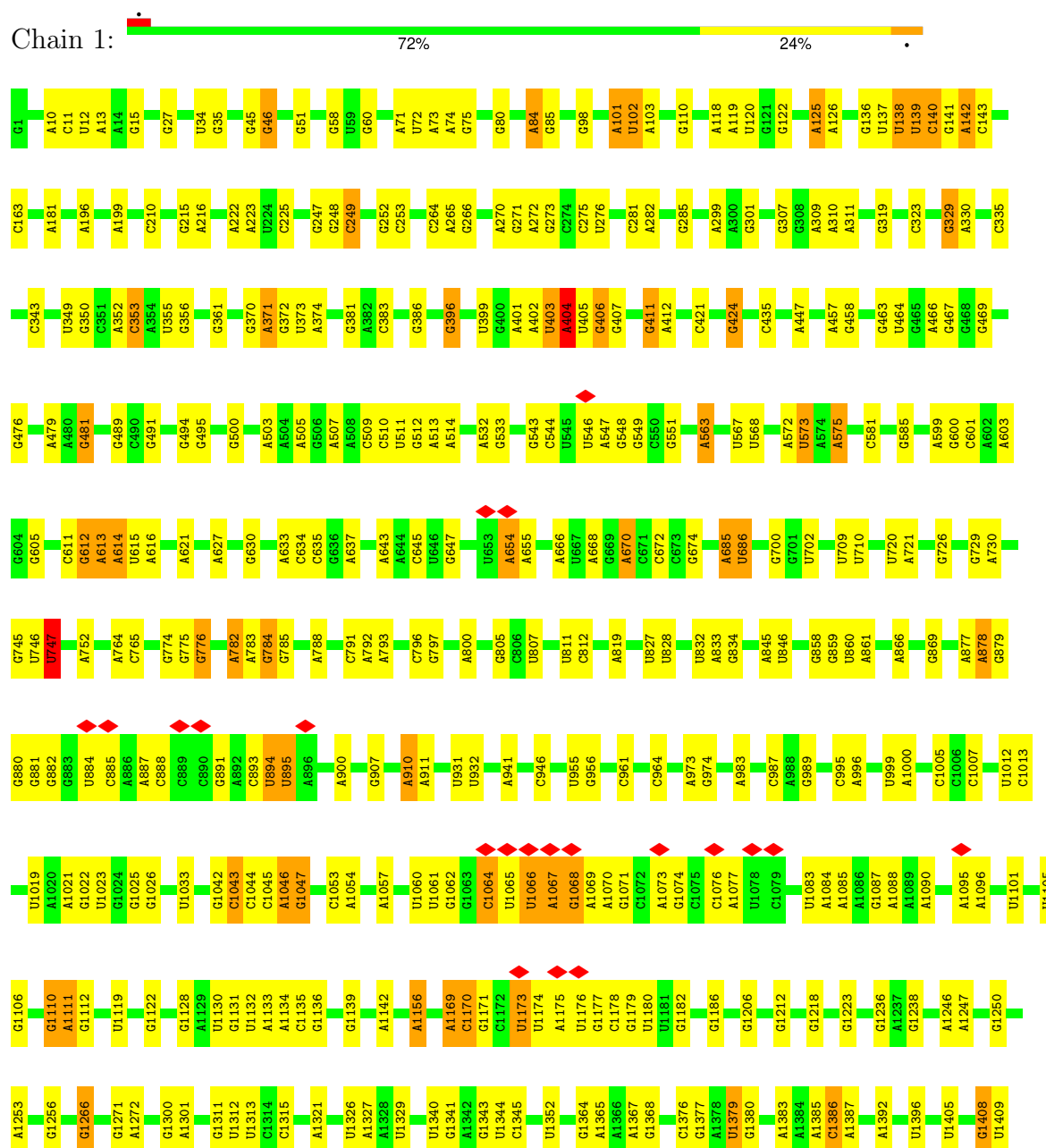
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

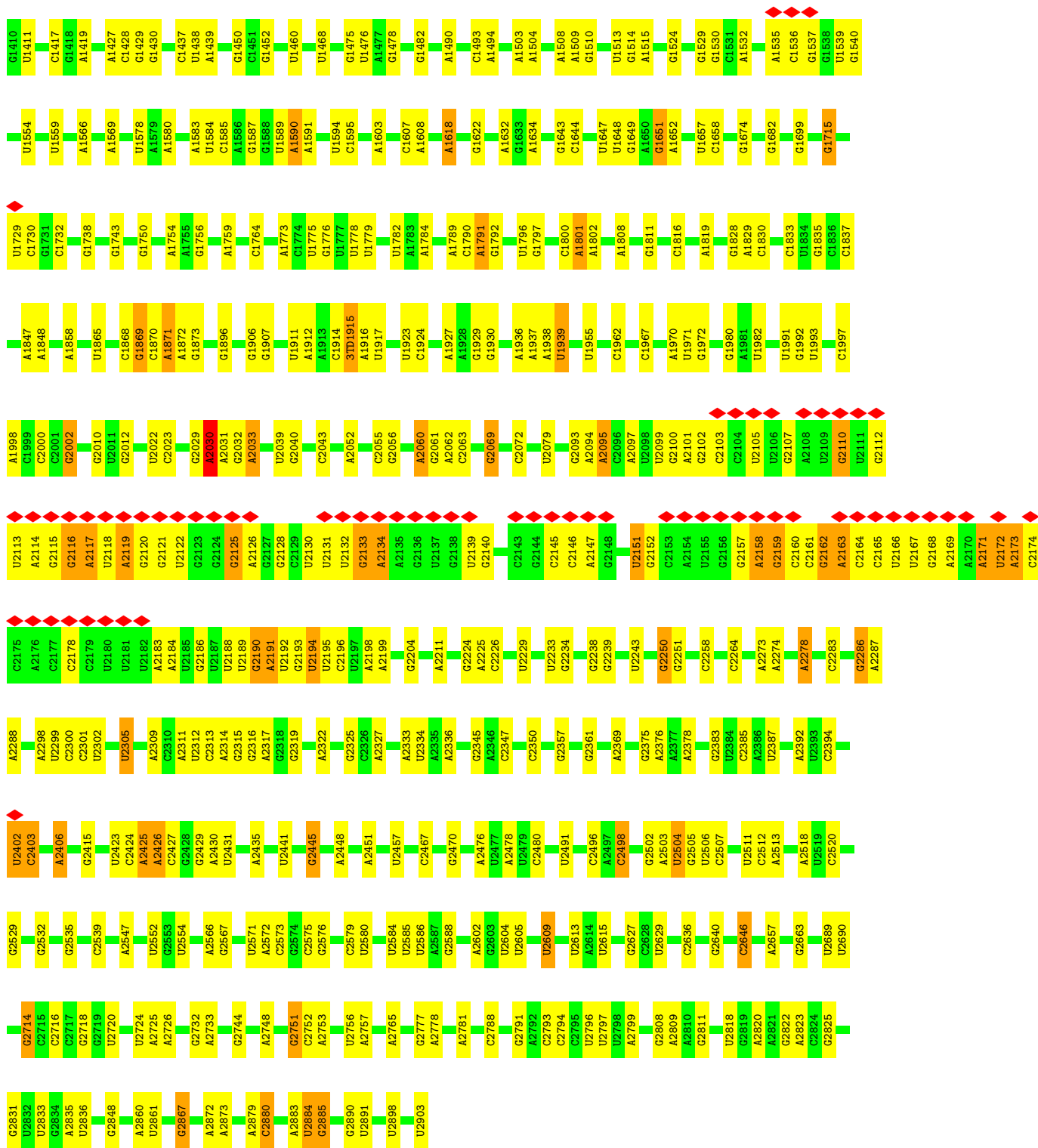
Mol	Chain	Residues	Atoms		AltConf
57	a	1	Total 1	Zn 1	0
57	f	1	Total 1	Zn 1	0

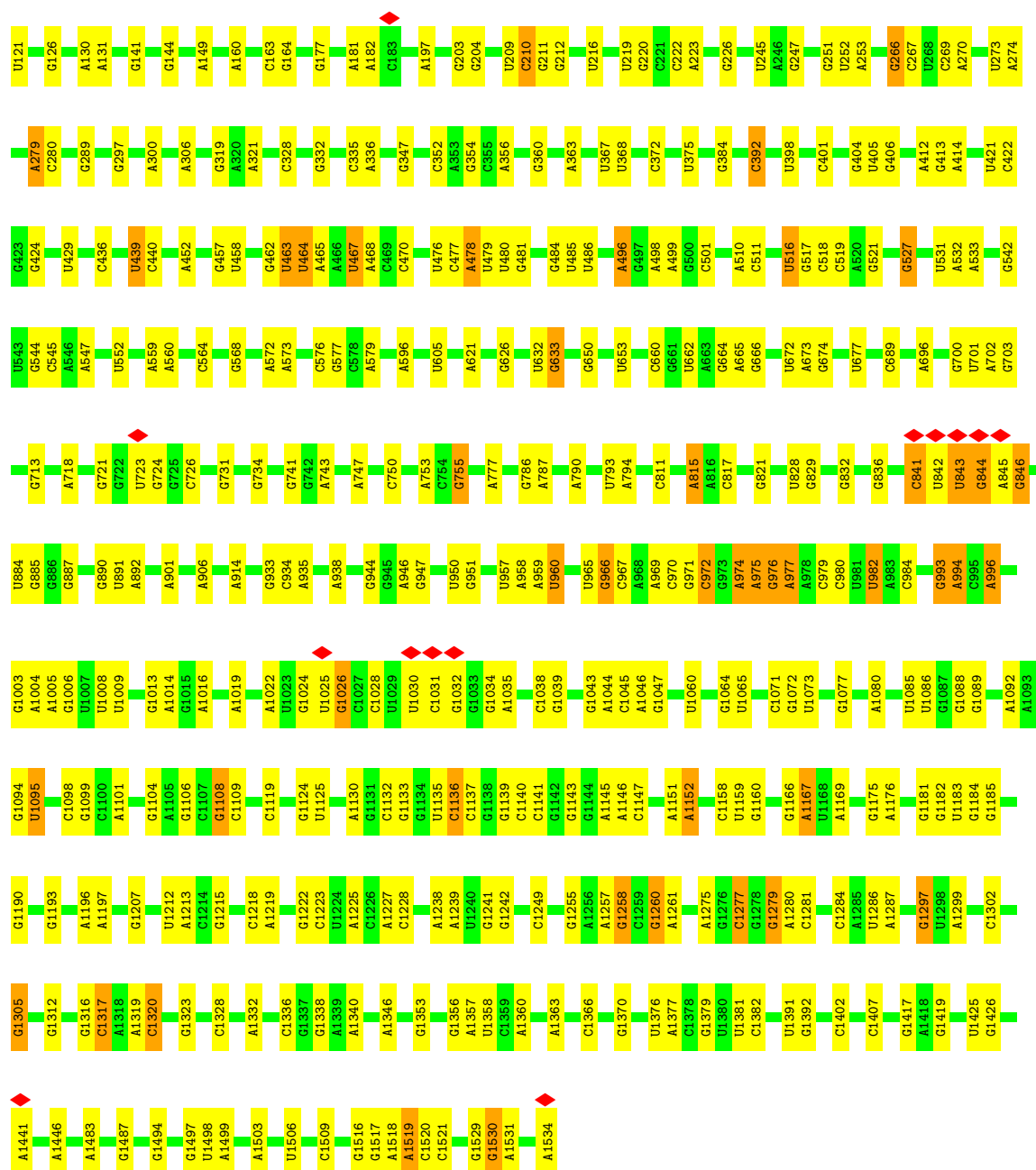
3 Residue-property plots

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

• Molecule 1: 23S ribosomal RNA







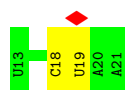
• Molecule 3: 5S ribosomal RNA

Chain 3: 82% 18%



• Molecule 4: RNA (5'-R(P*UP*UP*CP*UP*UP*CP*UP*AP*A)-3')

Chain 4: 11% 78% 22%



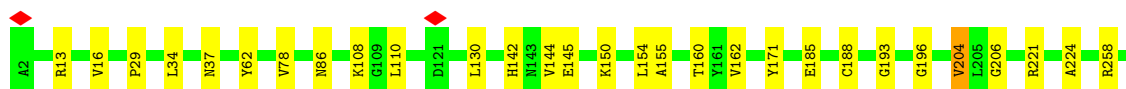
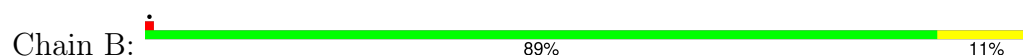
- Molecule 5: P-tRNA



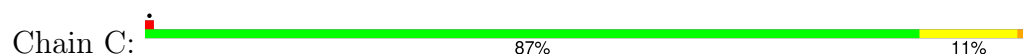
- Molecule 6: FME-PHE-PHE



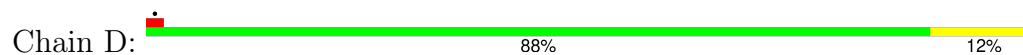
- Molecule 7: 50S ribosomal protein L2



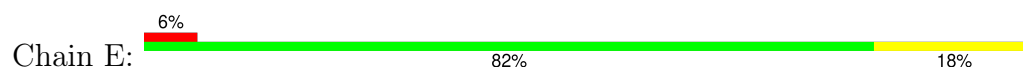
- Molecule 8: 50S ribosomal protein L3

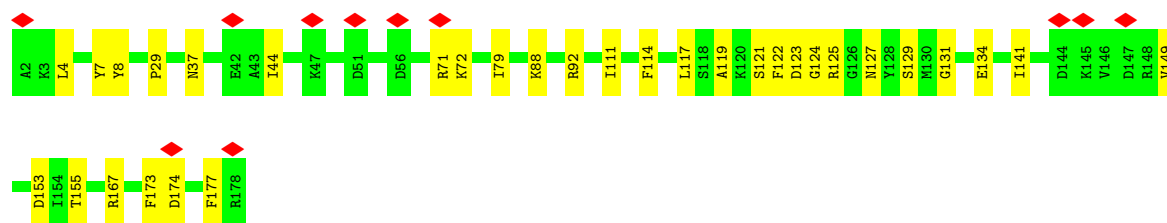


- Molecule 9: 50S ribosomal protein L4

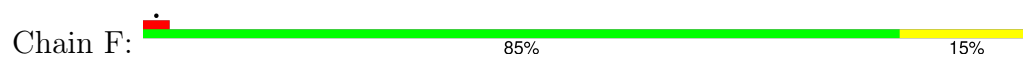


- Molecule 10: 50S ribosomal protein L5

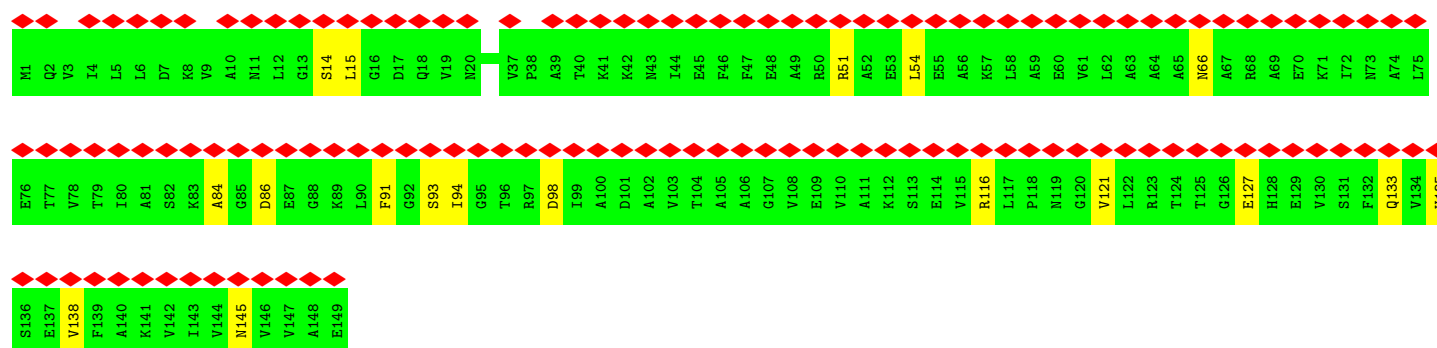
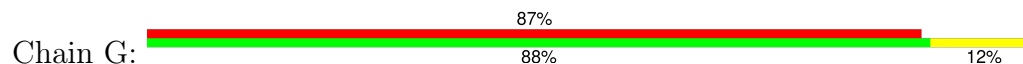




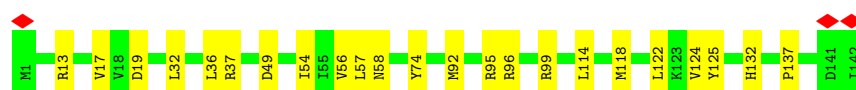
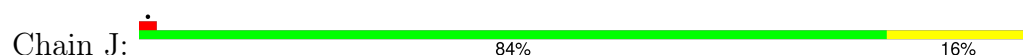
- Molecule 11: 50S ribosomal protein L6



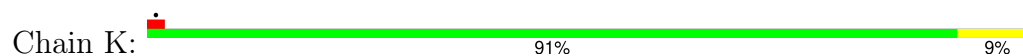
- Molecule 12: 50S ribosomal protein L9



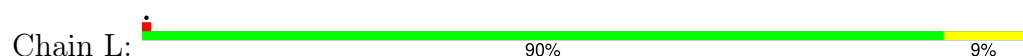
- Molecule 13: 50S ribosomal protein L13



- Molecule 14: 50S ribosomal protein L14



- Molecule 15: 50S ribosomal protein L15





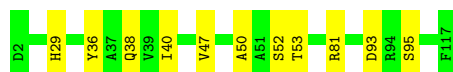
- Molecule 16: 50S ribosomal protein L16



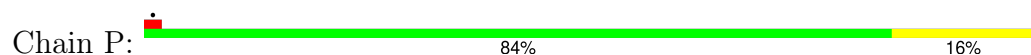
- Molecule 17: 50S ribosomal protein L17



- Molecule 18: 50S ribosomal protein L18



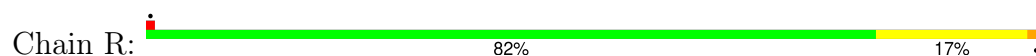
- Molecule 19: 50S ribosomal protein L19



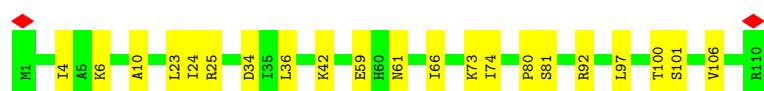
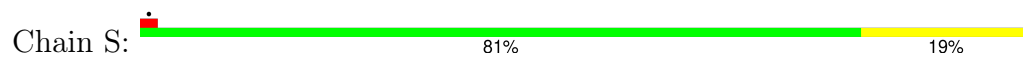
- Molecule 20: 50S ribosomal protein L20



- Molecule 21: 50S ribosomal protein L21



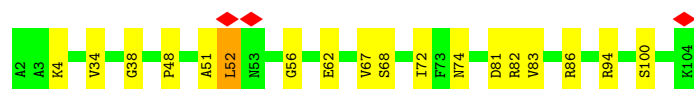
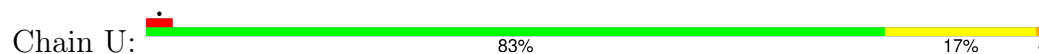
- Molecule 22: 50S ribosomal protein L22



- Molecule 23: 50S ribosomal protein L23



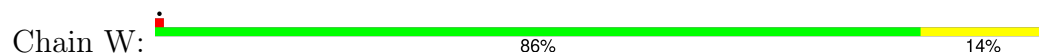
- Molecule 24: 50S ribosomal protein L24



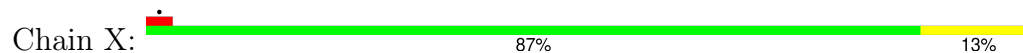
- Molecule 25: 50S ribosomal protein L25



- Molecule 26: 50S ribosomal protein L27



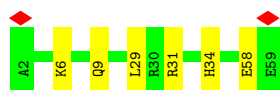
- Molecule 27: 50S ribosomal protein L28



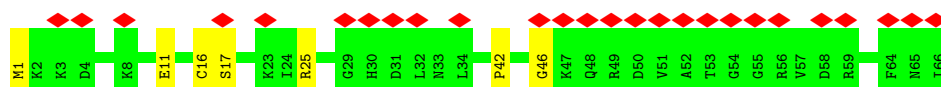
- Molecule 28: 50S ribosomal protein L29



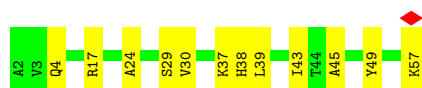
• Molecule 29: 50S ribosomal protein L30

Chain Z:  90% 10%

• Molecule 30: 50S ribosomal protein L31

Chain a:  39% 89% 11%

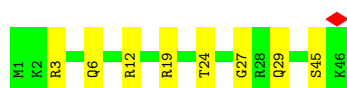
• Molecule 31: 50S ribosomal protein L32

Chain b:  79% 21%

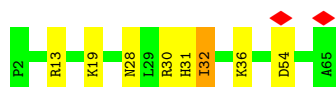
• Molecule 32: 50S ribosomal protein L33

Chain c:  87% 13%

• Molecule 33: 50S ribosomal protein L34

Chain d:  83% 17%

• Molecule 34: 50S ribosomal protein L35

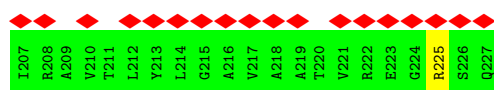
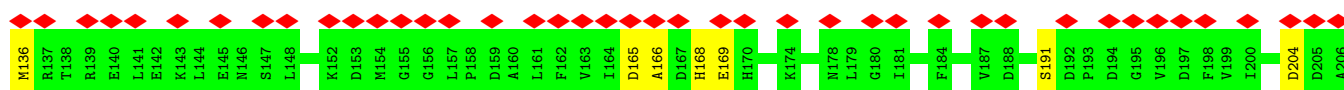
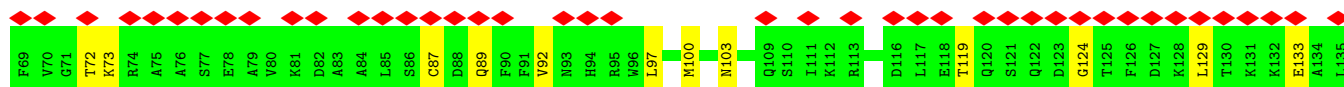
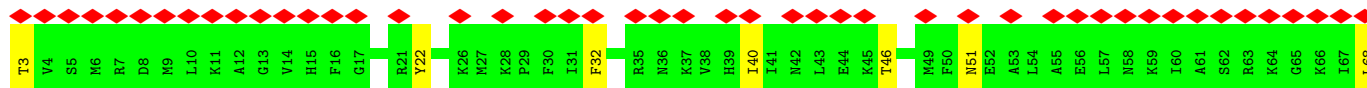
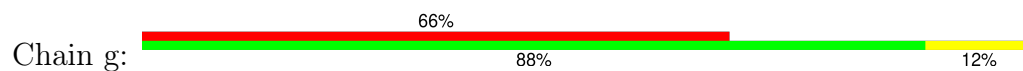
Chain e:  88% 11%

• Molecule 35: 50S ribosomal protein L36

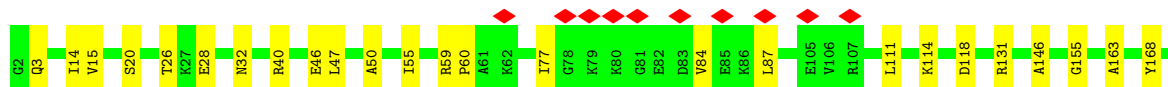
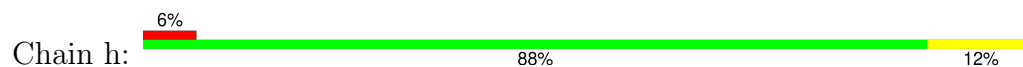
Chain f:  82% 18%



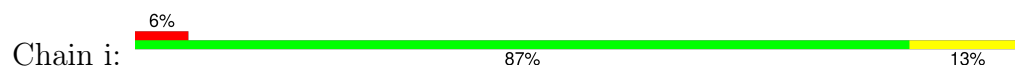
- Molecule 36: 30S ribosomal protein S2



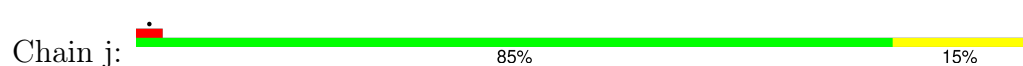
- Molecule 37: 30S ribosomal protein S3

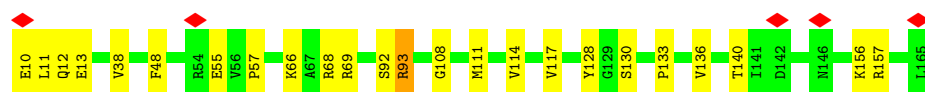


- Molecule 38: 30S ribosomal protein S4

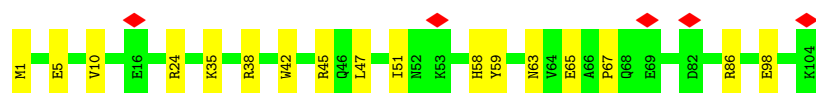
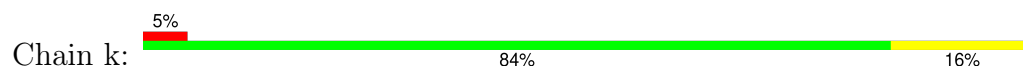


- Molecule 39: 30S ribosomal protein S5

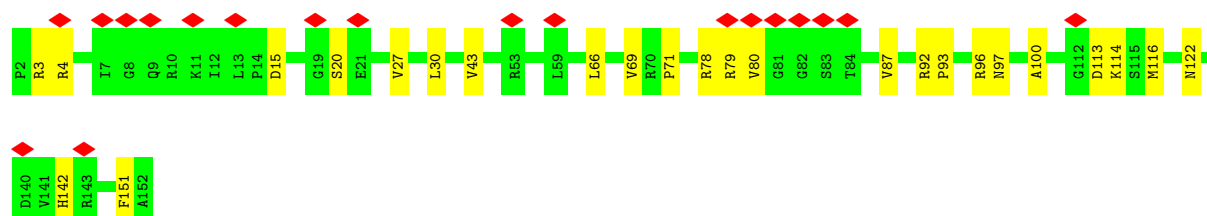
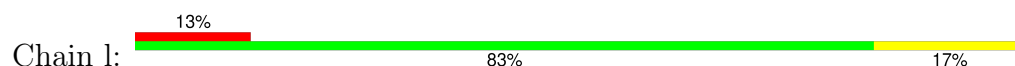




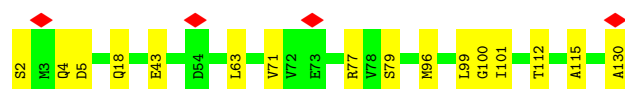
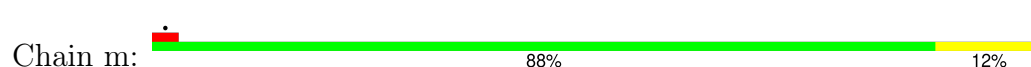
- Molecule 40: 30S ribosomal protein S6



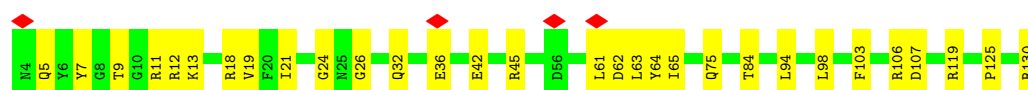
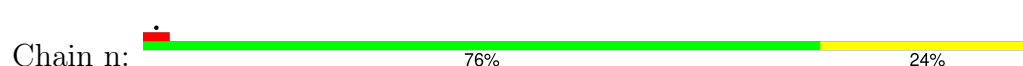
- Molecule 41: 30S ribosomal protein S7



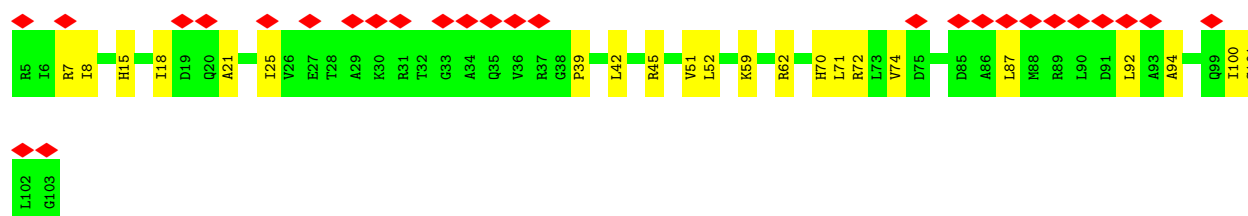
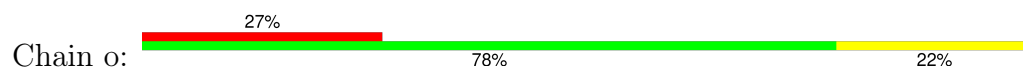
- Molecule 42: 30S ribosomal protein S8



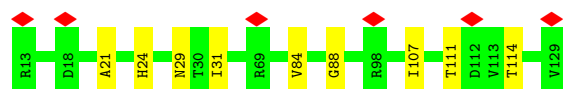
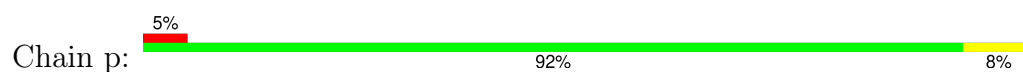
- Molecule 43: 30S ribosomal protein S9



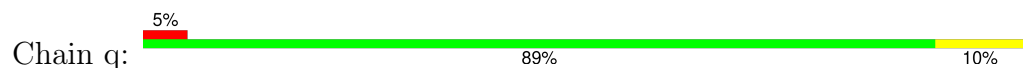
- Molecule 44: 30S ribosomal protein S10



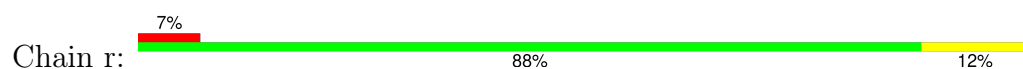
- Molecule 45: 30S ribosomal protein S11



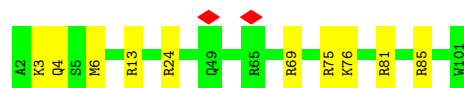
- Molecule 46: 30S ribosomal protein S12



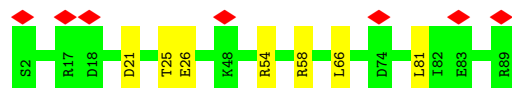
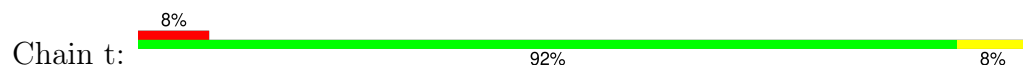
- Molecule 47: 30S ribosomal protein S13



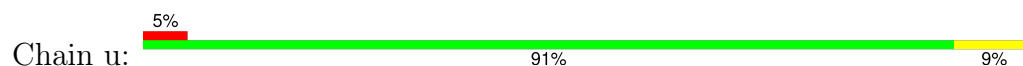
- Molecule 48: 30S ribosomal protein S14



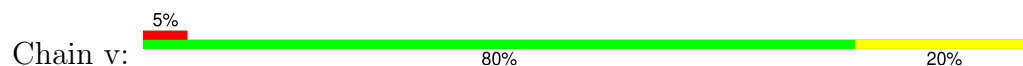
- Molecule 49: 30S ribosomal protein S15



- Molecule 50: 30S ribosomal protein S16

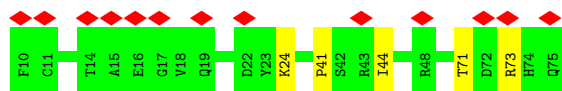
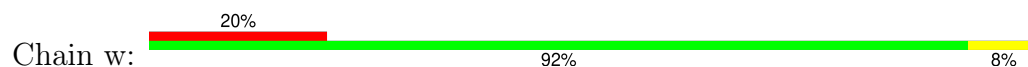


- Molecule 51: 30S ribosomal protein S17

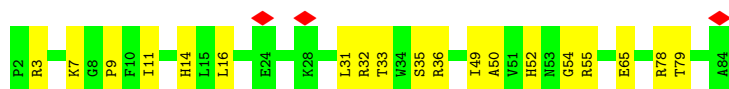




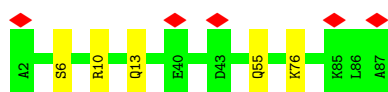
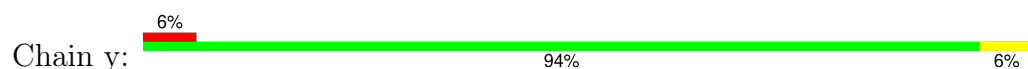
- Molecule 52: 30S ribosomal protein S18



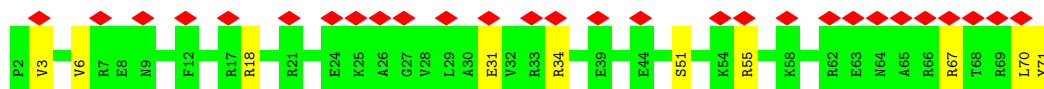
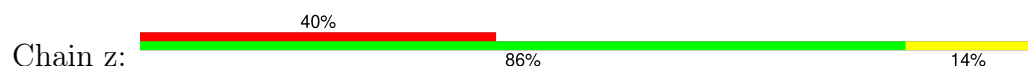
- Molecule 53: 30S ribosomal protein S19



- Molecule 54: 30S ribosomal protein S20



- Molecule 55: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.028	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	475.008, 475.008, 475.008	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.237, 1.237, 1.237	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, OMC, 2MG, 5MC, H2U, PSU, OMU, 3TD, 0TD, 5MU, G7M, 1MG, 4SU, ZN, 2MA, 6MZ, OMG, MG, 4OC, UR3, FME

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	1	0.44	0/69286	0.36	3/108087 (0.0%)
2	2	0.35	0/36590	0.32	0/57074
3	3	0.37	0/2872	0.33	0/4478
4	4	0.26	0/203	0.33	0/312
5	5	0.30	0/1704	0.35	1/2654 (0.0%)
6	A	0.52	0/23	0.44	0/29
7	B	0.45	0/2121	0.54	0/2852
8	C	0.45	0/1586	0.58	0/2134
9	D	0.40	0/1571	0.49	0/2113
10	E	0.32	0/1434	0.50	0/1926
11	F	0.30	0/1333	0.45	0/1805
12	G	0.20	0/1122	0.48	0/1515
13	J	0.42	0/1152	0.48	0/1551
14	K	0.41	0/955	0.52	0/1279
15	L	0.43	0/1062	0.64	2/1413 (0.1%)
16	M	0.41	0/1093	0.49	0/1460
17	N	0.44	0/964	0.58	0/1289
18	O	0.35	0/902	0.50	0/1209
19	P	0.42	0/929	0.49	0/1242
20	Q	0.47	0/960	0.53	0/1278
21	R	0.43	0/829	0.58	0/1107
22	S	0.43	0/864	0.48	0/1156
23	T	0.36	0/752	0.47	0/1005
24	U	0.37	0/796	0.59	0/1062
25	V	0.35	0/766	0.47	0/1025
26	W	0.44	0/589	0.52	0/779
27	X	0.41	0/635	0.48	0/848
28	Y	0.34	0/502	0.41	0/667
29	Z	0.39	0/452	0.50	0/605
30	a	0.22	0/531	0.43	0/709
31	b	0.43	0/450	0.56	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.35	0/433	0.49	0/576
33	d	0.46	0/380	0.60	0/498
34	e	0.50	0/513	0.60	0/676
35	f	0.41	0/303	0.50	0/397
36	g	0.24	0/1791	0.54	4/2413 (0.2%)
37	h	0.31	0/1663	0.48	0/2241
38	i	0.28	0/1665	0.44	0/2227
39	j	0.37	0/1165	0.57	0/1568
40	k	0.32	0/867	0.54	0/1171
41	l	0.27	0/1195	0.48	0/1602
42	m	0.33	0/989	0.47	0/1326
43	n	0.30	0/1034	0.55	0/1375
44	o	0.29	0/800	0.51	0/1082
45	p	0.32	0/893	0.44	0/1205
46	q	0.34	0/960	0.56	0/1286
47	r	0.30	0/909	0.55	0/1215
48	s	0.33	0/817	0.46	0/1088
49	t	0.32	0/722	0.49	0/964
50	u	0.32	0/659	0.51	0/884
51	v	0.29	0/657	0.49	0/881
52	w	0.31	0/553	0.44	0/743
53	x	0.27	0/680	0.47	0/915
54	y	0.31	0/675	0.42	0/895
55	z	0.25	0/597	0.43	0/792
All	All	0.40	0/155948	0.39	10/233282 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	36	LYS	CA-C-N	-8.19	115.14	122.43
15	L	36	LYS	C-N-CA	-8.19	115.14	122.43
5	5	17	U	C4'-C3'-O3'	5.98	118.37	109.40
1	1	894	U	C2'-C3'-O3'	5.67	118.01	109.50
36	g	46	THR	CA-C-N	5.43	124.68	120.33
36	g	46	THR	C-N-CA	5.43	124.68	120.33
1	1	404	A	C4'-C3'-O3'	5.43	117.54	109.40
36	g	87	CYS	CA-C-N	5.34	131.73	121.54
36	g	87	CYS	C-N-CA	5.34	131.73	121.54
1	1	1379	U	C2'-C3'-O3'	5.19	121.49	113.70

There are no chirality outliers.

There are no planarity outliers.

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	1	62336	0	31371	428	0
2	2	32929	0	16586	164	0
3	3	2569	0	1301	6	0
4	4	184	0	95	0	0
5	5	1627	0	831	7	0
6	A	32	0	28	5	0
7	B	2082	0	2154	20	0
8	C	1565	0	1616	23	0
9	D	1552	0	1619	15	0
10	E	1410	0	1444	26	0
11	F	1313	0	1358	13	0
12	G	1111	0	1148	10	0
13	J	1129	0	1162	12	0
14	K	946	0	1023	7	0
15	L	1053	0	1129	15	0
16	M	1074	0	1157	8	0
17	N	951	0	994	7	0
18	O	892	0	923	6	0
19	P	917	0	962	12	0
20	Q	947	0	1019	7	0
21	R	816	0	839	19	0
22	S	857	0	922	15	0
23	T	746	0	811	3	0
24	U	788	0	843	11	0
25	V	753	0	780	5	0
26	W	582	0	599	8	0
27	X	625	0	652	8	0
28	Y	501	0	531	3	0
29	Z	448	0	488	3	0
30	a	522	0	520	4	0
31	b	444	0	458	9	0
32	c	426	0	464	5	0
33	d	377	0	418	6	0
34	e	504	0	572	11	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	f	302	0	340	5	0
36	g	1760	0	1787	13	0
37	h	1636	0	1710	17	0
38	i	1643	0	1707	18	0
39	j	1152	0	1196	14	0
40	k	848	0	846	12	0
41	l	1181	0	1238	16	0
42	m	979	0	1031	11	0
43	n	1022	0	1070	18	0
44	o	790	0	831	15	0
45	p	877	0	887	6	0
46	q	957	0	1017	11	0
47	r	900	0	965	11	0
48	s	805	0	844	11	0
49	t	714	0	734	5	0
50	u	649	0	666	5	0
51	v	648	0	691	10	0
52	w	544	0	560	3	0
53	x	663	0	688	13	0
54	y	669	0	719	4	0
55	z	589	0	629	8	0
56	1	290	0	0	0	0
56	2	126	0	0	0	0
56	3	8	0	0	0	0
56	5	4	0	0	0	0
56	B	1	0	0	0	0
56	C	1	0	0	0	0
56	Q	1	0	0	0	0
56	b	2	0	0	0	0
56	f	1	0	0	0	0
56	i	1	0	0	0	0
56	r	1	0	0	0	0
57	a	1	0	0	0	0
57	f	1	0	0	0	0
All	All	144774	0	96973	954	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 (954) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:402:A:C2'	1:1:403:U:H5'	1.34	1.52
1:1:402:A:H2'	1:1:403:U:C5'	1.40	1.48
1:1:2313:C:H2'	1:1:2314:A:C8	1.67	1.30
1:1:2313:C:N4	1:1:2314:A:N6	1.93	1.16
1:1:2313:C:C4	1:1:2314:A:N6	2.13	1.16
21:R:52:PRO:HD2	21:R:53:PHE:H	1.07	1.13
8:C:151:THR:CG2	8:C:152:PRO:HD3	1.79	1.12
1:1:2190:G:C6	1:1:2191:A:C6	2.40	1.09
21:R:52:PRO:O	21:R:53:PHE:CD2	2.06	1.08
1:1:2190:G:C6	1:1:2191:A:N6	2.22	1.06
21:R:52:PRO:CD	21:R:53:PHE:H	1.70	1.04
1:1:2097:A:N3	1:1:2193:G:C6	2.26	1.03
8:C:151:THR:HG23	8:C:152:PRO:CD	1.92	0.99
1:1:2190:G:O6	1:1:2191:A:N6	1.96	0.99
1:1:402:A:C3'	1:1:403:U:H5'	1.93	0.98
10:E:173:PHE:O	10:E:174:ASP:OD1	1.81	0.97
1:1:402:A:C2'	1:1:403:U:C5'	2.15	0.97
8:C:151:THR:HG23	8:C:152:PRO:HD3	0.98	0.96
21:R:52:PRO:O	21:R:53:PHE:CG	2.19	0.96
1:1:2097:A:C2	1:1:2193:G:C6	2.54	0.94
1:1:2313:C:H2'	1:1:2314:A:H8	1.12	0.94
1:1:611:C:C2'	1:1:612:G:H5'	2.01	0.91
21:R:52:PRO:HD2	21:R:53:PHE:N	1.87	0.89
1:1:2584:U:H2'	1:1:2585:U:C2	2.11	0.86
1:1:2190:G:N1	1:1:2191:A:C6	2.44	0.85
1:1:2097:A:C4	1:1:2193:G:O6	2.30	0.85
10:E:123:ASP:OD2	10:E:127:ASN:HB2	1.78	0.84
1:1:611:C:H2'	1:1:612:G:H5'	1.57	0.83
1:1:2190:G:H2'	1:1:2191:A:C8	2.15	0.82
1:1:599:A:H2'	1:1:600:G:H8	1.45	0.82
1:1:1042:G:O2'	1:1:1043:C:H5''	1.81	0.81
1:1:2190:G:C4	1:1:2191:A:N7	2.50	0.80
1:1:404:A:H5'	1:1:406:G:O4'	1.82	0.80
1:1:2190:G:C2	1:1:2191:A:C5	2.71	0.79
1:1:2313:C:N4	1:1:2314:A:H61	1.80	0.79
1:1:27:G:N2	1:1:512:G:H1'	1.97	0.78
1:1:2190:G:H2'	1:1:2191:A:H8	1.48	0.77
1:1:2571:U:O2'	8:C:151:THR:HG21	1.84	0.77
1:1:2751:G:H5'	1:1:2752:C:C5	2.19	0.77
1:1:2125:G:N2	1:1:2173:A:H62	1.83	0.76
1:1:1047:G:HO2'	1:1:1110:G:H1	1.31	0.76
1:1:599:A:H2'	1:1:600:G:C8	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:496:A:N3	2:2:496:A:H2'	2.00	0.75
1:1:404:A:H5'	1:1:406:G:C1'	2.17	0.75
1:1:139:U:OP2	1:1:140:C:N4	2.17	0.73
1:1:2063:C:H1'	6:A:77:PHE:HB2	1.70	0.73
1:1:2125:G:H21	1:1:2173:A:H62	1.36	0.73
1:1:2511:U:O4	1:1:2512:C:N4	2.22	0.73
1:1:2190:G:N1	1:1:2191:A:C5	2.58	0.72
1:1:403:U:H4'	1:1:406:G:O2'	1.90	0.72
1:1:2313:C:C2	1:1:2314:A:N7	2.58	0.71
21:R:52:PRO:CD	21:R:53:PHE:N	2.37	0.71
1:1:2511:U:C4	1:1:2512:C:N4	2.58	0.71
1:1:27:G:H22	1:1:512:G:H1'	1.54	0.70
1:1:2190:G:C2	1:1:2191:A:C4	2.79	0.70
2:2:993:G:O6	2:2:1045:C:N3	2.25	0.70
1:1:1408:G:O6	1:1:1594:U:N3	2.20	0.70
1:1:599:A:N1	1:1:600:G:C6	2.58	0.70
1:1:2190:G:C6	1:1:2191:A:C5	2.80	0.69
1:1:2097:A:C2	1:1:2193:G:C5	2.80	0.69
1:1:402:A:H2'	1:1:403:U:H5''	1.66	0.69
45:p:88:GLY:H	45:p:114:THR:HG22	1.58	0.69
1:1:599:A:C6	1:1:600:G:O6	2.46	0.68
1:1:585:G:N7	20:Q:6:ARG:NH1	2.41	0.68
1:1:138:U:H1'	1:1:141:G:O6	1.94	0.68
1:1:599:A:C2	1:1:600:G:C5	2.82	0.68
2:2:993:G:H2'	2:2:993:G:N3	2.06	0.68
21:R:51:VAL:HB	21:R:52:PRO:HD3	1.75	0.68
1:1:1343:G:C6	1:1:1344:U:O4	2.47	0.67
2:2:1106:G:H5''	37:h:172:ARG:HB3	1.77	0.67
1:1:1312:U:O4'	1:1:1313:U:N3	2.26	0.67
1:1:563:A:N3	20:Q:37:GLN:NE2	2.43	0.67
1:1:252:G:C4	1:1:253:C:C5	2.82	0.67
47:r:25:VAL:HG12	47:r:29:ARG:HD2	1.77	0.67
53:x:33:THR:HG22	53:x:35:SER:H	1.60	0.67
1:1:2392:A:P	34:e:31:HIS:HE2	2.17	0.67
12:G:84:ALA:HA	12:G:91:PHE:H	1.60	0.67
1:1:2316:G:H2'	1:1:2317:A:H8	1.60	0.66
1:1:601:C:O5'	1:1:601:C:H6	1.78	0.66
1:1:402:A:H2'	1:1:403:U:H5'	0.68	0.66
20:Q:44:GLN:HE21	21:R:77:PHE:HB3	1.61	0.66
1:1:11:C:O5'	1:1:11:C:H6	1.78	0.66
2:2:950:U:H3'	47:r:101:ARG:HH22	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2192:U:O5'	1:1:2192:U:H6	1.79	0.66
29:Z:31:ARG:HD2	29:Z:34:HIS:HB2	1.76	0.66
8:C:33:ARG:HH22	8:C:74:GLU:HB3	1.60	0.66
2:2:1086:U:H3	2:2:1099:G:H22	1.43	0.66
1:1:1584:U:H5'	1:1:1585:C:C6	2.30	0.65
9:D:149:ILE:HG22	9:D:170:ARG:HB2	1.77	0.65
1:1:464:U:H1'	1:1:686:U:H5	1.61	0.65
1:1:1478:G:H1	1:1:1513:U:H3	1.45	0.65
1:1:2160:C:O5'	1:1:2160:C:H6	1.79	0.65
2:2:209:U:H3'	2:2:210:C:O2	1.97	0.65
2:2:841:C:H2'	2:2:843:U:H5'	1.79	0.65
1:1:599:A:O2'	1:1:600:G:H5'	1.98	0.64
1:1:252:G:C6	1:1:253:C:C4	2.86	0.64
1:1:2097:A:C4	1:1:2193:G:C6	2.85	0.64
1:1:2097:A:N3	1:1:2193:G:O6	2.29	0.64
1:1:2099:U:O2	1:1:2191:A:N1	2.30	0.64
1:1:2316:G:H2'	1:1:2317:A:C8	2.33	0.64
2:2:107:G:N7	54:y:10:ARG:NH2	2.45	0.64
1:1:402:A:C2'	1:1:403:U:H5''	2.23	0.63
2:2:664:G:H22	2:2:741:G:H1	1.44	0.63
1:1:2392:A:OP2	34:e:31:HIS:NE2	2.30	0.63
39:j:55:GLU:HG3	39:j:57:PRO:HD2	1.81	0.63
1:1:2126:A:O2'	1:1:2162:G:N2	2.31	0.63
1:1:2402:U:O2'	1:1:2403:C:H5''	1.98	0.63
2:2:1135:U:O2'	2:2:1136:C:O2	2.09	0.63
1:1:2097:A:C2	1:1:2193:G:O6	2.51	0.63
1:1:2193:G:H5''	1:1:2194:U:H5	1.64	0.63
2:2:501:C:OP1	46:q:114:ARG:NH2	2.31	0.63
36:g:89:GLN:HE21	36:g:225:ARG:HH12	1.47	0.63
1:1:686:U:H6	1:1:788:A:N1	1.96	0.62
37:h:14:ILE:HG22	37:h:15:VAL:HG13	1.80	0.62
44:o:21:ALA:HB1	44:o:92:LEU:HD23	1.81	0.62
1:1:136:G:C6	1:1:137:U:C4	2.86	0.62
13:J:74:TYR:HD2	13:J:92:MET:HG3	1.63	0.62
1:1:495:G:H21	22:S:61:ASN:HD21	1.47	0.62
1:1:2314:A:OP1	10:E:88:LYS:NZ	2.32	0.62
1:1:2584:U:H2'	1:1:2585:U:O2	1.98	0.62
50:u:4:ILE:HG12	50:u:21:VAL:HG22	1.80	0.62
1:1:1869:G:N2	1:1:1871:A:O2'	2.33	0.61
1:1:2880:C:O5'	1:1:2880:C:H6	1.82	0.61
1:1:402:A:C3'	1:1:403:U:C5'	2.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2305:U:H5''	10:E:131:GLY:HA3	1.81	0.61
1:1:783:A:H2'	1:1:783:A:N3	2.14	0.61
2:2:1060:U:OP1	48:s:85:ARG:NH1	2.33	0.61
3:3:43:C:O2	10:E:92:ARG:NH2	2.33	0.61
7:B:144:VAL:HB	7:B:154:LEU:HB2	1.81	0.61
1:1:568:U:H1'	1:1:2030:6MZ:H9C1	1.81	0.61
43:n:84:THR:HG21	43:n:103:PHE:HB3	1.82	0.61
51:v:61:ILE:HA	51:v:75:LEU:HA	1.82	0.61
15:L:58:TYR:O	34:e:13:ARG:NH2	2.34	0.61
1:1:2126:A:N1	1:1:2163:A:H5'	2.16	0.61
8:C:152:PRO:O	8:C:154:LYS:N	2.34	0.61
18:O:40:ILE:HG12	18:O:47:VAL:HG12	1.81	0.61
1:1:807:U:OP1	15:L:36:LYS:HE2	2.01	0.60
1:1:2313:C:N3	1:1:2314:A:C6	2.69	0.60
1:1:2168:G:O5'	1:1:2168:G:H8	1.84	0.60
42:m:96:MET:HE3	42:m:130:ALA:HB1	1.83	0.60
1:1:796:C:OP1	9:D:57:LYS:NZ	2.34	0.60
1:1:1068:G:N2	1:1:1095:A:N3	2.49	0.60
1:1:2224:G:H4'	1:1:2226:C:C2	2.36	0.60
10:E:122:PHE:O	10:E:123:ASP:OD1	2.19	0.60
2:2:951:G:OP2	47:r:101:ARG:NH2	2.34	0.60
37:h:40:ARG:NH1	37:h:55:ILE:O	2.35	0.60
2:2:1026:G:N1	2:2:1035:A:N1	2.47	0.60
47:r:11:ASP:HA	47:r:45:ILE:HB	1.83	0.60
33:d:24:THR:HG23	33:d:27:GLY:H	1.65	0.59
39:j:66:LYS:HA	39:j:69:ARG:HE	1.67	0.59
1:1:654:A:H61	34:e:19:LYS:HE2	1.67	0.59
1:1:2392:A:P	34:e:31:HIS:NE2	2.75	0.59
1:1:686:U:O4	33:d:12:ARG:HD3	2.02	0.59
2:2:958:A:OP1	53:x:55:ARG:NH1	2.35	0.59
7:B:37:ASN:HB2	7:B:62:TYR:HB2	1.85	0.59
7:B:258:ARG:NH2	7:B:263:THR:OG1	2.36	0.59
1:1:2451:A:C2	6:A:78:PHE:CE1	2.91	0.59
2:2:203:G:O2'	2:2:465:A:N1	2.36	0.59
44:o:7:ARG:HB2	44:o:101:SER:HB2	1.85	0.59
1:1:2403:C:N4	1:1:2415:G:N1	2.51	0.59
1:1:2579:C:O2'	8:C:136:ASN:ND2	2.36	0.59
40:k:10:VAL:HB	40:k:58:HIS:HB3	1.85	0.59
51:v:25:ILE:HD11	51:v:61:ILE:HD11	1.85	0.59
53:x:31:LEU:HB2	53:x:49:ILE:HG22	1.85	0.59
2:2:974:A:OP1	48:s:69:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:153:GLY:O	8:C:154:LYS:HB3	2.03	0.59
1:1:125:A:OP2	33:d:19:ARG:NH2	2.34	0.58
19:P:33:VAL:HG22	19:P:38:LYS:HG2	1.84	0.58
2:2:1147:C:H1'	43:n:18:ARG:HH21	1.69	0.58
1:1:2159:G:H2'	1:1:2160:C:C6	2.37	0.58
1:1:2301:C:H6	1:1:2301:C:O5'	1.87	0.58
30:a:11:GLU:HA	30:a:25:ARG:HA	1.85	0.58
46:q:46:ASN:ND2	46:q:89:0TD:SB	2.77	0.58
1:1:2511:U:N3	1:1:2512:C:C4	2.71	0.58
2:2:1377:A:OP1	41:l:92:ARG:NH1	2.35	0.58
1:1:301:G:OP2	24:U:82:ARG:NH1	2.36	0.58
12:G:135:HIS:HB3	12:G:138:VAL:H	1.69	0.58
1:1:1007:C:OP1	13:J:37:ARG:NH2	2.36	0.58
1:1:2511:U:C4	1:1:2512:C:C4	2.92	0.58
22:S:59:GLU:HB2	22:S:66:ILE:HD11	1.86	0.58
1:1:2105:U:H3	1:1:2184:A:H61	1.52	0.58
30:a:16:CYS:SG	30:a:17:SER:N	2.76	0.57
40:k:38:ARG:NH1	40:k:98:GLU:O	2.37	0.57
1:1:494:G:H4'	22:S:6:LYS:HB2	1.85	0.57
1:1:685:A:N7	1:1:774:G:C2	2.72	0.57
1:1:2403:C:C4	1:1:2415:G:C2	2.93	0.57
12:G:94:ILE:HG23	12:G:98:ASP:HB3	1.86	0.57
5:5:7:U:O2'	5:5:21:A:N1	2.33	0.57
43:n:42:GLU:OE2	43:n:45:ARG:NH1	2.37	0.57
1:1:613:A:O4'	1:1:614:A:C8	2.58	0.57
1:1:1408:G:N2	1:1:1595:C:H1'	2.19	0.57
2:2:50:A:O2'	2:2:360:G:N2	2.37	0.57
5:5:8:4SU:HN3	5:5:23:C:H41	1.52	0.57
8:C:181:ASP:OD2	8:C:184:ARG:NH2	2.38	0.57
15:L:74:THR:HG22	15:L:107:PHE:HB2	1.86	0.57
46:q:68:GLY:O	46:q:99:ARG:NH1	2.38	0.57
2:2:993:G:O2'	2:2:994:A:N7	2.38	0.57
7:B:29:PRO:HG2	7:B:34:LEU:HD11	1.87	0.57
1:1:599:A:C4	1:1:600:G:N7	2.72	0.57
2:2:666:G:H5'	2:2:726:C:H1'	1.86	0.57
41:l:66:LEU:HD21	41:l:97:ASN:HD21	1.70	0.57
1:1:1998:A:HO2'	1:1:2724:U:HO2'	1.49	0.57
2:2:463:U:C5	2:2:464:U:C4	2.93	0.57
2:2:1305:G:H21	2:2:1332:A:H2	1.52	0.57
1:1:352:A:C6	1:1:353:C:C4	2.93	0.57
2:2:405:U:O4	38:i:2:ALA:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:396:G:OP2	27:X:10:LYS:NZ	2.38	0.57
1:1:668:A:H2'	1:1:670:A:H62	1.70	0.57
1:1:1584:U:C5'	1:1:1585:C:C6	2.88	0.57
1:1:2193:G:H3'	1:1:2194:U:C5	2.40	0.57
1:1:2313:C:C2'	1:1:2314:A:H8	2.02	0.57
2:2:375:U:O2	50:u:28:ARG:NH2	2.37	0.57
1:1:402:A:H2'	1:1:403:U:C4'	2.26	0.56
1:1:2151:U:H2'	1:1:2152:G:H8	1.70	0.56
1:1:2314:A:O4'	10:E:155:THR:HG21	2.05	0.56
28:Y:49:ASP:OD1	28:Y:52:ARG:NH2	2.38	0.56
42:m:5:ASP:OD2	42:m:77:ARG:NH1	2.38	0.56
41:l:93:PRO:HA	41:l:96:ARG:HD3	1.87	0.56
51:v:76:VAL:HG23	51:v:77:ARG:HG2	1.88	0.56
1:1:138:U:H6	1:1:141:G:H1	1.53	0.56
1:1:1173:U:H4'	1:1:1174:U:H5'	1.88	0.56
2:2:1193:G:O6	37:h:3:GLN:NE2	2.38	0.56
1:1:1066:U:H2'	1:1:1067:A:H2'	1.87	0.56
2:2:462:G:H1	2:2:470:C:H42	1.54	0.56
9:D:97:ASN:ND2	9:D:100:MET:SD	2.78	0.56
11:F:69:ARG:NH1	11:F:73:ASN:OD1	2.38	0.56
7:B:258:ARG:NH1	7:B:264:ASP:OD1	2.36	0.56
18:O:50:ALA:O	18:O:81:ARG:NH2	2.39	0.56
1:1:404:A:C2	1:1:421:C:C4	2.94	0.56
1:1:1364:G:OP2	27:X:2:SER:N	2.39	0.56
1:1:210:C:OP1	33:d:29:GLN:NE2	2.39	0.56
1:1:881:G:H1	1:1:895:U:H3	1.53	0.56
1:1:1584:U:H5''	1:1:1585:C:O4'	2.05	0.56
2:2:279:A:H5''	2:2:280:C:H3'	1.88	0.56
27:X:37:ARG:HG2	27:X:48:THR:HG22	1.88	0.55
1:1:309:A:N3	1:1:329:G:O2'	2.39	0.55
16:M:50:ARG:HD3	16:M:65:ILE:HD11	1.87	0.55
22:S:10:ALA:HB3	22:S:101:SER:HB2	1.87	0.55
44:o:8:ILE:HG12	44:o:100:ILE:HG22	1.87	0.55
1:1:252:G:H2'	1:1:253:C:C6	2.41	0.55
2:2:35:G:N3	46:q:115:SER:OG	2.39	0.55
1:1:404:A:C2	1:1:406:G:N1	2.75	0.55
1:1:2313:C:N3	1:1:2314:A:N6	2.51	0.55
5:5:32:4OC:HM22	5:5:33:U:H5'	1.88	0.55
5:5:50:U:H3	5:5:64:G:H1	1.54	0.55
1:1:2313:C:C4	1:1:2314:A:C6	2.94	0.55
1:1:1819:A:H5''	7:B:160:THR:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1130:A:O2'	43:n:5:GLN:NE2	2.40	0.55
1:1:643:A:N1	1:1:2369:A:O2'	2.39	0.55
1:1:1791:A:N6	1:1:1828:G:O2'	2.38	0.55
2:2:811:C:O2'	2:2:901:A:N1	2.39	0.55
1:1:12:U:H2'	1:1:13:A:H5'	1.89	0.54
1:1:1776:G:H2'	1:1:1776:G:N3	2.22	0.54
1:1:2190:G:C5	1:1:2191:A:N7	2.75	0.54
2:2:1297:G:O2'	41:l:114:LYS:NZ	2.37	0.54
1:1:12:U:H2'	1:1:12:U:O2	2.07	0.54
2:2:1382:C:O2'	41:l:79:ARG:NH1	2.40	0.54
38:i:172:GLU:HB2	38:i:183:LYS:HD2	1.90	0.54
1:1:252:G:C5	1:1:253:C:C4	2.95	0.54
2:2:755:G:H21	42:m:4:GLN:HE22	1.54	0.54
1:1:599:A:N6	1:1:600:G:O6	2.39	0.54
1:1:729:G:OP1	7:B:13:ARG:HG2	2.07	0.54
55:z:6:VAL:HA	55:z:18:ARG:HH22	1.73	0.54
1:1:1044:C:O2'	1:1:1111:A:N1	2.40	0.54
1:1:2375:G:N2	1:1:2378:A:OP2	2.38	0.54
2:2:297:G:N2	2:2:300:A:OP2	2.38	0.54
2:2:544:G:OP1	38:i:56:ARG:NH2	2.34	0.54
25:V:58:SER:O	25:V:73:LYS:NZ	2.41	0.54
1:1:2584:U:C2'	1:1:2585:U:C2	2.89	0.54
1:1:143:C:H2'	1:1:143:C:O2	2.08	0.54
1:1:370:G:O2'	1:1:424:G:OP1	2.26	0.54
1:1:729:G:H2'	1:1:1775:U:H1'	1.88	0.54
1:1:2403:C:C4	1:1:2415:G:N1	2.75	0.54
1:1:635:C:O5'	1:1:635:C:H6	1.91	0.54
1:1:2103:C:H42	1:1:2186:G:H1	1.54	0.54
1:1:2720:U:OP1	19:P:53:ARG:NH2	2.41	0.54
2:2:1073:U:O2	36:g:103:ASN:ND2	2.41	0.54
33:d:3:ARG:O	33:d:6:GLN:NE2	2.36	0.53
1:1:2130:U:O3'	1:1:2158:A:N6	2.42	0.53
3:3:43:C:H5''	30:a:1:MET:HG2	1.90	0.53
1:1:2298:A:OP1	10:E:71:ARG:NH2	2.40	0.53
1:1:634:C:H6	1:1:634:C:O5'	1.92	0.53
2:2:559:A:H4'	2:2:560:A:H3'	1.91	0.53
21:R:34:GLU:HG2	21:R:60:LYS:HG2	1.89	0.53
1:1:567:U:OP2	15:L:29:LYS:NZ	2.41	0.53
2:2:1297:G:H21	41:l:114:LYS:HB3	1.74	0.53
9:D:148:ILE:HB	9:D:169:VAL:HG22	1.88	0.53
12:G:116:ARG:NE	12:G:133:GLN:OE1	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:21:LEU:HD21	26:W:41:ARG:HH21	1.73	0.53
15:L:29:LYS:HG3	15:L:30:THR:HG23	1.90	0.53
1:1:1779:U:OP2	1:1:1784:A:N6	2.38	0.53
1:1:2403:C:N4	1:1:2415:G:C6	2.77	0.53
2:2:972:C:OP2	44:o:59:LYS:NZ	2.38	0.53
1:1:2167:U:O5'	1:1:2167:U:H6	1.92	0.53
1:1:2646:C:OP2	1:1:2732:G:O2'	2.26	0.53
2:2:108:G:H5'	2:2:109:A:H5''	1.91	0.53
31:b:45:ALA:O	31:b:57:LYS:NZ	2.39	0.53
1:1:1266:G:O2'	1:1:2012:G:O6	2.27	0.52
2:2:392:C:OP1	50:u:8:ARG:NH2	2.42	0.52
9:D:176:ASP:OD1	9:D:176:ASP:N	2.40	0.52
40:k:5:GLU:OE2	52:w:24:LYS:NZ	2.40	0.52
54:y:55:GLN:HG3	54:y:76:LYS:HE2	1.91	0.52
1:1:72:U:O4	28:Y:58:ASN:ND2	2.42	0.52
1:1:2099:U:O2	1:1:2191:A:C2	2.62	0.52
32:c:8:LYS:HA	32:c:24:THR:HA	1.91	0.52
10:E:121:SER:OG	10:E:129:SER:O	2.28	0.52
46:q:56:ARG:NE	46:q:62:GLU:OE1	2.36	0.52
14:K:121:GLU:OE1	19:P:65:SER:OG	2.26	0.52
1:1:355:U:H2'	1:1:356:G:H8	1.74	0.52
1:1:563:A:OP2	21:R:79:ARG:NH2	2.39	0.52
1:1:2313:C:H42	1:1:2314:A:N6	2.01	0.52
2:2:1152:A:OP1	44:o:70:HIS:ND1	2.42	0.52
2:2:1255:G:OP2	44:o:45:ARG:NH1	2.40	0.52
35:f:25:VAL:HB	35:f:35:GLN:HB2	1.91	0.52
1:1:84:A:N1	1:1:98:G:O2'	2.40	0.52
2:2:439:U:N3	2:2:440:C:C4	2.77	0.52
2:2:439:U:N3	2:2:440:C:C5	2.77	0.52
7:B:142:HIS:ND1	7:B:193:GLY:O	2.35	0.52
12:G:127:GLU:HA	12:G:145:ASN:HA	1.91	0.52
40:k:42:TRP:HB2	40:k:59:TYR:HB2	1.92	0.52
1:1:1658:C:O5'	1:1:1658:C:H6	1.92	0.52
1:1:2640:G:OP1	13:J:95:ARG:NH2	2.37	0.52
8:C:49:GLN:HE21	8:C:79:LEU:HB3	1.74	0.52
38:i:95:GLU:HA	38:i:100:ASN:HD22	1.75	0.52
47:r:83:LEU:HD21	53:x:65:GLU:HB2	1.91	0.52
1:1:2190:G:N3	1:1:2191:A:C8	2.78	0.52
18:O:52:SER:OG	18:O:53:THR:N	2.42	0.52
19:P:30:VAL:HG12	19:P:81:VAL:HG12	1.91	0.52
1:1:252:G:H2'	1:1:253:C:H6	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2097:A:N3	1:1:2193:G:N1	2.58	0.52
1:1:2314:A:H2'	1:1:2315:G:C8	2.45	0.52
24:U:74:ASN:ND2	24:U:81:ASP:OD2	2.39	0.52
37:h:155:GLY:HA2	37:h:163:ALA:HB1	1.92	0.52
1:1:2313:C:C2	1:1:2314:A:C5	2.98	0.51
3:3:77:U:OP1	25:V:21:ARG:NH1	2.42	0.51
14:K:43:ILE:HD12	14:K:56:ASP:HB2	1.92	0.51
1:1:783:A:N3	1:1:783:A:C2'	2.73	0.51
1:1:1053:C:H2'	1:1:1054:A:H8	1.74	0.51
2:2:477:C:H2'	2:2:478:A:C8	2.46	0.51
2:2:673:A:H4'	40:k:86:ARG:HH12	1.76	0.51
2:2:1092:A:OP2	41:l:4:ARG:NH2	2.44	0.51
44:o:25:ILE:HG13	44:o:87:LEU:HD11	1.91	0.51
49:t:25:THR:HG23	49:t:66:LEU:HD12	1.92	0.51
2:2:959:A:HO2'	2:2:984:C:HO2'	1.58	0.51
11:F:24:ILE:HD11	11:F:43:VAL:HG11	1.90	0.51
19:P:14:LYS:HE2	19:P:77:HIS:HA	1.92	0.51
39:j:38:VAL:HA	39:j:48:PHE:HA	1.92	0.51
2:2:452:A:H62	2:2:480:U:H3	1.57	0.51
24:U:72:ILE:HD12	24:U:83:VAL:HG21	1.93	0.51
55:z:51:SER:OG	55:z:55:ARG:NH2	2.43	0.51
2:2:1320:C:N3	53:x:36:ARG:NH1	2.58	0.51
11:F:89:LEU:HD23	11:F:94:TYR:HB3	1.91	0.51
16:M:14:LYS:O	16:M:71:LYS:NZ	2.37	0.51
21:R:52:PRO:C	21:R:53:PHE:CG	2.88	0.51
22:S:73:LYS:HB2	22:S:106:VAL:HB	1.91	0.51
37:h:46:GLU:HG2	37:h:87:LEU:HD21	1.92	0.51
39:j:111:MET:HG3	39:j:140:THR:HG21	1.93	0.51
47:r:97:VAL:HG23	47:r:109:ARG:HH22	1.75	0.51
1:1:510:C:C2'	1:1:511:U:H5'	2.41	0.51
11:F:88:GLN:HE21	11:F:163:ARG:HD2	1.75	0.51
41:l:15:ASP:OD1	41:l:20:SER:N	2.44	0.51
1:1:2097:A:H1'	1:1:2193:G:H1	1.76	0.51
1:1:2199:A:OP1	27:X:37:ARG:NH1	2.43	0.51
11:F:101:ASN:HB2	11:F:117:LEU:HB2	1.91	0.51
37:h:32:ASN:OD1	37:h:59:ARG:NH1	2.43	0.51
38:i:15:GLU:HG3	38:i:19:LEU:HD11	1.93	0.51
43:n:36:GLU:OE1	43:n:45:ARG:NH1	2.44	0.51
1:1:404:A:H2	1:1:421:C:C4	2.29	0.51
1:1:568:U:OP1	15:L:36:LYS:HD3	2.11	0.51
1:1:2110:G:N7	1:1:2172:U:O4	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:979:C:OP1	2:2:1223:C:N4	2.44	0.51
24:U:48:PRO:HG3	24:U:56:GLY:HA3	1.92	0.51
1:1:2392:A:OP2	34:e:31:HIS:CE1	2.64	0.51
9:D:6:LYS:O	9:D:9:GLN:NE2	2.42	0.51
11:F:35:ARG:NH1	11:F:75:MET:SD	2.84	0.51
36:g:68:LEU:HD11	36:g:92:VAL:HG23	1.92	0.51
1:1:1652:A:OP1	17:N:8:ARG:NH2	2.42	0.51
12:G:51:ARG:HA	12:G:54:LEU:HB3	1.93	0.51
1:1:142:A:C6	1:1:143:C:C4	2.98	0.50
1:1:2885:G:O6	31:b:29:SER:OG	2.28	0.50
1:1:1450:G:N2	1:1:1452:G:O6	2.40	0.50
1:1:1789:A:OP2	7:B:221:ARG:NH1	2.44	0.50
1:1:2584:U:C2'	1:1:2585:U:O2	2.59	0.50
8:C:5:VAL:H	8:C:32:ASN:HD21	1.57	0.50
45:p:24:HIS:HB3	45:p:31:ILE:HB	1.94	0.50
1:1:247:G:OP2	1:1:249:C:N4	2.43	0.50
1:1:611:C:H2'	1:1:612:G:C5'	2.37	0.50
2:2:1166:G:O2'	2:2:1169:A:N6	2.43	0.50
2:2:1222:G:H5''	53:x:78:ARG:HD2	1.93	0.50
1:1:1047:G:O2'	1:1:1110:G:N1	2.32	0.50
11:F:155:GLU:HG2	11:F:157:TYR:H	1.76	0.50
20:Q:76:TYR:OH	20:Q:92:ARG:NH1	2.45	0.50
24:U:86:ARG:NH1	24:U:100:SER:OG	2.44	0.50
1:1:956:G:O6	16:M:14:LYS:NZ	2.45	0.50
29:Z:6:LYS:HB2	29:Z:58:GLU:HB3	1.93	0.50
1:1:1170:C:H5''	1:1:1170:C:H6	1.77	0.50
1:1:2029:G:N1	1:1:2033:A:OP2	2.35	0.50
2:2:1417:G:O2'	2:2:1483:A:N6	2.45	0.50
31:b:38:HIS:ND1	31:b:39:LEU:O	2.39	0.50
34:e:28:ASN:O	34:e:36:LYS:NZ	2.42	0.50
1:1:500:G:N1	1:1:503:A:OP2	2.45	0.50
1:1:2403:C:H2'	1:1:2403:C:O2	2.12	0.50
2:2:662:U:O2'	2:2:836:G:OP1	2.29	0.50
13:J:13:ARG:NH1	13:J:49:ASP:O	2.44	0.50
22:S:4:ILE:HG12	22:S:106:VAL:HG22	1.94	0.50
1:1:335:C:O2	24:U:68:SER:OG	2.29	0.50
1:1:2114:A:C8	1:1:2167:U:H4'	2.47	0.50
2:2:970:C:N4	43:n:130:ARG:O	2.45	0.50
11:F:123:ALA:HA	11:F:133:LEU:HA	1.93	0.50
55:z:31:GLU:OE2	55:z:34:ARG:NH2	2.44	0.50
1:1:102:U:H5''	1:1:102:U:O2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:496:A:N3	2:2:496:A:C2'	2.73	0.50
1:1:2032:G:O2'	8:C:150:GLN:NE2	2.45	0.49
2:2:1360:A:OP2	48:s:75:ARG:NH2	2.45	0.49
8:C:136:ASN:HD21	8:C:139:SER:HB2	1.75	0.49
1:1:1083:U:O2'	1:1:1085:A:OP2	2.28	0.49
13:J:17:VAL:HG23	13:J:137:PRO:HB2	1.94	0.49
21:R:52:PRO:O	21:R:53:PHE:CE2	2.61	0.49
1:1:630:G:N2	1:1:633:A:OP2	2.41	0.49
1:1:674:G:H1'	9:D:69:ARG:HD3	1.94	0.49
45:p:21:ALA:HB3	45:p:84:VAL:HG22	1.95	0.49
1:1:573:U:O2'	1:1:575:A:OP1	2.29	0.49
1:1:2301:C:H2'	1:1:2302:U:C6	2.47	0.49
12:G:86:ASP:OD2	40:k:24:ARG:NH1	2.46	0.49
15:L:76:GLU:HB2	15:L:111:ILE:HD13	1.95	0.49
43:n:94:LEU:HB3	43:n:98:LEU:HD13	1.94	0.49
2:2:126:G:OP1	2:2:605:U:O2'	2.26	0.49
7:B:130:LEU:N	7:B:130:LEU:HD23	2.28	0.49
22:S:34:ASP:OD2	31:b:37:LYS:NZ	2.39	0.49
24:U:34:VAL:HG13	24:U:67:VAL:HG22	1.95	0.49
1:1:476:G:N1	1:1:479:A:OP2	2.45	0.49
1:1:811:U:H2'	15:L:21:ARG:HA	1.94	0.49
1:1:1915:3TD:H2'	1:1:1916:A:O4'	2.12	0.49
11:F:84:THR:OG1	11:F:134:LYS:NZ	2.40	0.49
26:W:21:LEU:HD11	26:W:41:ARG:HE	1.78	0.49
1:1:600:G:H2'	1:1:601:C:C6	2.48	0.49
1:1:807:U:O2'	1:1:2060:A:N1	2.44	0.49
27:X:68:LEU:HD23	27:X:71:LEU:HD12	1.95	0.49
1:1:2532:G:O2'	1:1:2657:A:N1	2.44	0.49
2:2:269:C:H2'	2:2:270:A:C8	2.48	0.49
2:2:982:U:H5''	48:s:6:MET:HE2	1.93	0.49
2:2:1005:A:N6	2:2:1024:G:O2'	2.46	0.49
11:F:60:ASP:HB2	11:F:63:ALA:HB3	1.95	0.49
1:1:1939:5MU:OP1	1:1:2604:U:O2'	2.29	0.49
1:1:2311:A:O2'	1:1:2312:U:O4'	2.30	0.49
14:K:7:MET:HE1	14:K:44:LYS:HG3	1.93	0.49
44:o:42:LEU:HB2	44:o:71:LEU:HB3	1.94	0.49
1:1:2313:C:O4'	10:E:37:ASN:ND2	2.46	0.49
2:2:404:G:O6	38:i:2:ALA:N	2.46	0.49
2:2:1328:C:O2'	47:r:29:ARG:NH1	2.46	0.49
7:B:145:GLU:HB2	7:B:188:CYS:HB3	1.95	0.49
37:h:131:ARG:NH2	37:h:168:TYR:OH	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:112:THR:HG23	42:m:115:ALA:H	1.77	0.49
1:1:599:A:C6	1:1:600:G:C6	3.01	0.48
1:1:613:A:O4'	1:1:614:A:H8	1.96	0.48
1:1:2300:C:H2'	1:1:2301:C:C6	2.48	0.48
1:1:1069:A:O2'	1:1:1074:G:N1	2.44	0.48
1:1:2315:G:H2'	1:1:2316:G:C8	2.48	0.48
2:2:696:A:N3	2:2:786:G:O2'	2.42	0.48
5:5:15:C:H5''	5:5:15:C:O2	2.13	0.48
21:R:36:ALA:HA	21:R:58:VAL:HG23	1.94	0.48
38:i:192:SER:OG	38:i:194:ASP:OD1	2.29	0.48
1:1:270:A:H5'	1:1:271:G:H5''	1.94	0.48
1:1:568:U:OP1	15:L:36:LYS:CD	2.61	0.48
1:1:685:A:C8	1:1:774:G:N1	2.81	0.48
1:1:1392:A:N6	23:T:18:GLU:OE1	2.46	0.48
2:2:81:A:N6	2:2:88:U:O4	2.39	0.48
2:2:632:U:O2	2:2:632:U:H3'	2.12	0.48
2:2:980:C:O2'	48:s:13:ARG:NH1	2.46	0.48
22:S:24:ILE:HD13	22:S:36:LEU:HD11	1.94	0.48
1:1:252:G:C5	1:1:253:C:C5	3.01	0.48
1:1:1801:A:OP2	7:B:150:LYS:NZ	2.39	0.48
1:1:2190:G:C4	1:1:2191:A:C8	3.00	0.48
2:2:273:U:O4	2:2:274:A:N6	2.46	0.48
37:h:77:ILE:HA	37:h:84:VAL:HG23	1.95	0.48
52:w:71:THR:HG23	52:w:73:ARG:H	1.78	0.48
1:1:672:C:OP2	15:L:42:SER:OG	2.29	0.48
1:1:2097:A:C5	1:1:2193:G:O6	2.67	0.48
13:J:32:LEU:HD22	13:J:54:ILE:HG21	1.95	0.48
1:1:101:A:N3	1:1:101:A:H2'	2.28	0.48
1:1:700:G:O2'	1:1:1632:A:N3	2.42	0.48
2:2:401:C:O2'	2:2:621:A:N3	2.44	0.48
2:2:1098:C:O2'	55:z:71:TYR:O	2.30	0.48
23:T:8:LEU:HD23	23:T:50:LEU:HD21	1.95	0.48
2:2:363:A:N6	46:q:27:CYS:SG	2.87	0.48
35:f:30:GLU:HG3	35:f:32:LYS:H	1.79	0.48
1:1:747:5MU:O2'	22:S:92:ARG:NH1	2.47	0.48
1:1:1313:U:H3'	1:1:1313:U:O2	2.13	0.48
1:1:2002:G:H5'	17:N:13:ASN:HA	1.94	0.48
2:2:677:U:H3	2:2:713:G:H22	1.61	0.48
10:E:111:ILE:HB	10:E:114:PHE:HB2	1.95	0.48
1:1:634:C:H2'	1:1:635:C:C6	2.49	0.48
13:J:114:LEU:HG	13:J:118:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:87:PHE:HD1	17:N:90:ARG:HD3	1.79	0.48
48:s:3:LYS:HB2	48:s:6:MET:HG2	1.96	0.48
3:3:7:G:O2'	18:O:38:GLN:NE2	2.46	0.48
21:R:43:ASN:HB3	21:R:46:GLU:HB3	1.95	0.48
26:W:37:ILE:HG22	26:W:38:VAL:HG23	1.96	0.48
43:n:19:VAL:HG22	43:n:65:ILE:HG12	1.96	0.48
1:1:84:A:N1	1:1:103:A:C5	2.82	0.47
1:1:1340:U:OP1	23:T:84:TYR:OH	2.29	0.47
1:1:2313:C:N3	1:1:2314:A:C5	2.82	0.47
2:2:977:A:O2'	2:2:979:C:OP2	2.27	0.47
7:B:155:ALA:HB2	7:B:162:VAL:HG23	1.95	0.47
15:L:62:PRO:HB2	34:e:30:ARG:HH11	1.78	0.47
43:n:106:ARG:NH1	43:n:107:ASP:O	2.47	0.47
1:1:2751:G:H5'	1:1:2752:C:C6	2.48	0.47
2:2:1167:A:O2'	2:2:1169:A:N7	2.46	0.47
13:J:125:TYR:OH	13:J:132:HIS:NE2	2.43	0.47
1:1:1682:G:OP2	1:1:1699:G:N2	2.46	0.47
1:1:1792:G:H5'	7:B:204:VAL:HG23	1.95	0.47
24:U:51:ALA:O	24:U:52:LEU:CB	2.62	0.47
1:1:138:U:O2'	1:1:139:U:H5''	2.14	0.47
1:1:1312:U:H4'	1:1:1313:U:C2	2.50	0.47
2:2:4:U:H3'	2:2:4:U:O2	2.13	0.47
2:2:104:G:OP2	54:y:13:GLN:NE2	2.40	0.47
8:C:13:ARG:HH11	19:P:56:HIS:HA	1.78	0.47
36:g:22:TYR:OH	55:z:67:ARG:NH1	2.47	0.47
43:n:26:GLY:N	43:n:62:ASP:OD1	2.46	0.47
1:1:1429:G:H2'	1:1:1430:G:H8	1.80	0.47
2:2:626:G:O3'	50:u:51:ARG:NH1	2.44	0.47
7:B:108:LYS:HA	7:B:196:GLY:HA2	1.95	0.47
37:h:20:SER:OG	37:h:40:ARG:NH2	2.46	0.47
1:1:447:A:OP1	20:Q:5:LYS:NZ	2.40	0.47
1:1:2134:A:O2'	1:1:2159:G:N3	2.46	0.47
1:1:2224:G:O2'	1:1:2226:C:C4	2.68	0.47
39:j:93:ARG:HG2	39:j:128:TYR:HB2	1.97	0.47
1:1:877:A:O2'	1:1:900:A:N6	2.48	0.47
1:1:1169:A:H62	1:1:1180:U:H3	1.61	0.47
1:1:2387:U:OP1	26:W:55:ARG:NH2	2.45	0.47
1:1:2822:G:OP1	8:C:164:GLN:NE2	2.43	0.47
2:2:35:G:O2'	46:q:115:SER:O	2.33	0.47
2:2:1249:C:O3'	43:n:75:GLN:NE2	2.47	0.47
2:2:1520:C:H2'	2:2:1521:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:38:ARG:HE	40:k:63:ASN:ND2	2.13	0.47
41:l:27:VAL:HG12	41:l:43:VAL:HG21	1.97	0.47
1:1:2403:C:N3	1:1:2415:G:C2	2.83	0.47
2:2:467:U:O2	2:2:467:U:H5''	2.15	0.47
43:n:32:GLN:NE2	43:n:64:TYR:OH	2.47	0.47
1:1:752:A:H62	1:1:2609:U:H3	1.63	0.47
1:1:2313:C:C2'	1:1:2314:A:C8	2.63	0.47
32:c:15:ALA:HB2	32:c:47:VAL:HG11	1.97	0.47
1:1:307:G:N1	1:1:310:A:OP2	2.45	0.47
1:1:404:A:C2	1:1:421:C:N3	2.83	0.47
1:1:463:G:N2	1:1:466:A:OP2	2.45	0.47
1:1:511:U:H2'	1:1:512:G:H5'	1.97	0.47
1:1:2190:G:C5	1:1:2191:A:C5	3.03	0.47
45:p:111:THR:HG23	55:z:3:VAL:HG22	1.95	0.47
1:1:2576:G:O2'	1:1:2579:C:OP2	2.29	0.46
2:2:1013:G:N2	2:2:1016:A:OP2	2.44	0.46
15:L:57:LEU:HD22	34:e:54:ASP:HB3	1.97	0.46
17:N:2:ARG:HD2	17:N:5:LYS:HB2	1.96	0.46
36:g:3:THR:N	36:g:51:ASN:OD1	2.47	0.46
1:1:252:G:C6	1:1:253:C:N4	2.83	0.46
1:1:797:G:OP1	9:D:55:SER:OG	2.32	0.46
1:1:2315:G:H2'	1:1:2316:G:H8	1.81	0.46
11:F:86:LYS:HG2	11:F:132:VAL:HG22	1.97	0.46
18:O:29:HIS:HB3	18:O:36:TYR:HB2	1.97	0.46
1:1:411:G:OP2	1:1:2406:A:O2'	2.25	0.46
2:2:439:U:C2	2:2:440:C:C5	3.02	0.46
1:1:27:G:C2	1:1:512:G:N3	2.83	0.46
1:1:686:U:C6	1:1:788:A:N1	2.81	0.46
24:U:4:LYS:O	24:U:94:ARG:NH2	2.45	0.46
1:1:404:A:H2	1:1:421:C:N4	2.13	0.46
1:1:2250:G:C8	1:1:2496:C:H5''	2.50	0.46
2:2:579:A:O2'	49:t:54:ARG:NH1	2.44	0.46
2:2:632:U:H5''	2:2:633:G:C8	2.50	0.46
2:2:1530:G:H2'	2:2:1531:A:C8	2.51	0.46
8:C:3:GLY:HA3	8:C:204:LYS:HG2	1.96	0.46
12:G:93:SER:OG	12:G:121:VAL:O	2.31	0.46
1:1:72:U:OP2	28:Y:54:LYS:NZ	2.49	0.46
1:1:987:C:O2'	1:1:1000:A:N3	2.45	0.46
2:2:8:A:N6	38:i:202:GLU:O	2.46	0.46
2:2:1038:C:N4	2:2:1039:G:O6	2.49	0.46
11:F:95:ARG:HB2	11:F:128:GLN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:116:GLN:HE21	38:i:120:HIS:CE1	2.34	0.46
1:1:1045:C:O2	1:1:1047:G:N1	2.49	0.46
1:1:1607:C:N4	1:1:1622:G:OP2	2.36	0.46
2:2:73:C:H5''	2:2:73:C:H6	1.80	0.46
2:2:1316:G:N1	2:2:1319:A:OP2	2.48	0.46
1:1:601:C:O2'	1:1:605:G:OP1	2.33	0.46
1:1:1266:G:OP2	31:b:17:ARG:NE	2.41	0.46
1:1:2788:C:O2'	1:1:2809:A:N3	2.47	0.46
2:2:41:G:H2'	2:2:42:G:H8	1.81	0.46
2:2:356:A:N3	2:2:368:U:O2'	2.42	0.46
2:2:1277:C:O2'	2:2:1279:G:H8	1.99	0.46
19:P:71:GLU:OE2	19:P:101:ARG:NE	2.46	0.46
38:i:58:LYS:NZ	38:i:69:GLU:OE1	2.49	0.46
1:1:11:C:H2'	1:1:12:U:H5'	1.97	0.46
1:1:458:G:O2'	1:1:469:G:O6	2.28	0.46
1:1:782:A:O4'	1:1:783:A:C6	2.68	0.46
1:1:910:A:N3	1:1:2264:C:O2'	2.44	0.46
1:1:2094:A:C4	1:1:2095:A:C8	3.04	0.46
1:1:2299:U:OP1	10:E:72:LYS:NZ	2.43	0.46
1:1:2063:C:C1'	6:A:77:PHE:HB2	2.44	0.46
1:1:2278:A:OP2	26:W:12:ASN:ND2	2.45	0.46
2:2:689:C:OP1	45:p:29:ASN:ND2	2.46	0.46
2:2:1425:U:H2'	2:2:1426:G:H8	1.81	0.46
29:Z:9:GLN:HB2	29:Z:29:LEU:HD13	1.97	0.46
2:2:673:A:O3'	40:k:86:ARG:NH2	2.44	0.45
10:E:119:ALA:O	10:E:167:ARG:NH2	2.38	0.45
1:1:1223:G:OP1	21:R:68:ARG:NH2	2.50	0.45
1:1:1343:G:N2	1:1:1405:U:C2	2.84	0.45
1:1:2166:U:H5''	1:1:2166:U:H6	1.80	0.45
1:1:2194:U:H2'	1:1:2195:U:C6	2.51	0.45
9:D:98:LYS:HB3	9:D:102:ARG:HH22	1.80	0.45
14:K:71:ARG:NH2	14:K:123:LEU:O	2.46	0.45
37:h:28:GLU:O	37:h:32:ASN:ND2	2.50	0.45
1:1:2258:C:O2'	1:1:2427:C:OP2	2.35	0.45
39:j:156:LYS:HG2	42:m:71:VAL:HG13	1.98	0.45
42:m:43:GLU:HG2	42:m:101:ILE:HG12	1.98	0.45
43:n:119:ARG:HG3	43:n:125:PRO:HG3	1.98	0.45
1:1:514:A:N3	1:1:581:C:O2'	2.43	0.45
1:1:878:A:H3'	1:1:879:G:H8	1.82	0.45
1:1:1043:C:H5''	1:1:1043:C:H6	1.81	0.45
1:1:2394:C:H5''	15:L:63:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:993:G:H22	2:2:996:A:H62	1.64	0.45
2:2:1077:G:N2	2:2:1080:A:OP2	2.38	0.45
41:l:69:VAL:HG23	41:l:100:ALA:HB1	1.99	0.45
44:o:52:LEU:HD23	44:o:62:ARG:HG2	1.99	0.45
2:2:222:C:H2'	2:2:223:A:C8	2.52	0.45
36:g:72:THR:OG1	36:g:169:GLU:OE2	2.26	0.45
42:m:77:ARG:NE	42:m:79:SER:O	2.50	0.45
1:1:833:A:H2'	1:1:834:G:C8	2.50	0.45
1:1:1019:U:O2'	1:1:1021:A:N7	2.46	0.45
1:1:2315:G:H4'	10:E:127:ASN:ND2	2.31	0.45
34:e:32:ILE:HG22	34:e:32:ILE:O	2.17	0.45
36:g:97:LEU:H	36:g:100:MET:HE3	1.82	0.45
1:1:1343:G:C6	1:1:1344:U:C4	3.05	0.45
1:1:2313:C:H2'	1:1:2314:A:N7	2.22	0.45
2:2:1218:C:H2'	2:2:1219:A:C8	2.51	0.45
2:2:1279:G:O2'	2:2:1281:C:OP2	2.31	0.45
10:E:123:ASP:O	10:E:125:ARG:N	2.50	0.45
37:h:26:THR:OG1	48:s:76:LYS:NZ	2.50	0.45
1:1:353:C:H5''	1:1:353:C:H6	1.82	0.45
1:1:1076:C:H2'	1:1:1077:A:H8	1.81	0.45
1:1:2010:G:H5''	22:S:42:LYS:HB2	1.98	0.45
2:2:266:G:H3'	51:v:69:LYS:HB2	1.99	0.45
2:2:439:U:H3'	2:2:439:U:O2	2.17	0.45
37:h:111:LEU:HD22	37:h:146:ALA:HB2	1.97	0.45
1:1:1326:U:H2'	1:1:1327:A:H8	1.80	0.45
1:1:2101:A:N6	1:1:2188:U:O4	2.50	0.45
2:2:1003:G:N2	2:2:1005:A:O5'	2.46	0.45
21:R:38:VAL:HG13	21:R:54:VAL:HB	1.99	0.45
27:X:40:VAL:HG12	27:X:43:GLU:H	1.82	0.45
53:x:32:ARG:HA	53:x:50:ALA:HB3	1.98	0.45
1:1:2539:C:H5'	35:f:3:VAL:HG11	1.98	0.45
2:2:41:G:H2'	2:2:42:G:C8	2.52	0.45
2:2:552:U:O2'	46:q:83:ARG:O	2.27	0.45
22:S:80:PRO:O	22:S:100:THR:OG1	2.30	0.45
47:r:98:ARG:HB2	47:r:100:GLN:HE22	1.82	0.45
1:1:58:G:O2'	1:1:73:A:N1	2.42	0.44
1:1:1796:U:H2'	1:1:1797:G:H8	1.81	0.44
26:W:18:ALA:O	26:W:20:ARG:NH1	2.50	0.44
1:1:281:C:H2'	1:1:282:A:H8	1.82	0.44
2:2:542:G:O3'	38:i:14:ARG:NH2	2.44	0.44
2:2:1328:C:H5''	47:r:28:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:38:GLY:N	24:U:62:GLU:OE2	2.49	0.44
51:v:17:MET:HG3	51:v:20:SER:HB2	1.99	0.44
2:2:1136:C:O2	2:2:1136:C:H5''	2.18	0.44
7:B:16:VAL:HG22	7:B:206:GLY:HA3	1.98	0.44
13:J:36:LEU:HD11	13:J:122:LEU:HB2	1.99	0.44
36:g:165:ASP:HB3	36:g:168:HIS:HB3	1.99	0.44
44:o:15:HIS:HA	44:o:18:ILE:HG22	2.00	0.44
2:2:1241:G:H2'	2:2:1242:G:H8	1.83	0.44
7:B:62:TYR:HA	7:B:86:ASN:HD21	1.82	0.44
19:P:25:THR:N	19:P:88:ARG:O	2.44	0.44
6:A:78:PHE:O	6:A:78:PHE:CD1	2.70	0.44
10:E:4:LEU:HA	10:E:7:TYR:HB3	2.00	0.44
1:1:720:U:H2'	1:1:721:A:C8	2.52	0.44
1:1:1105:U:H2'	1:1:1106:G:H8	1.83	0.44
13:J:56:VAL:HB	13:J:124:VAL:HG12	2.00	0.44
2:2:976:G:OP2	2:2:1358:U:O2'	2.36	0.44
9:D:106:LYS:HG3	9:D:200:LEU:HD23	1.99	0.44
17:N:28:LEU:HD23	17:N:48:VAL:HG21	1.98	0.44
22:S:81:SER:HB3	22:S:97:LEU:HD12	2.00	0.44
37:h:114:LYS:NZ	37:h:118:ASP:OD2	2.44	0.44
1:1:126:A:OP1	33:d:45:SER:OG	2.29	0.44
1:1:1376:C:N4	1:1:1377:G:C6	2.86	0.44
1:1:1475:G:O2'	1:1:1514:G:O6	2.35	0.44
2:2:464:U:N3	2:2:467:U:OP2	2.34	0.44
22:S:23:LEU:HD22	31:b:24:ALA:HB2	2.00	0.44
39:j:92:SER:OG	39:j:130:SER:O	2.28	0.44
46:q:72:HIS:HB2	46:q:74:LEU:HD23	1.99	0.44
1:1:510:C:H2'	1:1:511:U:H5'	2.00	0.44
1:1:2250:G:N3	1:1:2250:G:H5'	2.33	0.44
2:2:673:A:H2'	2:2:674:G:C8	2.53	0.44
2:2:844:G:N1	2:2:846:G:H1'	2.33	0.44
47:r:101:ARG:HG2	47:r:103:LYS:H	1.82	0.44
2:2:1005:A:H3'	2:2:1006:G:C8	2.52	0.43
1:1:299:A:N3	1:1:319:G:O2'	2.47	0.43
1:1:788:A:OP1	1:1:791:C:N4	2.43	0.43
1:1:1311:G:H21	1:1:1603:A:H62	1.67	0.43
1:1:1539:U:H2'	1:1:1540:G:H8	1.83	0.43
1:1:2314:A:C1'	10:E:155:THR:HG21	2.48	0.43
1:1:2575:C:H5'	8:C:149:ASN:HB2	1.98	0.43
2:2:1260:G:OP1	2:2:1284:C:O2'	2.34	0.43
26:W:33:ALA:N	26:W:64:ASP:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:c:8:LYS:HB3	32:c:24:THR:HG22	2.00	0.43
39:j:12:GLN:HG3	39:j:117:VAL:HG12	2.01	0.43
44:o:71:LEU:O	44:o:72:ARG:NH1	2.44	0.43
46:q:54:ARG:HD2	46:q:62:GLU:HG3	2.00	0.43
1:1:2039:U:H2'	1:1:2040:G:C8	2.53	0.43
1:1:2425:A:H4'	1:1:2426:A:H5''	1.99	0.43
21:R:52:PRO:HD2	21:R:53:PHE:O	2.18	0.43
51:v:59:VAL:HG23	51:v:78:VAL:HG22	2.00	0.43
1:1:2753:A:O2'	35:f:15:LYS:NZ	2.37	0.43
2:2:750:C:H4'	49:t:21:ASP:HA	2.00	0.43
10:E:117:LEU:N	10:E:177:PHE:O	2.47	0.43
10:E:123:ASP:C	10:E:125:ARG:H	2.27	0.43
10:E:173:PHE:C	10:E:174:ASP:OD1	2.58	0.43
13:J:19:ASP:OD1	13:J:58:ASN:ND2	2.42	0.43
14:K:38:ILE:HD11	14:K:112:PHE:HZ	1.84	0.43
35:f:2:LYS:NZ	35:f:32:LYS:O	2.49	0.43
50:u:45:GLU:HG2	50:u:46:LYS:HG2	2.00	0.43
53:x:52:HIS:CD2	53:x:54:GLY:H	2.37	0.43
1:1:1046:A:H5'	1:1:1047:G:C8	2.53	0.43
1:1:1053:C:H2'	1:1:1054:A:C8	2.52	0.43
1:1:1385:A:O2'	1:1:1396:U:O2	2.35	0.43
1:1:1643:G:C2	1:1:1644:C:C2	3.06	0.43
1:1:2286:G:O6	32:c:23:THR:OG1	2.31	0.43
2:2:1255:G:O2'	2:2:1258:G:N3	2.41	0.43
8:C:4:LEU:HB2	8:C:101:PHE:HE2	1.83	0.43
16:M:41:LEU:HD22	16:M:124:LEU:HD22	2.01	0.43
22:S:25:ARG:NH1	22:S:74:ILE:O	2.51	0.43
38:i:102:VAL:HG13	38:i:107:PHE:HB2	1.99	0.43
41:l:113:ASP:OD2	41:l:122:ASN:ND2	2.48	0.43
1:1:381:G:OP1	27:X:18:ARG:NH2	2.50	0.43
2:2:216:U:H4'	2:2:464:U:O2'	2.18	0.43
2:2:252:U:O4	2:2:253:A:N6	2.51	0.43
2:2:938:A:N3	2:2:1376:U:O2'	2.41	0.43
2:2:1088:G:H4'	55:z:70:LEU:HD23	1.99	0.43
2:2:1119:C:OP2	43:n:11:ARG:NH1	2.49	0.43
39:j:10:GLU:HG2	39:j:11:LEU:HD12	2.00	0.43
1:1:404:A:N1	1:1:421:C:N3	2.66	0.43
1:1:2425:A:H4'	1:1:2426:A:O5'	2.19	0.43
1:1:2808:G:O2'	1:1:2890:G:O6	2.27	0.43
16:M:30:SER:H	16:M:106:ASP:HB3	1.82	0.43
25:V:86:LEU:HD13	25:V:89:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:95:GLU:HA	38:i:100:ASN:ND2	2.34	0.43
1:1:371:A:H61	1:1:401:A:H3'	1.84	0.43
1:1:1980:G:O2'	1:1:1982:U:OP2	2.29	0.43
1:1:2627:G:O2'	1:1:2781:A:N1	2.43	0.43
42:m:2:SER:HB2	42:m:4:GLN:HE21	1.84	0.43
1:1:138:U:H3'	1:1:138:U:O2	2.19	0.43
1:1:666:A:H4'	15:L:48:ARG:HD2	2.01	0.43
1:1:1750:G:O2'	1:1:2860:A:N1	2.48	0.43
44:o:51:VAL:HB	48:s:81:ARG:HB2	2.01	0.43
1:1:323:C:O2	1:1:323:C:H5'	2.19	0.43
1:1:1408:G:C2	1:1:1595:C:O2	2.72	0.43
1:1:2125:G:H21	1:1:2173:A:N6	2.10	0.43
1:1:2467:C:O2	16:M:123:LYS:NZ	2.51	0.43
2:2:269:C:H2'	2:2:270:A:H8	1.84	0.43
39:j:157:ARG:NH2	42:m:99:LEU:O	2.51	0.43
44:o:100:ILE:H	44:o:100:ILE:HG13	1.69	0.43
1:1:783:A:H8	1:1:1778:U:O2'	2.01	0.42
1:1:1651:G:H4'	17:N:39:PRO:HG2	2.01	0.42
1:1:2120:G:OP1	1:1:2172:U:H5	2.02	0.42
1:1:2315:G:O5'	1:1:2315:G:H8	2.02	0.42
2:2:842:U:H4'	2:2:846:G:C6	2.54	0.42
1:1:782:A:O2'	7:B:224:ALA:O	2.36	0.42
1:1:2128:G:O6	1:1:2161:C:O2	2.37	0.42
1:1:2615:U:C2	31:b:4:GLN:HA	2.55	0.42
2:2:933:G:O6	41:l:3:ARG:NH2	2.49	0.42
2:2:1317:C:OP1	48:s:24:ARG:NH2	2.42	0.42
5:5:21:A:O2'	5:5:46:A:N6	2.52	0.42
25:V:51:GLN:OE1	25:V:57:TYR:OH	2.35	0.42
37:h:26:THR:HG23	48:s:76:LYS:HG3	2.01	0.42
1:1:1156:A:C8	20:Q:51:ARG:HG2	2.53	0.42
2:2:467:U:O2	2:2:467:U:H3'	2.19	0.42
2:2:743:A:OP1	49:t:58:ARG:NH2	2.42	0.42
2:2:1356:G:H2'	2:2:1357:A:C8	2.55	0.42
3:3:5:U:OP1	3:3:61:G:O2'	2.32	0.42
7:B:78:VAL:HG21	7:B:110:LEU:HD21	2.00	0.42
10:E:4:LEU:O	10:E:8:TYR:N	2.51	0.42
16:M:47:GLU:OE2	16:M:51:ARG:NE	2.52	0.42
47:r:17:ILE:O	47:r:20:THR:OG1	2.30	0.42
1:1:1246:A:H4'	9:D:40:ARG:HH12	1.83	0.42
1:1:1796:U:H2'	1:1:1797:G:C8	2.54	0.42
1:1:2193:G:H5''	1:1:2194:U:C5	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:335:C:H2'	2:2:336:A:C8	2.55	0.42
2:2:891:U:H2'	2:2:892:A:H8	1.84	0.42
2:2:1064:G:O2'	2:2:1190:G:N2	2.53	0.42
14:K:80:ASP:OD2	19:P:62:ARG:NH1	2.50	0.42
38:i:57:GLU:HG2	38:i:199:LEU:HB2	2.00	0.42
43:n:12:ARG:HG3	43:n:13:LYS:H	1.83	0.42
53:x:11:ILE:HD13	53:x:16:LEU:HD13	2.01	0.42
2:2:545:C:OP1	38:i:58:LYS:NZ	2.52	0.42
12:G:66:ASN:ND2	12:G:135:HIS:HB2	2.35	0.42
51:v:68:SER:OG	51:v:69:LYS:N	2.52	0.42
1:1:352:A:C2	1:1:353:C:C2	3.08	0.42
1:1:1754:A:O3'	19:P:103:ARG:NH2	2.52	0.42
1:1:1759:A:O2'	1:1:2714:G:O2'	2.35	0.42
1:1:2425:A:H4'	1:1:2426:A:C5'	2.49	0.42
1:1:2636:C:O2'	8:C:45:TYR:OH	2.36	0.42
2:2:975:A:N1	2:2:1366:C:O2'	2.43	0.42
1:1:137:U:H2'	1:1:138:U:H5'	2.02	0.42
1:1:223:A:N1	1:1:407:G:O2'	2.51	0.42
1:1:964:C:O2'	1:1:2273:A:N3	2.44	0.42
1:1:1386:C:H2'	1:1:1387:A:C8	2.54	0.42
1:1:1438:U:H2'	1:1:1439:A:H8	1.85	0.42
1:1:2193:G:H3'	1:1:2194:U:C6	2.55	0.42
2:2:222:C:H2'	2:2:223:A:H8	1.84	0.42
2:2:1520:C:H2'	2:2:1521:C:H6	1.84	0.42
9:D:119:ILE:HB	9:D:187:VAL:HG22	2.02	0.42
10:E:8:TYR:OH	10:E:29:PRO:O	2.32	0.42
24:U:51:ALA:O	24:U:52:LEU:HB3	2.19	0.42
1:1:102:U:O2	1:1:102:U:H3'	2.20	0.42
1:1:137:U:C2'	1:1:138:U:H5'	2.50	0.42
1:1:2000:C:OP1	17:N:5:LYS:NZ	2.42	0.42
2:2:1047:G:H5''	48:s:4:GLN:HG3	2.02	0.42
9:D:189:THR:HG22	9:D:191:ASP:H	1.85	0.42
12:G:14:SER:OG	12:G:15:LEU:N	2.53	0.42
42:m:18:GLN:HE21	42:m:63:LEU:HD22	1.84	0.42
45:p:107:ILE:HG23	55:z:6:VAL:HG21	2.01	0.42
1:1:2125:G:N2	1:1:2173:A:N6	2.59	0.42
1:1:2848:G:O2'	1:1:2867:G:N2	2.35	0.42
2:2:61:G:N7	54:y:6:SER:OG	2.53	0.42
2:2:1183:U:O2'	2:2:1185:G:OP2	2.37	0.42
6:A:78:PHE:CD1	6:A:78:PHE:C	2.98	0.42
22:S:97:LEU:HD13	22:S:97:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:96:MET:HB3	42:m:100:GLY:H	1.85	0.42
1:1:784:G:OP1	1:1:2588:G:H5''	2.20	0.41
1:1:1364:G:N2	1:1:1367:A:OP2	2.50	0.41
2:2:672:U:H2'	2:2:673:A:C8	2.55	0.41
25:V:35:GLU:OE1	25:V:93:ARG:NE	2.53	0.41
36:g:73:LYS:HE3	36:g:204:ASP:HB2	2.02	0.41
36:g:119:THR:O	36:g:124:GLY:N	2.42	0.41
38:i:106:GLY:HA3	38:i:162:ALA:HB2	2.02	0.41
51:v:11:ARG:HD2	51:v:58:VAL:HG22	2.02	0.41
1:1:45:G:H5''	1:1:46:G:H5'	2.01	0.41
1:1:352:A:N6	1:1:353:C:N4	2.68	0.41
1:1:510:C:OP1	1:1:512:G:O6	2.37	0.41
1:1:2512:C:H1'	8:C:145:SER:O	2.20	0.41
11:F:38:ASN:HD22	11:F:39:ASP:H	1.68	0.41
49:t:26:GLU:HG3	49:t:81:LEU:HD22	2.02	0.41
1:1:1042:G:HO2'	1:1:1043:C:H6	1.65	0.41
8:C:25:THR:HG21	8:C:193:VAL:HG22	2.02	0.41
13:J:96:ARG:HH21	13:J:99:ARG:HG2	1.84	0.41
19:P:90:GLY:O	19:P:113:ARG:NH1	2.53	0.41
43:n:21:ILE:HD12	43:n:61:LEU:HD13	2.01	0.41
1:1:510:C:C4	1:1:511:U:C4	3.09	0.41
1:1:1584:U:H4'	1:1:1585:C:H5''	2.02	0.41
1:1:2117:A:O2'	1:1:2119:A:OP1	2.35	0.41
1:1:2190:G:C4	1:1:2191:A:C5	3.08	0.41
1:1:2193:G:H2'	1:1:2194:U:H5'	2.02	0.41
1:1:2831:G:O2'	1:1:2884:U:OP1	2.23	0.41
2:2:944:G:N1	2:2:1338:G:OP2	2.50	0.41
2:2:1181:G:O2'	2:2:1182:G:N7	2.47	0.41
8:C:25:THR:OG1	8:C:191:GLY:O	2.32	0.41
31:b:43:ILE:HG22	31:b:49:TYR:HB2	2.03	0.41
53:x:3:ARG:HH21	53:x:7:LYS:HD3	1.84	0.41
1:1:2173:A:C6	1:1:2174:C:C4	3.09	0.41
2:2:1071:C:H2'	2:2:1072:G:C8	2.55	0.41
2:2:1391:U:H2'	2:2:1392:G:C8	2.55	0.41
9:D:83:VAL:HB	9:D:86:ALA:HB2	2.02	0.41
18:O:93:ASP:OD2	18:O:95:SER:OG	2.35	0.41
36:g:32:PHE:N	36:g:40:ILE:O	2.50	0.41
41:l:30:LEU:HD11	41:l:116:MET:HE2	2.03	0.41
1:1:832:U:H2'	1:1:833:A:C8	2.56	0.41
1:1:2160:C:H6	1:1:2160:C:P	2.44	0.41
2:2:790:A:OP1	5:5:38:A:O2'	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:890:G:O2'	2:2:906:A:N6	2.54	0.41
2:2:946:A:H2'	2:2:947:G:C8	2.56	0.41
8:C:101:PHE:HD1	8:C:104:VAL:HG21	1.84	0.41
14:K:105:ARG:NH1	19:P:34:GLU:OE1	2.53	0.41
38:i:78:GLU:OE2	38:i:81:ARG:NH1	2.38	0.41
41:l:78:ARG:HG2	41:l:80:VAL:HG13	2.01	0.41
1:1:11:C:C2'	1:1:12:U:H5'	2.50	0.41
1:1:481:G:O2'	1:1:507:A:N1	2.49	0.41
1:1:1837:C:O2'	1:1:1927:A:N3	2.49	0.41
1:1:2162:G:H5''	1:1:2173:A:H5''	2.01	0.41
2:2:1095:U:OP1	2:2:1108:G:N1	2.46	0.41
15:L:30:THR:HG21	15:L:35:HIS:NE2	2.36	0.41
36:g:166:ALA:HB3	36:g:191:SER:HB3	2.02	0.41
53:x:3:ARG:NH1	53:x:9:PRO:O	2.54	0.41
1:1:142:A:C5	1:1:143:C:C5	3.09	0.41
1:1:910:A:H2'	1:1:911:A:C8	2.56	0.41
1:1:1376:C:H6	1:1:1376:C:H5''	1.85	0.41
1:1:1429:G:H2'	1:1:1430:G:C8	2.55	0.41
2:2:9:G:H5'	39:j:108:GLY:HA3	2.03	0.41
2:2:815:A:N7	2:2:1509:C:O2'	2.52	0.41
2:2:960:U:H2'	2:2:1225:A:H62	1.86	0.41
2:2:1319:A:O2'	2:2:1323:G:N7	2.52	0.41
30:a:42:PRO:HB2	30:a:46:GLY:HA3	2.03	0.41
1:1:776:G:N7	1:1:793:A:O2'	2.46	0.41
1:1:860:U:H2'	1:1:861:A:H8	1.86	0.41
1:1:1076:C:H2'	1:1:1077:A:C8	2.56	0.41
1:1:1313:U:O4	1:1:1603:A:N1	2.53	0.41
1:1:1715:G:O2'	1:1:1743:G:O6	2.32	0.41
1:1:2079:U:O2'	27:X:23:ASN:OD1	2.38	0.41
1:1:2193:G:H3'	1:1:2194:U:H5	1.83	0.41
2:2:219:U:H2'	2:2:220:G:H8	1.85	0.41
2:2:1014:A:H4'	53:x:14:HIS:CE1	2.56	0.41
3:3:49:C:H2'	3:3:50:A:C8	2.55	0.41
10:E:44:ILE:H	10:E:44:ILE:HG13	1.64	0.41
10:E:131:GLY:HA2	10:E:153:ASP:HA	2.03	0.41
16:M:42:THR:HG22	16:M:93:VAL:HG12	2.03	0.41
20:Q:53:ARG:HH11	20:Q:53:ARG:HD2	1.76	0.41
32:c:37:LYS:HA	32:c:48:ILE:HA	2.02	0.41
36:g:133:GLU:HA	36:g:136:MET:HB2	2.02	0.41
37:h:47:LEU:HB3	37:h:50:ALA:HB3	2.03	0.41
38:i:107:PHE:HB3	38:i:145:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:133:PRO:HA	39:j:136:VAL:HG12	2.02	0.41
40:k:35:LYS:HB2	40:k:65:GLU:HB3	2.03	0.41
51:v:31:HIS:HA	51:v:32:PRO:HD3	1.96	0.41
1:1:349:U:H2'	1:1:350:G:H8	1.86	0.41
1:1:1064:C:H42	1:1:1074:G:H22	1.68	0.41
1:1:1657:U:H2'	1:1:1658:C:C6	2.56	0.41
1:1:2195:U:O2'	1:1:2196:C:H5'	2.21	0.41
31:b:30:VAL:HG22	31:b:37:LYS:HG2	2.03	0.41
40:k:47:LEU:HD13	40:k:51:ILE:HG12	2.03	0.41
1:1:2116:G:N7	1:1:2171:A:N6	2.68	0.40
2:2:404:G:O2'	2:2:498:A:N1	2.50	0.40
2:2:439:U:H2'	2:2:440:C:O4'	2.21	0.40
37:h:60:PRO:HB3	44:o:94:ALA:HB2	2.03	0.40
39:j:38:VAL:HG21	39:j:114:VAL:HG23	2.03	0.40
41:l:87:VAL:HG12	41:l:151:PHE:HB3	2.03	0.40
43:n:24:GLY:H	43:n:61:LEU:HA	1.86	0.40
1:1:352:A:C6	1:1:353:C:N3	2.89	0.40
1:1:404:A:N1	1:1:421:C:C2	2.89	0.40
1:1:1315:C:O2'	1:1:1392:A:N3	2.51	0.40
1:1:1790:C:H2'	1:1:1791:A:C5	2.57	0.40
1:1:2273:A:H2'	1:1:2274:A:C8	2.56	0.40
26:W:23:VAL:HG13	26:W:38:VAL:HG22	2.04	0.40
40:k:45:ARG:HD3	40:k:59:TYR:CE2	2.57	0.40
41:l:71:PRO:HA	41:l:142:HIS:HE1	1.87	0.40
44:o:39:PRO:HA	44:o:74:VAL:HG22	2.02	0.40
51:v:68:SER:HB3	51:v:71:LYS:HB3	2.02	0.40
52:w:41:PRO:HD2	52:w:44:ILE:HD12	2.02	0.40
1:1:142:A:N1	1:1:143:C:C4	2.89	0.40
1:1:373:U:H2'	1:1:374:A:H8	1.87	0.40
1:1:613:A:H4'	1:1:614:A:OP1	2.19	0.40
1:1:1779:U:H5	1:1:1784:A:N7	2.19	0.40
1:1:2133:G:O2'	1:1:2157:G:N2	2.54	0.40
2:2:72:A:C6	2:2:73:C:N3	2.89	0.40
7:B:171:TYR:HE1	7:B:185:GLU:HG2	1.87	0.40
34:e:31:HIS:ND1	34:e:32:ILE:HG13	2.37	0.40
39:j:13:GLU:OE2	39:j:68:ARG:NH1	2.54	0.40
43:n:7:TYR:HH	43:n:9:THR:HG1	1.61	0.40
46:q:89:OTD:H4	46:q:89:OTD:H8	1.88	0.40
1:1:572:A:OP2	21:R:80:ARG:NH2	2.44	0.40
1:1:2039:U:H2'	1:1:2040:G:H8	1.86	0.40
1:1:2233:U:H2'	1:1:2234:G:C8	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:7:ASP:OD1	9:D:7:ASP:N	2.48	0.40
10:E:44:ILE:HG21	10:E:79:ILE:HG22	2.02	0.40
1:1:404:A:N3	1:1:406:G:C6	2.90	0.40
1:1:611:C:O2'	1:1:612:G:H5'	2.19	0.40
1:1:1590:A:H2'	1:1:1591:A:C8	2.56	0.40
1:1:1792:G:O2'	1:1:1830:C:OP1	2.39	0.40
2:2:957:U:H4'	53:x:79:THR:HG23	2.04	0.40
10:E:134:GLU:HG3	10:E:149:VAL:HG13	2.04	0.40
21:R:5:PHE:HB3	21:R:59:ILE:HD12	2.04	0.40
40:k:1:MET:HE2	40:k:67:PRO:HD3	2.03	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	
6	A	1/3 (33%)	1 (100%)	0	0	100	100
7	B	269/271 (99%)	257 (96%)	12 (4%)	0	100	100
8	C	207/209 (99%)	201 (97%)	3 (1%)	3 (1%)	9	30
9	D	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
10	E	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	21	51
11	F	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
12	G	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
13	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
14	K	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
15	L	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
16	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
17	N	117/119 (98%)	114 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	O	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
19	P	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
20	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
21	R	101/103 (98%)	93 (92%)	6 (6%)	2 (2%)	6	22
22	S	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
23	T	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	U	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
25	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
26	W	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
27	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
28	Y	60/62 (97%)	60 (100%)	0	0	100	100
29	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	a	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
31	b	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
32	c	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
33	d	44/46 (96%)	44 (100%)	0	0	100	100
34	e	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
35	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
36	g	223/225 (99%)	208 (93%)	15 (7%)	0	100	100
37	h	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
38	i	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
39	j	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
40	k	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
41	l	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
42	m	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
43	n	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
44	o	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
45	p	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
46	q	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
47	r	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
48	s	98/100 (98%)	97 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	t	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
50	u	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
51	v	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
52	w	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
53	x	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
54	y	84/86 (98%)	84 (100%)	0	0	100	100
55	z	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
All	All	5609/5710 (98%)	5415 (96%)	188 (3%)	6 (0%)	49	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	C	152	PRO
8	C	153	GLY
8	C	154	LYS
21	R	52	PRO
21	R	53	PHE
10	E	124	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A	2/2 (100%)	0	2 (100%)	0	0
7	B	216/216 (100%)	215 (100%)	1 (0%)	81	93
8	C	164/164 (100%)	162 (99%)	2 (1%)	63	86
9	D	165/165 (100%)	165 (100%)	0	100	100
10	E	148/148 (100%)	147 (99%)	1 (1%)	76	92
11	F	136/136 (100%)	136 (100%)	0	100	100
12	G	114/114 (100%)	114 (100%)	0	100	100
13	J	116/116 (100%)	115 (99%)	1 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	K	104/104 (100%)	104 (100%)	0	100	100
15	L	103/103 (100%)	102 (99%)	1 (1%)	68	89
16	M	109/109 (100%)	109 (100%)	0	100	100
17	N	99/99 (100%)	99 (100%)	0	100	100
18	O	86/86 (100%)	86 (100%)	0	100	100
19	P	99/99 (100%)	99 (100%)	0	100	100
20	Q	89/89 (100%)	89 (100%)	0	100	100
21	R	84/84 (100%)	82 (98%)	2 (2%)	43	75
22	S	93/93 (100%)	93 (100%)	0	100	100
23	T	81/81 (100%)	81 (100%)	0	100	100
24	U	84/84 (100%)	83 (99%)	1 (1%)	63	86
25	V	78/78 (100%)	78 (100%)	0	100	100
26	W	58/58 (100%)	58 (100%)	0	100	100
27	X	67/67 (100%)	67 (100%)	0	100	100
28	Y	54/54 (100%)	54 (100%)	0	100	100
29	Z	48/48 (100%)	48 (100%)	0	100	100
30	a	59/59 (100%)	59 (100%)	0	100	100
31	b	47/47 (100%)	47 (100%)	0	100	100
32	c	47/47 (100%)	47 (100%)	0	100	100
33	d	38/38 (100%)	38 (100%)	0	100	100
34	e	51/51 (100%)	50 (98%)	1 (2%)	48	78
35	f	34/34 (100%)	34 (100%)	0	100	100
36	g	187/187 (100%)	186 (100%)	1 (0%)	81	93
37	h	171/171 (100%)	171 (100%)	0	100	100
38	i	172/172 (100%)	171 (99%)	1 (1%)	78	93
39	j	119/119 (100%)	118 (99%)	1 (1%)	73	90
40	k	91/91 (100%)	91 (100%)	0	100	100
41	l	124/124 (100%)	124 (100%)	0	100	100
42	m	104/104 (100%)	104 (100%)	0	100	100
43	n	105/105 (100%)	104 (99%)	1 (1%)	68	89
44	o	86/86 (100%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	p	90/90 (100%)	90 (100%)	0	100	100
46	q	102/102 (100%)	102 (100%)	0	100	100
47	r	94/94 (100%)	94 (100%)	0	100	100
48	s	83/83 (100%)	83 (100%)	0	100	100
49	t	76/76 (100%)	76 (100%)	0	100	100
50	u	65/65 (100%)	65 (100%)	0	100	100
51	v	74/74 (100%)	74 (100%)	0	100	100
52	w	57/57 (100%)	57 (100%)	0	100	100
53	x	72/72 (100%)	72 (100%)	0	100	100
54	y	65/65 (100%)	65 (100%)	0	100	100
55	z	60/60 (100%)	60 (100%)	0	100	100
All	All	4670/4670 (100%)	4654 (100%)	16 (0%)	84	96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	78	PHE
6	A	77	PHE
7	B	204	VAL
8	C	33	ARG
8	C	151	THR
10	E	141	ILE
13	J	57	LEU
15	L	111	ILE
21	R	10	LYS
21	R	48	LYS
24	U	52	LEU
34	e	32	ILE
36	g	129	LEU
38	i	143	VAL
39	j	93	ARG
43	n	63	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
7	B	53	HIS

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Mol	Chain	Res	Type
7	B	86	ASN
7	B	153	GLN
7	B	243	HIS
7	B	260	ASN
8	C	32	ASN
8	C	49	GLN
8	C	136	ASN
8	C	150	GLN
8	C	173	GLN
9	D	92	HIS
9	D	136	GLN
9	D	163	ASN
11	F	38	ASN
11	F	88	GLN
12	G	11	ASN
12	G	66	ASN
14	K	9	ASN
15	L	104	GLN
16	M	60	GLN
17	N	9	GLN
17	N	31	HIS
17	N	73	ASN
18	O	19	GLN
18	O	29	HIS
18	O	38	GLN
18	O	98	GLN
18	O	100	HIS
19	P	115	ASN
20	Q	44	GLN
20	Q	52	GLN
21	R	86	GLN
22	S	61	ASN
25	V	24	ASN
25	V	75	GLN
26	W	76	ASN
27	X	36	HIS
29	Z	20	HIS
29	Z	34	HIS
30	a	20	ASN
31	b	5	GLN
32	c	19	HIS
34	e	26	HIS

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Mol	Chain	Res	Type
36	g	39	HIS
36	g	177	ASN
38	i	116	GLN
39	j	132	ASN
40	k	63	ASN
40	k	94	HIS
41	l	97	ASN
43	n	32	GLN
45	p	119	ASN
46	q	5	ASN
49	t	20	ASN
50	u	29	ASN
53	x	52	HIS
53	x	57	HIS
54	y	3	ASN
54	y	52	ASN
55	z	56	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2903 (99%)	496 (17%)	9 (0%)
2	2	1532/1534 (99%)	256 (16%)	3 (0%)
3	3	119/120 (99%)	15 (12%)	0
4	4	8/9 (88%)	2 (25%)	0
5	5	75/76 (98%)	17 (22%)	1 (1%)
All	All	4636/4642 (99%)	786 (16%)	13 (0%)

All (786) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	51	G
1	1	60	G
1	1	71	A
1	1	74	A
1	1	75	G

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Mol	Chain	Res	Type
1	1	80	G
1	1	84	A
1	1	85	G
1	1	101	A
1	1	102	U
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U
1	1	122	G
1	1	125	A
1	1	138	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	248	G
1	1	249	C
1	1	264	C
1	1	265	A
1	1	266	G
1	1	272	A
1	1	273	G
1	1	275	C
1	1	276	U
1	1	285	G
1	1	311	A
1	1	329	G
1	1	330	A
1	1	343	C
1	1	353	C
1	1	361	G
1	1	371	A
1	1	372	G
1	1	383	C

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Mol	Chain	Res	Type
1	1	386	G
1	1	396	G
1	1	399	U
1	1	403	U
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	435	C
1	1	457	A
1	1	467	G
1	1	481	G
1	1	489	G
1	1	491	G
1	1	505	A
1	1	509	C
1	1	513	A
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	573	U
1	1	575	A
1	1	603	A
1	1	612	G
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	621	A
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G
1	1	654	A

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Mol	Chain	Res	Type
1	1	655	A
1	1	670	A
1	1	685	A
1	1	686	U
1	1	702	U
1	1	709	U
1	1	710	U
1	1	726	G
1	1	730	A
1	1	747	5MU
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	792	A
1	1	800	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	866	A
1	1	869	G
1	1	878	A
1	1	880	G
1	1	882	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	893	C
1	1	895	U
1	1	907	G
1	1	910	A

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Mol	Chain	Res	Type
1	1	931	U
1	1	932	U
1	1	941	A
1	1	946	C
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1096	A
1	1	1101	U
1	1	1110	G

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Mol	Chain	Res	Type
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1122	G
1	1	1128	G
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1136	G
1	1	1139	G
1	1	1142	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1171	G
1	1	1173	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1182	G
1	1	1186	G
1	1	1206	G
1	1	1212	G
1	1	1218	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1250	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1300	G
1	1	1301	A
1	1	1321	A
1	1	1329	U

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Mol	Chain	Res	Type
1	1	1341	G
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1408	G
1	1	1409	U
1	1	1411	U
1	1	1417	C
1	1	1419	A
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1460	U
1	1	1468	U
1	1	1476	U
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1494	A
1	1	1503	A
1	1	1504	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1532	A
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U

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Mol	Chain	Res	Type
1	1	1580	A
1	1	1583	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1608	A
1	1	1618	6MZ
1	1	1634	A
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1756	G
1	1	1764	C
1	1	1773	A
1	1	1782	U
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1802	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1865	U
1	1	1868	C
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1896	G

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Mol	Chain	Res	Type
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1914	C
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A
1	1	1938	A
1	1	1955	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2030	6MZ
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2072	C
1	1	2093	G
1	1	2095	A
1	1	2100	G
1	1	2102	G
1	1	2107	G
1	1	2110	G
1	1	2112	G

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Mol	Chain	Res	Type
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2121	G
1	1	2122	U
1	1	2125	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2140	G
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2151	U
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2178	C
1	1	2183	A
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2211	A
1	1	2225	A
1	1	2229	U
1	1	2238	G
1	1	2239	G

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Mol	Chain	Res	Type
1	1	2243	U
1	1	2250	G
1	1	2278	A
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2305	U
1	1	2309	A
1	1	2319	G
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2426	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G
1	1	2476	A
1	1	2478	A
1	1	2480	C

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Mol	Chain	Res	Type
1	1	2491	U
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2586	U
1	1	2602	A
1	1	2609	U
1	1	2613	U
1	1	2629	U
1	1	2646	C
1	1	2663	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2725	A
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2757	A
1	1	2765	A
1	1	2777	G
1	1	2778	A
1	1	2791	G
1	1	2793	C

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Mol	Chain	Res	Type
1	1	2794	C
1	1	2796	U
1	1	2797	U
1	1	2799	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2825	G
1	1	2833	U
1	1	2835	A
1	1	2836	U
1	1	2861	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2898	U
1	1	2903	U
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	66	A
2	2	68	G
2	2	69	G
2	2	70	U
2	2	71	A
2	2	72	A

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Mol	Chain	Res	Type
2	2	73	C
2	2	74	A
2	2	75	G
2	2	76	G
2	2	81	A
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	92	U
2	2	120	A
2	2	121	U
2	2	130	A
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A
2	2	160	A
2	2	163	C
2	2	164	G
2	2	177	G
2	2	181	A
2	2	182	A
2	2	197	A
2	2	204	G
2	2	210	C
2	2	211	G
2	2	212	G
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	266	G
2	2	267	C
2	2	279	A
2	2	289	G
2	2	306	A
2	2	319	G
2	2	321	A
2	2	328	C
2	2	332	G

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Mol	Chain	Res	Type
2	2	347	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	372	C
2	2	384	G
2	2	392	C
2	2	398	U
2	2	406	G
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	436	C
2	2	439	U
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	476	U
2	2	478	A
2	2	479	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	496	A
2	2	499	A
2	2	510	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	519	C
2	2	521	G
2	2	527	G7M
2	2	531	U
2	2	532	A

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Mol	Chain	Res	Type
2	2	533	A
2	2	547	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	633	G
2	2	650	G
2	2	653	U
2	2	660	C
2	2	665	A
2	2	700	G
2	2	701	U
2	2	702	A
2	2	703	G
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	753	A
2	2	755	G
2	2	777	A
2	2	787	A
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
2	2	821	G
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	843	U
2	2	844	G
2	2	845	A
2	2	846	G

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Mol	Chain	Res	Type
2	2	884	U
2	2	885	G
2	2	887	G
2	2	914	A
2	2	934	C
2	2	935	A
2	2	960	U
2	2	965	U
2	2	966	2MG
2	2	969	A
2	2	971	G
2	2	972	C
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	982	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1004	A
2	2	1008	U
2	2	1009	U
2	2	1019	A
2	2	1022	A
2	2	1025	U
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1034	G
2	2	1043	G
2	2	1044	A
2	2	1046	A
2	2	1065	U
2	2	1085	U
2	2	1089	G
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1104	G

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Mol	Chain	Res	Type
2	2	1108	G
2	2	1124	G
2	2	1125	U
2	2	1132	C
2	2	1133	G
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1145	A
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1212	U
2	2	1213	A
2	2	1215	G
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1277	C
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G

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Mol	Chain	Res	Type
2	2	1299	A
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1336	C
2	2	1340	A
2	2	1346	A
2	2	1353	G
2	2	1363	A
2	2	1370	G
2	2	1379	G
2	2	1381	U
2	2	1419	G
2	2	1441	A
2	2	1446	A
2	2	1487	G
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1519	MA6
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	13	G
3	3	24	G
3	3	31	C
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A

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Mol	Chain	Res	Type
3	3	109	A
4	4	18	C
4	4	19	U
5	5	8	4SU
5	5	15	C
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	20	H2U
5	5	21	A
5	5	30	G
5	5	43	A
5	5	47	U
5	5	48	C
5	5	49	G
5	5	55	PSU
5	5	58	A
5	5	74	C
5	5	76	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	613	A
1	1	784	G
1	1	894	U
1	1	1379	U
1	1	2146	C
1	1	2189	U
1	1	2425	A
1	1	2756	U
2	2	516	PSU
2	2	1109	C
2	2	1145	A
5	5	17	U

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

40 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$
1	5MU	1	747	1	19,22,23	4.61	7 (36%)	27,32,35	3.76	10 (37%)
2	2MG	2	1207	2	23,26,27	2.93	7 (30%)	33,38,41	2.23	11 (33%)
2	MA6	2	1519	2	23,26,27	1.57	4 (17%)	33,38,41	2.73	13 (39%)
1	PSU	1	2457	1	18,21,22	1.09	3 (16%)	21,30,33	2.19	5 (23%)
2	2MG	2	966	2	23,26,27	2.95	7 (30%)	33,38,41	2.43	9 (27%)
1	PSU	1	2504	56,1	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
1	5MC	1	1962	1	19,22,23	3.71	8 (42%)	26,32,35	1.09	2 (7%)
5	5MU	5	54	5	19,22,23	4.76	7 (36%)	27,32,35	3.60	9 (33%)
1	3TD	1	1915	56,1	19,22,23	4.38	5 (26%)	23,32,35	1.89	4 (17%)
1	OMG	1	2251	5,1	23,26,27	2.35	8 (34%)	32,38,41	1.89	8 (25%)
2	G7M	2	527	2	23,26,27	3.60	12 (52%)	34,39,42	1.66	7 (20%)
5	PSU	5	55	5	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
6	FME	A	79	6	8,9,10	0.69	0	8,9,11	1.29	1 (12%)
1	PSU	1	2580	1	18,21,22	1.09	3 (16%)	21,30,33	1.96	5 (23%)
2	PSU	2	516	56,2	18,21,22	1.36	2 (11%)	21,30,33	2.10	5 (23%)
2	UR3	2	1498	2	19,22,23	2.57	7 (36%)	26,32,35	1.54	2 (7%)
1	2MG	1	1835	1	23,26,27	2.85	7 (30%)	33,38,41	2.40	9 (27%)
2	5MC	2	1407	2	19,22,23	3.78	8 (42%)	26,32,35	1.02	3 (11%)
1	PSU	1	955	56,1	18,21,22	1.09	2 (11%)	21,30,33	1.91	4 (19%)
1	OMU	1	2552	1	19,22,23	2.78	8 (42%)	25,31,34	1.95	5 (20%)
2	MA6	2	1518	2	23,26,27	1.59	4 (17%)	33,38,41	2.81	12 (36%)
1	PSU	1	1917	1	18,21,22	1.10	1 (5%)	21,30,33	1.84	4 (19%)
1	OMC	1	2498	56,1	19,22,23	2.71	7 (36%)	25,31,34	1.06	1 (4%)
1	6MZ	1	2030	1	22,25,26	2.92	6 (27%)	29,36,39	4.61	14 (48%)
1	G7M	1	2069	1	23,26,27	2.57	7 (30%)	34,39,42	2.43	10 (29%)
1	5MU	1	1939	56,1	19,22,23	4.61	7 (36%)	27,32,35	3.82	10 (37%)
1	2MG	1	2445	1	23,26,27	2.86	9 (39%)	33,38,41	2.40	11 (33%)
1	PSU	1	2605	1	18,21,22	1.04	2 (11%)	21,30,33	1.93	4 (19%)
2	2MG	2	1516	2	23,26,27	2.90	8 (34%)	33,38,41	2.35	11 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	4OC	5	32	5	20,23,24	2.96	8 (40%)	25,32,35	0.93	0
5	4SU	5	8	5	18,21,22	3.72	8 (44%)	25,30,33	2.32	7 (28%)
2	5MC	2	967	2	19,22,23	3.79	8 (42%)	26,32,35	1.06	2 (7%)
5	H2U	5	20	5	18,21,22	3.21	5 (27%)	19,30,33	1.40	3 (15%)
46	0TD	q	89	46	8,9,10	1.91	1 (12%)	6,11,13	1.07	0
2	4OC	2	1402	2	20,23,24	2.93	8 (40%)	25,32,35	0.96	2 (8%)
1	2MA	1	2503	56,1	22,25,26	3.64	10 (45%)	32,37,40	2.27	8 (25%)
1	PSU	1	746	56,1	18,21,22	1.06	2 (11%)	21,30,33	1.90	4 (19%)
1	PSU	1	1911	1	18,21,22	1.09	2 (11%)	21,30,33	1.91	4 (19%)
1	1MG	1	745	1	23,26,27	2.75	7 (30%)	33,39,42	2.03	8 (24%)
1	6MZ	1	1618	1	22,25,26	2.88	6 (27%)	29,36,39	4.37	13 (44%)

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
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	0/9/27/28	0/3/3/3
2	MA6	2	1519	2	-	3/11/29/30	0/3/3/3
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
2	2MG	2	966	2	-	2/9/27/28	0/3/3/3
1	PSU	1	2504	56,1	-	2/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
5	5MU	5	54	5	-	0/7/25/26	0/2/2/2
1	3TD	1	1915	56,1	-	2/7/25/26	0/2/2/2
1	OMG	1	2251	5,1	-	0/9/27/28	0/3/3/3
2	G7M	2	527	2	-	3/7/25/26	0/3/3/3
5	PSU	5	55	5	-	2/7/25/26	0/2/2/2
6	FME	A	79	6	-	2/7/9/11	-
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
2	PSU	2	516	56,2	-	2/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/9/27/28	0/3/3/3
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	PSU	1	955	56,1	-	0/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MA6	2	1518	2	-	0/11/29/30	0/3/3/3
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	56,1	-	1/9/27/28	0/2/2/2
1	6MZ	1	2030	1	-	2/9/27/28	0/3/3/3
1	G7M	1	2069	1	-	1/7/25/26	0/3/3/3
1	5MU	1	1939	56,1	-	0/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
5	4OC	5	32	5	-	0/9/29/30	0/2/2/2
5	4SU	5	8	5	-	3/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
5	H2U	5	20	5	-	4/7/38/39	0/2/2/2
46	0TD	q	89	46	-	2/7/12/14	-
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
1	2MA	1	2503	56,1	-	2/7/25/26	0/3/3/3
1	PSU	1	746	56,1	-	1/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/7/25/26	0/3/3/3
1	6MZ	1	1618	1	-	2/9/27/28	0/3/3/3

All (223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	13.69	1.50	1.35
1	1	1618	6MZ	C6-N6	11.33	1.47	1.34
1	1	2030	6MZ	C6-N6	11.01	1.46	1.34
1	1	2503	2MA	C4-N3	10.95	1.48	1.34
5	5	54	5MU	C2-N1	10.87	1.55	1.38
2	2	527	G7M	C8-N7	10.49	1.51	1.33
1	1	747	5MU	C2-N1	10.25	1.54	1.38
5	5	54	5MU	C6-N1	10.20	1.55	1.38
5	5	20	H2U	C2-N1	10.12	1.49	1.35
1	1	1915	3TD	C2-N1	9.96	1.49	1.37
1	1	1939	5MU	C2-N1	9.94	1.54	1.38
5	5	54	5MU	C4-C5	9.84	1.60	1.44
1	1	1939	5MU	C6-N1	9.84	1.54	1.38
1	1	747	5MU	C6-N1	9.82	1.54	1.38
1	1	1939	5MU	C4-C5	9.37	1.60	1.44
2	2	1407	5MC	C6-C5	9.15	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	747	5MU	C4-C5	9.03	1.59	1.44
2	2	967	5MC	C6-C5	8.97	1.49	1.34
1	1	1962	5MC	C6-C5	8.96	1.49	1.34
1	1	747	5MU	C4-N3	-8.45	1.23	1.38
1	1	1939	5MU	C4-N3	-8.33	1.23	1.38
5	5	8	4SU	C2-N1	8.17	1.51	1.38
5	5	54	5MU	C4-N3	-7.94	1.24	1.38
5	5	8	4SU	C4-N3	7.88	1.45	1.37
2	2	1207	2MG	C2-N3	7.26	1.45	1.32
2	2	966	2MG	C2-N3	7.24	1.45	1.32
1	1	745	1MG	C2-N2	7.18	1.46	1.34
1	1	1962	5MC	C4-N3	7.14	1.45	1.34
2	2	967	5MC	C4-N3	7.09	1.45	1.34
2	2	1516	2MG	C2-N3	6.93	1.45	1.32
5	5	32	4OC	C4-N3	6.88	1.44	1.32
1	1	1835	2MG	C2-N3	6.85	1.45	1.32
2	2	1407	5MC	C4-N3	6.83	1.45	1.34
1	1	2445	2MG	C2-N3	6.82	1.45	1.32
2	2	1402	4OC	C4-N3	6.80	1.44	1.32
2	2	966	2MG	C4-N3	6.78	1.49	1.34
1	1	2503	2MA	C2-N3	6.77	1.45	1.34
5	5	20	H2U	C2-N3	6.68	1.49	1.38
2	2	966	2MG	C2-N2	6.60	1.47	1.33
1	1	745	1MG	C2-N3	6.52	1.43	1.33
2	2	1207	2MG	C4-N3	6.47	1.49	1.34
2	2	1207	2MG	C2-N2	6.40	1.46	1.33
1	1	2069	G7M	C4-N3	6.39	1.48	1.34
2	2	1516	2MG	C2-N2	6.37	1.46	1.33
1	1	2552	OMU	C2-N3	6.36	1.49	1.38
2	2	1516	2MG	C4-N3	6.36	1.48	1.34
1	1	2445	2MG	C4-N3	6.35	1.48	1.34
1	1	1835	2MG	C4-N3	6.34	1.48	1.34
1	1	745	1MG	C4-N3	6.27	1.48	1.34
2	2	1498	UR3	C2-N1	6.25	1.47	1.38
2	2	967	5MC	C2-N3	6.20	1.48	1.36
1	1	1835	2MG	C2-N2	6.15	1.46	1.33
2	2	1407	5MC	C2-N3	6.13	1.48	1.36
1	1	2445	2MG	C2-N2	6.07	1.46	1.33
1	1	2251	OMG	C4-N3	6.06	1.48	1.34
2	2	1498	UR3	C6-C5	5.98	1.48	1.35
1	1	1915	3TD	C6-N1	5.92	1.46	1.36
1	1	1962	5MC	C2-N3	5.89	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	32	4OC	C2-N3	5.89	1.48	1.36
1	1	2498	OMC	C6-C5	5.89	1.48	1.35
5	5	8	4SU	C6-C5	5.88	1.48	1.35
2	2	1402	4OC	C6-C5	5.86	1.48	1.35
1	1	2552	OMU	C2-N1	5.81	1.47	1.38
5	5	32	4OC	C6-C5	5.77	1.48	1.35
2	2	967	5MC	C5-C4	5.76	1.48	1.44
2	2	527	G7M	C2-N3	5.75	1.47	1.33
2	2	1402	4OC	C2-N3	5.73	1.47	1.36
5	5	8	4SU	C2-N3	5.69	1.47	1.38
1	1	2498	OMC	C2-N3	5.68	1.47	1.36
5	5	54	5MU	C6-C5	5.67	1.43	1.34
1	1	2069	G7M	C5-N7	-5.63	1.32	1.39
5	5	8	4SU	C4-S4	-5.63	1.58	1.68
1	1	2503	2MA	C2-N1	5.56	1.43	1.34
2	2	527	G7M	C8-N9	5.51	1.50	1.35
2	2	527	G7M	C4-N3	5.47	1.46	1.34
1	1	747	5MU	C6-C5	5.43	1.43	1.34
1	1	2503	2MA	C6-N1	5.40	1.42	1.35
1	1	1939	5MU	C6-C5	5.39	1.43	1.34
1	1	2552	OMU	C6-C5	5.39	1.47	1.35
1	1	1962	5MC	C5-C4	5.31	1.48	1.44
2	2	1407	5MC	C5-C4	5.28	1.48	1.44
1	1	2251	OMG	C2-N3	5.04	1.45	1.33
1	1	2069	G7M	C2-N3	5.03	1.45	1.33
1	1	1915	3TD	C2-N3	5.02	1.49	1.38
1	1	2498	OMC	C4-N3	5.01	1.44	1.34
5	5	20	H2U	C4-N3	4.88	1.45	1.37
2	2	967	5MC	C4-N4	4.85	1.46	1.34
1	1	1962	5MC	C4-N4	4.81	1.46	1.34
2	2	1407	5MC	C4-N4	4.80	1.46	1.34
2	2	527	G7M	C5-N7	4.73	1.44	1.39
2	2	527	G7M	C2-N2	4.72	1.45	1.34
2	2	1407	5MC	C6-N1	4.52	1.45	1.38
1	1	2251	OMG	C2-N2	4.50	1.44	1.34
2	2	1498	UR3	C2-N3	4.50	1.47	1.39
2	2	1516	2MG	C2-N1	4.32	1.43	1.36
2	2	967	5MC	C6-N1	4.26	1.45	1.38
2	2	1207	2MG	C2-N1	4.21	1.43	1.36
1	1	2069	G7M	C2-N2	4.18	1.44	1.34
2	2	1407	5MC	C2-N1	4.14	1.48	1.40
1	1	2030	6MZ	C5-C4	-4.13	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	966	2MG	C2-N1	4.12	1.43	1.36
1	1	2503	2MA	C5-C6	4.04	1.52	1.41
2	2	967	5MC	C2-N1	4.02	1.48	1.40
1	1	2030	6MZ	C8-N9	-4.00	1.30	1.37
1	1	1835	2MG	C2-N1	3.98	1.43	1.36
1	1	1962	5MC	C6-N1	3.97	1.44	1.38
1	1	2445	2MG	C2-N1	3.91	1.42	1.36
5	5	32	4OC	C4-N4	3.91	1.44	1.36
5	5	32	4OC	C2-N1	3.85	1.48	1.40
1	1	2445	2MG	O6-C6	-3.81	1.16	1.23
2	2	1402	4OC	C4-N4	3.79	1.43	1.36
1	1	1962	5MC	C2-N1	3.73	1.47	1.40
1	1	2445	2MG	C5-N7	-3.71	1.31	1.39
1	1	2503	2MA	C6-N6	-3.70	1.24	1.34
1	1	1835	2MG	C5-N7	-3.69	1.31	1.39
2	2	1518	MA6	C6-N6	3.69	1.47	1.36
1	1	2503	2MA	C5-N7	-3.68	1.32	1.39
2	2	516	PSU	C6-C5	3.66	1.39	1.35
46	q	89	0TD	CB-CA	-3.63	1.53	1.54
1	1	2552	OMU	C4-N3	3.62	1.44	1.38
1	1	1835	2MG	O6-C6	-3.61	1.16	1.23
1	1	2069	G7M	C5-C6	3.61	1.53	1.43
2	2	1402	4OC	C2-N1	3.60	1.47	1.40
1	1	1618	6MZ	C5-C4	-3.58	1.32	1.39
2	2	966	2MG	C5-N7	-3.57	1.31	1.39
2	2	1516	2MG	C5-N7	-3.56	1.31	1.39
2	2	1207	2MG	C5-N7	-3.54	1.32	1.39
2	2	966	2MG	O6-C6	-3.53	1.16	1.23
2	2	1519	MA6	C6-N6	3.53	1.46	1.36
5	5	55	PSU	C6-C5	3.53	1.39	1.35
2	2	1207	2MG	O6-C6	-3.52	1.16	1.23
2	2	1518	MA6	C8-N9	-3.51	1.31	1.37
1	1	2498	OMC	C4-N4	3.49	1.42	1.33
1	1	1618	6MZ	C8-N9	-3.48	1.31	1.37
1	1	2498	OMC	C2-N1	3.48	1.47	1.40
2	2	1516	2MG	O6-C6	-3.48	1.17	1.23
1	1	745	1MG	C5-N7	-3.48	1.32	1.39
2	2	527	G7M	C2-N1	3.46	1.46	1.37
1	1	1962	5MC	O2-C2	-3.45	1.17	1.23
1	1	1917	PSU	C6-C5	3.44	1.39	1.35
2	2	1407	5MC	O2-C2	-3.43	1.17	1.23
2	2	527	G7M	C5-C6	3.37	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1519	MA6	C8-N9	-3.37	1.31	1.37
1	1	2030	6MZ	C4-N9	-3.37	1.30	1.37
5	5	32	4OC	C5-C4	3.36	1.48	1.41
1	1	2251	OMG	C5-N7	-3.33	1.32	1.39
2	2	1402	4OC	C5-C4	3.32	1.48	1.41
5	5	8	4SU	C5-C4	3.25	1.46	1.42
2	2	1518	MA6	C5-N7	-3.24	1.33	1.39
2	2	967	5MC	O2-C2	-3.24	1.17	1.23
1	1	1911	PSU	C6-C5	3.23	1.38	1.35
1	1	2504	PSU	C6-C5	3.19	1.38	1.35
2	2	1519	MA6	C5-N7	-3.17	1.33	1.39
2	2	1519	MA6	C5-C4	-3.17	1.33	1.39
1	1	2498	OMC	O2-C2	-3.17	1.17	1.23
1	1	2552	OMU	O4-C4	-3.12	1.18	1.24
2	2	1518	MA6	C5-C4	-3.11	1.33	1.39
2	2	1402	4OC	O2-C2	-3.09	1.18	1.23
1	1	2498	OMC	C6-N1	3.08	1.45	1.38
1	1	1939	5MU	O2-C2	-3.08	1.17	1.23
1	1	1939	5MU	O4-C4	-3.06	1.17	1.23
1	1	2552	OMU	O2-C2	-3.02	1.17	1.23
1	1	747	5MU	O4-C4	-2.99	1.17	1.23
1	1	955	PSU	C6-C5	2.94	1.38	1.35
1	1	747	5MU	O2-C2	-2.94	1.17	1.23
1	1	745	1MG	C2-N1	2.92	1.42	1.37
1	1	2251	OMG	O6-C6	-2.91	1.18	1.23
5	5	32	4OC	O2-C2	-2.89	1.18	1.23
1	1	1915	3TD	C4-N3	2.86	1.46	1.40
1	1	2069	G7M	O6-C6	-2.85	1.18	1.23
5	5	32	4OC	C6-N1	2.85	1.44	1.38
1	1	2605	PSU	C6-C5	2.80	1.38	1.35
2	2	1402	4OC	C6-N1	2.80	1.44	1.38
2	2	527	G7M	C6-N1	2.77	1.44	1.38
1	1	1618	6MZ	C4-N9	-2.77	1.31	1.37
1	1	2030	6MZ	C6-N1	-2.76	1.30	1.35
5	5	54	5MU	O4-C4	-2.75	1.18	1.23
2	2	527	G7M	O6-C6	-2.70	1.18	1.23
1	1	746	PSU	C6-C5	2.68	1.38	1.35
1	1	2457	PSU	C6-C5	2.67	1.38	1.35
1	1	2503	2MA	C4-N9	-2.66	1.32	1.37
1	1	2580	PSU	C6-C5	2.63	1.38	1.35
2	2	1498	UR3	C6-N1	2.62	1.44	1.38
5	5	8	4SU	O2-C2	-2.58	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1498	UR3	O4-C4	-2.54	1.18	1.23
5	5	54	5MU	O2-C2	-2.52	1.18	1.23
1	1	2503	2MA	C8-N9	-2.45	1.33	1.37
1	1	1618	6MZ	C6-N1	-2.43	1.31	1.35
1	1	2251	OMG	C4-N9	-2.42	1.31	1.38
2	2	1498	UR3	O2-C2	-2.41	1.18	1.22
5	5	20	H2U	O2-C2	-2.40	1.18	1.23
1	1	2552	OMU	C6-N1	2.35	1.43	1.38
1	1	2251	OMG	C2-N1	2.33	1.43	1.37
2	2	516	PSU	C4-N3	-2.33	1.34	1.38
5	5	20	H2U	O4-C4	-2.33	1.18	1.23
1	1	746	PSU	C4-C5	-2.28	1.38	1.44
1	1	2580	PSU	O4'-C1'	-2.25	1.40	1.43
1	1	2069	G7M	C2-N1	2.24	1.43	1.37
1	1	745	1MG	C5-C6	2.23	1.51	1.45
2	2	527	G7M	C4-N9	2.23	1.43	1.38
2	2	1516	2MG	C4-N9	-2.21	1.32	1.38
1	1	2445	2MG	C8-N9	-2.20	1.32	1.37
1	1	2457	PSU	C4-C5	-2.19	1.38	1.44
1	1	2030	6MZ	C5-C6	-2.18	1.36	1.41
2	2	1516	2MG	C5-C6	2.18	1.52	1.44
2	2	1207	2MG	C5-C6	2.17	1.52	1.44
1	1	2445	2MG	C5-C6	2.16	1.52	1.44
2	2	966	2MG	C5-C6	2.14	1.52	1.44
1	1	745	1MG	C4-N9	-2.13	1.32	1.38
1	1	2251	OMG	C5-C6	2.12	1.52	1.44
1	1	1618	6MZ	C5-C6	-2.11	1.36	1.41
1	1	1835	2MG	C5-C6	2.10	1.52	1.44
2	2	527	G7M	C5-C4	2.10	1.43	1.38
1	1	1911	PSU	C4-C5	-2.07	1.38	1.44
1	1	2445	2MG	C4-N9	-2.07	1.32	1.38
1	1	2605	PSU	C4-C5	-2.06	1.38	1.44
1	1	2580	PSU	C4-C5	-2.06	1.38	1.44
1	1	2552	OMU	C5-C4	2.06	1.48	1.43
1	1	955	PSU	C4-C5	-2.05	1.38	1.44
2	2	1498	UR3	C5-C4	2.04	1.49	1.43
1	1	2457	PSU	O4'-C1'	-2.03	1.41	1.43
1	1	2503	2MA	C5-C4	-2.01	1.35	1.39
5	5	8	4SU	C6-N1	2.00	1.42	1.38

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2030	6MZ	C4-N9-C8	14.71	121.18	105.74
1	1	1618	6MZ	C4-N9-C8	13.41	119.81	105.74
1	1	1939	5MU	C5-C4-N3	12.52	126.20	115.32
1	1	747	5MU	C5-C4-N3	12.27	125.99	115.32
5	5	54	5MU	C5-C4-N3	11.94	125.70	115.32
1	1	2030	6MZ	N9-C8-N7	-11.00	98.34	113.94
1	1	1939	5MU	C5-C6-N1	-10.57	111.83	123.31
1	1	747	5MU	C5-C6-N1	-10.49	111.91	123.31
1	1	1618	6MZ	N9-C8-N7	-10.08	99.64	113.94
5	5	54	5MU	C5-C6-N1	-9.53	112.96	123.31
1	1	1618	6MZ	C5-C6-N1	8.65	127.44	118.15
2	2	1518	MA6	N1-C6-N6	-8.60	106.38	116.86
1	1	2030	6MZ	C5-C6-N1	8.40	127.17	118.15
2	2	1519	MA6	N1-C6-N6	-8.36	106.67	116.86
2	2	966	2MG	C2-N3-C4	7.33	121.17	112.00
5	5	8	4SU	C4-N3-C2	-7.03	120.58	127.31
1	1	2503	2MA	C5-C4-N3	-6.95	119.86	127.18
1	1	1835	2MG	C2-N3-C4	6.73	120.42	112.00
1	1	2445	2MG	C2-N3-C4	6.58	120.23	112.00
2	2	966	2MG	C5-C4-N3	-6.56	117.95	128.39
1	1	2069	G7M	CN7-N7-C5	6.49	134.89	126.80
1	1	1618	6MZ	N3-C4-N9	6.47	138.16	127.17
2	2	1516	2MG	C2-N3-C4	6.20	119.75	112.00
2	2	1518	MA6	N1-C2-N3	-6.19	119.21	128.58
2	2	1207	2MG	C2-N3-C4	6.16	119.71	112.00
2	2	1519	MA6	N1-C2-N3	-6.08	119.37	128.58
1	1	2552	OMU	C4-N3-C2	-6.07	119.08	126.61
1	1	2030	6MZ	N3-C4-N9	5.95	137.29	127.17
1	1	1835	2MG	C5-C4-N3	-5.82	119.13	128.39
1	1	2030	6MZ	N1-C2-N3	-5.76	119.86	128.58
1	1	2445	2MG	C5-C4-N3	-5.74	119.25	128.39
2	2	1518	MA6	C5-C6-N6	5.72	134.39	125.33
2	2	516	PSU	N1-C2-N3	5.67	121.15	115.17
1	1	1618	6MZ	N1-C2-N3	-5.62	120.08	128.58
1	1	747	5MU	O4-C4-C5	-5.61	118.50	124.92
1	1	2457	PSU	N1-C2-N3	5.58	121.06	115.17
1	1	1939	5MU	O4-C4-C5	-5.51	118.61	124.92
2	2	1207	2MG	C5-C4-N3	-5.49	119.66	128.39
5	5	54	5MU	O4-C4-C5	-5.47	118.66	124.92
2	2	1498	UR3	C4-N3-C2	-5.44	120.20	124.58
1	1	2503	2MA	N3-C4-N9	5.42	133.87	126.99
1	1	1939	5MU	C4-N3-C2	-5.41	120.25	127.34
1	1	1915	3TD	N1-C2-N3	5.37	120.04	116.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2457	PSU	C4-N3-C2	-5.37	118.98	126.37
2	2	1519	MA6	C5-C6-N6	5.28	133.69	125.33
1	1	2030	6MZ	C9-N6-C6	-5.24	117.99	122.85
1	1	745	1MG	C5-C4-N3	-5.22	120.08	128.39
5	5	8	4SU	C5-C4-N3	5.18	119.57	114.75
1	1	747	5MU	C4-N3-C2	-5.15	120.59	127.34
1	1	2030	6MZ	C5-C4-N9	-5.14	100.21	105.81
2	2	1516	2MG	C5-C4-N3	-5.14	120.21	128.39
1	1	746	PSU	C4-N3-C2	-5.11	119.34	126.37
1	1	2605	PSU	C4-N3-C2	-5.10	119.34	126.37
1	1	2251	OMG	C5-C4-N3	-5.10	120.27	128.39
1	1	2069	G7M	CN7-N7-C8	-5.10	117.07	124.79
1	1	2069	G7M	C2-N3-C4	5.09	121.06	112.30
1	1	2580	PSU	N1-C2-N3	5.06	120.51	115.17
1	1	1618	6MZ	C5-C4-N9	-5.02	100.34	105.81
1	1	1911	PSU	C4-N3-C2	-5.01	119.46	126.37
1	1	1835	2MG	C2-N1-C6	-5.00	118.51	124.55
1	1	745	1MG	C1'-N9-C4	-5.00	111.73	126.49
1	1	2503	2MA	N9-C8-N7	-4.94	106.93	113.94
1	1	2445	2MG	C2-N1-C6	-4.93	118.58	124.55
1	1	2069	G7M	C5-C4-N3	-4.91	118.87	128.15
1	1	955	PSU	N1-C2-N3	4.91	120.34	115.17
1	1	2580	PSU	C4-N3-C2	-4.90	119.62	126.37
1	1	2504	PSU	N1-C2-N3	4.87	120.31	115.17
1	1	955	PSU	C4-N3-C2	-4.87	119.67	126.37
2	2	966	2MG	C2-N1-C6	-4.85	118.68	124.55
1	1	2605	PSU	N1-C2-N3	4.82	120.26	115.17
1	1	1911	PSU	N1-C2-N3	4.79	120.22	115.17
1	1	1917	PSU	N1-C2-N3	4.78	120.21	115.17
1	1	1917	PSU	C4-N3-C2	-4.75	119.83	126.37
5	5	55	PSU	N1-C2-N3	4.74	120.17	115.17
1	1	1939	5MU	N3-C2-N1	4.69	120.99	114.89
2	2	966	2MG	N9-C4-N3	4.66	135.28	125.95
1	1	746	PSU	N1-C2-N3	4.64	120.06	115.17
5	5	54	5MU	C4-N3-C2	-4.62	121.28	127.34
2	2	1518	MA6	N9-C8-N7	-4.62	107.38	113.94
5	5	55	PSU	C4-N3-C2	-4.61	120.02	126.37
1	1	747	5MU	N3-C2-N1	4.58	120.85	114.89
2	2	1207	2MG	C2-N1-C6	-4.56	119.03	124.55
2	2	527	G7M	C2-N3-C4	4.54	120.12	112.30
1	1	2030	6MZ	C5-N7-C8	4.53	110.56	103.45
1	1	745	1MG	C1'-N9-C8	4.49	139.47	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2504	PSU	C4-N3-C2	-4.47	120.22	126.37
1	1	2251	OMG	C2-N3-C4	4.45	119.96	112.30
2	2	1516	2MG	N1-C2-N2	4.42	121.07	116.56
2	2	1519	MA6	N9-C8-N7	-4.38	107.72	113.94
2	2	1516	2MG	C2-N1-C6	-4.38	119.25	124.55
1	1	1618	6MZ	C9-N6-C6	-4.37	118.80	122.85
1	1	1915	3TD	C1'-C5-C4	4.36	124.22	117.61
2	2	1519	MA6	C5-C4-N3	-4.29	120.80	126.72
2	2	1518	MA6	C5-C4-N3	-4.25	120.87	126.72
5	5	54	5MU	N3-C2-N1	4.24	120.41	114.89
1	1	2069	G7M	C5-C6-N1	4.22	120.56	111.84
1	1	2552	OMU	N3-C2-N1	4.20	120.36	114.89
1	1	1618	6MZ	C1'-N9-C8	-4.16	117.87	127.09
1	1	1915	3TD	C4-N3-C2	-4.14	120.23	124.61
1	1	1618	6MZ	C5-N7-C8	4.10	109.90	103.45
5	5	8	4SU	C1'-N1-C2	4.09	124.94	117.59
2	2	516	PSU	O3'-C3'-C4'	4.08	122.80	111.08
1	1	2503	2MA	C4-N9-C8	4.06	110.00	105.74
2	2	527	G7M	C5-C4-N3	-4.05	120.49	128.15
2	2	527	G7M	C5-C6-N1	3.94	119.98	111.84
1	1	1835	2MG	N1-C2-N2	3.93	120.57	116.56
1	1	2445	2MG	N1-C2-N2	3.89	120.53	116.56
2	2	1518	MA6	C2-N1-C6	3.87	121.29	111.83
1	1	2552	OMU	C5-C4-N3	3.83	120.17	114.80
1	1	1835	2MG	N9-C4-N3	3.83	133.60	125.95
1	1	2069	G7M	N9-C4-N3	3.82	133.59	125.95
1	1	1618	6MZ	C5-C4-N3	-3.79	121.49	126.72
1	1	2445	2MG	N9-C4-N3	3.73	133.40	125.95
5	5	54	5MU	C5M-C5-C4	3.72	122.75	118.78
2	2	1519	MA6	C2-N1-C6	3.69	120.84	111.83
2	2	516	PSU	C4-N3-C2	-3.66	121.33	126.37
1	1	2030	6MZ	C1'-N9-C8	-3.64	119.02	127.09
2	2	1498	UR3	C5-C4-N3	3.64	119.83	115.04
5	5	54	5MU	C5M-C5-C6	-3.62	117.95	122.85
5	5	8	4SU	N3-C2-N1	3.62	119.61	114.89
1	1	1618	6MZ	C2-N3-C4	3.60	120.62	111.83
1	1	745	1MG	C2-N3-C4	3.55	119.97	111.98
2	2	1207	2MG	N9-C4-N3	3.52	133.00	125.95
2	2	967	5MC	C5-C6-N1	-3.49	119.52	123.31
5	5	20	H2U	N3-C2-N1	3.45	120.12	116.65
5	5	8	4SU	C5-C4-S4	-3.44	120.37	124.31
1	1	747	5MU	C5M-C5-C6	-3.42	118.22	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2069	G7M	C2-N1-C6	-3.41	118.93	125.11
2	2	1518	MA6	C4-C5-C6	3.39	119.42	115.91
1	1	2030	6MZ	C2-N3-C4	3.36	120.04	111.83
2	2	1518	MA6	C2-N3-C4	3.35	120.01	111.83
2	2	1519	MA6	C4-C5-C6	3.34	119.37	115.91
1	1	1962	5MC	C5-C6-N1	-3.34	119.69	123.31
2	2	1519	MA6	C2-N3-C4	3.34	119.98	111.83
1	1	1939	5MU	C5M-C5-C6	-3.33	118.34	122.85
1	1	2251	OMG	C2-N1-C6	-3.31	119.10	125.11
1	1	745	1MG	N9-C8-N7	-3.29	107.30	113.40
1	1	2251	OMG	N9-C8-N7	-3.29	107.31	113.40
1	1	2504	PSU	C6-N1-C2	-3.28	119.65	122.69
1	1	1835	2MG	CM2-N2-C2	-3.27	116.62	123.65
2	2	1518	MA6	C5-N7-C8	3.27	108.59	103.45
1	1	745	1MG	N9-C4-N3	3.26	132.47	125.95
2	2	516	PSU	O2-C2-N1	-3.24	119.45	122.79
1	1	2069	G7M	O6-C6-C5	-3.21	120.85	128.01
2	2	1516	2MG	C1'-N9-C4	-3.20	117.04	126.49
1	1	2030	6MZ	C6-C5-N7	3.17	135.89	132.43
2	2	966	2MG	N1-C2-N2	3.14	119.77	116.56
1	1	2457	PSU	O2-C2-N1	-3.11	119.58	122.79
1	1	2445	2MG	CM2-N2-C2	-3.09	117.01	123.65
1	1	2552	OMU	O4-C4-C5	-3.08	119.84	125.16
1	1	2030	6MZ	C5-C4-N3	-3.06	122.51	126.72
1	1	2251	OMG	N9-C4-N3	3.05	132.05	125.95
1	1	2552	OMU	O2-C2-N1	-3.04	118.84	122.80
1	1	746	PSU	O2-C2-N1	-3.03	119.66	122.79
2	2	1519	MA6	C5-N7-C8	3.02	108.20	103.45
1	1	2445	2MG	N9-C8-N7	-3.01	107.83	113.40
1	1	1939	5MU	O2-C2-N1	-3.00	118.89	122.80
5	5	55	PSU	O2-C2-N1	-3.00	119.69	122.79
5	5	20	H2U	C5-C6-N1	3.00	120.59	111.52
1	1	2504	PSU	O2-C2-N1	-2.98	119.72	122.79
1	1	2069	G7M	C1'-N9-C4	-2.95	117.78	126.49
2	2	1516	2MG	N9-C8-N7	-2.94	107.94	113.40
2	2	1207	2MG	N9-C8-N7	-2.94	107.94	113.40
1	1	2503	2MA	C5-N7-C8	2.94	108.07	103.45
1	1	1939	5MU	C5M-C5-C4	2.94	121.92	118.78
2	2	966	2MG	C5-C6-N1	2.92	120.69	113.25
2	2	1516	2MG	N9-C4-N3	2.92	131.80	125.95
2	2	1516	2MG	CM2-N2-C2	-2.92	117.37	123.65
1	1	2030	6MZ	C4-N9-C1'	-2.92	119.80	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1835	2MG	N9-C8-N7	-2.91	108.00	113.40
1	1	2030	6MZ	C4-C5-C6	-2.87	114.39	116.78
2	2	966	2MG	O6-C6-C5	-2.86	118.98	126.53
1	1	2503	2MA	N3-C2-N1	-2.86	120.73	125.77
1	1	1835	2MG	C5-C6-N1	2.85	120.52	113.25
2	2	1516	2MG	C1'-N9-C8	2.85	134.84	126.73
1	1	2445	2MG	C5-C6-N1	2.84	120.49	113.25
2	2	1207	2MG	N1-C2-N2	2.84	119.46	116.56
1	1	2580	PSU	O2-C2-N1	-2.82	119.88	122.79
2	2	527	G7M	C2-N1-C6	-2.81	120.01	125.11
1	1	747	5MU	C5M-C5-C4	2.81	121.78	118.78
2	2	1518	MA6	C4-N9-C8	2.81	108.69	105.74
1	1	2580	PSU	C6-N1-C2	-2.80	120.09	122.69
1	1	2251	OMG	C5-C6-N1	2.80	120.37	113.25
1	1	2498	OMC	O2-C2-N3	-2.78	117.95	122.33
1	1	1911	PSU	O2-C2-N1	-2.75	119.95	122.79
2	2	1518	MA6	C4-C5-N7	-2.74	107.45	110.58
5	5	20	H2U	C5-C4-N3	2.73	119.59	116.69
1	1	2457	PSU	C6-N1-C2	-2.70	120.19	122.69
5	5	55	PSU	C6-N1-C2	-2.69	120.20	122.69
1	1	1835	2MG	O6-C6-C5	-2.69	119.44	126.53
2	2	1207	2MG	C5-C6-N1	2.68	120.08	113.25
1	1	955	PSU	O2-C2-N1	-2.67	120.04	122.79
2	2	1516	2MG	C5-C6-N1	2.63	119.95	113.25
1	1	745	1MG	C5-C6-N1	2.63	119.88	115.02
1	1	1939	5MU	O4-C4-N3	-2.62	115.18	120.11
2	2	1207	2MG	C1'-N9-C4	-2.62	118.76	126.49
2	2	1519	MA6	C4-C5-N7	-2.61	107.59	110.58
2	2	527	G7M	O6-C6-C5	-2.60	122.20	128.01
1	1	2457	PSU	C6-C5-C4	2.58	119.92	118.17
2	2	1207	2MG	O6-C6-C5	-2.58	119.72	126.53
1	1	955	PSU	C6-N1-C2	-2.56	120.31	122.69
1	1	2251	OMG	O6-C6-C5	-2.55	119.81	126.53
1	1	2605	PSU	O2-C2-N1	-2.54	120.17	122.79
2	2	966	2MG	N9-C8-N7	-2.54	108.69	113.40
1	1	747	5MU	O2-C2-N1	-2.52	119.52	122.80
2	2	1519	MA6	C4-N9-C8	2.51	108.38	105.74
2	2	516	PSU	O4'-C4'-C3'	-2.51	100.17	105.15
2	2	1516	2MG	O6-C6-C5	-2.50	119.94	126.53
2	2	1407	5MC	C5-C6-N1	-2.49	120.61	123.31
1	1	1911	PSU	C6-N1-C2	-2.48	120.39	122.69
1	1	2445	2MG	C1'-N9-C4	-2.46	119.21	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2445	2MG	O6-C6-C5	-2.46	120.03	126.53
1	1	747	5MU	O4-C4-N3	-2.45	115.52	120.11
1	1	1917	PSU	C6-N1-C2	-2.43	120.44	122.69
2	2	527	G7M	N9-C8-N7	-2.41	106.62	112.48
1	1	2503	2MA	C6-C5-C4	2.40	120.46	117.18
1	1	747	5MU	C6-C5-C4	2.40	120.00	118.02
2	2	1518	MA6	N3-C4-N9	2.40	131.25	127.17
5	5	54	5MU	O4-C4-N3	-2.38	115.64	120.11
1	1	2503	2MA	N6-C6-N1	2.37	120.23	117.03
1	1	1917	PSU	O2-C2-N1	-2.36	120.35	122.79
5	5	8	4SU	O2-C2-N3	-2.34	117.18	121.49
1	1	1618	6MZ	C4-C5-C6	-2.33	114.84	116.78
2	2	1207	2MG	CM2-N2-C2	-2.31	118.67	123.65
2	2	1519	MA6	N3-C4-N9	2.30	131.08	127.17
1	1	2605	PSU	C6-N1-C2	-2.27	120.59	122.69
2	2	527	G7M	C5-C4-N9	2.26	110.71	105.88
1	1	2069	G7M	C1'-N9-C8	2.24	134.30	126.74
1	1	1618	6MZ	C6-C5-N7	2.23	134.86	132.43
1	1	745	1MG	C8-N7-C5	2.19	108.16	104.26
1	1	2251	OMG	C8-N7-C5	2.16	108.11	104.26
1	1	746	PSU	C6-N1-C2	-2.16	120.69	122.69
2	2	1207	2MG	C1'-N9-C8	2.15	132.84	126.73
2	2	1402	4OC	C6-C5-C4	2.14	119.58	117.00
5	5	54	5MU	O2-C2-N1	-2.11	120.05	122.80
2	2	1519	MA6	C5-C4-N9	2.11	108.11	105.81
1	1	2445	2MG	C8-N7-C5	2.11	108.01	104.26
6	A	79	FME	O1-CN-N	-2.10	119.89	125.32
1	1	1939	5MU	C6-C5-C4	2.09	119.74	118.02
1	1	2580	PSU	O4'-C1'-C2'	2.07	108.02	105.15
2	2	1407	5MC	C5-C4-N3	-2.07	119.63	121.75
2	2	1402	4OC	CM4-N4-C4	-2.05	118.44	122.45
1	1	1915	3TD	O4-C4-N3	-2.04	116.63	120.36
5	5	8	4SU	C1'-N1-C6	-2.04	116.42	120.78
2	2	966	2MG	N1-C2-N3	-2.03	120.25	123.68
1	1	1962	5MC	CM5-C5-C6	-2.03	120.11	122.85
2	2	1407	5MC	O2-C2-N3	-2.02	119.14	122.33
2	2	967	5MC	CM5-C5-C6	-2.02	120.12	122.85

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2504	PSU	O4'-C4'-C5'-O5'
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	1519	MA6	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C6
6	A	79	FME	O1-CN-N-CA
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
5	5	20	H2U	C3'-C4'-C5'-O5'
6	A	79	FME	CA-CB-CG-SD
1	1	1835	2MG	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
1	1	1835	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	1402	4OC	C3'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C2
46	q	89	0TD	CG-CB-SB-CSB
1	1	2503	2MA	O4'-C4'-C5'-O5'
46	q	89	0TD	SB-CB-CG-OD1
2	2	527	G7M	C4'-C5'-O5'-P
5	5	8	4SU	O4'-C1'-N1-C6
5	5	55	PSU	C3'-C4'-C5'-O5'
5	5	55	PSU	C4'-C5'-O5'-P
1	1	2498	OMC	O4'-C4'-C5'-O5'
1	1	2503	2MA	C3'-C4'-C5'-O5'
1	1	746	PSU	O4'-C1'-C5-C6
5	5	8	4SU	O4'-C1'-N1-C2
1	1	2069	G7M	O4'-C4'-C5'-O5'
5	5	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	747	5MU	1	0
1	1	1915	3TD	1	0
1	1	2030	6MZ	1	0
1	1	1939	5MU	1	0
5	5	32	4OC	1	0
5	5	8	4SU	1	0
46	q	89	0TD	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 438 ligands modelled in this entry, 438 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

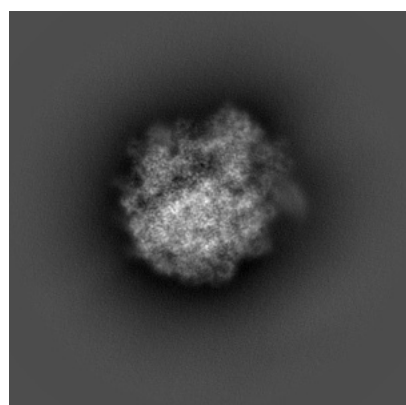
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20173. These allow visual inspection of the internal detail of the map and identification of artifacts.

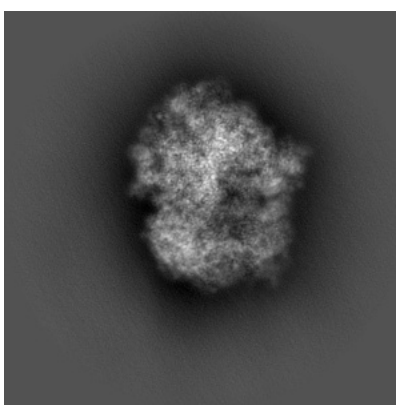
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

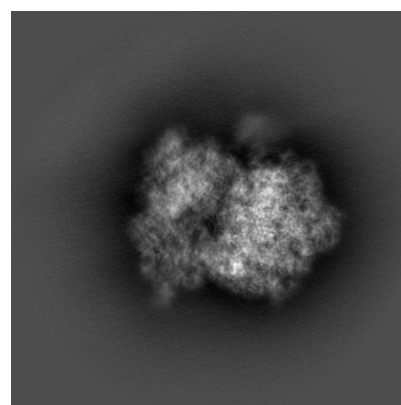
6.1.1 Primary map



X



Y

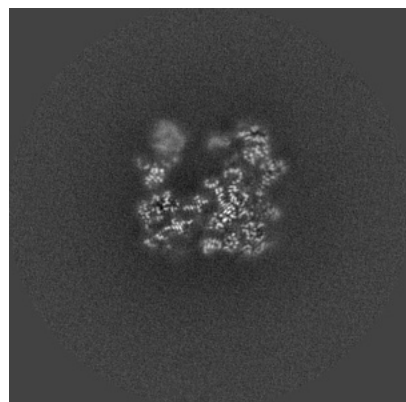


Z

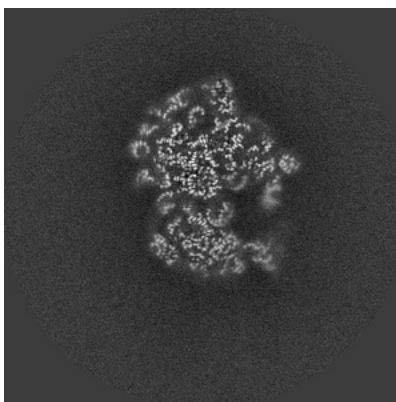
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

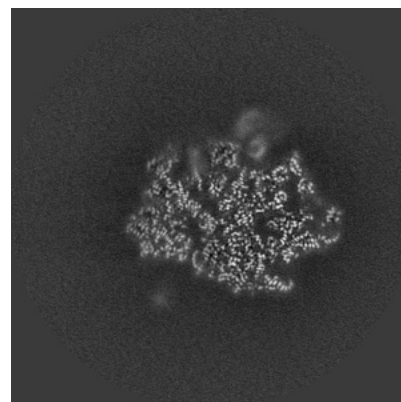
6.2.1 Primary map



X Index: 192



Y Index: 192

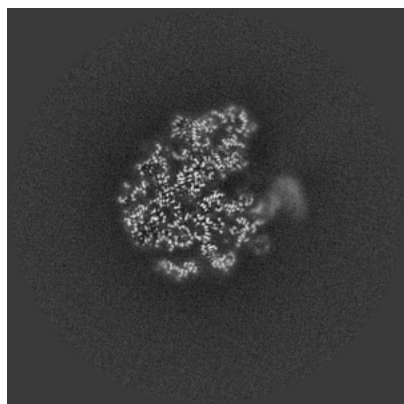


Z Index: 192

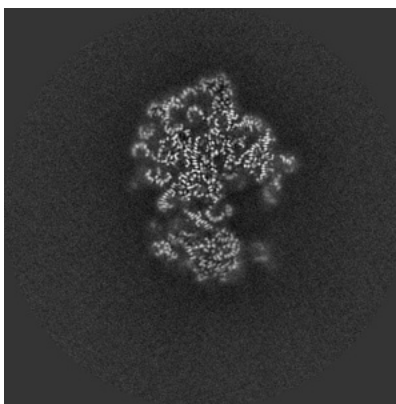
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

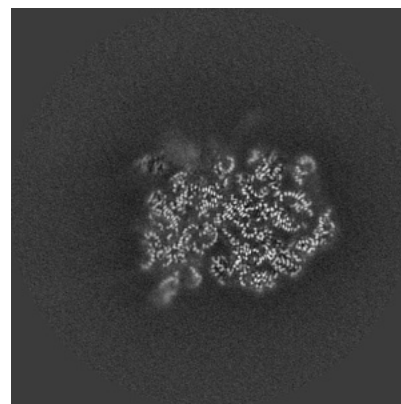
6.3.1 Primary map



X Index: 236



Y Index: 188

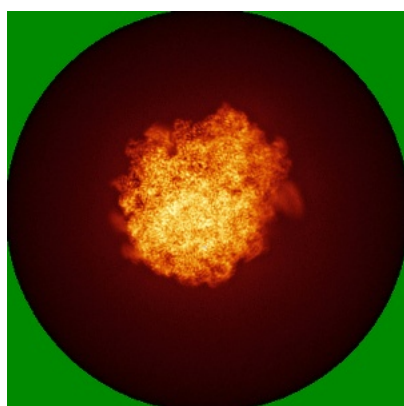


Z Index: 179

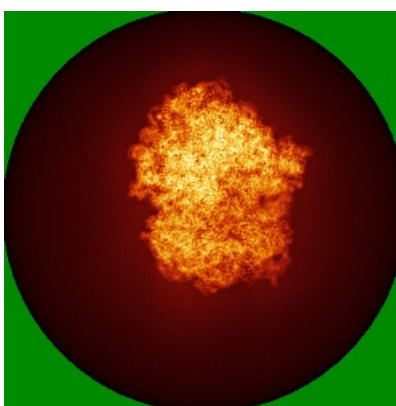
The images above show the largest variance slices of the map in three orthogonal directions.

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

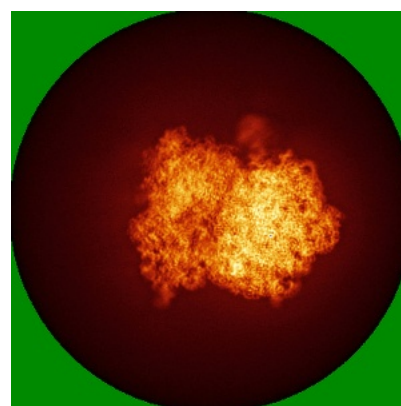
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

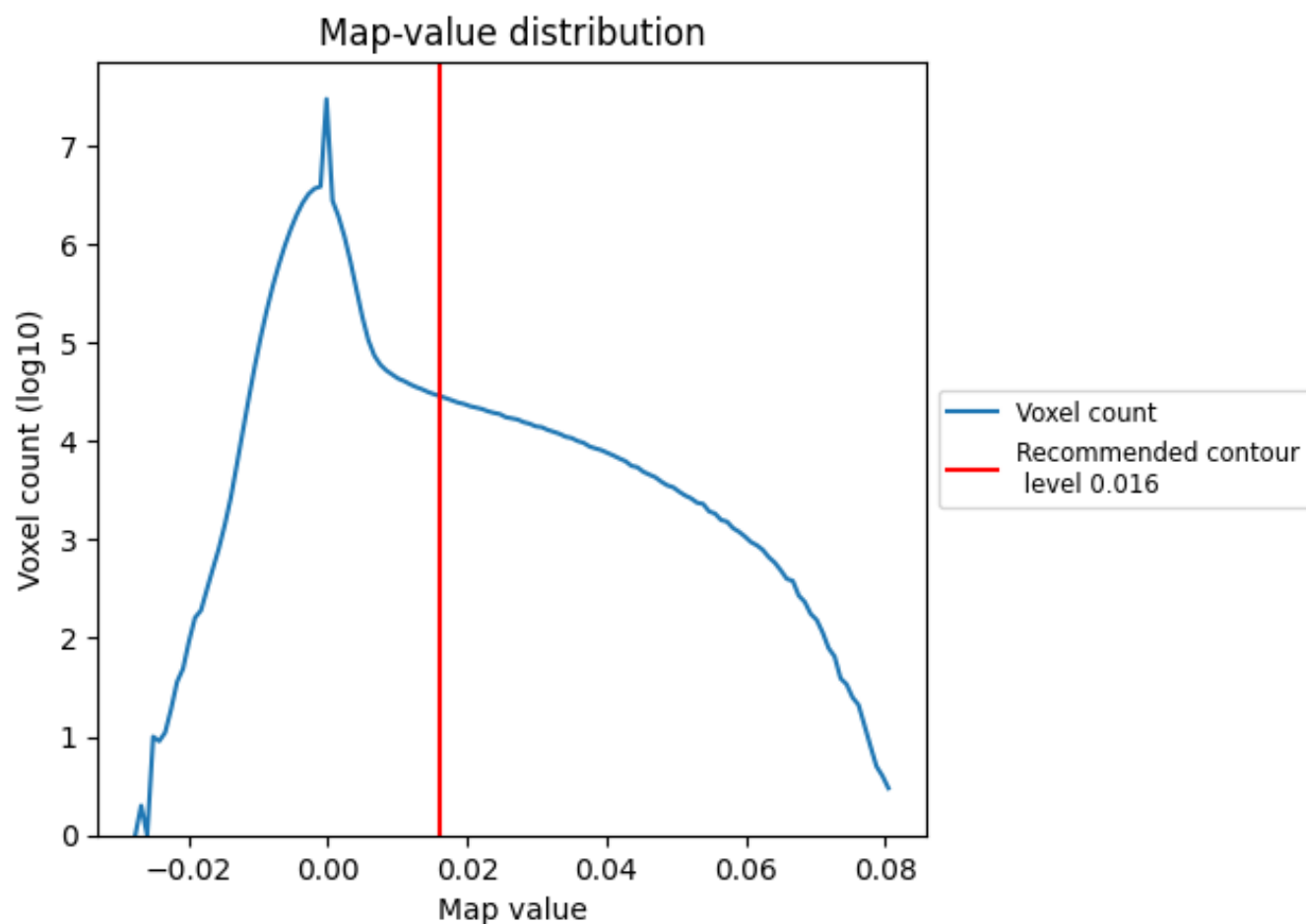
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

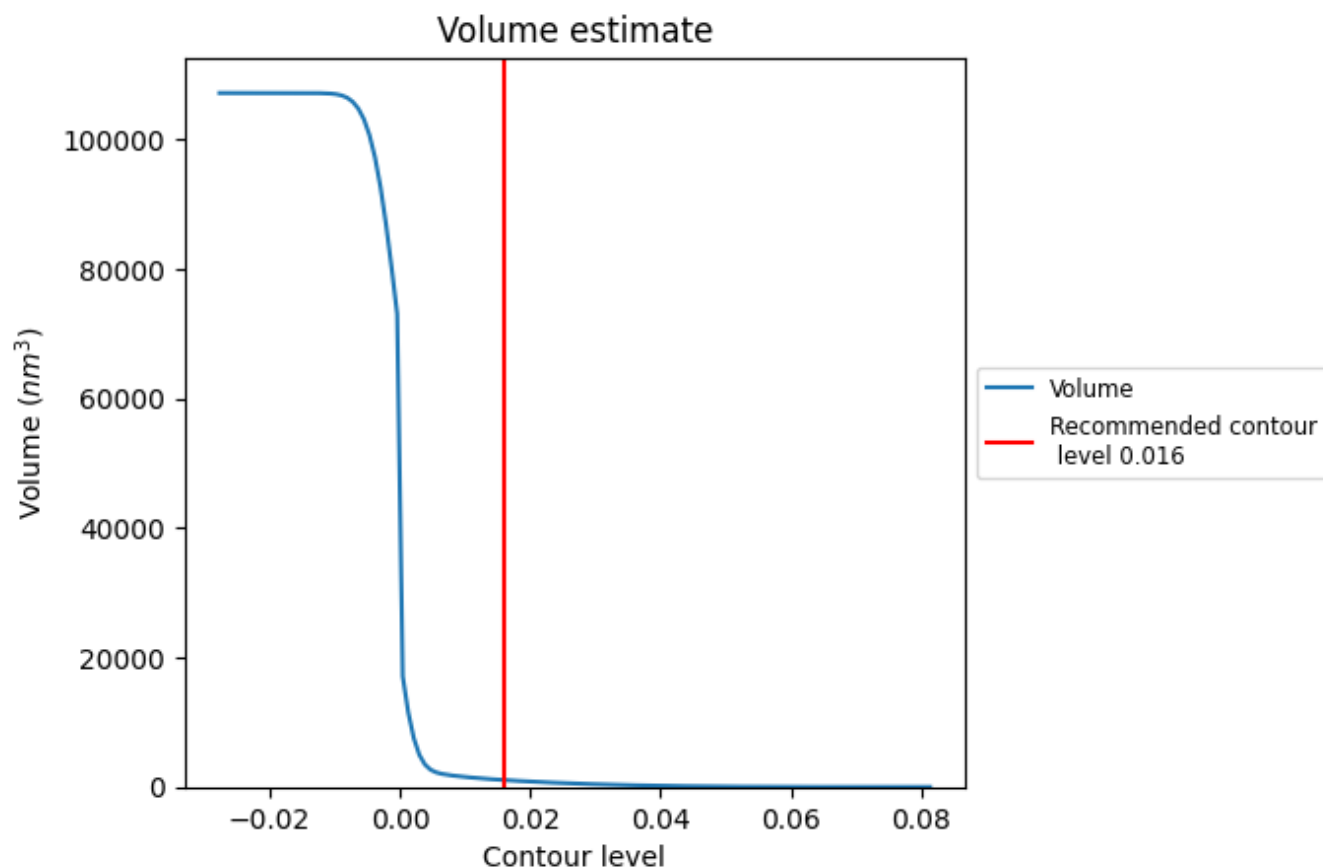
This section contains the results of statistical analysis of the map.

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.

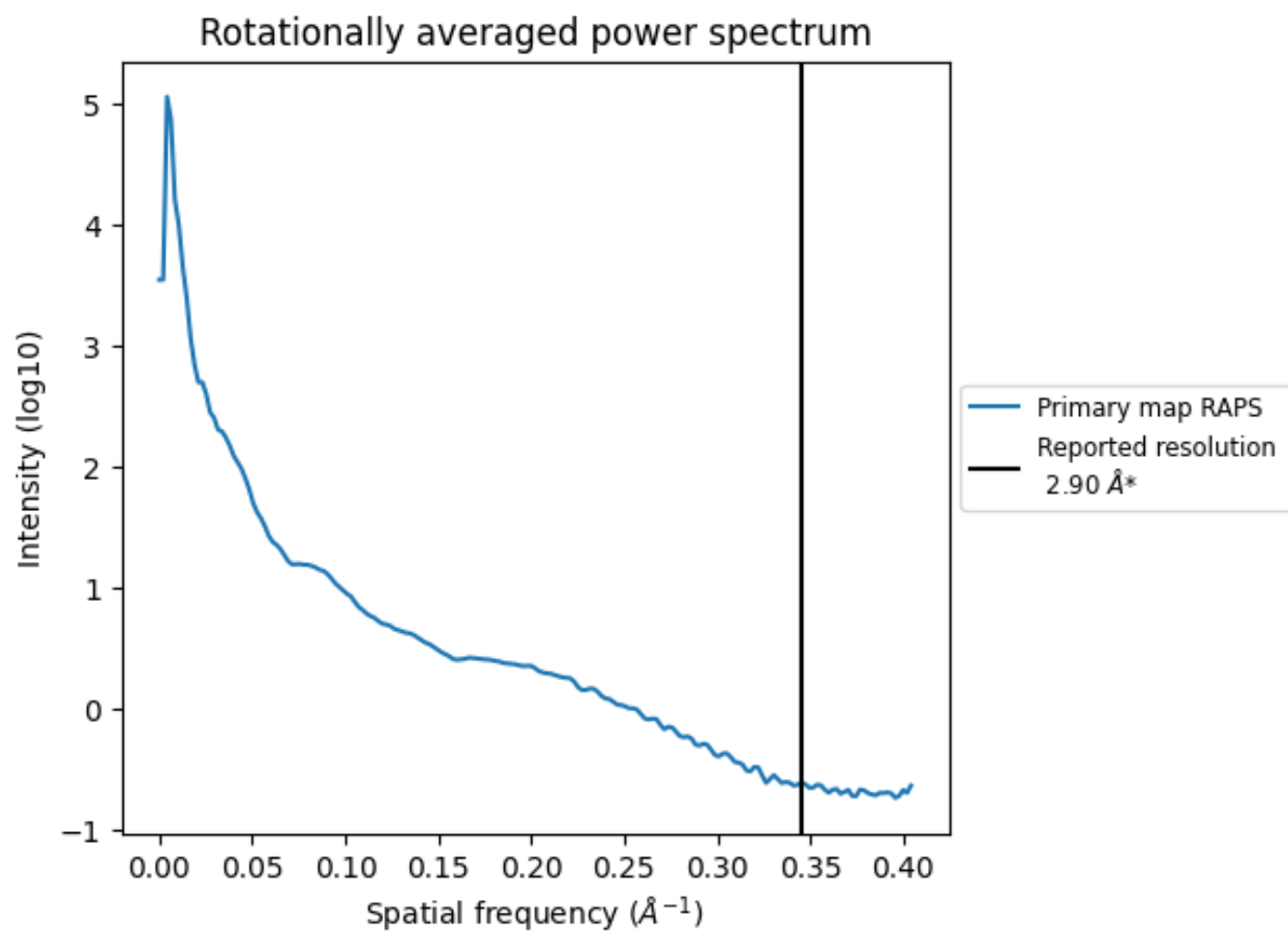
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1068 nm^3 ; this corresponds to an approximate mass of 965 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 0.345 Å⁻¹

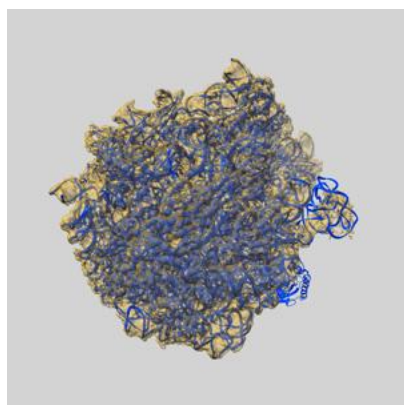
8 Fourier-Shell correlation

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

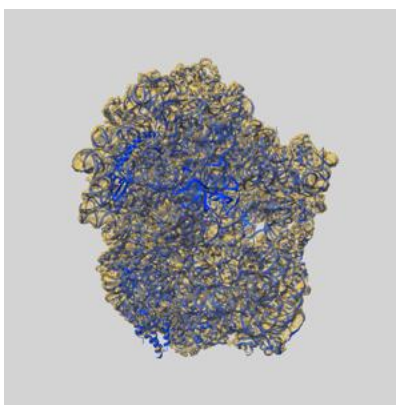
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20173 and PDB model 6ORE. Per-residue inclusion information can be found in section [3](#) on page [15](#).

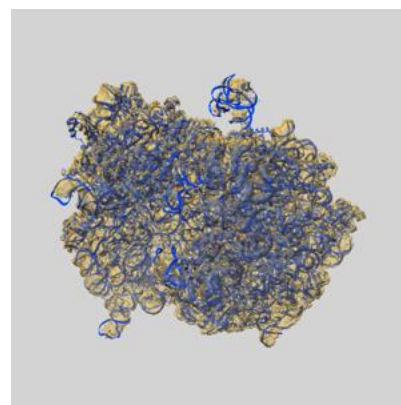
9.1 Map-model overlay [i](#)



X



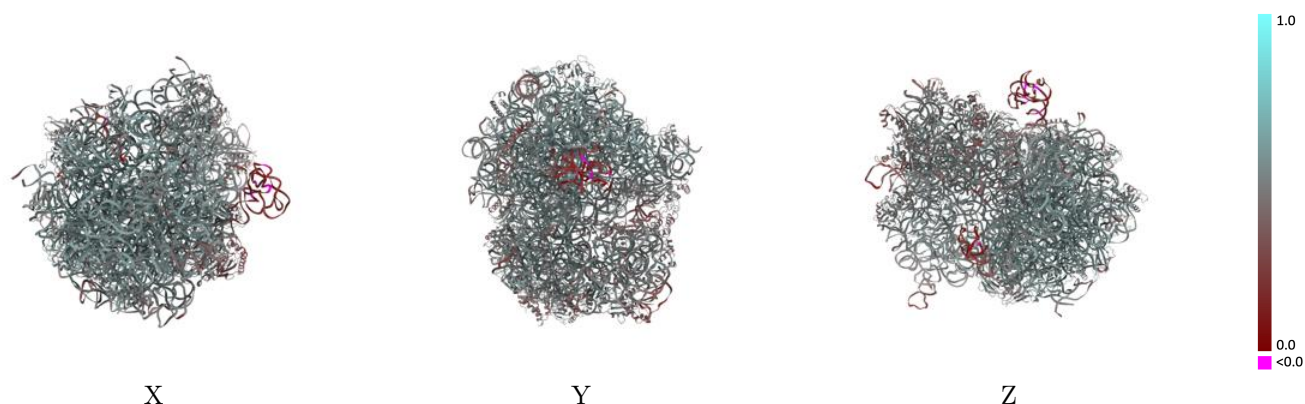
Y



Z

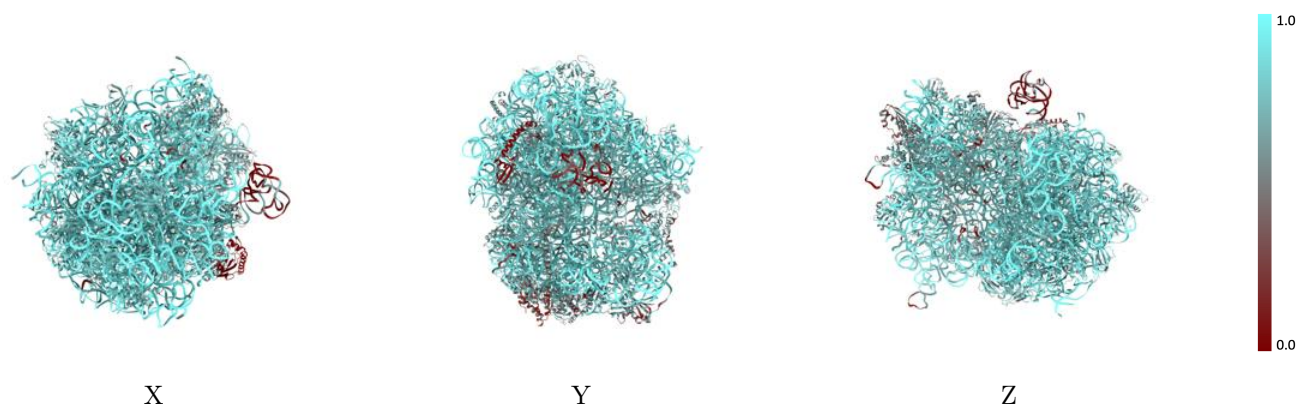
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



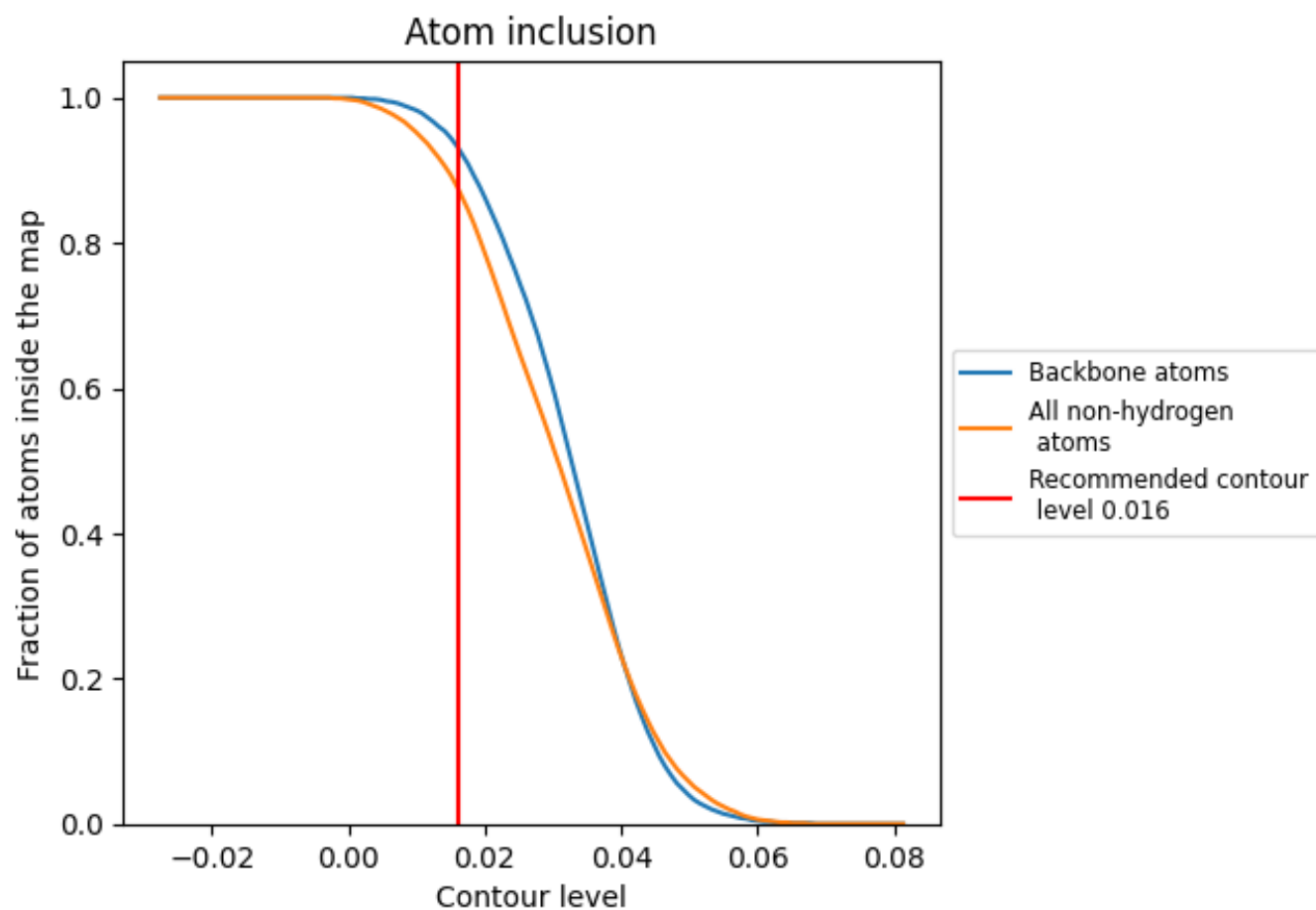
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.5160
1	 0.9460	 0.5310
2	 0.9460	 0.5070
3	 0.9760	 0.5190
4	 0.7120	 0.4110
5	 0.7980	 0.4820
A	 0.2500	 0.4220
B	 0.8240	 0.5620
C	 0.8360	 0.5540
D	 0.7860	 0.5280
E	 0.7020	 0.4570
F	 0.7540	 0.4840
G	 0.1070	 0.3720
J	 0.8380	 0.5550
K	 0.7570	 0.5390
L	 0.8290	 0.5390
M	 0.8190	 0.5380
N	 0.8630	 0.5610
O	 0.8150	 0.5040
P	 0.8090	 0.5500
Q	 0.8650	 0.5530
R	 0.8320	 0.5420
S	 0.7740	 0.5480
T	 0.7730	 0.5250
U	 0.7850	 0.5230
V	 0.7940	 0.5180
W	 0.8320	 0.5570
X	 0.8050	 0.5480
Y	 0.7550	 0.4860
Z	 0.8260	 0.5410
a	 0.4630	 0.4090
b	 0.8140	 0.5490
c	 0.7580	 0.5220
d	 0.8560	 0.5710
e	 0.8470	 0.5750



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Chain	Atom inclusion	Q-score
f	 0.8130	 0.5490
g	 0.3320	 0.4320
h	 0.6830	 0.4840
i	 0.7000	 0.4820
j	 0.7380	 0.5100
k	 0.6720	 0.4500
l	 0.6330	 0.4430
m	 0.7440	 0.5120
n	 0.7210	 0.4680
o	 0.5620	 0.4410
p	 0.6930	 0.4870
q	 0.7220	 0.5160
r	 0.6810	 0.4600
s	 0.7290	 0.4860
t	 0.7200	 0.4750
u	 0.7620	 0.5040
v	 0.6920	 0.4850
w	 0.6370	 0.4910
x	 0.6910	 0.4780
y	 0.7510	 0.4890
z	 0.4790	 0.4210