



Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 01:06 AM EDT

PDB ID : 8UTJ / pdb_00008utj
EMDB ID : EMD-42541
Title : E. coli 70S ribosome with unmodified lys-tRNA^{Pro}(GGG) bound to slippery P-site CCC-C codon in the 0 frame
Authors : Kimbrough, E.M.; Dunham, C.M.; Nguyen, H.A.
Deposited on : 2023-10-31
Resolution : 3.50 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.dev133
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) : 2.50

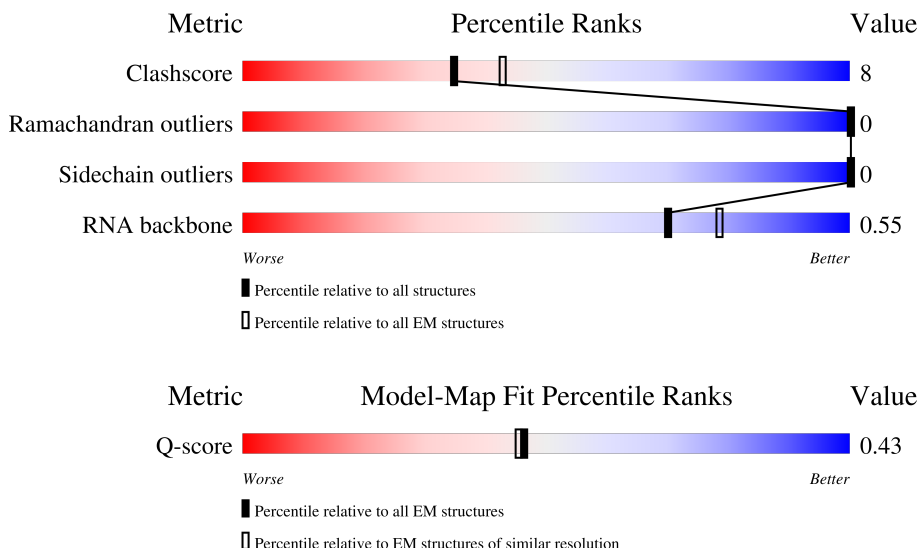
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



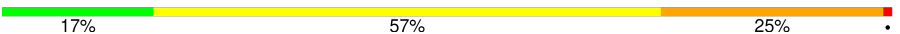
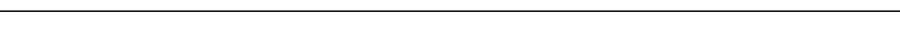
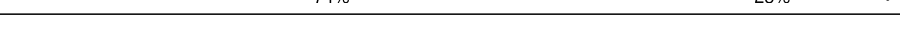
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	2904	
2	2	1540	
3	3	120	

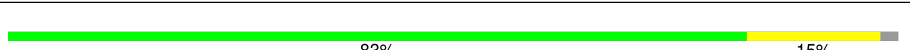
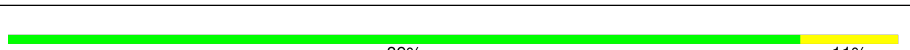
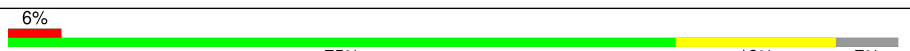
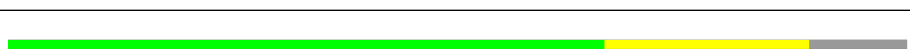
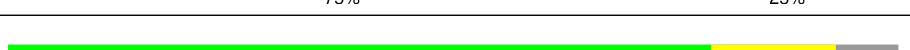
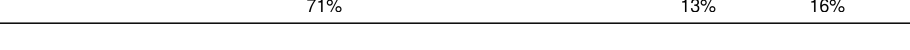
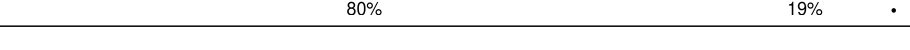
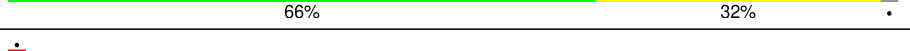
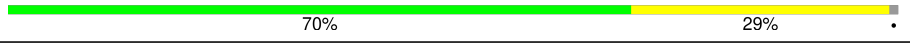
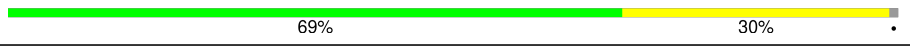
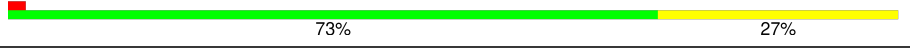
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Mol	Chain	Length	Quality of chain
4	4	18	
5	5	77	
6	A	232	
7	B	273	
8	C	209	
9	D	201	
10	E	179	
11	F	177	
12	G	149	
13	J	142	
14	K	123	
15	L	144	
16	M	136	
17	N	127	
18	O	117	
19	P	115	
20	Q	118	
21	R	103	
22	S	110	
23	T	100	
24	U	104	
25	V	94	
26	W	84	
27	X	78	
28	Y	63	

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Mol	Chain	Length	Quality of chain
29	Z	59	
30	a	70	
31	b	57	
32	c	55	
33	d	46	
34	e	65	
35	f	38	
36	g	241	
37	h	233	
38	i	206	
39	j	167	
40	k	135	
41	l	179	
42	m	130	
43	n	130	
44	o	103	
45	p	129	
46	q	124	
47	r	118	
48	s	101	
49	t	89	
50	u	82	
51	v	84	
52	w	75	
53	x	92	

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Mol	Chain	Length	Quality of chain
54	y	87	 84%15%•
55	z	71	 86%13%•

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 146133 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
			62334	27814	11470	20147	2903		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	887	A	U	conflict	GB 2577360273

- 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 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	8	Total	C	N	O	P	0	0
			168	75	29	56	8		

- Molecule 5 is a RNA chain called Lys-tRNA^{pro}L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	77	Total	C	N	O	P	0	0
			1648	733	297	541	77		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	67	Total	C	N	O	S	0	0
			507	321	90	95	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 Large ribosomal subunit protein uL13.

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 Large ribosomal subunit protein uL18.

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 Large ribosomal subunit protein bL19.

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 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 Large ribosomal subunit protein bL25.

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 Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	78	Total	C	N	O	S	0	0
			592	365	119	107	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 Large ribosomal subunit protein uL29.

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 Small ribosomal subunit protein uS8.

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 Small ribosomal subunit protein uS9.

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 Small ribosomal subunit protein uS10.

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 Small ribosomal subunit protein uS12.

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 Small ribosomal subunit protein uS14.

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 Small ribosomal subunit protein uS17.

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 Small ribosomal subunit protein uS19.

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).

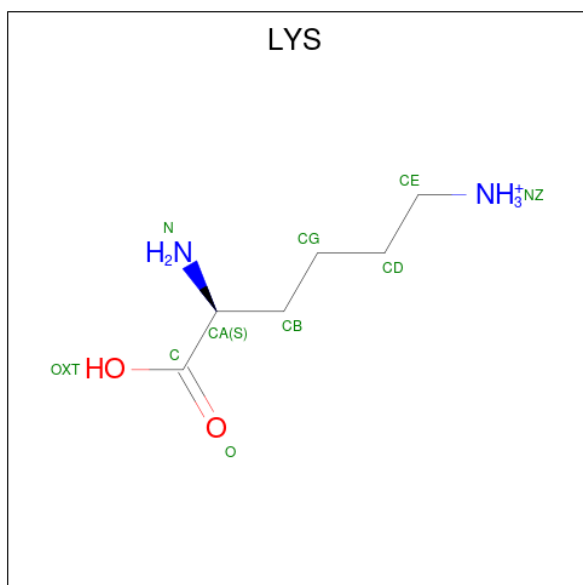
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			355	355	
56	2	145	Total	Mg	0
			145	145	
56	3	7	Total	Mg	0
			7	7	
56	B	1	Total	Mg	0
			1	1	
56	D	2	Total	Mg	0
			2	2	
56	L	1	Total	Mg	0
			1	1	
56	O	1	Total	Mg	0
			1	1	
56	P	2	Total	Mg	0
			2	2	
56	Q	2	Total	Mg	0
			2	2	
56	S	1	Total	Mg	0
			1	1	
56	U	1	Total	Mg	0
			1	1	
56	V	1	Total	Mg	0
			1	1	
56	X	1	Total	Mg	0
			1	1	
56	b	1	Total	Mg	0
			1	1	
56	e	1	Total	Mg	0
			1	1	
56	f	3	Total	Mg	0
			3	3	
56	i	1	Total	Mg	0
			1	1	
56	l	1	Total	Mg	0
			1	1	
56	m	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
56	n	1	Total	Mg	0
			1	1	
56	y	1	Total	Mg	0
			1	1	

- Molecule 57 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
57	5	1	Total	C	N	O	0
			9	6	2	1	

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	1	498	Total	O	0
			498	498	
58	2	203	Total	O	0
			203	203	
58	3	3	Total	O	0
			3	3	
58	5	1	Total	O	0
			1	1	
58	A	13	Total	O	0
			13	13	
58	B	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
58	C	2	Total 2	O 2	0
58	D	2	Total 2	O 2	0
58	E	2	Total 2	O 2	0
58	F	2	Total 2	O 2	0
58	G	1	Total 1	O 1	0
58	K	1	Total 1	O 1	0
58	L	2	Total 2	O 2	0
58	M	1	Total 1	O 1	0
58	O	1	Total 1	O 1	0
58	Q	1	Total 1	O 1	0
58	S	1	Total 1	O 1	0
58	T	1	Total 1	O 1	0
58	V	1	Total 1	O 1	0
58	W	1	Total 1	O 1	0
58	Y	1	Total 1	O 1	0
58	a	1	Total 1	O 1	0
58	b	1	Total 1	O 1	0
58	d	1	Total 1	O 1	0
58	g	4	Total 4	O 4	0
58	h	4	Total 4	O 4	0
58	i	1	Total 1	O 1	0

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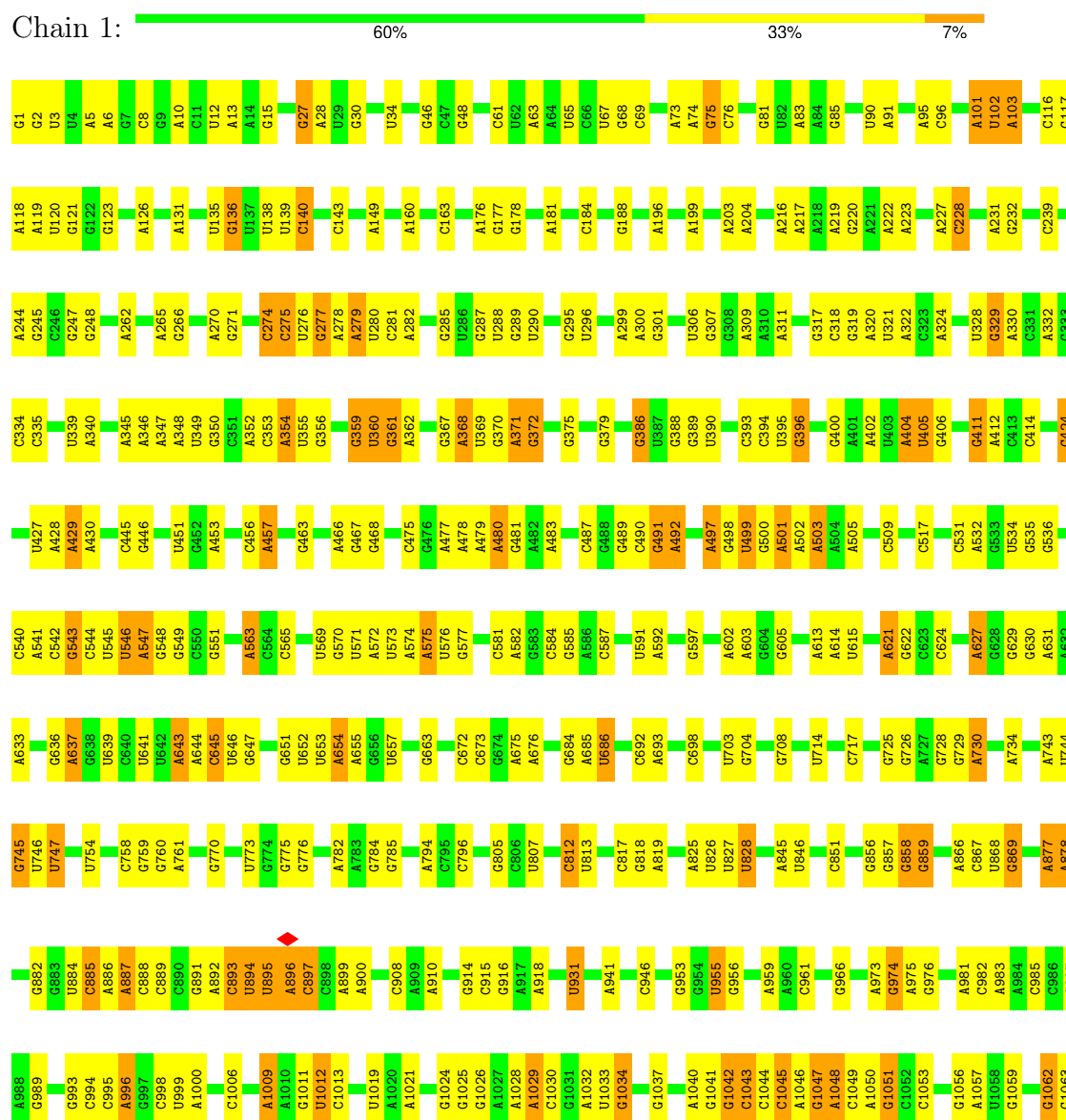
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Mol	Chain	Residues	Atoms		AltConf
58	k	2	Total 2	O 2	0
58	l	4	Total 4	O 4	0
58	n	1	Total 1	O 1	0
58	o	1	Total 1	O 1	0
58	q	1	Total 1	O 1	0
58	r	1	Total 1	O 1	0
58	t	2	Total 2	O 2	0
58	u	3	Total 3	O 3	0
58	v	2	Total 2	O 2	0
58	w	1	Total 1	O 1	0
58	z	1	Total 1	O 1	0

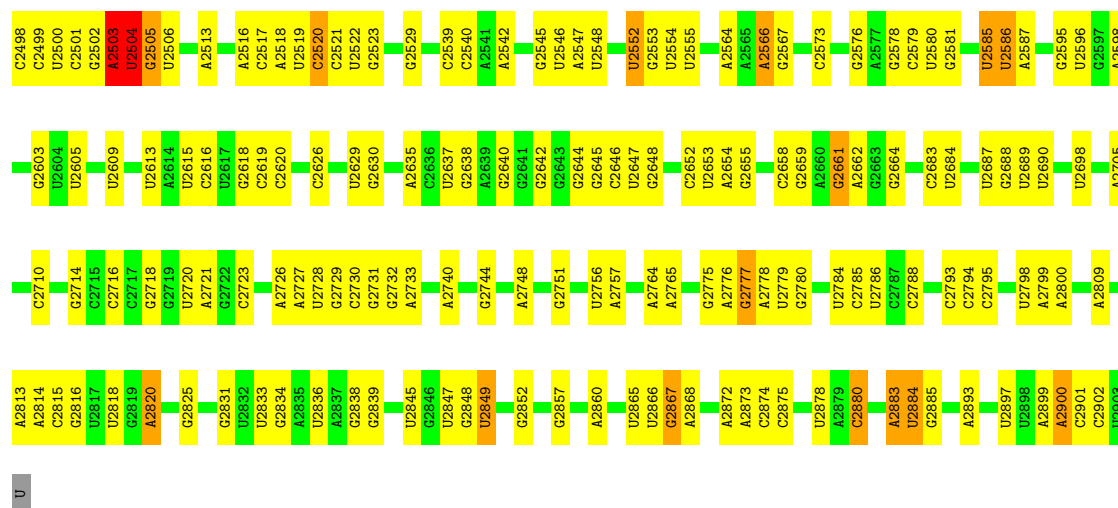
3 Residue-property plots

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.

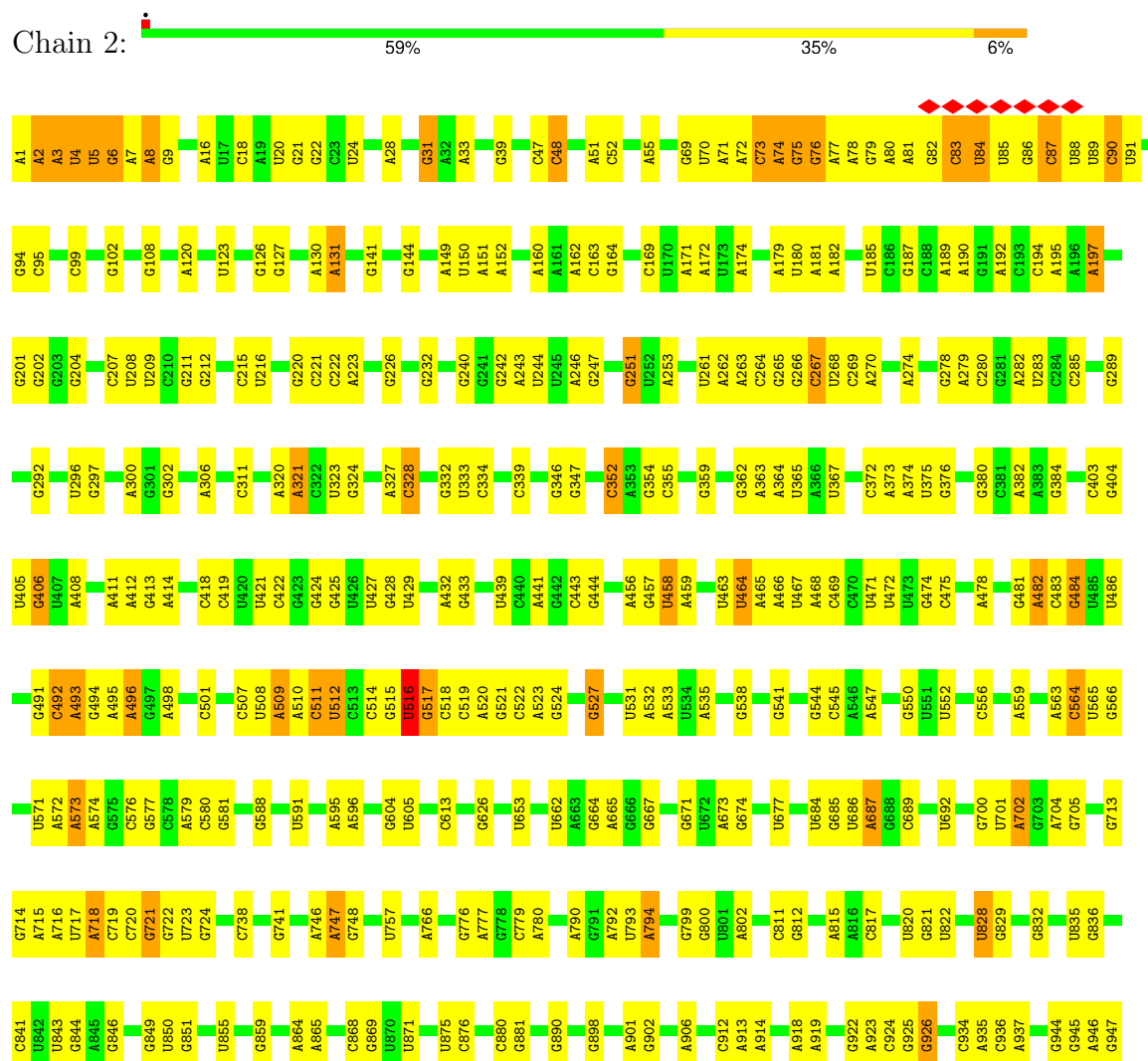
• Molecule 1: 23S ribosomal RNA

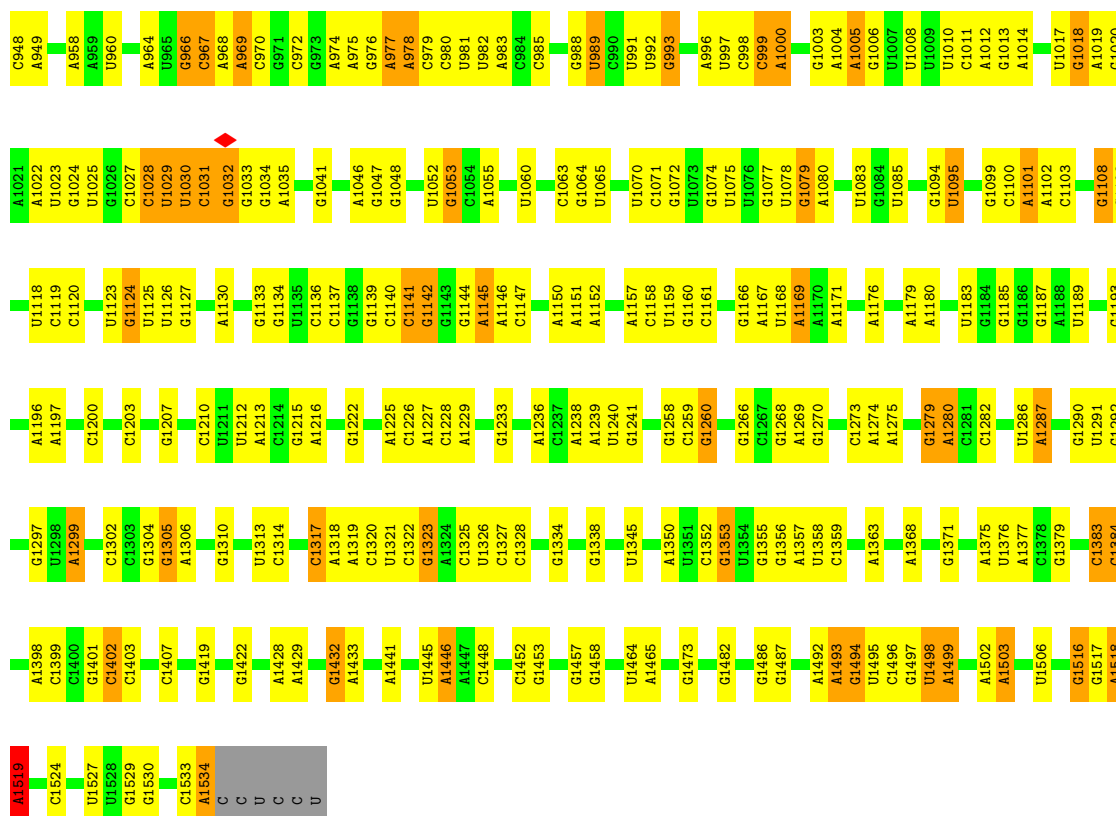






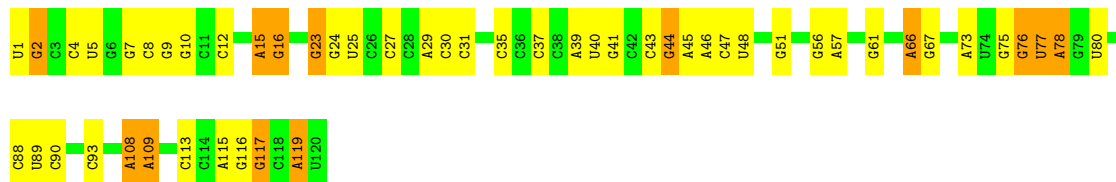
• Molecule 2: 16S ribosomal RNA





• Molecule 3: 5S ribosomal RNA

Chain 3: 57% 32% 11%



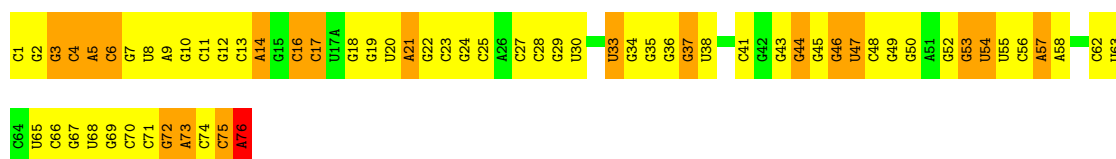
• Molecule 4: mRNA

Chain 4: 6% 28% 11% 56%

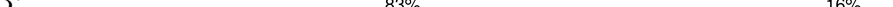


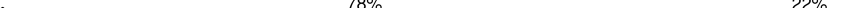
• Molecule 5: Lys-tRNA^{proL}

Chain 5: 17% 57% 25%



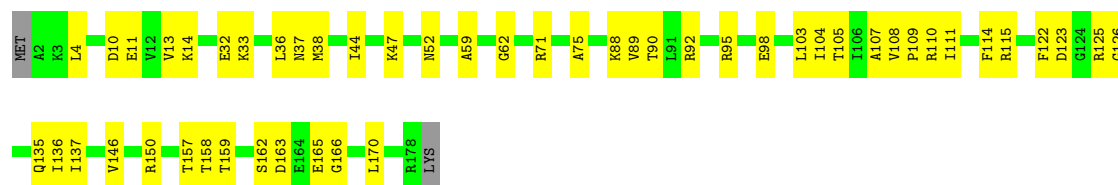
- [illegible]

- Chain B:  83% 16%
- Met A2 H15 H16 V17 K28 N45 N46 T49 D66 K71 A76 R80 R81 L81 E82 V94 L95 E100 R101 R102 P107 K108 G109 L110 Q115 S118 K125 K147 R156 S157 T160 V165 D168 M181 E194 E199 V204
- L205 A210 G241 T246 P247 W248 G249 V250 K253 K256 T257 R258 V288 R269 R270 R271 S272 Lys

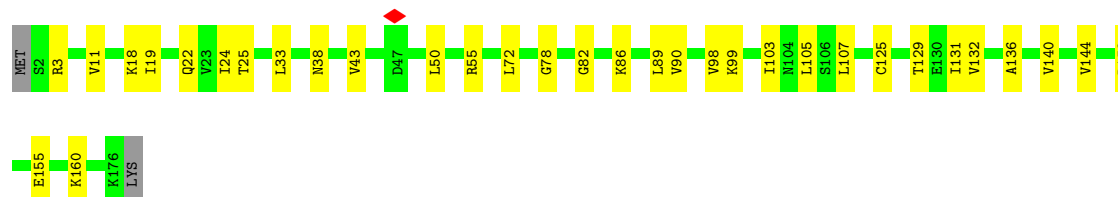
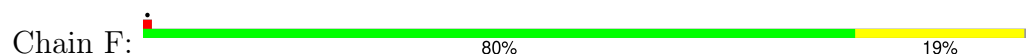
- Chain C:  78% 22%
- 
- 

- Chain D: 77% 23%
-
- | Label | Color |
|-------|--------|
| M1 | Yellow |
| K6 | Yellow |
| D7 | Yellow |
| A8 | Yellow |
| Q9 | Yellow |
| S15 | Yellow |
| E16 | Yellow |
| T17 | Yellow |
| T18 | Yellow |
| F19 | Yellow |
| G20 | Green |
| R21 | Yellow |
| N24 | Yellow |
| V28 | Yellow |
| E51 | Yellow |
| K57 | Yellow |
| X58 | Green |
| P59 | Yellow |
| Q62 | Yellow |
| R69 | Yellow |
| L73 | Yellow |
| K74 | Yellow |
| S75 | Yellow |
| P76 | Yellow |
| L77 | Yellow |
| W78 | Yellow |
| R88 | Yellow |
| V96 | Yellow |
| K99 | Yellow |
| K106 | Yellow |
| S107 | Green |
| I108 | Yellow |
| R114 | Yellow |
| R117 | Yellow |
| L118 | Yellow |
| E127 | Yellow |
| A128 | Yellow |
| P129 | Green |
| K130 | Yellow |
| T131 | Yellow |
| K132 | Yellow |
| L133 | Green |
| L134 | Yellow |
| L138 | Yellow |
| E144 | Yellow |
| L153 | Yellow |
| F158 | Yellow |
| R162 | Yellow |
| M163 | Yellow |
| D171 | Yellow |
| A172 | Yellow |
| D176 | Yellow |
| S179 | Yellow |
| L180 | Yellow |
| M188 | Yellow |
| T189 | Yellow |
| A190 | Green |
| D191 | Yellow |
| A201 | Green |

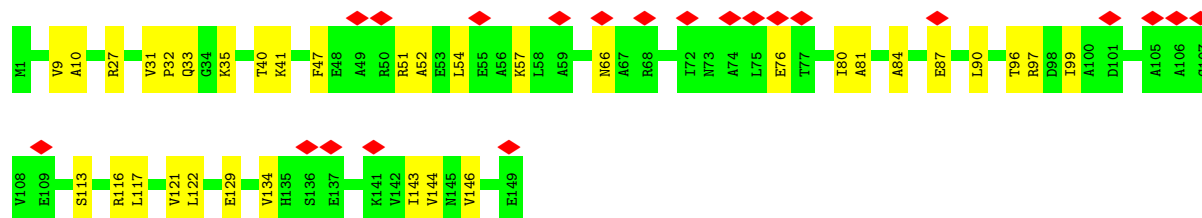
- Chain E: 71% 28%



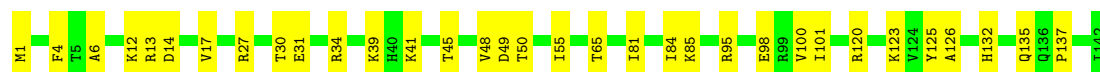
- Molecule 11: 50S ribosomal protein L6



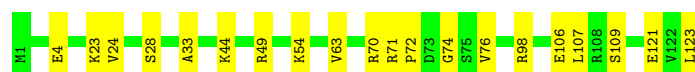
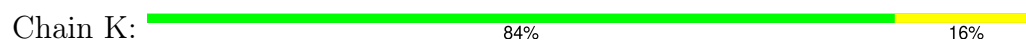
- Molecule 12: 50S ribosomal protein L9



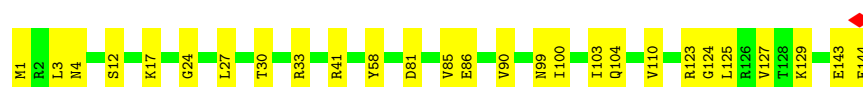
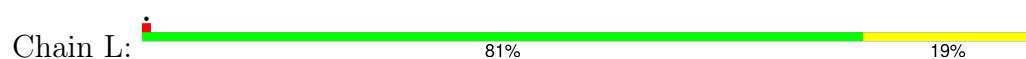
- Molecule 13: Large ribosomal subunit protein uL13



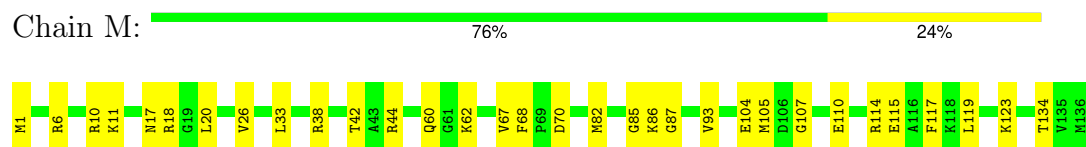
- Molecule 14: 50S ribosomal protein L14



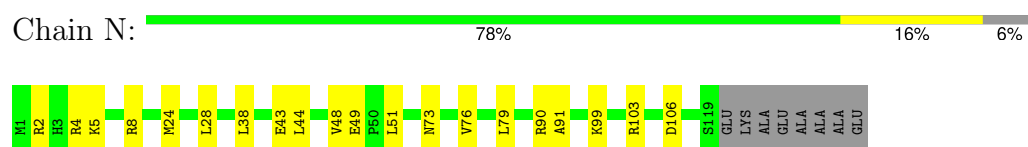
- Molecule 15: 50S ribosomal protein L15



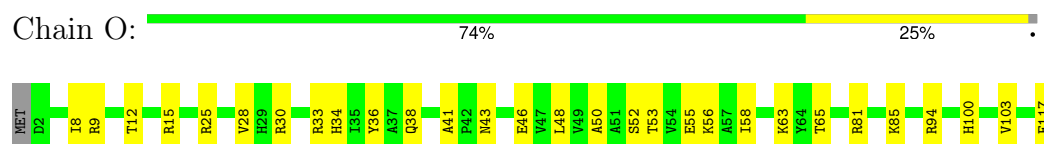
- Molecule 16: 50S ribosomal protein L16



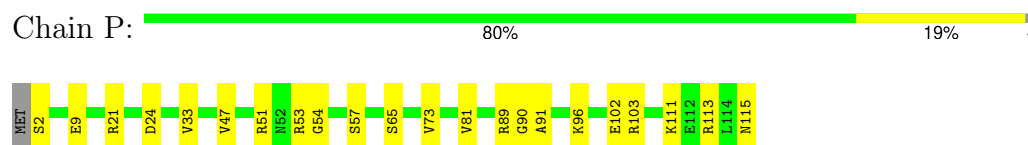
- Molecule 17: 50S ribosomal protein L17



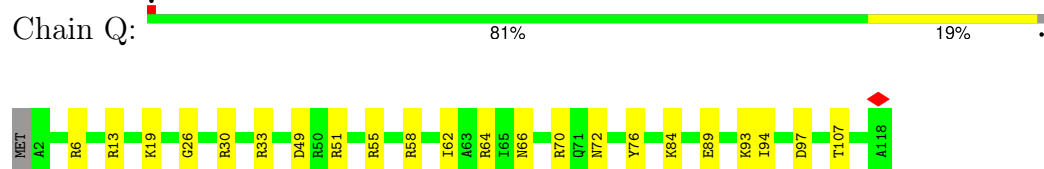
- Molecule 18: Large ribosomal subunit protein uL18



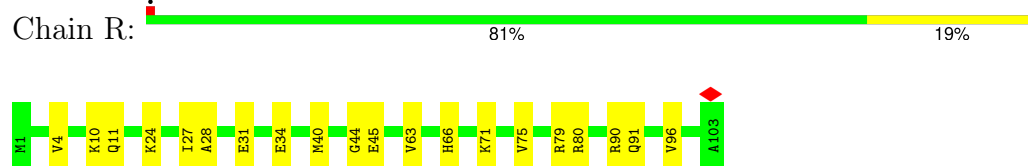
- Molecule 19: Large ribosomal subunit protein bL19



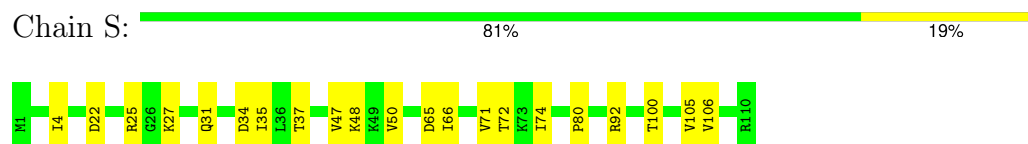
- Molecule 20: 50S ribosomal protein L20



- Molecule 21: Ribosomal protein L21



- Molecule 22: 50S ribosomal protein L22



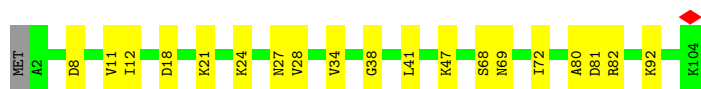
- Molecule 23: 50S ribosomal protein L23

Chain T:  79% 15% 6%



- Molecule 24: 50S ribosomal protein L24

Chain U:  81% 18%



- Molecule 25: Large ribosomal subunit protein bL25

Chain V:  78% 22%



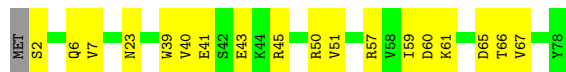
- Molecule 26: Large ribosomal subunit protein bL27

Chain W:  65% 27% 7%



- Molecule 27: 50S ribosomal protein L28

Chain X:  76% 23%



- Molecule 28: Large ribosomal subunit protein uL29

Chain Y:  84% 14%

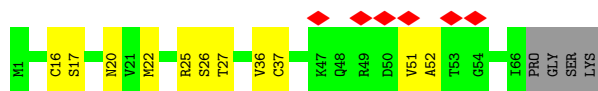
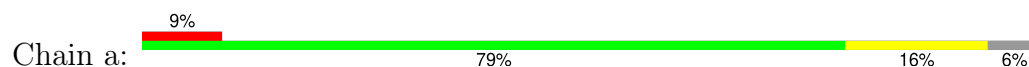


- Molecule 29: 50S ribosomal protein L30

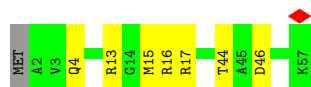
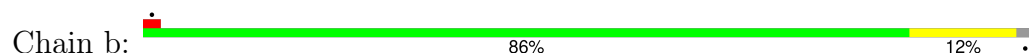
Chain Z:  80% 19%



- Molecule 30: 50S ribosomal protein L31



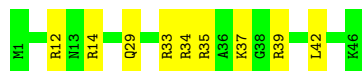
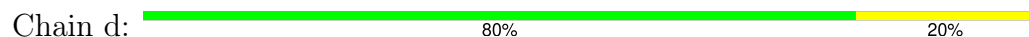
- Molecule 31: 50S ribosomal protein L32



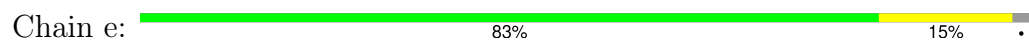
- Molecule 32: 50S ribosomal protein L33



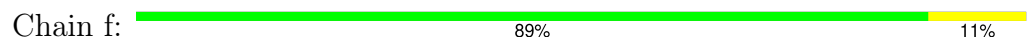
- Molecule 33: 50S ribosomal protein L34



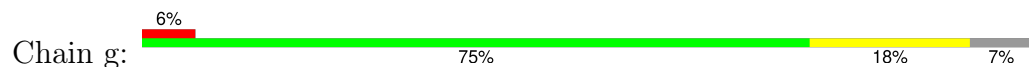
- Molecule 34: 50S ribosomal protein L35

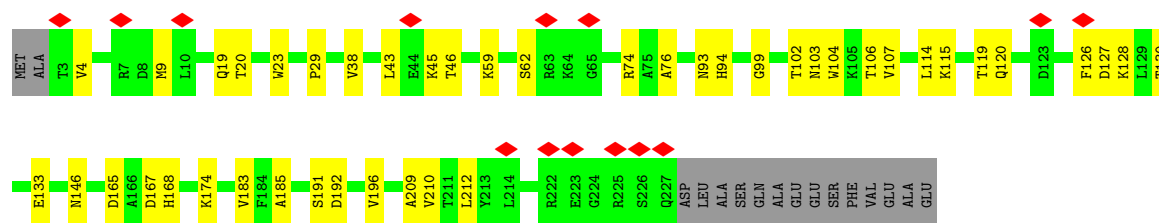


- Molecule 35: 50S ribosomal protein L36

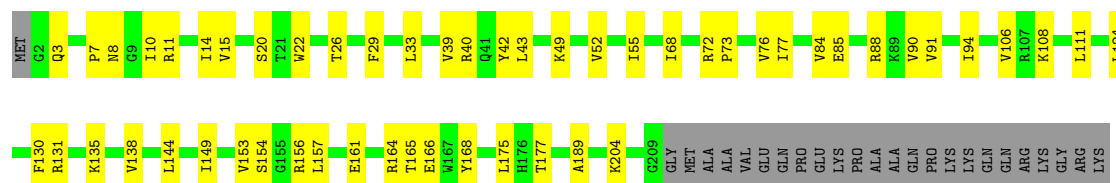


- Molecule 36: 30S ribosomal protein S2

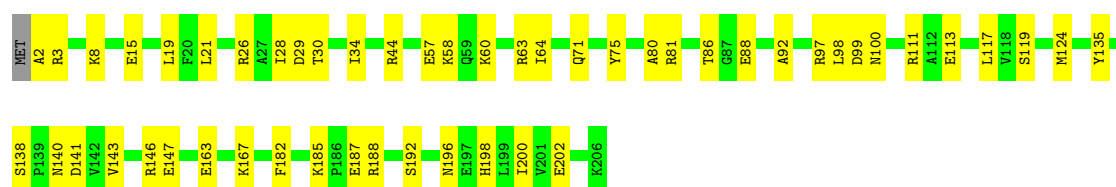




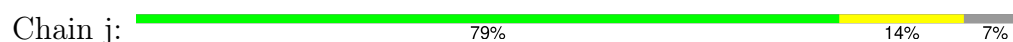
• Molecule 37: 30S ribosomal protein S3



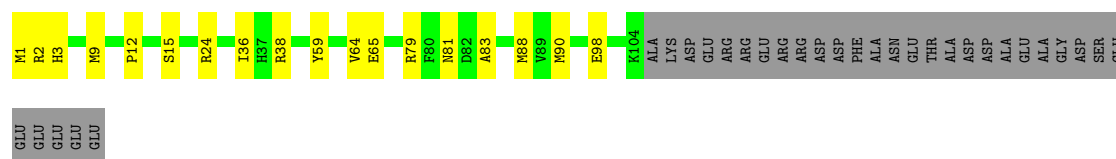
• Molecule 38: 30S ribosomal protein S4



• Molecule 39: 30S ribosomal protein S5

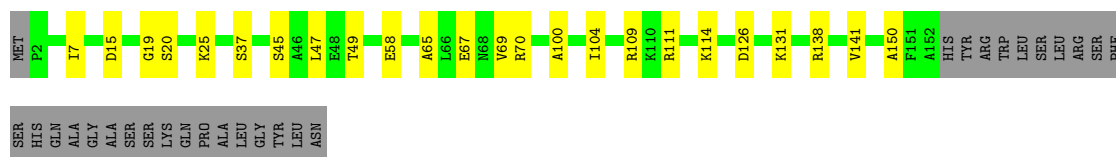


• Molecule 40: 30S ribosomal protein S6



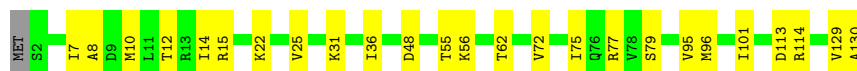
• Molecule 41: 30S ribosomal protein S7





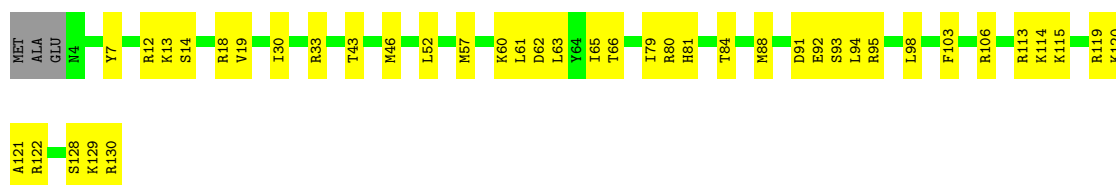
- Molecule 42: Small ribosomal subunit protein uS8

Chain m: 80% 19% .



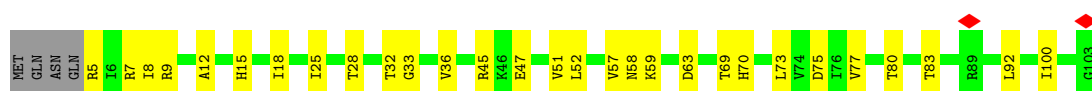
- Molecule 43: Small ribosomal subunit protein uS9

Chain n: 66% 32% .



- Molecule 44: Small ribosomal subunit protein uS10

Chain o: 68% 28% .



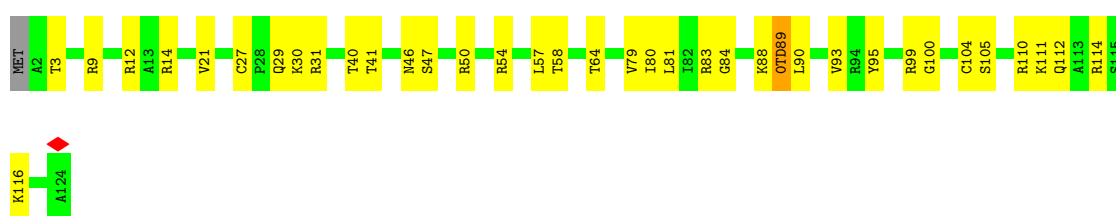
- Molecule 45: 30S ribosomal protein S11

Chain p: 77% 14% 9%



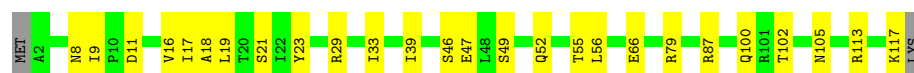
- Molecule 46: Small ribosomal subunit protein uS12

Chain q: 69% 29% .



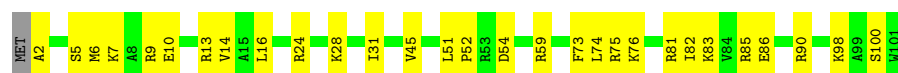
- Molecule 47: 30S ribosomal protein S13

Chain r:  76% 22%



- Molecule 48: Small ribosomal subunit protein uS14

Chain s:  70% 29%



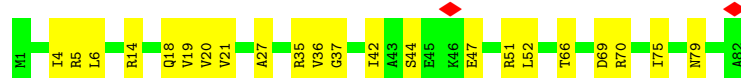
- Molecule 49: 30S ribosomal protein S15

Chain t:  69% 30%



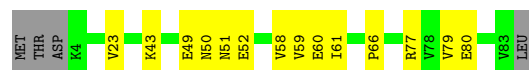
- Molecule 50: 30S ribosomal protein S16

Chain u:  73% 27%



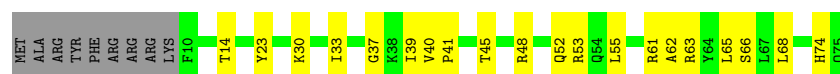
- Molecule 51: Small ribosomal subunit protein uS17

Chain v:  79% 17% 5%



- Molecule 52: 30S ribosomal protein S18

Chain w:  61% 27% 12%

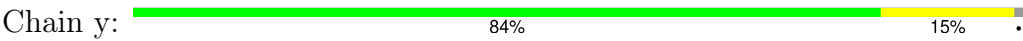


- Molecule 53: Small ribosomal subunit protein uS19

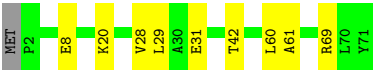
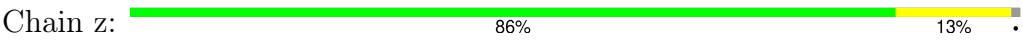
Chain x:  72% 18% 10%



- 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	70298	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.23	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	547.3792, 547.3792, 547.3792	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0691, 1.0691, 1.0691	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, G7M, PSU, 2MG, OMU, MA6, 2MA, 4OC, 0TD, OMC, 5MC, 6MZ, MG, UR3, 5MU, 1MG, 7MG

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	0.13	0/69335	0.25	0/108168
2	2	0.12	0/36590	0.24	0/57074
3	3	0.11	0/2872	0.22	0/4478
4	4	0.39	0/186	0.68	0/287
5	5	0.22	0/1841	0.42	2/2870 (0.1%)
6	A	0.13	0/511	0.30	0/685
7	B	0.20	0/2121	0.34	0/2852
8	C	0.19	0/1586	0.34	0/2134
9	D	0.17	0/1571	0.31	0/2113
10	E	0.16	0/1434	0.35	0/1926
11	F	0.15	0/1333	0.32	0/1805
12	G	0.16	0/1122	0.36	0/1515
13	J	0.18	0/1152	0.30	0/1551
14	K	0.18	0/955	0.30	0/1279
15	L	0.20	0/1062	0.33	0/1413
16	M	0.18	0/1093	0.31	0/1460
17	N	0.20	0/964	0.35	0/1289
18	O	0.16	0/902	0.33	0/1209
19	P	0.18	0/929	0.32	0/1242
20	Q	0.17	0/960	0.29	0/1278
21	R	0.18	0/829	0.38	0/1107
22	S	0.19	0/864	0.32	0/1156
23	T	0.17	0/752	0.30	0/1005
24	U	0.15	0/796	0.32	0/1062
25	V	0.17	0/766	0.33	0/1025
26	W	0.18	0/599	0.33	0/792
27	X	0.18	0/635	0.34	0/848
28	Y	0.15	0/502	0.27	0/667
29	Z	0.17	0/452	0.32	0/605
30	a	0.16	0/531	0.32	0/709
31	b	0.17	0/450	0.30	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.18	0/433	0.28	0/576
33	d	0.19	0/380	0.32	0/498
34	e	0.40	0/513	0.48	0/676
35	f	0.20	0/303	0.33	0/397
36	g	0.15	0/1791	0.35	0/2413
37	h	0.17	0/1663	0.34	0/2241
38	i	0.15	0/1665	0.31	0/2227
39	j	0.17	0/1165	0.34	0/1568
40	k	0.16	0/867	0.35	0/1171
41	l	0.14	0/1195	0.33	0/1602
42	m	0.17	0/989	0.29	0/1326
43	n	0.17	0/1034	0.36	0/1375
44	o	0.16	0/800	0.35	0/1082
45	p	0.16	0/893	0.32	0/1205
46	q	0.17	0/960	0.34	0/1286
47	r	0.15	0/909	0.34	0/1215
48	s	0.15	0/817	0.30	0/1088
49	t	0.14	0/722	0.29	0/964
50	u	0.18	0/659	0.34	0/884
51	v	0.16	0/657	0.36	0/881
52	w	0.16	0/553	0.33	0/743
53	x	0.14	0/680	0.31	0/915
54	y	0.15	0/675	0.28	0/895
55	z	0.15	0/597	0.31	0/792
All	All	0.14	0/156615	0.27	2/234223 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	76	A	C2'-C3'-O3'	6.79	119.68	109.50
5	5	76	A	C1'-C2'-O2'	5.74	120.40	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62334	0	31368	712	0
2	2	32929	0	16587	409	0
3	3	2569	0	1301	41	0
4	4	168	0	88	6	0
5	5	1648	0	833	65	0
6	A	507	0	542	10	0
7	B	2082	0	2154	32	0
8	C	1565	0	1616	41	0
9	D	1552	0	1619	32	0
10	E	1410	0	1444	39	0
11	F	1313	0	1358	19	0
12	G	1111	0	1148	24	0
13	J	1129	0	1162	26	0
14	K	946	0	1023	18	0
15	L	1053	0	1129	23	0
16	M	1074	0	1157	24	0
17	N	951	0	994	17	0
18	O	892	0	923	23	0
19	P	917	0	962	22	0
20	Q	947	0	1019	20	0
21	R	816	0	839	17	0
22	S	857	0	922	13	0
23	T	746	0	811	11	0
24	U	788	0	844	15	0
25	V	753	0	780	15	0
26	W	592	0	607	17	0
27	X	625	0	652	15	0
28	Y	501	0	531	8	0
29	Z	448	0	488	9	0
30	a	522	0	524	12	0
31	b	444	0	458	6	0
32	c	426	0	464	13	0
33	d	377	0	418	8	0
34	e	504	0	572	10	0
35	f	302	0	343	4	0
36	g	1760	0	1787	30	0
37	h	1636	0	1710	41	0
38	i	1643	0	1707	39	0
39	j	1152	0	1196	25	0
40	k	848	0	846	15	0
41	l	1181	0	1238	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	m	979	0	1031	19	0
43	n	1022	0	1070	35	0
44	o	790	0	831	26	0
45	p	877	0	887	17	0
46	q	957	0	1017	28	0
47	r	900	0	965	21	0
48	s	805	0	844	30	0
49	t	714	0	734	20	0
50	u	649	0	666	19	0
51	v	648	0	691	11	0
52	w	544	0	560	16	0
53	x	663	0	688	10	0
54	y	669	0	719	12	0
55	z	589	0	629	7	0
56	1	355	0	0	0	0
56	2	145	0	0	0	0
56	3	7	0	0	0	0
56	B	1	0	0	0	0
56	D	2	0	0	0	0
56	L	1	0	0	0	0
56	O	1	0	0	0	0
56	P	2	0	0	0	0
56	Q	2	0	0	0	0
56	S	1	0	0	0	0
56	U	1	0	0	0	0
56	V	1	0	0	0	0
56	X	1	0	0	0	0
56	b	1	0	0	0	0
56	e	1	0	0	0	0
56	f	3	0	0	0	0
56	i	1	0	0	0	0
56	l	1	0	0	0	0
56	m	1	0	0	0	0
56	n	1	0	0	0	0
56	y	1	0	0	0	0
57	5	9	0	12	3	0
58	1	498	0	0	43	0
58	2	203	0	0	24	0
58	3	3	0	0	0	0
58	5	1	0	0	1	0
58	A	13	0	0	2	0
58	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	C	2	0	0	0	0
58	D	2	0	0	1	0
58	E	2	0	0	2	0
58	F	2	0	0	1	0
58	G	1	0	0	0	0
58	K	1	0	0	0	0
58	L	2	0	0	0	0
58	M	1	0	0	0	0
58	O	1	0	0	0	0
58	Q	1	0	0	2	0
58	S	1	0	0	0	0
58	T	1	0	0	0	0
58	V	1	0	0	0	0
58	W	1	0	0	0	0
58	Y	1	0	0	0	0
58	a	1	0	0	0	0
58	b	1	0	0	0	0
58	d	1	0	0	0	0
58	g	4	0	0	0	0
58	h	4	0	0	1	0
58	i	1	0	0	0	0
58	k	2	0	0	0	0
58	l	4	0	0	0	0
58	n	1	0	0	0	0
58	o	1	0	0	0	0
58	q	1	0	0	0	0
58	r	1	0	0	0	0
58	t	2	0	0	0	0
58	u	3	0	0	1	0
58	v	2	0	0	0	0
58	w	1	0	0	0	0
58	z	1	0	0	0	0
All	All	146133	0	97508	1866	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 8.

All (1866) 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)
2:2:493:A:O2'	2:2:494:G:O4'	1.79	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1779:U:OP2	1:1:1784:A:N6	2.02	0.92
1:1:2585:U:H3	57:5:101:LYS:C	1.78	0.92
2:2:1032:G:N2	2:2:1033:G:O4'	2.03	0.91
2:2:1147:C:HO2'	43:n:7:TYR:HH	1.19	0.90
2:2:297:G:N2	2:2:300:A:OP2	2.05	0.89
1:1:2646:C:OP2	1:1:2732:G:O2'	1.88	0.89
2:2:552:U:O2'	46:q:83:ARG:O	1.89	0.88
1:1:1219:U:OP2	20:Q:19:LYS:NZ	2.07	0.88
2:2:363:A:N6	46:q:27:CYS:SG	2.47	0.87
2:2:980:C:O2'	48:s:13:ARG:NH1	2.08	0.87
2:2:1403:C:O2	2:2:1499:A:N6	2.08	0.87
1:1:395:U:O2'	1:1:396:G:N7	2.08	0.86
1:1:1954:G:O2'	1:1:1956:U:O4	1.93	0.86
2:2:507:C:OP2	2:2:508:U:O2'	1.94	0.86
2:2:263:A:OP1	54:y:74:ARG:NH1	2.09	0.85
37:h:49:LYS:O	37:h:72:ARG:NH2	2.09	0.85
1:1:270:A:N6	1:1:369:U:O2	2.09	0.85
1:1:2286:G:O6	32:c:23:THR:OG1	1.94	0.85
1:1:2731:G:O3'	8:C:208:LYS:NZ	2.10	0.85
1:1:1582:C:O2'	1:1:1583:A:O4'	1.95	0.85
2:2:1130:A:OP1	43:n:18:ARG:NH2	2.11	0.84
2:2:1124:G:O2'	2:2:1145:A:N6	2.10	0.84
47:r:11:ASP:O	47:r:46:SER:OG	1.95	0.84
1:1:282:A:N6	1:1:359:G:O6	2.10	0.84
1:1:2847:U:OP1	19:P:96:LYS:NZ	2.10	0.84
1:1:61:C:OP2	28:Y:47:ARG:NH2	2.11	0.83
1:1:2121:G:O2'	6:A:166:ASP:OD1	1.96	0.83
2:2:126:G:OP1	2:2:605:U:O2'	1.95	0.83
36:g:130:THR:OG1	36:g:133:GLU:OE1	1.97	0.83
1:1:489:G:N2	1:1:491:G:OP1	2.12	0.83
1:1:2014:A:O2'	1:1:2015:A:O4'	1.97	0.83
2:2:565:U:OP2	2:2:566:G:O2'	1.96	0.83
1:1:645:C:N4	1:1:2349:G:N3	2.27	0.83
1:1:1715:G:O2'	1:1:1743:G:O6	1.97	0.82
1:1:463:G:N2	1:1:466:A:OP2	2.12	0.82
38:i:163:GLU:O	38:i:167:LYS:NZ	2.13	0.82
40:k:38:ARG:NH1	40:k:98:GLU:O	2.13	0.82
1:1:2250:G:O2'	1:1:2496:C:OP1	1.98	0.82
1:1:2296:U:OP2	18:O:9:ARG:NH2	2.12	0.82
2:2:718:A:O2'	55:z:31:GLU:OE2	1.98	0.82
1:1:1328:A:O2'	1:1:1329:U:O5'	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1364:G:OP2	27:X:2:SER:N	2.13	0.81
2:2:1280:A:OP1	44:o:9:ARG:NH2	2.12	0.81
1:1:956:G:O2'	16:M:82:MET:SD	2.39	0.81
48:s:86:GLU:OE1	48:s:90:ARG:NH2	2.12	0.81
1:1:244:A:OP2	34:e:8:ARG:NH2	2.13	0.81
2:2:1028:C:O2'	2:2:1029:U:O4'	1.97	0.81
1:1:1992:G:N2	1:1:1996:C:O2'	2.14	0.80
31:b:44:THR:OG1	31:b:46:ASP:OD1	1.99	0.80
2:2:339:C:OP2	14:K:98:ARG:NH1	2.14	0.80
9:D:189:THR:OG1	9:D:191:ASP:OD1	1.99	0.80
18:O:50:ALA:O	18:O:81:ARG:NH1	2.14	0.80
40:k:59:TYR:OH	52:w:66:SER:OG	2.00	0.80
10:E:162:SER:OG	10:E:165:GLU:OE1	2.00	0.80
1:1:1858:A:O2'	1:1:1859:U:O4'	1.97	0.80
2:2:292:G:O6	58:2:1801:HOH:O	2.00	0.80
2:2:1233:G:OP1	43:n:119:ARG:NH2	2.15	0.80
1:1:2122:U:O2	1:1:2176:A:N6	2.14	0.80
2:2:1063:C:OP2	2:2:1064:G:O2'	2.00	0.80
1:1:2619:C:OP1	8:C:157:LYS:NZ	2.14	0.80
1:1:918:A:N3	3:3:80:U:O2'	2.15	0.80
26:W:26:PHE:N	26:W:29:GLU:OE1	2.14	0.80
1:1:2308:G:O2'	1:1:2309:A:OP1	1.99	0.80
1:1:324:A:OP2	1:1:1205:A:N6	2.15	0.79
1:1:894:U:O2'	1:1:895:U:O5'	1.98	0.79
1:1:2377:A:O2'	18:O:117:PHE:O	2.00	0.79
1:1:2141:G:N2	1:1:2150:C:O2	2.15	0.79
46:q:31:ARG:O	46:q:58:THR:OG1	1.99	0.79
1:1:400:G:OP2	27:X:57:ARG:NH2	2.14	0.79
25:V:10:LYS:NZ	25:V:41:GLU:OE2	2.14	0.79
1:1:1818:U:OP2	7:B:156:ARG:NH1	2.16	0.79
1:1:2387:U:O2'	26:W:41:ARG:NH2	2.16	0.79
2:2:1006:G:N2	58:2:1815:HOH:O	2.15	0.79
12:G:113:SER:O	12:G:116:ARG:NH1	2.14	0.79
1:1:1341:G:OP2	1:1:1394:U:O2'	2.00	0.79
2:2:912:C:O2'	58:2:1802:HOH:O	2.00	0.79
1:1:370:G:O2'	1:1:424:G:OP1	2.01	0.79
1:1:887:A:OP2	58:1:3401:HOH:O	2.00	0.79
1:1:994:C:O2	21:R:10:LYS:NZ	2.16	0.79
1:1:1814:G:OP2	1:1:1815:A:O2'	2.00	0.78
2:2:152:A:N6	2:2:169:C:O2	2.16	0.78
2:2:71:A:N6	2:2:99:C:O2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2188:U:C4	1:1:2189:U:O4	2.36	0.78
1:1:2788:C:O2'	1:1:2809:A:N3	2.15	0.78
2:2:1338:G:N3	5:5:41:C:O2'	2.15	0.78
2:2:1270:G:HO2'	2:2:1313:U:HO2'	1.13	0.78
1:1:1084:A:O2'	1:1:1085:A:O4'	2.01	0.78
2:2:1338:G:N2	5:5:41:C:O2	2.17	0.78
28:Y:9:LYS:NZ	28:Y:13:GLU:OE2	2.16	0.77
1:1:475:C:O2	1:1:479:A:N6	2.17	0.77
3:3:5:U:OP1	3:3:61:G:O2'	2.02	0.77
1:1:2705:A:O2'	1:1:2852:G:OP1	2.01	0.77
52:w:14:THR:OG1	52:w:48:ARG:NH1	2.18	0.77
13:J:13:ARG:NH2	13:J:49:ASP:O	2.18	0.77
10:E:110:ARG:NH2	10:E:136:ILE:O	2.17	0.77
54:y:44:LYS:NZ	54:y:87:ALA:O	2.17	0.77
1:1:1072:C:O2	58:1:3402:HOH:O	2.00	0.77
10:E:10:ASP:OD1	10:E:11:GLU:N	2.17	0.77
1:1:2123:G:O2'	1:1:2124:G:N7	2.17	0.77
1:1:2564:A:OP1	1:1:2648:G:O2'	2.03	0.77
1:1:2784:U:OP1	58:1:3404:HOH:O	2.03	0.77
49:t:15:PHE:O	49:t:17:ARG:NH1	2.18	0.77
1:1:1521:G:OP2	1:1:1522:A:O2'	2.02	0.77
1:1:1754:A:N1	1:1:2716:C:O2'	2.16	0.77
22:S:80:PRO:O	22:S:100:THR:OG1	2.02	0.77
2:2:1030:U:O2'	2:2:1031:C:OP2	2.02	0.77
2:2:1350:A:OP2	43:n:120:LYS:NZ	2.17	0.76
10:E:98:GLU:OE2	30:a:25:ARG:NH1	2.18	0.76
1:1:2751:G:OP1	1:1:2751:G:N2	2.17	0.76
10:E:135:GLN:N	10:E:135:GLN:OE1	2.19	0.76
53:x:36:ARG:NH2	53:x:75:ALA:O	2.18	0.76
9:D:51:GLU:OE2	9:D:88:ARG:NH2	2.17	0.76
12:G:87:GLU:OE1	40:k:24:ARG:NH2	2.19	0.76
1:1:974:G:O2'	1:1:975:A:OP2	2.03	0.76
1:1:1837:C:O2'	1:1:1927:A:N3	2.18	0.76
2:2:876:C:OP2	58:2:1803:HOH:O	2.02	0.76
13:J:120:ARG:O	13:J:123:LYS:NZ	2.16	0.76
1:1:2141:G:N1	1:1:2150:C:N3	2.34	0.76
1:1:2585:U:N3	57:5:101:LYS:C	2.43	0.76
5:5:4:C:HO2'	5:5:5:A:H8	1.30	0.76
1:1:1034:G:N2	1:1:1121:C:O2	2.17	0.76
1:1:1437:C:HO2'	1:1:1516:G:HO2'	1.30	0.76
1:1:2616:C:OP1	58:1:3403:HOH:O	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:58:SER:O	25:V:73:LYS:NZ	2.18	0.76
1:1:2848:G:O2'	1:1:2867:G:N2	2.19	0.75
24:U:12:ILE:HD11	24:U:80:ALA:HB2	1.68	0.75
50:u:44:SER:N	50:u:47:GLU:OE2	2.18	0.75
1:1:1201:U:OP1	58:1:3407:HOH:O	2.05	0.75
1:1:1858:A:O2'	1:1:1859:U:O5'	2.05	0.75
1:1:2635:A:O2'	8:C:49:GLN:NE2	2.19	0.75
1:1:2645:G:OP2	1:1:2645:G:N2	2.16	0.75
13:J:1:MET:SD	58:Q:301:HOH:O	2.44	0.75
1:1:177:G:N2	1:1:177:G:OP2	2.20	0.75
1:1:2128:G:O6	1:1:2160:C:N4	2.20	0.75
1:1:1379:U:O2'	1:1:1380:G:OP1	2.04	0.75
2:2:509:A:O2'	2:2:510:A:O4'	2.01	0.75
25:V:48:MET:SD	25:V:51:GLN:NE2	2.60	0.75
6:A:159:GLY:N	58:A:301:HOH:O	2.20	0.74
38:i:15:GLU:OE2	38:i:63:ARG:NH1	2.19	0.74
9:D:176:ASP:OD1	9:D:179:SER:OG	2.03	0.74
2:2:323:U:OP1	54:y:21:ASN:ND2	2.19	0.74
2:2:671:G:O2'	40:k:79:ARG:NH2	2.21	0.74
1:1:976:G:HO2'	1:1:1155:A:HO2'	1.26	0.74
1:1:1064:C:O2'	1:1:1065:U:O5'	2.04	0.74
2:2:1060:U:O2'	44:o:58:ASN:OD1	2.05	0.74
2:2:1193:G:O6	37:h:3:GLN:NE2	2.20	0.74
42:m:48:ASP:OD1	42:m:62:THR:OG1	2.05	0.74
1:1:825:A:OP1	58:1:3406:HOH:O	2.04	0.74
41:l:67:GLU:OE2	41:l:70:ARG:NH1	2.20	0.74
2:2:977:A:O2'	2:2:979:C:OP2	2.04	0.74
46:q:110:ARG:NE	46:q:112:GLN:O	2.21	0.74
1:1:429:A:O2'	1:1:430:A:O4'	2.03	0.73
1:1:959:A:OP1	58:1:3408:HOH:O	2.05	0.73
19:P:90:GLY:O	19:P:113:ARG:NH1	2.21	0.73
1:1:1042:G:O2'	1:1:1043:C:OP2	2.05	0.73
25:V:26:PHE:CE1	25:V:47:VAL:HG21	2.23	0.73
1:1:1688:U:O4	58:1:3405:HOH:O	2.04	0.73
1:1:2730:C:O3'	8:C:174:SER:OG	2.05	0.73
2:2:876:C:H1'	42:m:12:THR:HG21	1.70	0.73
43:n:91:ASP:OD2	43:n:93:SER:OG	2.05	0.73
1:1:643:A:O2'	1:1:644:A:O4'	2.06	0.73
1:1:1417:C:O2'	1:1:1587:G:O2'	2.02	0.73
1:1:2506:U:O4	57:5:101:LYS:HA	1.88	0.73
1:1:2831:G:N2	1:1:2884:U:OP2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:368:A:O2'	1:1:369:U:O4'	2.06	0.73
2:2:1524:C:OP1	45:p:122:ARG:NH2	2.21	0.73
47:r:47:GLU:OE1	47:r:47:GLU:N	2.21	0.73
1:1:372:G:OP2	27:X:61:LYS:NZ	2.21	0.73
1:1:1125:G:OP2	1:1:1126:A:O2'	2.06	0.73
1:1:1202:G:N2	15:L:4:ASN:OD1	2.22	0.73
2:2:1358:U:OP2	2:2:1359:C:N4	2.22	0.73
38:i:19:LEU:HB3	38:i:64:ILE:HG22	1.70	0.73
1:1:2450:A:OP1	1:1:2497:A:O2'	2.04	0.72
2:2:1203:C:OP1	48:s:2:ALA:N	2.22	0.72
3:3:93:C:OP2	25:V:18:ARG:NH1	2.22	0.72
22:S:22:ASP:OD1	22:S:25:ARG:NH2	2.22	0.72
1:1:2839:G:O2'	17:N:49:GLU:OE1	2.04	0.72
2:2:949:A:N7	47:r:105:ASN:ND2	2.37	0.72
1:1:2875:C:O3'	19:P:2:SER:OG	2.07	0.72
20:Q:89:GLU:O	21:R:11:GLN:NE2	2.22	0.72
47:r:49:SER:OG	47:r:52:GLN:NE2	2.23	0.72
52:w:37:GLY:O	52:w:63:ARG:NH2	2.22	0.72
1:1:2540:C:O2'	1:1:2740:A:N3	2.23	0.72
2:2:1030:U:OP1	58:2:1804:HOH:O	2.07	0.72
1:1:993:G:OP2	20:Q:51:ARG:NH2	2.22	0.72
20:Q:97:ASP:OD2	58:Q:301:HOH:O	2.07	0.72
51:v:52:GLU:OE1	51:v:52:GLU:N	2.23	0.72
1:1:2279:G:N7	26:W:14:ARG:NH2	2.37	0.72
7:B:17:VAL:HG12	7:B:204:VAL:HG22	1.70	0.72
2:2:1240:U:O4	41:l:109:ARG:NH1	2.23	0.72
1:1:1706:C:OP2	58:1:3410:HOH:O	2.07	0.72
1:1:411:G:OP2	1:1:2406:A:O2'	2.07	0.71
1:1:2168:G:O6	58:1:3409:HOH:O	2.06	0.71
1:1:2576:G:O2'	1:1:2579:C:OP2	2.08	0.71
14:K:70:ARG:NH2	14:K:74:GLY:O	2.23	0.71
2:2:81:A:N6	2:2:88:U:O4	2.19	0.71
2:2:1229:A:O2'	5:5:30:U:OP1	2.07	0.71
1:1:335:C:O2	24:U:68:SER:OG	2.08	0.71
1:1:1131:G:O2'	1:1:2025:C:O2'	2.08	0.71
1:1:2258:C:O2'	1:1:2427:C:OP2	2.08	0.71
47:r:79:ARG:NH1	53:x:65:GLU:OE1	2.23	0.71
1:1:319:G:OP2	9:D:132:LYS:NZ	2.24	0.71
8:C:24:VAL:HG12	8:C:178:VAL:HG21	1.71	0.71
1:1:1712:U:OP2	1:1:1713:A:O2'	2.04	0.71
24:U:18:ASP:OD1	24:U:21:LYS:NZ	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:o:7:ARG:NH1	44:o:75:ASP:OD2	2.23	0.71
1:1:1288:G:OP2	1:1:1288:G:N2	2.23	0.71
10:E:10:ASP:O	10:E:14:LYS:NZ	2.21	0.71
5:5:9:A:O2'	5:5:10:G:N7	2.23	0.71
12:G:33:GLN:OE1	12:G:35:LYS:NZ	2.24	0.71
25:V:26:PHE:HE1	25:V:47:VAL:HG21	1.55	0.71
29:Z:7:ILE:HD13	29:Z:48:ILE:HD11	1.72	0.71
2:2:520:A:OP2	46:q:50:ARG:NH2	2.24	0.71
22:S:37:THR:OG1	22:S:48:LYS:NZ	2.24	0.71
2:2:766:A:OP2	2:2:812:G:N2	2.24	0.70
51:v:60:GLU:OE2	51:v:77:ARG:NH1	2.23	0.70
9:D:6:LYS:O	9:D:9:GLN:NE2	2.24	0.70
13:J:17:VAL:HG12	13:J:55:ILE:HB	1.73	0.70
1:1:629:G:N3	1:1:639:U:O2'	2.24	0.70
1:1:2043:C:OP1	1:1:2777:G:O2'	2.08	0.70
9:D:76:PRO:O	58:D:401:HOH:O	2.08	0.70
1:1:2111:U:H3	1:1:2145:C:HO2'	1.39	0.70
2:2:16:A:N3	2:2:1080:A:O2'	2.21	0.70
2:2:1226:C:OP2	47:r:102:THR:HG21	1.92	0.70
1:1:974:G:OP1	1:1:1187:G:O2'	2.07	0.70
1:1:2167:U:O2	1:1:2170:A:N7	2.25	0.70
2:2:33:A:N3	46:q:29:GLN:NE2	2.39	0.70
2:2:738:C:OP1	40:k:2:ARG:NH2	2.24	0.70
2:2:1003:G:O2'	58:2:1805:HOH:O	2.10	0.70
2:2:1383:C:O2'	2:2:1384:C:OP1	2.10	0.70
1:1:372:G:O2'	1:1:400:G:O6	2.07	0.70
20:Q:94:ILE:HG21	21:R:4:VAL:HG21	1.74	0.70
1:1:123:G:O2'	58:1:3412:HOH:O	2.09	0.69
1:1:2820:A:OP2	17:N:2:ARG:NH2	2.25	0.69
1:1:987:C:O2'	1:1:1000:A:N3	2.23	0.69
1:1:2581:G:OP2	1:1:2581:G:N2	2.22	0.69
2:2:1077:G:O2'	2:2:1079:G:O6	2.09	0.69
8:C:183:GLU:OE1	8:C:183:GLU:N	2.25	0.69
1:1:985:C:O2	58:1:3411:HOH:O	2.08	0.69
1:1:2585:U:O4	5:5:76:A:H3'	1.92	0.69
2:2:352:C:O2	2:2:355:C:N4	2.25	0.69
3:3:76:G:O2'	3:3:77:U:O4'	2.10	0.69
13:J:41:LYS:NZ	13:J:50:THR:O	2.17	0.69
1:1:1065:U:O4	1:1:1074:G:O6	2.08	0.69
1:1:1096:A:N1	58:1:3440:HOH:O	2.24	0.69
1:1:2262:U:OP2	26:W:16:SER:OG	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:979:C:O2	48:s:59:ARG:NE	2.25	0.69
1:1:1117:C:OP1	58:1:3413:HOH:O	2.09	0.69
3:3:51:G:OP1	18:O:63:LYS:NZ	2.26	0.69
10:E:44:ILE:O	10:E:47:LYS:NZ	2.25	0.69
37:h:156:ARG:NH1	37:h:161:GLU:OE1	2.25	0.69
1:1:2578:G:N2	8:C:130:GLN:OE1	2.25	0.69
2:2:1355:G:OP2	58:2:1806:HOH:O	2.10	0.69
2:2:1027:C:O2'	2:2:1034:G:N2	2.25	0.69
43:n:115:LYS:NZ	43:n:121:ALA:O	2.20	0.69
1:1:714:U:OP1	49:t:89:ARG:NH1	2.25	0.69
1:1:981:A:OP2	1:1:982:C:N4	2.25	0.69
1:1:2278:A:OP1	16:M:10:ARG:NH2	2.25	0.69
3:3:15:A:O2'	3:3:16:G:O5'	2.06	0.69
5:5:43:G:H2'	5:5:44:G:C8	2.27	0.69
41:l:15:ASP:OD1	41:l:19:GLY:N	2.26	0.69
48:s:2:ALA:O	48:s:7:LYS:NZ	2.25	0.69
1:1:1416:G:O2'	1:1:1417:C:O5'	2.10	0.69
1:1:1912:A:O2'	2:2:1494:G:O2'	2.10	0.69
1:1:1190:G:OP1	15:L:30:THR:OG1	2.09	0.69
13:J:12:LYS:NZ	13:J:14:ASP:OD1	2.26	0.69
13:J:135:GLN:OE1	13:J:135:GLN:N	2.26	0.69
51:v:58:VAL:HG13	51:v:79:VAL:HG23	1.75	0.69
1:1:239:C:O2'	1:1:622:G:O2'	2.10	0.68
43:n:65:ILE:HD13	43:n:79:ILE:HG23	1.75	0.68
20:Q:66:ASN:OD1	20:Q:70:ARG:NH1	2.26	0.68
1:1:1011:G:OP2	20:Q:66:ASN:ND2	2.25	0.68
2:2:1141:C:O2'	2:2:1142:G:O5'	2.10	0.68
1:1:3:U:OP1	58:1:3415:HOH:O	2.11	0.68
1:1:2128:G:N3	1:1:2173:A:O2'	2.26	0.68
2:2:1473:G:OP1	58:2:1808:HOH:O	2.11	0.68
1:1:2134:A:N6	1:1:2156:G:O2'	2.27	0.68
2:2:701:U:OP1	2:2:702:A:O2'	2.11	0.68
18:O:8:ILE:O	18:O:12:THR:HG23	1.94	0.68
53:x:52:HIS:NE2	53:x:54:GLY:O	2.26	0.68
1:1:2175:C:OP1	58:1:3414:HOH:O	2.10	0.68
49:t:44:ALA:O	49:t:47:LYS:NZ	2.27	0.68
1:1:887:A:O2'	1:1:889:C:OP2	2.11	0.68
1:1:2785:C:O3'	8:C:70:LYS:NZ	2.26	0.68
2:2:197:A:N1	2:2:220:G:O2'	2.27	0.68
1:1:265:A:N1	1:1:427:U:O2'	2.26	0.67
1:1:301:G:OP2	24:U:82:ARG:NH2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2365:G:N7	34:e:39:LYS:NZ	2.42	0.67
1:1:369:U:OP2	58:1:3416:HOH:O	2.11	0.67
1:1:265:A:O2'	1:1:428:A:N6	2.26	0.67
2:2:283:U:OP1	58:2:1807:HOH:O	2.11	0.67
19:P:102:GLU:N	19:P:102:GLU:OE2	2.27	0.67
1:1:1109:C:O2'	1:1:1110:G:O4'	2.12	0.67
2:2:1322:C:O2'	2:2:1323:G:OP2	2.11	0.67
14:K:71:ARG:NH2	14:K:123:LEU:O	2.27	0.67
46:q:46:ASN:ND2	46:q:89:0TD:OD1	2.27	0.67
1:1:2126:A:O2'	1:1:2162:G:N2	2.26	0.67
2:2:1527:U:OP2	55:z:42:THR:OG1	2.03	0.67
10:E:126:GLY:O	10:E:158:THR:OG1	2.10	0.67
32:c:32:GLU:OE1	32:c:32:GLU:N	2.28	0.67
1:1:320:A:N3	9:D:163:ASN:ND2	2.42	0.67
1:1:517:C:OP1	31:b:13:ARG:NH2	2.28	0.67
1:1:1079:C:OP1	58:1:3417:HOH:O	2.12	0.67
1:1:1266:G:OP1	31:b:16:ARG:NE	2.28	0.67
1:1:2728:U:OP2	58:1:3418:HOH:O	2.13	0.67
1:1:2405:G:O2'	1:1:2406:A:OP1	2.12	0.66
2:2:923:A:O2'	2:2:1399:C:OP2	2.12	0.66
2:2:1171:A:OP2	58:2:1812:HOH:O	2.13	0.66
1:1:2478:A:OP2	35:f:2:LYS:NZ	2.28	0.66
32:c:9:ILE:HD12	32:c:51:GLU:HG3	1.77	0.66
1:1:69:C:O2	1:1:73:A:O2'	2.11	0.66
1:1:575:A:OP2	1:1:2499:C:O2'	2.13	0.66
1:1:1174:U:O2'	1:1:1177:G:N7	2.26	0.66
3:3:48:U:OP1	18:O:30:ARG:NH2	2.27	0.66
20:Q:72:ASN:OD1	20:Q:107:THR:HG22	1.94	0.66
2:2:403:C:OP2	38:i:71:GLN:NE2	2.29	0.66
1:1:574:A:N6	1:1:2034:U:OP1	2.29	0.66
1:1:2553:G:O2'	58:1:3420:HOH:O	2.14	0.66
2:2:297:G:O6	58:2:1809:HOH:O	2.12	0.66
1:1:2052:A:O2'	8:C:148:GLN:O	2.10	0.66
2:2:359:G:OP2	58:2:1810:HOH:O	2.12	0.66
11:F:22:GLN:NE2	11:F:38:ASN:O	2.29	0.66
2:2:835:U:OP1	52:w:53:ARG:NH2	2.28	0.66
5:5:9:A:O2'	5:5:45:G:N2	2.28	0.66
2:2:626:G:O3'	50:u:51:ARG:NH2	2.29	0.65
2:2:1157:A:N7	2:2:1180:A:N6	2.44	0.65
7:B:71:LYS:O	7:B:118:SER:OG	2.13	0.65
49:t:29:VAL:HG21	49:t:81:LEU:HD21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:117:G:OP2	1:1:119:A:O2'	2.12	0.65
1:1:966:G:O4'	1:1:2267:A:N6	2.29	0.65
1:1:2266:A:N6	1:1:2273:A:OP2	2.29	0.65
37:h:73:PRO:HA	37:h:76:VAL:HG22	1.78	0.65
49:t:26:GLU:OE1	49:t:77:ARG:NH2	2.29	0.65
1:1:636:G:OP1	15:L:129:LYS:NZ	2.29	0.65
3:3:76:G:O2'	3:3:77:U:O5'	2.11	0.65
37:h:43:LEU:HD12	37:h:55:ILE:HD11	1.77	0.65
1:1:2124:G:N2	1:1:2172:U:OP1	2.30	0.65
10:E:62:GLY:O	10:E:95:ARG:NH2	2.30	0.65
22:S:34:ASP:OD2	22:S:35:ILE:N	2.29	0.65
36:g:29:PRO:O	36:g:45:LYS:NZ	2.28	0.65
8:C:131:ASP:O	8:C:136:ASN:ND2	2.29	0.65
1:1:1124:G:N3	35:f:37:GLN:NE2	2.45	0.65
1:1:1535:A:N6	58:1:3450:HOH:O	2.30	0.65
2:2:1095:U:OP1	2:2:1108:G:N2	2.28	0.65
1:1:889:C:OP2	58:1:3422:HOH:O	2.14	0.65
18:O:48:LEU:O	18:O:85:LYS:NZ	2.29	0.65
2:2:362:G:N2	2:2:365:U:OP2	2.30	0.65
1:1:675:A:O2'	9:D:62:GLN:OE1	2.14	0.64
27:X:6:GLN:OE1	27:X:50:ARG:N	2.30	0.64
15:L:123:ARG:NE	15:L:143:GLU:OE2	2.30	0.64
2:2:285:C:O2'	58:2:1816:HOH:O	2.15	0.64
37:h:40:ARG:NH1	37:h:55:ILE:O	2.30	0.64
1:1:95:A:O2'	28:Y:41:HIS:ND1	2.26	0.64
1:1:621:A:OP2	15:L:99:ASN:ND2	2.30	0.64
2:2:91:U:OP2	58:2:1813:HOH:O	2.14	0.64
2:2:1377:A:C6	41:l:7:ILE:HD11	2.32	0.64
44:o:45:ARG:NH1	44:o:47:GLU:OE1	2.30	0.64
2:2:1482:G:OP2	58:2:1814:HOH:O	2.14	0.64
44:o:51:VAL:HG13	48:s:81:ARG:HB2	1.80	0.64
1:1:2519:U:O4'	1:1:2542:A:N6	2.31	0.64
2:2:1152:A:OP1	44:o:70:HIS:ND1	2.29	0.64
2:2:201:G:O2'	2:2:469:C:O2'	2.05	0.64
2:2:1321:U:O2'	53:x:78:ARG:NH1	2.30	0.64
11:F:89:LEU:O	11:F:129:THR:OG1	2.14	0.64
41:l:45:SER:O	41:l:49:THR:HG23	1.97	0.64
1:1:276:U:O2'	1:1:277:G:N7	2.31	0.64
1:1:2635:A:O2'	8:C:81:GLU:OE1	2.15	0.64
1:1:1799:G:OP1	7:B:258:ARG:NH1	2.30	0.64
1:1:1844:C:O3'	7:B:256:LYS:NZ	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2874:C:OP1	17:N:4:ARG:NH1	2.31	0.64
5:5:33:U:N3	5:5:36:G:OP2	2.31	0.64
7:B:66:ASP:OD2	7:B:102:ARG:NH1	2.31	0.64
20:Q:26:GLY:O	20:Q:30:ARG:NH1	2.31	0.64
53:x:30:PRO:HA	53:x:48:THR:HG23	1.80	0.64
1:1:428:A:O2'	1:1:429:A:O5'	2.16	0.63
1:1:1090:A:O2'	58:1:3427:HOH:O	2.15	0.63
1:1:1681:G:O2'	1:1:1762:A:N3	2.28	0.63
1:1:2865:U:OP2	1:1:2866:U:O2'	2.06	0.63
1:1:2878:U:O4	58:1:3419:HOH:O	2.13	0.63
2:2:1368:A:OP1	43:n:113:ARG:NH2	2.31	0.63
5:5:23:C:H2'	5:5:24:G:C8	2.33	0.63
50:u:19:VAL:HG21	50:u:52:LEU:CD2	2.28	0.63
8:C:156:PHE:CE1	13:J:81:ILE:HD13	2.33	0.63
47:r:18:ALA:O	47:r:21:SER:OG	2.10	0.63
2:2:408:A:OP1	38:i:8:LYS:NZ	2.31	0.63
43:n:63:LEU:HD21	43:n:65:ILE:HD11	1.80	0.63
1:1:896:A:O2'	1:1:897:C:OP2	2.08	0.63
1:1:1559:U:O4	58:1:3423:HOH:O	2.15	0.63
1:1:2816:G:N3	1:1:2883:A:O2'	2.30	0.63
1:1:692:C:OP2	58:1:3425:HOH:O	2.15	0.63
38:i:140:ASN:N	38:i:182:PHE:O	2.32	0.63
1:1:188:G:O2'	58:1:3426:HOH:O	2.15	0.63
1:1:2467:C:O2	16:M:123:LYS:NZ	2.30	0.63
2:2:811:C:O2'	2:2:901:A:N1	2.31	0.63
5:5:7:G:OP1	5:5:16:C:N4	2.32	0.63
2:2:958:A:N3	2:2:985:C:O2'	2.30	0.63
2:2:1070:U:O3'	39:j:54:ARG:NH2	2.31	0.63
1:1:1094:U:N3	1:1:1097:U:OP2	2.32	0.63
2:2:83:C:O2'	2:2:86:G:N1	2.31	0.63
2:2:374:A:O3'	50:u:70:ARG:NH2	2.31	0.63
39:j:100:SER:O	39:j:103:THR:HG22	1.99	0.62
2:2:1099:G:O2'	55:z:69:ARG:NH1	2.31	0.62
5:5:18:G:H1	5:5:55:U:H6	1.45	0.62
6:A:165:ASN:OD1	6:A:166:ASP:N	2.32	0.62
1:1:2013:A:N6	1:1:2014:A:N1	2.47	0.62
10:E:115:ARG:NH2	58:E:202:HOH:O	2.25	0.62
40:k:81:ASN:OD1	40:k:83:ALA:N	2.32	0.62
1:1:675:A:N3	1:1:2443:C:O2'	2.31	0.62
2:2:24:U:HO2'	2:2:524:G:HO2'	1.48	0.62
1:1:1475:G:O2'	1:1:1514:G:O6	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:427:U:OP2	2:2:428:G:O2'	2.12	0.62
50:u:5:ARG:NH2	50:u:27:ALA:O	2.32	0.62
2:2:1310:G:OP2	47:r:87:ARG:NH2	2.32	0.62
1:1:591:U:HO2'	34:e:2:PRO:N	1.97	0.62
1:1:1044:C:N4	58:1:3453:HOH:O	2.31	0.62
1:1:1437:C:O2'	1:1:1516:G:O2'	2.08	0.62
1:1:2249:U:N3	1:1:2253:G:OP2	2.31	0.62
3:3:8:C:O3'	18:O:25:ARG:NH2	2.33	0.62
8:C:179:ARG:HB3	8:C:188:LEU:HD13	1.82	0.62
37:h:131:ARG:NH2	39:j:55:GLU:OE2	2.31	0.62
2:2:1047:G:HO2'	2:2:1215:G:HO2'	1.46	0.62
48:s:24:ARG:HH11	48:s:51:LEU:HD23	1.65	0.62
1:1:324:A:N6	1:1:339:U:O4'	2.33	0.62
2:2:677:U:O2	2:2:777:A:O2'	2.18	0.62
27:X:43:GLU:OE2	27:X:45:ARG:NH2	2.33	0.62
1:1:545:U:O2'	1:1:548:G:O6	2.05	0.62
1:1:643:A:N1	32:c:44:ARG:NE	2.47	0.62
2:2:31:G:O2'	2:2:48:C:N4	2.31	0.62
38:i:138:SER:OG	38:i:141:ASP:OD2	2.16	0.62
37:h:164:ARG:NE	37:h:166:GLU:OE2	2.33	0.61
3:3:43:C:O2	10:E:92:ARG:NH1	2.31	0.61
39:j:13:GLU:HB3	39:j:39:VAL:HG12	1.82	0.61
51:v:23:VAL:HG11	51:v:61:ILE:HD13	1.82	0.61
1:1:2595:G:N2	1:1:2598:A:OP2	2.29	0.61
2:2:84:U:O4	2:2:87:C:O2'	2.18	0.61
38:i:147:GLU:N	38:i:147:GLU:OE1	2.34	0.61
1:1:1600:C:OP1	23:T:81:LYS:NZ	2.33	0.61
1:1:2523:G:HO2'	1:1:2764:A:HO2'	1.48	0.61
1:1:1469:A:OP2	1:1:1522:A:N6	2.33	0.61
2:2:187:G:N2	2:2:190:A:OP2	2.33	0.61
2:2:1270:G:N7	58:2:1827:HOH:O	2.31	0.61
1:1:1730:C:O2	1:1:1731:G:N1	2.33	0.61
2:2:185:U:O4'	54:y:69:LYS:NZ	2.26	0.61
37:h:11:ARG:NH1	37:h:177:THR:O	2.34	0.61
49:t:29:VAL:CG2	49:t:81:LEU:HD21	2.31	0.61
1:1:1155:A:O3'	20:Q:55:ARG:NH2	2.34	0.61
2:2:181:A:N6	2:2:195:A:OP2	2.34	0.61
9:D:144:GLU:OE1	9:D:144:GLU:N	2.33	0.61
1:1:290:U:O2	1:1:350:G:O6	2.17	0.61
44:o:52:LEU:O	48:s:81:ARG:NH1	2.34	0.61
1:1:90:U:OP2	1:1:91:A:O2'	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2065:C:O2	1:1:2446:G:N2	2.33	0.61
2:2:944:G:N1	2:2:1338:G:OP2	2.31	0.61
7:B:157:SER:OG	7:B:160:THR:HG23	2.01	0.61
50:u:42:ILE:O	50:u:42:ILE:HG23	2.01	0.61
2:2:1183:U:O2'	2:2:1185:G:OP2	2.19	0.60
1:1:483:A:OP1	24:U:47:LYS:NZ	2.34	0.60
10:E:111:ILE:HD11	10:E:114:PHE:HD1	1.66	0.60
1:1:1339:G:OP1	23:T:82:LYS:NZ	2.33	0.60
2:2:380:G:O6	58:2:1811:HOH:O	2.13	0.60
53:x:56:GLN:NE2	53:x:57:HIS:O	2.34	0.60
1:1:931:U:OP1	29:Z:30:ARG:NH2	2.35	0.60
1:1:1534:U:O2'	1:1:1537:G:O6	2.17	0.60
2:2:1291:U:OP1	41:l:37:SER:OG	2.16	0.60
1:1:299:A:N3	1:1:319:G:O2'	2.28	0.60
1:1:2596:U:O2'	7:B:241:GLY:O	2.20	0.60
2:2:123:U:OP1	2:2:311:C:O2'	2.19	0.60
1:1:2653:U:OP2	1:1:2654:A:O2'	2.12	0.60
2:2:492:C:H4'	2:2:493:A:OP1	2.01	0.60
2:2:327:A:O2'	2:2:328:C:O4'	2.18	0.60
2:2:828:U:OP1	42:m:22:LYS:NZ	2.23	0.60
2:2:875:U:O2'	42:m:15:ARG:NH1	2.34	0.60
37:h:8:ASN:ND2	48:s:90:ARG:O	2.34	0.60
1:1:730:A:OP1	1:1:1775:U:O2'	2.14	0.60
12:G:47:PHE:O	12:G:52:ALA:N	2.35	0.60
13:J:13:ARG:NH2	13:J:49:ASP:OD1	2.33	0.60
1:1:698:C:O2'	1:1:734:A:N6	2.35	0.60
19:P:24:ASP:OD1	19:P:90:GLY:N	2.34	0.60
40:k:12:PRO:O	40:k:15:SER:OG	2.18	0.60
50:u:19:VAL:HG22	50:u:37:GLY:C	2.27	0.60
1:1:2099:U:O2	1:1:2190:G:O6	2.19	0.59
1:1:2125:G:OP2	58:1:3424:HOH:O	2.15	0.59
2:2:719:C:O2'	52:w:39:ILE:O	2.12	0.59
2:2:1130:A:H61	2:2:1144:G:H1'	1.67	0.59
11:F:107:LEU:O	11:F:152:ARG:NH2	2.35	0.59
1:1:714:U:OP2	49:t:88:ARG:NH1	2.35	0.59
1:1:2836:U:OP2	58:1:3428:HOH:O	2.17	0.59
1:1:534:U:O2'	20:Q:49:ASP:OD2	2.04	0.59
10:E:111:ILE:HG22	10:E:137:ILE:HG21	1.84	0.59
26:W:17:GLU:O	26:W:19:LYS:NZ	2.34	0.59
1:1:1614:A:N6	22:S:92:ARG:O	2.35	0.59
2:2:1029:U:O2'	2:2:1030:U:O3'	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:59:PRO:HG3	9:D:73:ILE:HD13	1.83	0.59
42:m:96:MET:HE3	42:m:130:ALA:HB1	1.84	0.59
1:1:818:G:N1	1:1:1188:U:OP2	2.32	0.59
1:1:1069:A:O2'	1:1:1073:A:N6	2.34	0.59
5:5:22:G:N7	5:5:46:G:N2	2.41	0.59
7:B:115:GLN:O	7:B:125:LYS:NZ	2.36	0.59
15:L:58:TYR:O	34:e:13:ARG:NH1	2.35	0.59
24:U:38:GLY:HA2	24:U:41:LEU:HD11	1.84	0.59
47:r:8:ASN:OD1	47:r:9:ILE:N	2.35	0.59
1:1:807:U:OP2	15:L:41:ARG:NH2	2.36	0.59
2:2:278:G:OP2	51:v:43:LYS:NZ	2.35	0.59
3:3:30:C:H1'	3:3:57:A:H61	1.67	0.59
5:5:56:C:O2'	10:E:75:ALA:N	2.33	0.59
1:1:1266:G:OP2	31:b:17:ARG:NH2	2.34	0.59
1:1:1912:A:HO2'	2:2:1494:G:HO2'	1.39	0.59
2:2:87:C:O2'	2:2:88:U:O4'	2.20	0.59
17:N:24:MET:HG2	17:N:44:LEU:HD22	1.83	0.59
1:1:388:G:O6	1:1:390:U:O2'	2.17	0.59
3:3:24:G:N3	3:3:27:C:N4	2.42	0.59
1:1:546:U:O2'	1:1:547:A:OP2	2.16	0.59
1:1:1114:C:H2'	1:1:1115:G:H5'	1.83	0.59
1:1:2204:G:OP2	7:B:147:LYS:NZ	2.36	0.59
2:2:102:G:OP2	54:y:5:LYS:NZ	2.28	0.59
2:2:924:C:O2'	2:2:1502:A:N1	2.35	0.59
2:2:545:C:OP1	38:i:58:LYS:NZ	2.36	0.58
4:4:14:U:H3'	4:4:15:G:N7	2.18	0.58
19:P:24:ASP:O	19:P:47:VAL:HG12	2.03	0.58
21:R:28:ALA:O	21:R:63:VAL:HG21	2.02	0.58
22:S:27:LYS:O	22:S:71:VAL:HG12	2.03	0.58
37:h:26:THR:HG23	48:s:76:LYS:HD2	1.85	0.58
47:r:39:ILE:HD12	47:r:56:LEU:HD21	1.86	0.58
1:1:627:A:O4'	1:1:637:A:N6	2.36	0.58
2:2:1000:A:N6	2:2:1041:G:O6	2.36	0.58
22:S:74:ILE:HG22	22:S:105:VAL:HG22	1.85	0.58
43:n:88:MET:HE1	43:n:98:LEU:HB2	1.86	0.58
2:2:533:A:O2'	2:2:535:A:OP2	2.14	0.58
2:2:1080:A:H5''	39:j:21:VAL:HG21	1.86	0.58
25:V:35:GLU:OE1	25:V:35:GLU:N	2.36	0.58
43:n:128:SER:OG	43:n:129:LYS:N	2.36	0.58
1:1:1913:A:OP1	58:1:3430:HOH:O	2.17	0.58
2:2:483:C:OP2	2:2:484:G:O2'	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:25:U:O2	3:3:117:G:O2'	2.22	0.58
9:D:134:LEU:O	9:D:138:LEU:HD23	2.04	0.58
12:G:27:ARG:NH1	27:X:60:ASP:OD2	2.37	0.58
1:1:227:A:O2'	1:1:228:C:OP2	2.17	0.58
2:2:80:A:N1	2:2:90:C:N4	2.52	0.58
2:2:302:G:O2'	46:q:14:ARG:NH2	2.35	0.58
5:5:66:C:H2'	5:5:67:G:C8	2.39	0.58
10:E:37:ASN:OD1	10:E:38:MET:N	2.37	0.58
30:a:51:VAL:HG23	30:a:52:ALA:H	1.68	0.58
40:k:90:MET:HE1	52:w:23:TYR:OH	2.03	0.58
2:2:1078:U:N3	39:j:90:THR:HG21	2.19	0.58
1:1:1668:A:O2'	1:1:1674:G:N7	2.26	0.58
1:1:2548:U:O2'	14:K:4:GLU:OE1	2.22	0.58
23:T:48:GLN:OE1	23:T:55:VAL:N	2.36	0.58
1:1:13:A:O2'	1:1:15:G:N7	2.35	0.58
43:n:60:LYS:C	43:n:61:LEU:HD22	2.29	0.58
50:u:75:ILE:O	50:u:79:ASN:ND2	2.37	0.57
1:1:466:A:O3'	33:d:33:ARG:NH2	2.37	0.57
2:2:1118:U:H5''	43:n:106:ARG:HE	1.69	0.57
49:t:33:THR:HG22	49:t:63:ARG:HH11	1.69	0.57
1:1:685:A:O2'	1:1:773:U:O4	2.18	0.57
1:1:1365:A:N6	58:1:3426:HOH:O	2.37	0.57
2:2:1005:A:N6	2:2:1024:G:O2'	2.37	0.57
43:n:80:ARG:O	43:n:84:THR:HG23	2.04	0.57
37:h:138:VAL:HG23	37:h:149:ILE:HG23	1.85	0.57
2:2:1074:G:O2'	36:g:102:THR:OG1	2.23	0.57
49:t:25:THR:HG23	49:t:70:LEU:HD12	1.86	0.57
1:1:993:G:N3	21:R:91:GLN:NE2	2.53	0.57
46:q:99:ARG:NH2	46:q:105:SER:O	2.38	0.57
1:1:955:PSU:OP1	16:M:86:LYS:NZ	2.33	0.57
1:1:1029:A:N1	1:1:2465:C:O2'	2.26	0.57
1:1:1582:C:HO2'	1:1:1583:A:C1'	2.17	0.57
1:1:2683:C:OP1	19:P:51:ARG:NH2	2.38	0.57
2:2:664:G:H22	2:2:741:G:H1	1.52	0.57
3:3:15:A:HO2'	3:3:16:G:C5'	2.17	0.57
11:F:98:VAL:O	11:F:99:LYS:NZ	2.28	0.57
2:2:251:G:N7	58:2:1828:HOH:O	2.32	0.57
5:5:74:C:H2'	5:5:75:C:C6	2.40	0.57
9:D:21:ARG:O	9:D:114:ARG:NH2	2.37	0.57
47:r:52:GLN:O	47:r:55:THR:OG1	2.22	0.57
1:1:869:G:O3'	16:M:6:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1383:A:O2'	1:1:1384:A:O4'	2.15	0.56
2:2:993:G:OP2	58:2:1817:HOH:O	2.18	0.56
23:T:4:GLU:OE1	23:T:4:GLU:N	2.37	0.56
28:Y:46:VAL:O	28:Y:50:VAL:HG13	2.05	0.56
52:w:30:LYS:HA	52:w:33:ILE:HG22	1.86	0.56
2:2:375:U:H4'	50:u:6:LEU:HD12	1.86	0.56
2:2:859:G:OP2	2:2:869:G:N1	2.34	0.56
41:l:65:ALA:O	41:l:69:VAL:HG12	2.05	0.56
43:n:92:GLU:OE2	43:n:95:ARG:NH1	2.37	0.56
1:1:1012:U:OP2	20:Q:70:ARG:NH2	2.37	0.56
1:1:1065:U:N3	1:1:1074:G:N1	2.54	0.56
1:1:1067:A:O2'	1:1:1068:G:O4'	2.22	0.56
1:1:2566:A:N1	14:K:28:SER:OG	2.30	0.56
53:x:10:PHE:O	53:x:39:THR:HG22	2.04	0.56
1:1:453:A:N3	1:1:457:A:O2'	2.39	0.56
1:1:663:G:O3'	15:L:17:LYS:NZ	2.36	0.56
1:1:2522:U:O2'	1:1:2647:U:OP1	2.18	0.56
1:1:160:A:N3	1:1:2208:C:O2'	2.36	0.56
2:2:913:A:OP2	46:q:88:LYS:NZ	2.39	0.56
1:1:2880:C:O2'	17:N:90:ARG:NH2	2.38	0.56
2:2:1345:U:OP1	43:n:122:ARG:NH2	2.36	0.56
10:E:110:ARG:NH1	10:E:137:ILE:O	2.38	0.56
18:O:28:VAL:HG11	18:O:103:VAL:HG23	1.87	0.56
33:d:35:ARG:HG3	33:d:42:LEU:HD21	1.87	0.56
1:1:1088:A:N6	58:1:3466:HOH:O	2.39	0.56
1:1:1163:G:OP1	21:R:24:LYS:NZ	2.36	0.56
2:2:1383:C:HO2'	2:2:1384:C:P	2.25	0.56
2:2:1399:C:O2	2:2:1502:A:N6	2.39	0.56
30:a:16:CYS:SG	30:a:17:SER:N	2.78	0.56
37:h:135:LYS:NZ	58:h:301:HOH:O	2.32	0.56
38:i:60:LYS:O	38:i:64:ILE:HG23	2.06	0.56
1:1:65:U:O2'	1:1:456:C:N3	2.31	0.56
1:1:877:A:O2'	1:1:900:A:N6	2.39	0.56
1:1:1283:G:N1	1:1:1286:A:OP2	2.38	0.56
15:L:144:GLU:OE1	15:L:144:GLU:N	2.39	0.56
37:h:154:SER:OG	37:h:165:THR:HG22	2.04	0.56
49:t:21:ASP:O	49:t:22:THR:OG1	2.21	0.56
3:3:66:A:OP2	3:3:108:A:N6	2.35	0.56
21:R:4:VAL:HG12	21:R:40:MET:HB3	1.88	0.56
1:1:858:G:HO2'	1:1:2268:A:HO2'	1.49	0.56
45:p:29:ASN:OD1	45:p:30:THR:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1065:U:O2'	1:1:1066:U:O5'	2.24	0.55
2:2:24:U:O2'	2:2:524:G:O2'	2.20	0.55
2:2:373:A:N3	2:2:482:A:N6	2.54	0.55
39:j:99:ALA:HB1	39:j:103:THR:HG21	1.88	0.55
2:2:444:G:N1	2:2:491:G:O6	2.39	0.55
1:1:428:A:C2'	1:1:429:A:O5'	2.55	0.55
1:1:542:C:N4	1:1:543:G:O6	2.40	0.55
2:2:6:G:N2	39:j:103:THR:OG1	2.38	0.55
2:2:692:U:OP2	45:p:28:ASN:ND2	2.39	0.55
2:2:981:U:OP1	48:s:9:ARG:NH1	2.40	0.55
50:u:18:GLN:OE1	50:u:35:ARG:NE	2.37	0.55
1:1:274:C:H2'	1:1:275:C:C1'	2.37	0.55
2:2:673:A:H2'	2:2:674:G:C8	2.41	0.55
2:2:1047:G:O2'	2:2:1215:G:O2'	2.21	0.55
2:2:1187:G:N3	48:s:100:SER:OG	2.34	0.55
1:1:974:G:HO2'	1:1:975:A:P	2.27	0.55
1:1:2438:U:O2'	1:1:2440:C:OP1	2.23	0.55
1:1:2845:U:O3'	19:P:53:ARG:NH1	2.39	0.55
15:L:90:VAL:HG23	15:L:90:VAL:O	2.07	0.55
5:5:33:U:H5''	43:n:130:ARG:NH2	2.21	0.55
36:g:74:ARG:NH2	36:g:93:ASN:O	2.39	0.55
1:1:340:A:O2'	9:D:162:ARG:NH2	2.40	0.55
1:1:1962:5MC:O2'	1:1:1964:G:OP2	2.24	0.55
1:1:2141:G:O6	1:1:2150:C:N4	2.40	0.55
2:2:302:G:O3'	46:q:14:ARG:NH1	2.39	0.55
2:2:720:C:OP2	2:2:721:G:O2'	2.19	0.55
12:G:84:ALA:HB2	12:G:90:LEU:HD23	1.89	0.55
38:i:188:ARG:NH2	38:i:192:SER:O	2.37	0.55
1:1:585:G:N7	20:Q:6:ARG:NH2	2.53	0.55
2:2:501:C:OP1	46:q:114:ARG:NH2	2.36	0.55
29:Z:40:ASP:OD1	29:Z:45:ARG:NH1	2.40	0.55
42:m:8:ALA:O	42:m:12:THR:HG23	2.07	0.55
47:r:23:TYR:N	47:r:66:GLU:OE1	2.39	0.55
10:E:4:LEU:HD11	10:E:104:ILE:HD11	1.88	0.55
49:t:25:THR:CG2	49:t:70:LEU:HD12	2.37	0.54
50:u:6:LEU:CD2	50:u:19:VAL:HG12	2.38	0.54
10:E:105:THR:HB	30:a:22:MET:HE1	1.88	0.54
1:1:500:G:N1	1:1:503:A:OP2	2.39	0.54
15:L:124:GLY:O	15:L:125:LEU:HD23	2.08	0.54
37:h:91:VAL:HA	37:h:94:ILE:HG22	1.89	0.54
1:1:1475:G:O6	58:l:3429:HOH:O	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2102:G:C6	1:1:2188:U:N3	2.75	0.54
1:1:2313:C:O4'	10:E:37:ASN:ND2	2.40	0.54
4:4:14:U:H3'	4:4:15:G:C8	2.42	0.54
7:B:165:VAL:HG21	7:B:181:MET:HE1	1.88	0.54
52:w:41:PRO:O	52:w:45:THR:HG23	2.07	0.54
1:1:2253:G:N2	58:1:3477:HOH:O	2.41	0.54
5:5:9:A:O4'	5:5:46:G:H1'	2.07	0.54
8:C:8:LYS:HB2	8:C:201:LEU:HD11	1.88	0.54
10:E:105:THR:HG21	30:a:22:MET:HE1	1.88	0.54
12:G:80:ILE:HG22	12:G:81:ALA:N	2.23	0.54
36:g:19:GLN:HE22	36:g:38:VAL:HG22	1.72	0.54
46:q:46:ASN:OD1	46:q:47:SER:N	2.40	0.54
1:1:30:G:O2'	1:1:1214:A:N3	2.37	0.54
1:1:859:G:O2'	1:1:916:G:O6	2.21	0.54
5:5:74:C:O2'	5:5:75:C:H5'	2.08	0.54
1:1:2500:U:O2'	1:1:2504:PSU:OP1	2.23	0.54
7:B:205:LEU:HD12	7:B:210:ALA:CB	2.37	0.54
22:S:65:ASP:OD1	22:S:66:ILE:N	2.41	0.54
1:1:8:C:OP1	58:1:3431:HOH:O	2.19	0.54
1:1:1131:G:HO2'	1:1:2025:C:HO2'	1.43	0.54
1:1:1807:G:O2'	1:1:1809:A:N6	2.34	0.54
2:2:1266:G:N2	2:2:1269:A:OP2	2.30	0.54
5:5:27:C:H2'	5:5:28:C:H6	1.73	0.54
10:E:163:ASP:OD1	10:E:163:ASP:N	2.41	0.54
29:Z:7:ILE:CD1	29:Z:48:ILE:HD11	2.36	0.54
1:1:728:G:H3'	1:1:729:G:H5'	1.88	0.54
1:1:2193:G:HO2'	1:1:2194:U:P	2.30	0.54
1:1:2849:U:O4	19:P:21:ARG:NH1	2.40	0.54
2:2:667:G:N2	49:t:49:ASP:OD2	2.34	0.54
5:5:73:A:H4'	5:5:74:C:C5	2.42	0.54
16:M:1:MET:HE2	16:M:44:ARG:HG2	1.90	0.54
37:h:10:ILE:HG23	37:h:11:ARG:HD3	1.90	0.54
38:i:99:ASP:OD1	38:i:100:ASN:N	2.40	0.54
42:m:14:ILE:HG22	42:m:25:VAL:HG11	1.88	0.54
1:1:1909:C:H5'	5:5:12:G:OP1	2.07	0.54
42:m:75:ILE:HG22	42:m:129:VAL:HG22	1.88	0.54
26:W:27:GLY:HA2	26:W:67:VAL:HG23	1.89	0.53
2:2:261:U:OP2	54:y:74:ARG:NH2	2.33	0.53
2:2:689:C:OP1	45:p:29:ASN:ND2	2.35	0.53
3:3:1:U:HO2'	3:3:2:G:H8	1.56	0.53
37:h:43:LEU:HD12	37:h:55:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:s:31:ILE:HD13	48:s:45:VAL:HG23	1.90	0.53
2:2:1518:MA6:H103	2:2:1519:MA6:N6	2.24	0.53
5:5:66:C:H2'	5:5:67:G:H8	1.73	0.53
10:E:111:ILE:HD11	10:E:114:PHE:CD1	2.42	0.53
37:h:106:VAL:O	37:h:106:VAL:HG23	2.07	0.53
37:h:131:ARG:NE	37:h:168:TYR:OH	2.37	0.53
39:j:164:ILE:O	42:m:114:ARG:NH2	2.41	0.53
1:1:1798:U:OP2	7:B:271:ARG:NH2	2.36	0.53
1:1:2390:U:O5'	34:e:35:LYS:NZ	2.39	0.53
5:5:24:G:H2'	5:5:25:C:C6	2.43	0.53
17:N:103:ARG:NH2	17:N:106:ASP:OD2	2.41	0.53
41:l:126:ASP:O	41:l:131:LYS:N	2.40	0.53
1:1:262:A:N3	1:1:430:A:O2'	2.35	0.53
2:2:925:G:N2	2:2:1503:A:OP1	2.40	0.53
2:2:978:A:C2	2:2:1319:A:C4	2.96	0.53
11:F:22:GLN:OE1	11:F:55:ARG:NH1	2.42	0.53
14:K:106:GLU:OE1	14:K:106:GLU:N	2.42	0.53
19:P:89:ARG:O	19:P:113:ARG:N	2.39	0.53
1:1:1997:C:OP2	8:C:129:THR:OG1	2.26	0.53
1:1:2780:G:OP2	13:J:120:ARG:NE	2.38	0.53
49:t:78:TYR:OH	49:t:89:ARG:O	2.26	0.53
1:1:329:G:OP2	24:U:69:ASN:ND2	2.37	0.53
1:1:584:C:N4	1:1:585:G:O6	2.42	0.53
2:2:662:U:O2'	2:2:836:G:OP1	2.26	0.53
26:W:33:ALA:N	26:W:64:ASP:OD1	2.38	0.53
1:1:1028:A:OP2	1:1:1126:A:N6	2.42	0.53
1:1:2640:G:OP1	13:J:95:ARG:NH1	2.42	0.53
58:1:3455:HOH:O	5:5:76:A:H3'	2.07	0.53
3:3:12:C:O2'	26:W:74:PRO:O	2.22	0.53
10:E:105:THR:CG2	30:a:22:MET:HE1	2.39	0.53
22:S:72:THR:OG1	22:S:106:VAL:O	2.21	0.53
1:1:998:C:OP2	20:Q:58:ARG:NH2	2.40	0.53
1:1:1006:C:O4'	13:J:30:THR:OG1	2.27	0.53
2:2:83:C:O2	2:2:86:G:N1	2.42	0.53
2:2:544:G:OP2	38:i:63:ARG:NH2	2.41	0.53
2:2:1516:2MG:N2	2:2:1519:MA6:OP2	2.42	0.53
16:M:17:ASN:O	16:M:38:ARG:NH1	2.42	0.53
42:m:12:THR:HG22	42:m:15:ARG:HH12	1.74	0.53
1:1:996:A:OP2	20:Q:93:LYS:NZ	2.36	0.53
8:C:4:LEU:HD12	8:C:32:ASN:ND2	2.24	0.53
37:h:7:PRO:HA	37:h:10:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:8:LYS:HB3	38:i:21:LEU:HD23	1.89	0.53
38:i:187:GLU:OE1	38:i:187:GLU:N	2.42	0.53
45:p:17:SER:O	45:p:81:ASN:N	2.40	0.53
1:1:1857:G:O2'	1:1:1858:A:OP2	2.25	0.52
2:2:441:A:H61	2:2:494:G:H22	1.57	0.52
2:2:972:C:OP2	44:o:59:LYS:NZ	2.41	0.52
5:5:12:G:H2'	5:5:13:C:O4'	2.10	0.52
9:D:108:ILE:HD11	9:D:180:LEU:HD12	1.91	0.52
1:1:2193:G:O2'	1:1:2194:U:P	2.67	0.52
1:1:2901:C:H3'	1:1:2902:C:H6	1.75	0.52
2:2:1083:U:O2'	2:2:1102:A:OP2	2.26	0.52
10:E:105:THR:CB	30:a:22:MET:HE1	2.38	0.52
17:N:106:ASP:N	17:N:106:ASP:OD1	2.41	0.52
27:X:40:VAL:O	27:X:40:VAL:HG13	2.08	0.52
1:1:81:G:O2'	1:1:295:G:O2'	2.28	0.52
1:1:1024:G:OP2	1:1:1025:G:O2'	2.17	0.52
9:D:171:ASP:OD1	9:D:172:ALA:N	2.41	0.52
1:1:605:G:OP1	9:D:99:LYS:NZ	2.43	0.52
1:1:1050:A:C2'	1:1:1051:G:O5'	2.58	0.52
2:2:970:C:N4	43:n:130:ARG:OXT	2.42	0.52
39:j:52:LYS:O	39:j:62:LYS:NZ	2.29	0.52
43:n:84:THR:HG21	43:n:103:PHE:HB3	1.91	0.52
1:1:577:G:O2'	1:1:1254:A:OP1	2.28	0.52
2:2:130:A:O2'	2:2:131:A:O5'	2.26	0.52
1:1:1009:A:OP2	13:J:39:LYS:NZ	2.43	0.52
37:h:77:ILE:HA	37:h:84:VAL:HG13	1.91	0.52
1:1:1668:A:N3	1:1:1670:C:N4	2.58	0.52
1:1:2468:A:P	1:1:2476:A:H61	2.33	0.52
3:3:113:C:O2'	18:O:46:GLU:OE1	2.24	0.52
19:P:47:VAL:HG13	19:P:47:VAL:O	2.09	0.52
1:1:882:G:N2	1:1:895:U:O4'	2.43	0.52
1:1:2079:U:O2'	27:X:23:ASN:OD1	2.26	0.52
3:3:23:G:O2'	3:3:24:G:O4'	2.28	0.52
5:5:18:G:N2	5:5:58:A:O5'	2.41	0.52
28:Y:6:LEU:HD13	28:Y:9:LYS:HD2	1.92	0.52
1:1:637:A:N1	1:1:651:G:O2'	2.40	0.52
1:1:2652:C:H2'	1:1:2653:U:O4'	2.09	0.52
2:2:713:G:H2'	2:2:714:G:C8	2.45	0.52
3:3:76:G:HO2'	3:3:77:U:P	2.33	0.52
7:B:71:LYS:NZ	7:B:100:GLU:OE1	2.43	0.52
8:C:34:VAL:HG22	8:C:50:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:90:LEU:HD11	12:G:146:VAL:HG21	1.91	0.52
1:1:1028:A:N3	1:1:2486:C:O2'	2.34	0.51
1:1:2344:U:C6	32:c:36:LEU:HD11	2.45	0.51
2:2:4:U:O2'	2:2:5:U:OP1	2.21	0.51
2:2:424:G:H2'	2:2:425:G:C8	2.45	0.51
2:2:1239:A:H62	2:2:1299:A:N6	2.09	0.51
12:G:51:ARG:HE	12:G:54:LEU:HD21	1.75	0.51
14:K:70:ARG:HG2	14:K:76:VAL:HG12	1.92	0.51
24:U:11:VAL:HG12	24:U:72:ILE:HA	1.92	0.51
26:W:18:ALA:O	26:W:20:ARG:NH1	2.42	0.51
1:1:597:G:N2	15:L:12:SER:O	2.42	0.51
2:2:8:A:N1	39:j:112:ARG:NH1	2.58	0.51
9:D:117:ARG:NH1	15:L:1:MET:O	2.42	0.51
47:r:46:SER:O	47:r:47:GLU:C	2.53	0.51
1:1:565:C:OP2	21:R:80:ARG:N	2.38	0.51
1:1:672:C:H2'	1:1:673:C:C6	2.45	0.51
1:1:1724:G:N1	1:1:1736:U:O2'	2.41	0.51
1:1:1798:U:OP2	7:B:270:ARG:NH2	2.43	0.51
9:D:153:LEU:HD11	9:D:158:PHE:HB2	1.93	0.51
17:N:8:ARG:N	17:N:43:GLU:OE2	2.43	0.51
29:Z:41:THR:HG22	29:Z:43:ALA:H	1.74	0.51
39:j:99:ALA:CB	39:j:103:THR:HG21	2.40	0.51
2:2:579:A:O2'	49:t:54:ARG:NH1	2.43	0.51
19:P:89:ARG:NH2	19:P:113:ARG:O	2.44	0.51
51:v:59:VAL:HG22	51:v:60:GLU:N	2.26	0.51
1:1:445:C:H2'	1:1:446:G:O4'	2.10	0.51
1:1:468:G:N7	33:d:39:ARG:NH2	2.55	0.51
1:1:498:G:H2'	1:1:499:U:C1'	2.41	0.51
1:1:641:U:O2'	1:1:2350:C:OP1	2.28	0.51
1:1:1043:C:H2'	1:1:1044:C:C1'	2.41	0.51
1:1:1901:A:OP2	7:B:253:LYS:NZ	2.42	0.51
2:2:253:A:N6	2:2:274:A:N1	2.58	0.51
2:2:512:U:OP1	38:i:44:ARG:NH1	2.44	0.51
2:2:855:U:OP2	2:2:871:U:N3	2.34	0.51
32:c:25:LYS:NZ	32:c:30:LYS:O	2.42	0.51
36:g:9:MET:HE2	36:g:9:MET:HA	1.92	0.51
1:1:2489:U:H2'	1:1:2490:G:O4'	2.10	0.51
2:2:1458:G:HO2'	54:y:23:SER:HG	1.55	0.51
27:X:39:TRP:NE1	27:X:41:GLU:OE1	2.41	0.51
1:1:487:C:H42	1:1:492:A:H61	1.59	0.51
1:1:2091:C:OP2	1:1:2092:U:O2'	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:125:TYR:OH	13:J:132:HIS:NE2	2.35	0.51
17:N:28:LEU:HD22	17:N:44:LEU:HD21	1.92	0.51
21:R:34:GLU:N	21:R:34:GLU:OE1	2.44	0.51
46:q:21:VAL:HG23	46:q:95:TYR:CE1	2.45	0.51
5:5:5:A:N6	5:5:69:G:O6	2.44	0.51
7:B:157:SER:HG	7:B:160:THR:HG23	1.75	0.51
21:R:31:GLU:OE1	21:R:31:GLU:N	2.44	0.51
30:a:26:SER:OG	30:a:27:THR:N	2.43	0.51
41:l:69:VAL:HG22	41:l:69:VAL:O	2.11	0.51
37:h:29:PHE:O	37:h:33:LEU:HD23	2.10	0.51
44:o:69:THR:HG23	44:o:69:THR:O	2.11	0.51
1:1:1528:A:OP2	1:1:1543:G:N2	2.43	0.51
1:1:1872:A:N6	58:1:3474:HOH:O	2.40	0.51
2:2:686:U:O2'	2:2:687:A:OP2	2.29	0.51
17:N:73:ASN:HA	17:N:76:VAL:HG12	1.93	0.51
47:r:19:LEU:HD21	47:r:33:ILE:HG21	1.93	0.51
1:1:184:C:O2'	1:1:217:A:N3	2.42	0.50
36:g:76:ALA:HB2	36:g:210:VAL:HG11	1.93	0.50
48:s:24:ARG:NH1	48:s:51:LEU:HD23	2.25	0.50
1:1:1654:A:O2'	8:C:118:PHE:O	2.27	0.50
1:1:1999:C:O2	1:1:2687:U:O2'	2.28	0.50
1:1:2167:U:C2	1:1:2170:A:N7	2.79	0.50
2:2:898:G:N2	2:2:901:A:OP2	2.40	0.50
2:2:922:G:OP2	58:2:1818:HOH:O	2.19	0.50
5:5:36:G:O2'	5:5:37:G:O4'	2.30	0.50
44:o:25:ILE:HD11	44:o:92:LEU:HD21	1.92	0.50
1:1:587:C:O2	15:L:33:ARG:NH1	2.43	0.50
1:1:813:U:O2'	1:1:1225:G:O2'	2.25	0.50
1:1:2642:G:OP2	13:J:85:LYS:NZ	2.45	0.50
1:1:2723:C:OP1	8:C:114:LYS:NZ	2.34	0.50
2:2:580:C:H2'	2:2:581:G:O4'	2.11	0.50
3:3:7:G:O2'	18:O:38:GLN:NE2	2.45	0.50
54:y:42:GLY:HA2	54:y:86:LEU:HD11	1.92	0.50
1:1:630:G:N2	1:1:633:A:OP2	2.41	0.50
1:1:1024:G:HO2'	1:1:1144:A:HO2'	1.60	0.50
1:1:2122:U:O3'	1:1:2123:G:O4'	2.28	0.50
16:M:11:LYS:NZ	16:M:87:GLY:O	2.37	0.50
18:O:43:ASN:OD1	18:O:46:GLU:N	2.45	0.50
48:s:16:LEU:HD21	48:s:52:PRO:HB2	1.93	0.50
1:1:332:A:O2'	1:1:334:C:OP2	2.29	0.50
1:1:672:C:H2'	1:1:673:C:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1053:G:N2	58:2:1840:HOH:O	2.41	0.50
8:C:20:VAL:HG12	14:K:72:PRO:HB3	1.94	0.50
9:D:1:MET:HE1	9:D:19:PHE:C	2.36	0.50
36:g:4:VAL:HG21	36:g:9:MET:HE3	1.93	0.50
37:h:42:TYR:CZ	37:h:90:VAL:HG11	2.46	0.50
2:2:1027:C:OP2	2:2:1028:C:N4	2.45	0.50
2:2:1126:U:OP1	44:o:7:ARG:NH2	2.45	0.50
39:j:10:GLU:N	39:j:10:GLU:OE1	2.44	0.50
1:1:371:A:N6	1:1:402:A:OP2	2.45	0.50
1:1:2050:C:H2'	1:1:2051:A:O4'	2.12	0.50
5:5:27:C:H2'	5:5:28:C:C6	2.47	0.50
5:5:54:U:H2'	5:5:55:U:C2	2.46	0.50
11:F:103:ILE:HG22	11:F:105:LEU:CD2	2.42	0.50
13:J:31:GLU:OE2	13:J:34:ARG:NH1	2.45	0.50
18:O:41:ALA:HB3	18:O:43:ASN:HD22	1.76	0.50
49:t:12:VAL:HG21	49:t:22:THR:HG22	1.93	0.50
2:2:945:G:C2	2:2:946:A:C8	3.00	0.50
1:1:770:G:O3'	33:d:14:ARG:NH1	2.45	0.50
1:1:1900:A:O2'	1:1:1901:A:OP1	2.25	0.50
2:2:444:G:C6	2:2:491:G:O6	2.65	0.50
2:2:464:U:O2'	2:2:466:A:N7	2.34	0.50
2:2:550:G:O2'	46:q:116:LYS:NZ	2.45	0.50
2:2:1304:G:O3'	2:2:1305:G:O4'	2.29	0.50
49:t:81:LEU:HD12	49:t:85:LEU:HD23	1.93	0.50
1:1:379:G:N1	1:1:396:G:C6	2.80	0.49
1:1:394:C:H2'	1:1:395:U:O4'	2.12	0.49
1:1:1068:G:O2'	1:1:1096:A:N3	2.35	0.49
1:1:2291:U:O2'	1:1:2374:C:O2	2.29	0.49
1:1:2684:U:OP2	19:P:51:ARG:NH1	2.44	0.49
2:2:81:A:OP2	2:2:83:C:N4	2.41	0.49
5:5:1:C:N4	5:5:2:G:O6	2.44	0.49
11:F:24:ILE:HG21	11:F:72:LEU:HD21	1.94	0.49
34:e:7:VAL:HG23	34:e:7:VAL:O	2.11	0.49
38:i:29:ASP:OD2	38:i:30:THR:N	2.45	0.49
38:i:64:ILE:O	38:i:111:ARG:NH1	2.45	0.49
1:1:1062:G:H2'	1:1:1063:G:O4'	2.12	0.49
1:1:1866:A:H62	1:1:1875:G:H21	1.59	0.49
1:1:2503:2MA:O2'	1:1:2505:G:OP2	2.28	0.49
2:2:411:A:OP2	38:i:26:ARG:NH1	2.43	0.49
7:B:246:THR:HG22	7:B:250:VAL:HG12	1.93	0.49
11:F:18:LYS:HB2	11:F:25:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:114:LEU:O	36:g:114:LEU:HD23	2.12	0.49
1:1:300:A:O2'	1:1:318:C:O2	2.24	0.49
1:1:306:U:H2'	1:1:307:G:O4'	2.12	0.49
1:1:2555:U:O2'	58:1:3433:HOH:O	2.20	0.49
2:2:674:G:H21	45:p:118:HIS:HB2	1.77	0.49
2:2:1125:U:O2'	2:2:1126:U:O5'	2.27	0.49
3:3:29:A:H2'	3:3:30:C:O4'	2.12	0.49
11:F:78:GLY:O	11:F:82:GLY:N	2.45	0.49
13:J:17:VAL:HG13	13:J:137:PRO:HB2	1.94	0.49
14:K:121:GLU:OE2	19:P:65:SER:OG	2.20	0.49
33:d:29:GLN:OE1	33:d:33:ARG:NH1	2.45	0.49
46:q:54:ARG:HH11	46:q:64:THR:HG23	1.77	0.49
48:s:10:GLU:O	48:s:14:VAL:HG23	2.12	0.49
1:1:643:A:C2	32:c:44:ARG:NE	2.81	0.49
1:1:1379:U:O2'	1:1:1380:G:P	2.71	0.49
1:1:2618:G:H21	8:C:155:VAL:HG21	1.77	0.49
2:2:1074:G:O2'	2:2:1101:A:N1	2.40	0.49
2:2:1383:C:O2'	2:2:1384:C:P	2.69	0.49
8:C:73:VAL:HG12	8:C:74:GLU:N	2.27	0.49
12:G:57:LYS:N	12:G:57:LYS:HD3	2.27	0.49
18:O:36:TYR:HD1	18:O:52:SER:HG	1.59	0.49
20:Q:62:ILE:HD12	20:Q:76:TYR:CZ	2.47	0.49
30:a:36:VAL:O	30:a:36:VAL:HG13	2.13	0.49
43:n:63:LEU:CD2	43:n:65:ILE:HD11	2.42	0.49
1:1:693:A:O2'	1:1:1353:A:N3	2.40	0.49
1:1:1908:C:O2'	5:5:12:G:H5''	2.12	0.49
10:E:32:GLU:OE2	10:E:159:THR:N	2.45	0.49
43:n:62:ASP:OD1	43:n:63:LEU:N	2.45	0.49
44:o:32:THR:HG23	44:o:33:GLY:N	2.27	0.49
1:1:1062:G:H2'	1:1:1063:G:C8	2.47	0.49
1:1:1720:U:H2'	1:1:1721:G:O4'	2.13	0.49
1:1:2114:A:H62	1:1:2169:A:N6	2.10	0.49
14:K:24:VAL:HG13	14:K:33:ALA:HB2	1.94	0.49
38:i:124:MET:HE2	38:i:146:ARG:HE	1.77	0.49
50:u:6:LEU:HD23	50:u:19:VAL:HG12	1.95	0.49
1:1:321:U:OP1	9:D:130:LYS:NZ	2.38	0.49
1:1:631:A:N3	1:1:2415:G:O2'	2.40	0.49
2:2:405:U:O4	38:i:2:ALA:N	2.46	0.49
2:2:1052:U:O4	2:2:1200:C:O2'	2.17	0.49
37:h:111:LEU:O	37:h:204:LYS:NZ	2.40	0.49
1:1:1065:U:O2'	1:1:1066:U:P	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1416:G:O2'	1:1:1417:C:P	2.71	0.49
19:P:33:VAL:HG13	19:P:33:VAL:O	2.13	0.49
44:o:8:ILE:O	44:o:73:LEU:HD12	2.13	0.49
1:1:1:G:H2'	1:1:2:G:C8	2.47	0.49
1:1:1604:C:O2'	1:1:1610:A:N1	2.32	0.49
1:1:2102:G:N1	1:1:2188:U:N3	2.60	0.49
2:2:613:C:OP1	38:i:81:ARG:NH1	2.40	0.49
2:2:687:A:N6	2:2:701:U:O4'	2.46	0.49
2:2:1031:C:O5'	2:2:1032:G:N2	2.46	0.49
2:2:1319:A:C8	2:2:1323:G:C5	3.01	0.49
2:2:1328:C:O2'	47:r:29:ARG:NH2	2.46	0.49
36:g:185:ALA:HB3	36:g:196:VAL:HG21	1.94	0.49
1:1:998:C:OP1	20:Q:84:LYS:NZ	2.46	0.49
1:1:2124:G:O3'	6:A:217:THR:OG1	2.31	0.49
1:1:2655:G:O2'	1:1:2664:G:O6	2.20	0.49
2:2:563:A:O2'	2:2:566:G:O3'	2.31	0.49
2:2:978:A:N7	2:2:1318:A:N6	2.60	0.49
2:2:1432:G:O2'	2:2:1433:A:OP2	2.29	0.49
3:3:40:U:O2'	3:3:43:C:OP2	2.24	0.49
23:T:6:ARG:O	23:T:10:VAL:HG13	2.13	0.49
37:h:153:VAL:HG23	37:h:157:LEU:HD21	1.95	0.49
40:k:1:MET:N	40:k:1:MET:SD	2.82	0.49
1:1:2109:U:H2'	1:1:2110:G:C8	2.48	0.48
2:2:780:A:N6	58:2:1847:HOH:O	2.46	0.48
5:5:3:G:H1'	5:5:4:C:H5'	1.94	0.48
5:5:69:G:H2'	5:5:70:C:C6	2.48	0.48
10:E:158:THR:O	58:E:201:HOH:O	2.19	0.48
11:F:140:VAL:O	11:F:144:VAL:HG23	2.13	0.48
12:G:96:THR:HG23	12:G:97:ARG:CD	2.43	0.48
24:U:8:ASP:OD1	24:U:24:LYS:NZ	2.44	0.48
37:h:20:SER:OG	37:h:22:TRP:NE1	2.46	0.48
1:1:1019:U:O2'	1:1:1021:A:N7	2.35	0.48
2:2:20:U:H2'	2:2:21:G:O4'	2.13	0.48
5:5:10:G:H2'	5:5:11:C:C6	2.48	0.48
1:1:1073:A:N6	1:1:1074:G:O6	2.46	0.48
1:1:1754:A:O3'	19:P:103:ARG:NH2	2.45	0.48
2:2:1533:C:HO2'	2:2:1534:A:P	2.36	0.48
16:M:134:THR:HG23	16:M:134:THR:O	2.13	0.48
37:h:14:ILE:HG22	37:h:15:VAL:HG13	1.94	0.48
40:k:3:HIS:NE2	40:k:65:GLU:OE1	2.46	0.48
44:o:57:VAL:HG23	44:o:57:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:48:G:H22	1:1:177:G:P	2.37	0.48
1:1:1075:C:H2'	1:1:1076:C:C6	2.48	0.48
45:p:56:ARG:O	45:p:59:THR:HG22	2.13	0.48
54:y:54:MET:SD	54:y:55:GLN:N	2.86	0.48
1:1:279:A:C2	1:1:362:A:H4'	2.48	0.48
1:1:1059:G:O6	1:1:1080:A:N6	2.46	0.48
1:1:1203:U:O5'	1:1:1204:A:H5''	2.14	0.48
2:2:820:U:H4'	2:2:821:G:OP2	2.13	0.48
8:C:181:ASP:OD2	8:C:184:ARG:NE	2.47	0.48
38:i:88:GLU:OE1	38:i:88:GLU:N	2.46	0.48
39:j:46:VAL:HG12	39:j:47:GLY:N	2.28	0.48
44:o:5:ARG:HH22	44:o:77:VAL:HG22	1.78	0.48
44:o:28:THR:O	44:o:32:THR:HG22	2.14	0.48
1:1:76:C:OP1	28:Y:48:ARG:NE	2.46	0.48
1:1:908:C:O2'	16:M:70:ASP:OD2	2.21	0.48
1:1:1433:A:H2'	1:1:1434:A:O4'	2.14	0.48
2:2:926:G:C4	4:4:15:G:N2	2.81	0.48
2:2:1371:G:OP1	43:n:14:SER:OG	2.29	0.48
3:3:76:G:OP1	25:V:13:GLY:N	2.46	0.48
5:5:3:G:C4	5:5:4:C:C5	3.02	0.48
36:g:43:LEU:HA	36:g:46:THR:HG22	1.94	0.48
43:n:30:ILE:O	43:n:33:ARG:N	2.46	0.48
1:1:744:U:H2'	1:1:745:1MG:O4'	2.14	0.48
1:1:867:C:C2	1:1:868:U:C5	3.01	0.48
1:1:1069:A:OP1	58:1:3434:HOH:O	2.20	0.48
1:1:1364:G:OP2	27:X:50:ARG:NH1	2.37	0.48
2:2:427:U:O2'	2:2:541:G:OP1	2.32	0.48
2:2:1376:U:OP2	41:l:25:LYS:NZ	2.42	0.48
3:3:76:G:C2'	3:3:77:U:O4'	2.61	0.48
8:C:34:VAL:HA	8:C:50:VAL:HG12	1.96	0.48
37:h:157:LEU:HD22	37:h:166:GLU:OE1	2.14	0.48
50:u:19:VAL:HG23	50:u:36:VAL:HG13	1.96	0.48
1:1:280:U:O4	1:1:361:G:N2	2.47	0.48
1:1:367:G:H2'	1:1:367:G:N3	2.29	0.48
1:1:1965:C:OP1	1:1:1966:A:O2'	2.27	0.48
1:1:2276:G:OP2	16:M:85:GLY:N	2.46	0.48
1:1:2857:G:N2	1:1:2860:A:OP2	2.26	0.48
29:Z:47:MET:O	29:Z:51:VAL:HG22	2.14	0.48
30:a:20:ASN:ND2	30:a:37:CYS:SG	2.84	0.48
36:g:104:TRP:HA	36:g:107:VAL:HG22	1.96	0.48
42:m:72:VAL:O	42:m:72:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:w:52:GLN:NE2	52:w:55:LEU:HD11	2.29	0.48
1:1:892:A:H2'	1:1:893:C:C1'	2.43	0.48
1:1:1638:C:O2	1:1:2698:U:O2'	2.31	0.48
1:1:2756:U:OP2	35:f:19:ARG:NE	2.42	0.48
2:2:926:G:N9	4:4:15:G:N2	2.61	0.48
2:2:1078:U:C2	39:j:90:THR:HG21	2.48	0.48
14:K:63:VAL:HG12	14:K:107:LEU:HD21	1.96	0.48
48:s:31:ILE:CD1	48:s:45:VAL:HG23	2.44	0.48
1:1:1737:G:H2'	1:1:1738:G:C1'	2.44	0.48
1:1:2586:U:H2'	1:1:2587:A:O4'	2.13	0.48
7:B:205:LEU:HD12	7:B:210:ALA:HB1	1.95	0.48
8:C:136:ASN:ND2	8:C:139:SER:O	2.39	0.48
11:F:33:LEU:HD11	11:F:136:ALA:HB1	1.95	0.48
39:j:13:GLU:OE1	39:j:13:GLU:N	2.47	0.48
1:1:1095:A:O2'	1:1:1096:A:O5'	2.28	0.47
2:2:182:A:N1	2:2:223:A:O2'	2.47	0.47
5:5:2:G:H2'	58:5:201:HOH:O	2.13	0.47
5:5:14:A:H1'	5:5:22:G:N2	2.28	0.47
21:R:75:VAL:O	21:R:75:VAL:HG23	2.13	0.47
23:T:37:ASP:OD1	23:T:37:ASP:N	2.45	0.47
1:1:414:C:O3'	1:1:1878:G:N2	2.48	0.47
2:2:71:A:H61	2:2:99:C:H1'	1.79	0.47
8:C:24:VAL:CG1	8:C:178:VAL:HG21	2.43	0.47
15:L:110:VAL:HB	15:L:127:VAL:HG12	1.96	0.47
1:1:759:G:OP1	58:1:3432:HOH:O	2.20	0.47
1:1:1204:A:O4'	1:1:1206:G:C8	2.68	0.47
2:2:1125:U:C2	2:2:1127:G:C8	3.02	0.47
2:2:1287:A:N3	2:2:1353:G:O2'	2.42	0.47
22:S:71:VAL:HG13	22:S:71:VAL:O	2.14	0.47
46:q:30:LYS:HB3	46:q:57:LEU:HD12	1.96	0.47
1:1:279:A:H2'	1:1:280:U:O4'	2.14	0.47
2:2:418:C:H2'	2:2:419:C:O4'	2.15	0.47
2:2:493:A:H2'	2:2:494:G:C8	2.49	0.47
2:2:591:U:OP2	42:m:31:LYS:NZ	2.37	0.47
2:2:1493:A:O2'	2:2:1494:G:OP1	2.23	0.47
7:B:108:LYS:N	7:B:194:GLU:O	2.48	0.47
50:u:19:VAL:O	50:u:36:VAL:HG12	2.14	0.47
50:u:69:ASP:OD1	50:u:70:ARG:N	2.45	0.47
1:1:1328:A:O2'	1:1:1329:U:P	2.72	0.47
2:2:1124:G:N2	2:2:1125:U:O4	2.43	0.47
9:D:18:THR:HG22	9:D:106:LYS:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:38:LEU:HD13	17:N:99:LYS:HG2	1.96	0.47
37:h:55:ILE:O	37:h:55:ILE:HG23	2.14	0.47
1:1:758:C:O2'	1:1:1981:A:N3	2.47	0.47
1:1:807:U:O2	9:D:69:ARG:NH2	2.48	0.47
1:1:2049:G:N2	8:C:161:MET:SD	2.87	0.47
2:2:150:U:O2'	2:2:151:A:O4'	2.22	0.47
2:2:1130:A:C8	2:2:1146:A:N1	2.82	0.47
7:B:76:ALA:HB1	7:B:94:VAL:HG22	1.97	0.47
38:i:28:ILE:CG2	38:i:34:ILE:HD13	2.44	0.47
52:w:40:VAL:HG13	52:w:45:THR:CG2	2.44	0.47
1:1:265:A:C2'	1:1:428:A:H61	2.27	0.47
1:1:754:U:O2'	1:1:1272:A:N1	2.44	0.47
1:1:1141:U:OP2	13:J:65:THR:OG1	2.30	0.47
1:1:1952:A:OP1	14:K:44:LYS:NZ	2.39	0.47
1:1:2220:U:O3'	12:G:97:ARG:NH1	2.40	0.47
1:1:2756:U:H4'	1:1:2757:A:OP1	2.15	0.47
2:2:20:U:O2'	2:2:573:A:N6	2.48	0.47
2:2:204:G:C8	2:2:465:A:N1	2.82	0.47
2:2:406:G:O2'	38:i:3:ARG:NH2	2.47	0.47
2:2:716:A:O2'	2:2:717:U:O5'	2.31	0.47
2:2:978:A:C4	2:2:1319:A:C2	3.02	0.47
2:2:1496:C:H2'	2:2:1497:G:O4'	2.14	0.47
3:3:117:G:OP1	18:O:56:LYS:NZ	2.48	0.47
12:G:99:ILE:HD11	12:G:117:LEU:HD11	1.95	0.47
13:J:100:VAL:HG23	13:J:101:ILE:N	2.30	0.47
16:M:115:GLU:O	16:M:119:LEU:HD23	2.15	0.47
32:c:47:VAL:HG12	32:c:48:ILE:N	2.30	0.47
36:g:120:GLN:O	36:g:126:PHE:N	2.48	0.47
54:y:27:MET:O	54:y:30:THR:HG22	2.15	0.47
1:1:360:U:H5''	1:1:361:G:OP1	2.14	0.47
2:2:776:G:N2	2:2:802:A:OP2	2.45	0.47
5:5:36:G:HO2'	5:5:37:G:H8	1.63	0.47
40:k:9:MET:HE1	52:w:65:LEU:O	2.14	0.47
44:o:8:ILE:HD12	44:o:100:ILE:HG22	1.96	0.47
1:1:1949:G:H2'	1:1:1950:G:O4'	2.14	0.47
16:M:20:LEU:HD13	25:V:81:PRO:HG2	1.97	0.47
19:P:81:VAL:O	19:P:81:VAL:HG13	2.14	0.47
27:X:59:ILE:HD13	27:X:67:VAL:HG21	1.96	0.47
30:a:51:VAL:HG23	30:a:52:ALA:N	2.28	0.47
44:o:63:ASP:OD2	48:s:85:ARG:NH1	2.46	0.47
1:1:6:A:N3	13:J:135:GLN:NE2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:501:A:H2'	1:1:502:A:C8	2.50	0.47
1:1:1351:C:H2'	1:1:1352:U:O4'	2.15	0.47
1:1:2102:G:N1	1:1:2188:U:C2	2.83	0.47
6:A:212:VAL:HG23	6:A:212:VAL:O	2.15	0.47
24:U:81:ASP:OD1	24:U:82:ARG:N	2.48	0.47
40:k:88:MET:HG2	40:k:90:MET:HE2	1.96	0.47
45:p:94:GLU:OE2	55:z:20:LYS:HD3	2.15	0.47
1:1:2148:G:C2	1:1:2149:U:C4	3.03	0.46
2:2:3:A:H5''	2:2:4:U:O4'	2.15	0.46
2:2:573:A:O2'	2:2:574:A:O4'	2.11	0.46
2:2:1445:U:O2	2:2:1457:G:O6	2.33	0.46
2:2:1498:UR3:OP2	4:4:16:C:O2'	2.32	0.46
37:h:130:PHE:CE2	37:h:157:LEU:HD23	2.49	0.46
38:i:28:ILE:HG21	38:i:34:ILE:HD13	1.98	0.46
39:j:102:GLY:N	39:j:122:ASN:OD1	2.48	0.46
42:m:95:VAL:HG21	42:m:101:ILE:O	2.15	0.46
1:1:776:G:N2	1:1:2241:A:OP1	2.49	0.46
1:1:1065:U:O2'	1:1:1066:U:C6	2.68	0.46
1:1:1386:C:O2'	1:1:1469:A:N3	2.35	0.46
1:1:2283:C:O3'	32:c:4:GLY:N	2.48	0.46
2:2:564:C:OP2	46:q:12:ARG:NH2	2.48	0.46
2:2:1012:A:H2'	2:2:1013:G:O4'	2.15	0.46
2:2:1305:G:HO2'	2:2:1306:A:H8	1.63	0.46
5:5:72:G:O2'	5:5:73:A:O5'	2.24	0.46
10:E:103:LEU:HD12	10:E:107:ALA:HB3	1.96	0.46
49:t:21:ASP:N	49:t:21:ASP:OD1	2.47	0.46
1:1:389:G:C8	1:1:2413:G:H4'	2.50	0.46
1:1:686:U:O4	33:d:12:ARG:NH1	2.40	0.46
1:1:1009:A:N3	1:1:1153:C:O2'	2.46	0.46
1:1:1501:G:H4'	7:B:95:LEU:HD21	1.98	0.46
1:1:2333:A:OP1	26:W:77:ARG:NH1	2.47	0.46
3:3:75:G:N2	25:V:90:ASP:OD1	2.49	0.46
5:5:18:G:O2'	5:5:57:A:N1	2.38	0.46
5:5:53:G:N1	5:5:62:C:N3	2.64	0.46
8:C:3:GLY:C	8:C:4:LEU:HD22	2.41	0.46
8:C:112:THR:HG23	8:C:112:THR:O	2.14	0.46
12:G:96:THR:HG23	12:G:97:ARG:HD3	1.95	0.46
1:1:277:G:H21	1:1:361:G:H8	1.62	0.46
1:1:467:G:OP2	33:d:34:ARG:NH1	2.43	0.46
1:1:1232:G:C5	1:1:1233:C:C5	3.03	0.46
1:1:1274:A:N1	1:1:1644:C:O2'	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1951:U:OP1	14:K:54:LYS:NZ	2.44	0.46
1:1:2720:U:C2	1:1:2721:A:C8	3.03	0.46
2:2:1375:A:OP1	41:l:25:LYS:NZ	2.43	0.46
36:g:115:LYS:O	36:g:119:THR:HG23	2.15	0.46
45:p:59:THR:HG23	45:p:62:ALA:H	1.80	0.46
46:q:90:LEU:HD23	46:q:93:VAL:HG21	1.97	0.46
1:1:704:G:O2'	1:1:726:G:N2	2.48	0.46
1:1:2126:A:H4'	1:1:2127:G:OP1	2.15	0.46
5:5:16:C:H3'	5:5:17:C:C6	2.49	0.46
23:T:10:VAL:HG23	23:T:11:LEU:N	2.31	0.46
1:1:27:G:O2'	1:1:28:A:OP2	2.23	0.46
1:1:1176:U:O2'	1:1:1177:G:N7	2.48	0.46
1:1:2637:U:O4	1:1:2776:A:N7	2.49	0.46
5:5:70:C:H2'	5:5:71:C:C6	2.51	0.46
36:g:99:GLY:O	36:g:103:ASN:N	2.42	0.46
37:h:130:PHE:CD2	37:h:157:LEU:HD23	2.50	0.46
41:l:111:ARG:NH2	41:l:126:ASP:OD2	2.48	0.46
1:1:851:C:O2'	29:Z:43:ALA:O	2.33	0.46
1:1:1153:C:H2'	1:1:1154:G:O4'	2.16	0.46
2:2:1279:G:O2'	2:2:1282:C:N4	2.49	0.46
5:5:44:G:H2'	5:5:45:G:C8	2.51	0.46
11:F:19:ILE:HG22	11:F:24:ILE:HD12	1.98	0.46
24:U:28:VAL:HG12	24:U:34:VAL:HG23	1.98	0.46
26:W:23:VAL:HG22	26:W:38:VAL:HG12	1.97	0.46
42:m:77:ARG:NE	42:m:79:SER:O	2.49	0.46
1:1:203:A:OP2	1:1:204:A:O2'	2.21	0.46
1:1:1056:G:N1	1:1:1102:C:OP2	2.44	0.46
1:1:2122:U:H3'	1:1:2123:G:C8	2.50	0.46
1:1:2418:A:H2'	1:1:2419:U:O4'	2.16	0.46
1:1:2545:G:H2'	1:1:2546:U:O4'	2.16	0.46
2:2:458:U:H2'	2:2:459:A:C8	2.51	0.46
2:2:947:G:H2'	2:2:948:C:O4'	2.16	0.46
2:2:1326:U:C2	2:2:1327:C:C5	3.03	0.46
5:5:62:C:H2'	5:5:63:U:H6	1.81	0.46
44:o:80:THR:OG1	44:o:83:THR:OG1	2.24	0.46
1:1:497:A:H2'	1:1:498:G:H8	1.81	0.46
1:1:2548:U:O2	14:K:23:LYS:NZ	2.48	0.46
2:2:151:A:OP2	2:2:169:C:N4	2.40	0.46
2:2:215:C:H2'	2:2:216:U:O4'	2.15	0.46
2:2:333:U:C2	2:2:334:C:C5	3.03	0.46
3:3:9:G:OP2	18:O:15:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:169:GLY:N	58:A:303:HOH:O	2.48	0.46
15:L:85:VAL:HG11	15:L:90:VAL:HG12	1.98	0.46
1:1:480:A:N3	1:1:498:G:N2	2.64	0.46
1:1:569:U:H2'	1:1:570:G:O4'	2.15	0.46
1:1:2108:A:C5	1:1:2109:U:C5	3.04	0.46
11:F:43:VAL:HG22	11:F:50:LEU:HD12	1.97	0.46
22:S:4:ILE:HG22	22:S:106:VAL:HG22	1.97	0.46
47:r:16:VAL:HG23	47:r:17:ILE:N	2.31	0.46
1:1:67:U:C2	1:1:68:G:C8	3.04	0.45
1:1:275:C:N3	1:1:362:A:N6	2.65	0.45
1:1:728:G:H3'	1:1:729:G:C5'	2.47	0.45
1:1:1059:G:C6	1:1:1080:A:N6	2.84	0.45
1:1:1398:C:C2	1:1:1399:C:C5	3.04	0.45
2:2:946:A:H2'	2:2:947:G:C8	2.52	0.45
2:2:1401:G:H2'	2:2:1402:4OC:O4'	2.15	0.45
37:h:7:PRO:O	37:h:11:ARG:HG2	2.16	0.45
1:1:428:A:HO2'	1:1:429:A:P	2.39	0.45
1:1:1730:C:O2'	1:1:1731:G:O4'	2.34	0.45
2:2:1486:G:H2'	2:2:1487:G:O4'	2.15	0.45
13:J:45:THR:HB	13:J:48:VAL:HG12	1.99	0.45
24:U:27:ASN:OD1	24:U:27:ASN:N	2.49	0.45
34:e:32:ILE:HD12	34:e:32:ILE:HA	1.75	0.45
45:p:87:LYS:HB2	45:p:113:VAL:HG23	1.98	0.45
1:1:500:G:N2	1:1:503:A:OP2	2.43	0.45
1:1:953:G:OP2	16:M:18:ARG:NH2	2.42	0.45
1:1:989:G:OP2	29:Z:12:SER:OG	2.17	0.45
1:1:2122:U:H4'	1:1:2123:G:OP1	2.16	0.45
1:1:2357:G:N2	1:1:2360:G:OP2	2.49	0.45
1:1:2446:G:N2	1:1:2449:U:O2	2.41	0.45
2:2:1071:C:H2'	2:2:1072:G:H8	1.81	0.45
13:J:98:GLU:OE2	13:J:126:ALA:N	2.49	0.45
21:R:44:GLY:O	21:R:45:GLU:HB3	2.17	0.45
1:1:1179:G:OP2	1:1:1179:G:N2	2.47	0.45
1:1:1558:C:O4'	1:1:1560:G:C8	2.70	0.45
1:1:1858:A:C2'	1:1:1859:U:O4'	2.65	0.45
1:1:2107:G:C6	1:1:2183:A:C6	3.04	0.45
1:1:2521:C:C2	1:1:2545:G:N2	2.85	0.45
2:2:538:G:OP1	46:q:111:LYS:N	2.49	0.45
2:2:757:U:OP1	2:2:822:U:O2'	2.33	0.45
3:3:24:G:N7	3:3:56:G:O2'	2.42	0.45
7:B:49:ILE:HG23	7:B:49:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:n:94:LEU:HD13	43:n:98:LEU:HD13	1.98	0.45
46:q:83:ARG:NH1	46:q:84:GLY:O	2.50	0.45
1:1:282:A:C6	1:1:359:G:O6	2.70	0.45
1:1:497:A:C2	1:1:498:G:C5	3.04	0.45
1:1:652:U:OP2	1:1:654:A:N6	2.50	0.45
1:1:1370:C:H2'	1:1:1371:G:O4'	2.17	0.45
1:1:1839:G:C2	1:1:1840:G:C8	3.04	0.45
1:1:2149:U:H2'	1:1:2150:C:C6	2.51	0.45
2:2:441:A:H61	2:2:494:G:N2	2.14	0.45
2:2:946:A:OP1	47:r:113:ARG:NH1	2.42	0.45
15:L:124:GLY:C	15:L:125:LEU:HD23	2.42	0.45
49:t:53:ARG:O	49:t:57:LEU:HD23	2.16	0.45
1:1:885:C:N4	1:1:892:A:N6	2.65	0.45
1:1:1433:A:H2'	1:1:1434:A:C1'	2.47	0.45
1:1:1829:A:N3	7:B:15:HIS:NE2	2.64	0.45
1:1:2412:A:H2'	1:1:2413:G:O4'	2.17	0.45
2:2:1402:4OC:O5'	2:2:1402:4OC:H6	2.17	0.45
10:E:108:VAL:HB	10:E:109:PRO:HD3	1.99	0.45
28:Y:47:ARG:O	28:Y:50:VAL:HG22	2.16	0.45
48:s:73:PHE:C	48:s:74:LEU:HD12	2.42	0.45
55:z:28:VAL:HG23	55:z:29:LEU:N	2.31	0.45
1:1:271:G:C4	1:1:367:G:O6	2.70	0.45
1:1:1385:A:O2'	1:1:1396:U:O2	2.28	0.45
1:1:2298:A:OP1	10:E:71:ARG:NH1	2.50	0.45
1:1:2375:G:N2	1:1:2378:A:OP2	2.38	0.45
1:1:2484:G:O2'	16:M:123:LYS:O	2.31	0.45
2:2:16:A:O2'	39:j:21:VAL:HG23	2.16	0.45
2:2:380:G:C4	2:2:382:A:OP2	2.70	0.45
2:2:511:C:C2	2:2:512:U:C5	3.03	0.45
5:5:11:C:H2'	5:5:12:G:C8	2.51	0.45
7:B:80:ARG:NH2	7:B:82:GLU:OE1	2.50	0.45
10:E:59:ALA:O	30:a:27:THR:OG1	2.32	0.45
12:G:31:VAL:CG1	12:G:32:PRO:HD3	2.46	0.45
39:j:105:ILE:HD11	39:j:115:LEU:HB2	1.99	0.45
41:l:150:ALA:HB1	45:p:59:THR:HG21	1.99	0.45
1:1:371:A:O2'	27:X:61:LYS:NZ	2.34	0.45
1:1:744:U:OP1	8:C:138:LEU:HD12	2.16	0.45
1:1:2283:C:O5'	1:1:2389:G:O2'	2.35	0.45
2:2:982:U:H5''	48:s:6:MET:HE3	1.98	0.45
2:2:1055:A:N3	37:h:156:ARG:NH2	2.57	0.45
5:5:28:C:H2'	5:5:29:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:9:VAL:HG22	12:G:10:ALA:N	2.32	0.45
12:G:121:VAL:HG13	12:G:122:LEU:N	2.31	0.45
17:N:51:LEU:HB3	17:N:79:LEU:HD21	1.99	0.45
38:i:75:TYR:OH	38:i:97:ARG:NH1	2.49	0.45
1:1:468:G:OP2	33:d:37:LYS:NZ	2.48	0.45
36:g:4:VAL:CG2	36:g:9:MET:HE3	2.46	0.45
42:m:7:ILE:H	42:m:7:ILE:HD12	1.81	0.45
43:n:19:VAL:HG12	43:n:65:ILE:HG23	1.99	0.45
1:1:231:A:H2'	1:1:232:G:O4'	2.17	0.45
1:1:624:C:O2'	1:1:657:U:OP1	2.34	0.45
2:2:674:G:H21	45:p:118:HIS:CB	2.30	0.45
2:2:999:C:O2'	2:2:1000:A:O5'	2.32	0.45
2:2:1033:G:H2'	2:2:1034:G:O4'	2.17	0.45
8:C:181:ASP:OD2	8:C:184:ARG:NH2	2.49	0.45
39:j:105:ILE:HG23	39:j:105:ILE:O	2.17	0.45
43:n:57:MET:HB3	43:n:61:LEU:HD23	1.98	0.45
47:r:100:GLN:OE1	47:r:100:GLN:N	2.50	0.45
1:1:491:G:O2'	1:1:492:A:OP1	2.29	0.44
1:1:1050:A:N6	1:1:2751:G:C6	2.85	0.44
1:1:1218:G:N1	1:1:1232:G:N7	2.65	0.44
1:1:2176:A:O2'	6:A:221:GLY:N	2.50	0.44
1:1:2261:C:OP1	26:W:19:LYS:NZ	2.39	0.44
1:1:2364:C:H2'	1:1:2365:G:O4'	2.16	0.44
1:1:2867:G:O2'	1:1:2868:A:OP2	2.32	0.44
2:2:323:U:O4	2:2:327:A:N7	2.50	0.44
2:2:1075:U:O3'	36:g:174:LYS:NZ	2.48	0.44
36:g:114:LEU:HD23	36:g:114:LEU:C	2.42	0.44
43:n:12:ARG:HG3	43:n:13:LYS:H	1.82	0.44
48:s:54:ASP:OD1	48:s:59:ARG:NH1	2.50	0.44
51:v:49:GLU:O	51:v:50:ASN:C	2.60	0.44
1:1:1109:C:HO2'	1:1:1110:G:C1'	2.30	0.44
1:1:1378:A:O2'	1:1:1379:U:OP2	2.36	0.44
1:1:1990:C:H2'	1:1:1991:U:C1'	2.48	0.44
1:1:2813:A:C4	1:1:2814:A:C8	3.06	0.44
1:1:2838:G:C4	1:1:2839:G:C8	3.06	0.44
1:1:2899:A:C2	1:1:2900:A:C5	3.05	0.44
1:1:404:A:H1'	1:1:405:U:OP2	2.16	0.44
1:1:1833:C:O2'	1:1:1969:A:N1	2.44	0.44
1:1:1980:G:O2'	1:1:1982:U:OP2	2.29	0.44
2:2:82:G:H3'	2:2:83:C:C5'	2.47	0.44
2:2:983:A:OP1	48:s:6:MET:HE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:103:ILE:HG23	15:L:104:GLN:N	2.32	0.44
1:1:477:A:H2'	1:1:478:A:O4'	2.16	0.44
1:1:858:G:N2	1:1:2269:G:OP2	2.50	0.44
7:B:107:PRO:HD2	7:B:110:LEU:HD22	1.98	0.44
15:L:81:ASP:OD2	15:L:100:ILE:HG23	2.18	0.44
16:M:60:GLN:NE2	16:M:107:GLY:O	2.50	0.44
25:V:45:ASP:OD1	25:V:46:LYS:N	2.49	0.44
38:i:57:GLU:OE2	38:i:196:ASN:N	2.50	0.44
39:j:11:LEU:C	39:j:11:LEU:HD23	2.42	0.44
51:v:79:VAL:O	51:v:80:GLU:C	2.60	0.44
1:1:1275:A:O2'	1:1:1645:G:N2	2.47	0.44
1:1:1858:A:H2'	1:1:1859:U:C6	2.53	0.44
1:1:1909:C:N4	1:1:1922:G:O6	2.51	0.44
3:3:2:G:C6	3:3:119:A:N1	2.85	0.44
9:D:15:SER:HG	9:D:18:THR:HG1	1.63	0.44
37:h:138:VAL:HG23	37:h:149:ILE:CG2	2.48	0.44
44:o:32:THR:HG23	44:o:33:GLY:H	1.82	0.44
1:1:285:G:C6	1:1:356:G:C6	3.06	0.44
1:1:575:A:C2	1:1:576:U:C5	3.06	0.44
1:1:1733:G:H2'	1:1:1734:G:C8	2.52	0.44
1:1:1790:C:H2'	1:1:1791:A:C8	2.52	0.44
1:1:2093:G:N7	1:1:2225:A:H2'	2.33	0.44
1:1:2107:G:O6	1:1:2183:A:N6	2.50	0.44
2:2:404:G:O2'	2:2:498:A:N1	2.45	0.44
2:2:492:C:H2'	2:2:493:A:C4	2.53	0.44
2:2:684:U:H2'	2:2:685:G:O4'	2.17	0.44
2:2:1033:G:O6	58:2:1820:HOH:O	2.21	0.44
10:E:166:GLY:O	10:E:170:LEU:HD23	2.17	0.44
42:m:10:MET:HE2	42:m:36:ILE:CD1	2.47	0.44
1:1:140:C:O2	1:1:140:C:O4'	2.34	0.44
1:1:760:G:H2'	1:1:761:A:O4'	2.18	0.44
1:1:1201:U:C4	1:1:1202:G:C5	3.06	0.44
1:1:1360:G:C8	1:1:1361:G:C8	3.06	0.44
1:1:1462:C:C2	1:1:1463:C:C5	3.06	0.44
1:1:1922:G:O2'	1:1:1923:U:H5'	2.18	0.44
1:1:2180:U:H2'	1:1:2181:U:C6	2.53	0.44
2:2:880:C:C2	2:2:881:G:C8	3.06	0.44
5:5:18:G:H21	5:5:58:A:C5'	2.30	0.44
5:5:75:C:OP2	5:5:75:C:H6	2.01	0.44
12:G:31:VAL:HG13	12:G:32:PRO:HD3	1.99	0.44
1:1:48:G:N2	1:1:177:G:OP2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:633:A:O2'	1:1:2404:U:OP1	2.36	0.44
1:1:796:C:OP1	9:D:57:LYS:NZ	2.44	0.44
1:1:1399:C:C2	1:1:1400:U:C5	3.06	0.44
1:1:2450:A:N6	1:1:2501:C:O2	2.51	0.44
2:2:1027:C:N4	2:2:1034:G:O6	2.51	0.44
2:2:1297:G:O3'	41:l:114:LYS:NZ	2.51	0.44
7:B:168:ASP:N	7:B:168:ASP:OD1	2.50	0.44
9:D:191:ASP:OD1	9:D:191:ASP:N	2.51	0.44
11:F:90:VAL:HG23	11:F:160:LYS:HA	1.99	0.44
44:o:12:ALA:HB3	44:o:18:ILE:HG12	2.00	0.44
46:q:100:GLY:N	46:q:104:CYS:O	2.47	0.44
1:1:296:U:O3'	24:U:92:LYS:NZ	2.46	0.44
1:1:1064:C:H42	1:1:1075:C:H42	1.66	0.44
1:1:2316:G:H4'	10:E:125:ARG:CZ	2.48	0.44
2:2:296:U:O2'	2:2:556:C:O2	2.34	0.44
2:2:982:U:O2	2:2:1222:G:N2	2.51	0.44
1:1:1065:U:N3	1:1:1074:G:C6	2.86	0.43
1:1:1143:A:N7	13:J:27:ARG:NH1	2.66	0.43
1:1:1568:G:N7	7:B:28:LYS:NZ	2.65	0.43
1:1:2353:G:N2	26:W:34:GLY:O	2.42	0.43
1:1:2799:A:O2'	1:1:2800:A:H5''	2.18	0.43
2:2:264:C:O2'	51:v:66:PRO:O	2.29	0.43
2:2:269:C:H2'	2:2:270:A:H8	1.83	0.43
2:2:979:C:O2	2:2:979:C:H2'	2.18	0.43
9:D:16:GLU:OE2	9:D:16:GLU:N	2.48	0.43
38:i:58:LYS:HA	38:i:200:ILE:HD12	2.00	0.43
55:z:60:LEU:HD12	55:z:61:ALA:N	2.33	0.43
1:1:1882:U:C5	1:1:1883:U:O4	2.71	0.43
1:1:2404:U:H2'	1:1:2405:G:O4'	2.18	0.43
2:2:8:A:N6	38:i:202:GLU:O	2.49	0.43
2:2:507:C:P	2:2:508:U:HO2'	2.28	0.43
2:2:1077:G:N2	2:2:1080:A:OP2	2.34	0.43
2:2:1108:G:H2'	2:2:1108:G:N3	2.32	0.43
2:2:1166:G:O2'	2:2:1169:A:N6	2.51	0.43
2:2:1225:A:OP1	47:r:102:THR:HG22	2.18	0.43
2:2:1314:C:OP2	53:x:4:SER:OG	2.21	0.43
9:D:118:LEU:HD12	9:D:188:MET:CE	2.48	0.43
39:j:115:LEU:HD13	39:j:123:VAL:HG11	2.01	0.43
43:n:88:MET:HE3	43:n:95:ARG:HD2	1.99	0.43
1:1:894:U:O2'	1:1:895:U:H2'	2.18	0.43
1:1:1678:A:C4	1:1:1679:A:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2286:G:OP1	32:c:30:LYS:NZ	2.24	0.43
18:O:55:GLU:HB2	18:O:58:ILE:HD13	1.99	0.43
46:q:80:ILE:HG22	46:q:81:LEU:N	2.33	0.43
1:1:177:G:H3'	1:1:178:G:H8	1.83	0.43
1:1:281:C:N4	1:1:282:A:H62	2.16	0.43
1:1:571:U:N3	1:1:575:A:N7	2.66	0.43
1:1:2723:C:P	8:C:114:LYS:HZ3	2.39	0.43
2:2:181:A:N3	2:2:194:C:C4	2.86	0.43
2:2:890:G:O2'	2:2:906:A:N6	2.51	0.43
2:2:1179:A:H2'	2:2:1180:A:C8	2.54	0.43
3:3:78:A:OP2	16:M:20:LEU:HD12	2.17	0.43
36:g:94:HIS:NE2	36:g:146:ASN:OD1	2.51	0.43
38:i:92:ALA:O	38:i:185:LYS:NZ	2.47	0.43
44:o:8:ILE:CD1	44:o:100:ILE:HG22	2.48	0.43
48:s:82:ILE:HG23	48:s:83:LYS:N	2.34	0.43
1:1:685:A:C8	1:1:773:U:C4	3.06	0.43
1:1:1041:G:N2	1:1:1115:G:C6	2.86	0.43
2:2:220:G:C2	2:2:221:C:C6	3.07	0.43
2:2:232:G:O2'	2:2:263:A:N1	2.44	0.43
12:G:66:ASN:ND2	12:G:134:VAL:O	2.52	0.43
38:i:113:GLU:O	38:i:117:LEU:HD23	2.18	0.43
53:x:20:GLU:HA	53:x:23:VAL:HG12	2.00	0.43
1:1:866:A:C2	1:1:867:C:C6	3.06	0.43
1:1:886:A:C2'	1:1:887:A:O5'	2.66	0.43
1:1:1201:U:O2	1:1:1201:U:H2'	2.16	0.43
1:1:1856:U:O2	1:1:1885:A:N6	2.52	0.43
2:2:179:A:C5	2:2:180:U:C5	3.06	0.43
2:2:604:G:H2'	2:2:605:U:O4'	2.19	0.43
2:2:673:A:H2'	2:2:674:G:H8	1.81	0.43
2:2:864:A:H2'	2:2:865:A:C8	2.54	0.43
2:2:880:C:OP2	46:q:3:THR:HG21	2.19	0.43
2:2:991:U:N3	2:2:1212:U:O4'	2.51	0.43
12:G:76:GLU:OE1	12:G:76:GLU:HA	2.19	0.43
23:T:13:ALA:HB1	28:Y:33:ALA:CB	2.48	0.43
50:u:14:ARG:NH1	58:u:101:HOH:O	2.37	0.43
1:1:1053:C:C4	1:1:1107:G:C6	3.06	0.43
1:1:2539:C:H5'	35:f:3:VAL:HG21	2.00	0.43
2:2:1189:U:OP1	48:s:98:LYS:NZ	2.50	0.43
7:B:2:ALA:N	7:B:199:GLU:OE2	2.52	0.43
7:B:45:ASN:OD1	7:B:46:ASN:N	2.52	0.43
11:F:155:GLU:OE2	58:F:201:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:26:VAL:HG23	16:M:104:GLU:HG2	1.99	0.43
34:e:17:THR:HG21	34:e:49:MET:HE1	2.01	0.43
37:h:39:VAL:CG1	37:h:91:VAL:HG23	2.48	0.43
43:n:88:MET:HE1	43:n:98:LEU:CB	2.48	0.43
1:1:581:C:OP2	20:Q:33:ARG:NE	2.48	0.43
2:2:55:A:O4'	58:2:1819:HOH:O	2.21	0.43
2:2:160:A:H61	2:2:347:G:N2	2.17	0.43
10:E:33:LYS:HG2	10:E:157:THR:OG1	2.18	0.43
16:M:62:LYS:O	16:M:105:MET:HE3	2.18	0.43
18:O:41:ALA:HB2	18:O:48:LEU:HD21	2.01	0.43
41:l:69:VAL:HG13	41:l:100:ALA:HB1	1.99	0.43
1:1:1068:G:H21	1:1:1095:A:H1'	1.82	0.43
1:1:1991:U:H2'	1:1:1992:G:H5'	2.01	0.43
2:2:1:A:H2'	2:2:1:A:N3	2.33	0.43
2:2:2:A:H2'	2:2:3:A:C4	2.53	0.43
2:2:246:A:C2	2:2:282:A:C5	3.06	0.43
2:2:721:G:H4'	2:2:722:G:O4'	2.19	0.43
2:2:746:A:H2'	2:2:747:A:C1'	2.49	0.43
2:2:1317:C:O4'	48:s:24:ARG:NH2	2.52	0.43
3:3:39:A:C2	3:3:44:G:C2	3.07	0.43
9:D:24:ASN:O	9:D:28:VAL:HG12	2.19	0.43
21:R:63:VAL:HG12	21:R:96:VAL:HG12	2.01	0.43
45:p:77:TYR:HB2	45:p:79:ILE:HD11	2.01	0.43
1:1:966:G:C1'	1:1:2267:A:H62	2.30	0.43
1:1:1202:G:H21	15:L:3:LEU:C	2.27	0.43
1:1:2684:U:O4'	14:K:70:ARG:NH1	2.46	0.43
2:2:28:A:O2'	2:2:296:U:OP1	2.34	0.43
2:2:704:A:C4	2:2:705:G:C8	3.06	0.43
2:2:718:A:H2'	2:2:718:A:N3	2.34	0.43
2:2:868:C:H2'	2:2:869:G:O4'	2.19	0.43
8:C:12:THR:OG1	19:P:9:GLU:OE2	2.35	0.43
12:G:144:VAL:O	12:G:144:VAL:HG13	2.19	0.43
24:U:41:LEU:N	24:U:41:LEU:HD12	2.34	0.43
42:m:55:THR:HG23	42:m:56:LYS:N	2.34	0.43
1:1:319:G:H2'	1:1:320:A:O4'	2.19	0.42
1:1:813:U:OP2	15:L:24:GLY:N	2.42	0.42
1:1:1320:C:H2'	1:1:1329:U:OP1	2.18	0.42
1:1:1353:A:OP2	1:1:1377:G:N1	2.44	0.42
1:1:1736:U:H2'	1:1:1737:G:C4	2.54	0.42
2:2:418:C:H2'	2:2:419:C:C6	2.54	0.42
2:2:1458:G:P	54:y:30:THR:HG21	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:46:A:C5	3:3:47:C:C5	3.06	0.42
37:h:85:GLU:OE2	37:h:88:ARG:NH2	2.52	0.42
39:j:13:GLU:CB	39:j:39:VAL:HG12	2.48	0.42
43:n:65:ILE:HG22	43:n:66:THR:N	2.34	0.42
45:p:32:VAL:HG13	45:p:32:VAL:O	2.19	0.42
1:1:1287:A:O2'	1:1:1288:G:H5'	2.19	0.42
1:1:1432:G:H2'	1:1:1433:A:C8	2.55	0.42
1:1:2102:G:C2	1:1:2188:U:O2	2.72	0.42
1:1:2123:G:H4'	1:1:2124:G:OP1	2.18	0.42
1:1:2138:G:N1	1:1:2154:A:C6	2.87	0.42
1:1:2638:G:O2'	1:1:2775:G:N2	2.51	0.42
2:2:264:C:H2'	2:2:265:G:O4'	2.19	0.42
2:2:1291:U:O2	2:2:1292:G:C8	2.72	0.42
3:3:75:G:C6	3:3:76:G:N1	2.87	0.42
5:5:73:A:H4'	5:5:74:C:H5	1.83	0.42
9:D:127:GLU:HG2	9:D:128:ALA:N	2.34	0.42
19:P:91:ALA:N	19:P:111:LYS:O	2.50	0.42
38:i:57:GLU:O	38:i:60:LYS:HG2	2.20	0.42
38:i:143:VAL:HG13	38:i:143:VAL:O	2.18	0.42
46:q:21:VAL:HG23	46:q:95:TYR:HE1	1.84	0.42
1:1:1346:G:H2'	1:1:1347:A:O4'	2.19	0.42
1:1:1656:C:OP1	8:C:141:ARG:NH2	2.49	0.42
1:1:1752:C:OP2	58:1:3436:HOH:O	2.21	0.42
1:1:1839:G:C8	1:1:1927:A:C4	3.07	0.42
2:2:149:A:O2'	2:2:1446:A:N1	2.48	0.42
2:2:323:U:H2'	2:2:324:G:O4'	2.19	0.42
2:2:1055:A:O2'	37:h:161:GLU:O	2.30	0.42
36:g:165:ASP:OD1	36:g:168:HIS:N	2.51	0.42
37:h:11:ARG:NH2	37:h:175:LEU:O	2.52	0.42
48:s:28:LYS:HA	48:s:31:ILE:HG22	2.00	0.42
49:t:24:SER:O	49:t:27:VAL:HG22	2.20	0.42
53:x:12:ASP:OD1	53:x:35:SER:OG	2.35	0.42
1:1:563:A:OP2	21:R:79:ARG:NH1	2.50	0.42
1:1:896:A:O2'	1:1:897:C:H5'	2.19	0.42
1:1:1081:U:H2'	1:1:1082:U:C6	2.55	0.42
1:1:1349:C:C2	1:1:1350:C:C5	3.07	0.42
1:1:1857:G:HO2'	1:1:1858:A:P	2.42	0.42
1:1:2193:G:O2'	1:1:2194:U:OP1	2.34	0.42
1:1:2347:C:O2'	32:c:21:TYR:OH	1.99	0.42
1:1:2516:A:O2'	1:1:2517:C:H5'	2.19	0.42
2:2:404:G:N7	38:i:2:ALA:N	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1422:G:O3'	14:K:49:ARG:NH2	2.52	0.42
10:E:88:LYS:NZ	10:E:90:THR:OG1	2.53	0.42
1:1:1075:C:O2	58:1:3435:HOH:O	2.20	0.42
1:1:1298:C:H2'	1:1:1299:G:O4'	2.19	0.42
1:1:2045:C:O2'	31:b:15:MET:O	2.32	0.42
1:1:2124:G:H2'	1:1:2125:G:O4'	2.20	0.42
1:1:2552:OMU:O5'	1:1:2552:OMU:H6	2.20	0.42
1:1:2687:U:H2'	1:1:2688:G:O4'	2.19	0.42
2:2:982:U:H4'	2:2:983:A:O4'	2.20	0.42
3:3:37:C:O2	18:O:100:HIS:NE2	2.38	0.42
25:V:56:PHE:CE1	25:V:61:LEU:HD21	2.54	0.42
41:l:69:VAL:HG11	41:l:104:ILE:HD11	2.00	0.42
45:p:23:ILE:HD13	45:p:32:VAL:HG23	2.01	0.42
1:1:75:G:H2'	1:1:75:G:N3	2.35	0.42
1:1:1275:A:N1	1:1:1295:C:O2'	2.49	0.42
1:1:1857:G:H22	1:1:1884:G:H1'	1.85	0.42
1:1:1887:C:H2'	1:1:1888:G:O4'	2.19	0.42
1:1:2520:C:O2'	1:1:2521:C:H5'	2.20	0.42
2:2:162:A:H2'	2:2:163:C:O4'	2.19	0.42
2:2:269:C:H2'	2:2:270:A:C8	2.54	0.42
2:2:945:G:N2	2:2:1334:G:O2'	2.53	0.42
11:F:11:VAL:O	11:F:11:VAL:HG13	2.20	0.42
21:R:27:ILE:O	21:R:66:HIS:NE2	2.44	0.42
46:q:40:THR:HG22	46:q:41:THR:N	2.34	0.42
1:1:348:A:H2'	1:1:349:U:O4'	2.20	0.42
1:1:1201:U:C2	1:1:1202:G:C8	3.08	0.42
1:1:1453:A:N7	17:N:73:ASN:ND2	2.68	0.42
1:1:1520:U:H2'	1:1:1521:G:O4'	2.20	0.42
2:2:714:G:H2'	2:2:715:A:C8	2.55	0.42
2:2:1133:G:H2'	2:2:1134:G:C8	2.55	0.42
15:L:85:VAL:HG22	15:L:86:GLU:H	1.84	0.42
25:V:61:LEU:HD12	25:V:61:LEU:N	2.34	0.42
26:W:16:SER:OG	26:W:17:GLU:N	2.51	0.42
1:1:135:U:C2	1:1:136:G:C8	3.08	0.42
1:1:247:G:O2'	1:1:386:G:N1	2.48	0.42
1:1:998:C:H2'	1:1:999:U:O4'	2.20	0.42
1:1:1141:U:H4'	1:1:1142:A:O4'	2.19	0.42
1:1:1141:U:H4'	1:1:1142:A:O5'	2.19	0.42
1:1:1910:G:C2	1:1:1921:G:C2	3.08	0.42
2:2:268:U:C2	2:2:269:C:C5	3.07	0.42
2:2:1000:A:C6	2:2:1041:G:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1027:C:H2'	2:2:1028:C:C6	2.54	0.42
2:2:1216:A:O3'	48:s:5:SER:OG	2.36	0.42
4:4:17:C:H2'	4:4:18:C:C6	2.55	0.42
6:A:163:TYR:CD2	6:A:173:THR:HG23	2.55	0.42
10:E:146:VAL:O	10:E:146:VAL:HG13	2.19	0.42
13:J:84:ILE:HG23	13:J:84:ILE:O	2.20	0.42
16:M:110:GLU:O	16:M:114:ARG:HG2	2.20	0.42
42:m:10:MET:HE2	42:m:36:ILE:HD11	2.01	0.42
43:n:81:HIS:O	43:n:84:THR:OG1	2.32	0.42
1:1:676:A:O2'	1:1:2442:C:O2'	2.31	0.42
1:1:2188:U:O4	1:1:2189:U:O4	2.37	0.42
1:1:2450:A:P	1:1:2497:A:HO2'	2.31	0.42
2:2:374:A:C6	2:2:375:U:C4	3.08	0.42
2:2:439:U:O2	2:2:439:U:O4'	2.37	0.42
2:2:493:A:HO2'	2:2:494:G:C4'	2.14	0.42
2:2:493:A:C2'	2:2:494:G:O4'	2.66	0.42
2:2:779:C:H2'	2:2:780:A:O4'	2.19	0.42
2:2:1060:U:OP1	48:s:85:ARG:NH2	2.53	0.42
5:5:5:A:O2'	5:5:6:C:H6	2.03	0.42
19:P:89:ARG:NH2	19:P:115:ASN:OXT	2.53	0.42
24:U:41:LEU:HD12	24:U:41:LEU:H	1.84	0.42
1:1:487:C:H42	1:1:492:A:N6	2.18	0.42
1:1:1071:G:H2'	1:1:1072:C:C6	2.55	0.42
1:1:1319:C:N4	1:1:1334:G:O6	2.53	0.42
1:1:2070:A:H2'	1:1:2071:A:O4'	2.19	0.42
2:2:432:A:C4	2:2:433:G:C8	3.08	0.42
2:2:471:U:C2	2:2:472:U:C5	3.08	0.42
2:2:515:G:C6	2:2:516:PSU:C2	3.08	0.42
2:2:674:G:O3'	52:w:74:HIS:NE2	2.52	0.42
2:2:988:G:H3'	2:2:989:U:H5''	2.01	0.42
2:2:1018:G:H2'	2:2:1019:A:O4'	2.20	0.42
2:2:1078:U:H2'	2:2:1079:G:C4	2.55	0.42
5:5:21:A:N6	5:5:47:U:O2'	2.53	0.42
6:A:189:LEU:HD21	6:A:224:VAL:HG21	2.01	0.42
8:C:57:ALA:HA	8:C:60:VAL:HG12	2.02	0.42
26:W:56:ASP:OD1	26:W:58:THR:HG22	2.19	0.42
34:e:7:VAL:HG23	34:e:10:ALA:HB3	2.02	0.42
36:g:20:THR:O	36:g:23:TRP:CD1	2.72	0.42
38:i:196:ASN:OD1	38:i:198:HIS:NE2	2.53	0.42
1:1:245:G:O6	34:e:8:ARG:NH1	2.50	0.41
1:1:301:G:C6	1:1:317:G:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:602:A:O2'	1:1:655:A:N1	2.45	0.41
1:1:886:A:H2'	1:1:887:A:O5'	2.20	0.41
1:1:1465:G:H2'	1:1:1466:U:O4'	2.20	0.41
1:1:2294:G:OP2	18:O:94:ARG:NH2	2.52	0.41
1:1:2349:G:O6	1:1:2369:A:N6	2.53	0.41
2:2:790:A:OP1	5:5:38:U:O2'	2.34	0.41
2:2:1008:U:O4	2:2:1022:A:N6	2.53	0.41
27:X:7:VAL:HG12	27:X:51:VAL:HG23	2.02	0.41
29:Z:51:VAL:O	29:Z:55:VAL:HG22	2.20	0.41
36:g:104:TRP:HA	36:g:107:VAL:CG2	2.49	0.41
36:g:165:ASP:OD1	36:g:167:ASP:N	2.53	0.41
41:l:15:ASP:OD1	41:l:20:SER:N	2.43	0.41
1:1:498:G:H2'	1:1:499:U:O4'	2.19	0.41
1:1:1233:C:C2	1:1:1234:U:C5	3.08	0.41
1:1:1577:C:H2'	1:1:1578:U:C1'	2.49	0.41
1:1:1955:U:C5	1:1:2552:OMU:H1'	2.55	0.41
1:1:2620:C:O2'	8:C:162:ALA:O	2.27	0.41
1:1:2727:A:O2'	1:1:2728:U:H5'	2.19	0.41
1:1:2899:A:H2'	1:1:2900:A:C8	2.55	0.41
2:2:267:C:C2	2:2:268:U:C5	3.09	0.41
2:2:1119:C:H2'	2:2:1120:C:H6	1.85	0.41
3:3:45:A:C4	3:3:46:A:C8	3.08	0.41
8:C:24:VAL:HG21	8:C:188:LEU:HD23	2.02	0.41
12:G:143:ILE:H	12:G:143:ILE:HD12	1.84	0.41
37:h:108:LYS:HB3	37:h:144:LEU:HD23	2.02	0.41
50:u:4:ILE:HD12	50:u:66:THR:O	2.20	0.41
51:v:50:ASN:O	51:v:51:ASN:C	2.63	0.41
1:1:878:A:N6	1:1:899:A:O2'	2.52	0.41
1:1:1045:C:H5''	1:1:1047:G:O4'	2.20	0.41
1:1:1065:U:C4	1:1:1066:U:C2	3.08	0.41
1:1:1079:C:O2	1:1:1080:A:C8	2.73	0.41
1:1:1574:C:C2	1:1:1575:C:C5	3.08	0.41
1:1:1723:G:C4	1:1:1724:G:C8	3.07	0.41
2:2:75:G:H2'	2:2:76:G:H8	1.86	0.41
2:2:171:A:H2'	2:2:172:A:C8	2.55	0.41
2:2:242:G:H2'	2:2:243:A:H5'	2.02	0.41
2:2:439:U:O2'	38:i:119:SER:O	2.26	0.41
2:2:1432:G:HO2'	2:2:1433:A:P	2.42	0.41
8:C:91:THR:HG22	8:C:92:VAL:N	2.35	0.41
13:J:6:ALA:HB3	13:J:48:VAL:HG11	2.01	0.41
16:M:42:THR:HG22	16:M:93:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:n:52:LEU:HD12	43:n:52:LEU:N	2.35	0.41
43:n:84:THR:HG21	43:n:103:PHE:O	2.21	0.41
51:v:49:GLU:O	51:v:50:ASN:OD1	2.38	0.41
1:1:542:C:O2	1:1:551:G:N2	2.53	0.41
1:1:703:U:H2'	1:1:704:G:O4'	2.21	0.41
1:1:1079:C:C2	1:1:1080:A:N7	2.89	0.41
1:1:1263:U:O2'	31:b:4:GLN:NE2	2.53	0.41
1:1:1589:U:HO2'	1:1:1590:A:H8	1.64	0.41
1:1:1774:C:H4'	1:1:1979:U:O2	2.20	0.41
1:1:1790:C:C3'	1:1:1791:A:C8	3.03	0.41
1:1:2496:C:H2'	1:1:2497:A:O4'	2.20	0.41
1:1:2751:G:C8	11:F:3:ARG:HD2	2.55	0.41
1:1:2847:U:H2'	1:1:2848:G:O4'	2.20	0.41
2:2:78:A:H2'	2:2:79:G:H8	1.86	0.41
2:2:320:A:H2'	2:2:321:A:O4'	2.20	0.41
2:2:718:A:H5'	45:p:119:ASN:ND2	2.36	0.41
3:3:1:U:O2'	3:3:2:G:H8	2.03	0.41
16:M:70:ASP:OD1	16:M:70:ASP:N	2.52	0.41
23:T:23:ALA:HB1	23:T:29:THR:CG2	2.50	0.41
25:V:36:ALA:O	25:V:93:ARG:NH2	2.43	0.41
36:g:103:ASN:CG	36:g:106:THR:HG22	2.46	0.41
36:g:183:VAL:HG23	36:g:196:VAL:HG23	2.01	0.41
37:h:124:LEU:HD11	37:h:189:ALA:CB	2.51	0.41
1:1:1118:C:H2'	1:1:1119:U:O4'	2.21	0.41
1:1:1889:A:H2'	1:1:1890:A:O4'	2.21	0.41
2:2:77:A:H2'	2:2:78:A:O4'	2.20	0.41
2:2:849:G:H2'	2:2:850:U:O4'	2.21	0.41
2:2:936:C:C4	2:2:937:A:N7	2.88	0.41
9:D:75:SER:HG	9:D:78:TRP:CD1	2.38	0.41
11:F:86:LYS:HG2	11:F:132:VAL:HG12	2.03	0.41
11:F:125:CYS:SG	11:F:131:ILE:HD13	2.60	0.41
23:T:92:ASN:OD1	23:T:93:LEU:N	2.53	0.41
36:g:59:LYS:O	36:g:62:SER:OG	2.36	0.41
40:k:36:ILE:HG23	40:k:36:ILE:O	2.20	0.41
52:w:52:GLN:HE22	52:w:55:LEU:HD11	1.85	0.41
1:1:307:G:C4	1:1:309:A:OP2	2.73	0.41
1:1:1048:A:C2	1:1:1049:C:C5	3.08	0.41
1:1:1311:G:H21	1:1:1603:A:H62	1.68	0.41
1:1:1427:A:H4'	1:1:1428:C:O4'	2.20	0.41
1:1:1922:G:C2'	1:1:1923:U:H5'	2.50	0.41
1:1:1957:C:C2	1:1:1958:C:C5	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2000:C:OP1	17:N:5:LYS:NZ	2.44	0.41
2:2:363:A:H2'	2:2:364:A:O4'	2.21	0.41
2:2:918:A:H2'	2:2:919:A:O4'	2.21	0.41
2:2:1152:A:H4'	44:o:15:HIS:NE2	2.35	0.41
3:3:8:C:OP1	18:O:15:ARG:NH2	2.45	0.41
22:S:47:VAL:HA	22:S:50:VAL:HG12	2.01	0.41
36:g:59:LYS:N	36:g:59:LYS:HD2	2.35	0.41
38:i:98:LEU:N	38:i:135:TYR:O	2.54	0.41
41:l:138:ARG:O	41:l:141:VAL:HG12	2.20	0.41
48:s:16:LEU:HD23	48:s:54:ASP:HB2	2.02	0.41
1:1:5:A:H2'	1:1:6:A:H8	1.84	0.41
1:1:868:U:H2'	1:1:869:G:O4'	2.20	0.41
1:1:1059:G:C6	1:1:1080:A:C6	3.08	0.41
1:1:1066:U:O2	1:1:1069:A:C8	2.74	0.41
1:1:1680:U:H2'	1:1:1681:G:O4'	2.21	0.41
5:5:2:G:O2'	5:5:3:G:H2'	2.20	0.41
25:V:75:GLN:HB2	25:V:92:VAL:HG13	2.03	0.41
46:q:79:VAL:O	46:q:79:VAL:HG13	2.19	0.41
49:t:5:THR:OG1	49:t:6:GLU:OE2	2.39	0.41
1:1:287:G:H2'	1:1:288:U:C6	2.56	0.41
1:1:743:A:O2'	1:1:1659:G:OP1	2.35	0.41
1:1:817:C:H2'	1:1:818:G:O4'	2.20	0.41
1:1:1360:G:N7	1:1:1361:G:C8	2.89	0.41
1:1:1434:A:H61	1:1:1558:C:H42	1.69	0.41
1:1:1879:C:H2'	1:1:1880:U:O4'	2.19	0.41
1:1:2141:G:N2	1:1:2150:C:C2	2.84	0.41
2:2:73:C:C2'	2:2:74:A:H5'	2.51	0.41
2:2:75:G:H2'	2:2:76:G:C8	2.55	0.41
2:2:323:U:H5'	54:y:21:ASN:HD21	1.84	0.41
2:2:792:A:H1'	2:2:794:A:N7	2.36	0.41
2:2:997:U:H2'	2:2:998:C:O4'	2.20	0.41
2:2:1325:C:N3	2:2:1326:U:C5	2.89	0.41
3:3:9:G:C2	3:3:10:G:C8	3.09	0.41
7:B:246:THR:HG23	7:B:248:TRP:H	1.86	0.41
10:E:36:LEU:HB2	10:E:89:VAL:HG22	2.03	0.41
17:N:44:LEU:O	17:N:48:VAL:HG12	2.20	0.41
22:S:31:GLN:O	22:S:34:ASP:OD2	2.39	0.41
52:w:55:LEU:HD12	52:w:55:LEU:C	2.46	0.41
55:z:8:GLU:HA	55:z:8:GLU:OE1	2.21	0.41
1:1:12:U:O2	1:1:2626:C:H4'	2.21	0.41
1:1:83:A:O2'	1:1:103:A:N6	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:289:G:H2'	1:1:290:U:O4'	2.20	0.41
1:1:372:G:H5''	27:X:61:LYS:HZ2	1.86	0.41
1:1:394:C:O2'	1:1:395:U:H5'	2.21	0.41
1:1:826:U:H2'	1:1:828:U:O4'	2.20	0.41
1:1:867:C:N3	1:1:868:U:C5	2.89	0.41
1:1:1196:C:C2	1:1:1197:G:C8	3.08	0.41
1:1:1199:U:O2	1:1:1199:U:H2'	2.20	0.41
1:1:1722:A:C4	1:1:1723:G:C8	3.08	0.41
1:1:2282:G:H4'	1:1:2389:G:O2'	2.21	0.41
1:1:2286:G:H4'	1:1:2287:A:O4'	2.20	0.41
1:1:2661:G:H2'	1:1:2662:A:O4'	2.21	0.41
2:2:160:A:N6	2:2:346:G:O6	2.53	0.41
2:2:195:A:H1'	2:2:222:C:O2'	2.21	0.41
2:2:207:C:H2'	2:2:208:U:O4'	2.21	0.41
2:2:967:5MC:OP2	2:2:968:A:O2'	2.32	0.41
2:2:979:C:C5	2:2:980:C:C5	3.09	0.41
2:2:1145:A:H2	2:2:1147:C:H41	1.68	0.41
2:2:1259:C:H3'	2:2:1260:G:H5''	2.03	0.41
2:2:1494:G:C2	2:2:1495:U:C5	3.08	0.41
2:2:1497:G:H1'	2:2:1518:MA6:H2	2.03	0.41
5:5:2:G:O2'	5:5:3:G:OP2	2.32	0.41
5:5:46:G:C8	5:5:47:U:H1'	2.56	0.41
7:B:268:VAL:HG12	7:B:269:ARG:HG3	2.03	0.41
9:D:7:ASP:OD1	9:D:7:ASP:N	2.51	0.41
16:M:33:LEU:HD13	16:M:117:PHE:HB3	2.03	0.41
21:R:71:LYS:HA	21:R:90:ARG:HG2	2.03	0.41
36:g:127:ASP:O	36:g:128:LYS:C	2.64	0.41
38:i:80:ALA:HA	38:i:86:THR:HG22	2.03	0.41
39:j:39:VAL:HG23	39:j:71:MET:HE3	2.03	0.41
44:o:32:THR:HG21	44:o:83:THR:HA	2.03	0.41
1:1:1638:C:H4'	1:1:2710:C:O2	2.21	0.41
1:1:2493:U:C4	1:1:2494:G:C8	3.09	0.41
2:2:21:G:H2'	2:2:22:G:C8	2.56	0.41
2:2:496:A:N3	2:2:496:A:C2'	2.84	0.41
2:2:514:C:H2'	2:2:515:G:H8	1.86	0.41
2:2:1273:C:H2'	2:2:1274:A:O4'	2.20	0.41
2:2:1358:U:OP1	48:s:75:ARG:HG2	2.21	0.41
5:5:65:U:H2'	5:5:66:C:H6	1.86	0.41
12:G:40:THR:O	12:G:41:LYS:C	2.64	0.41
32:c:42:VAL:HG13	32:c:43:VAL:N	2.35	0.41
1:1:138:U:O2	1:1:138:U:O4'	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:581:C:H2'	1:1:582:A:H8	1.85	0.40
1:1:1376:C:H2'	1:1:1377:G:O4'	2.20	0.40
2:2:82:G:H22	2:2:84:U:H6	1.69	0.40
2:2:375:U:H2'	2:2:376:G:O4'	2.21	0.40
2:2:443:C:N4	2:2:492:C:H42	2.19	0.40
2:2:491:G:C6	2:2:492:C:N4	2.89	0.40
2:2:1352:C:H2'	2:2:1353:G:O4'	2.21	0.40
2:2:1464:U:C2	2:2:1465:A:C8	3.09	0.40
5:5:49:G:H2'	5:5:50:G:H8	1.85	0.40
5:5:54:U:H2'	5:5:55:U:N1	2.36	0.40
9:D:96:VAL:O	9:D:96:VAL:HG23	2.20	0.40
12:G:129:GLU:OE1	12:G:129:GLU:HA	2.21	0.40
32:c:9:ILE:HD12	32:c:51:GLU:CG	2.50	0.40
36:g:209:ALA:O	36:g:212:LEU:HG	2.21	0.40
40:k:90:MET:SD	52:w:61:ARG:NH1	2.87	0.40
1:1:101:A:O2'	1:1:102:U:H5'	2.21	0.40
1:1:116:C:H2'	1:1:117:G:O4'	2.21	0.40
1:1:299:A:N6	1:1:322:A:O2'	2.53	0.40
1:1:345:A:N3	1:1:347:A:N6	2.69	0.40
1:1:354:A:H2'	1:1:355:U:O4'	2.21	0.40
1:1:367:G:H3'	1:1:368:A:C8	2.56	0.40
1:1:535:G:H2'	1:1:536:G:O4'	2.21	0.40
1:1:856:G:H2'	1:1:857:G:C8	2.57	0.40
2:2:18:C:OP1	39:j:132:ASN:ND2	2.51	0.40
2:2:718:A:C8	45:p:118:HIS:CG	3.09	0.40
2:2:1305:G:HO2'	2:2:1306:A:C5'	2.34	0.40
2:2:1368:A:OP2	43:n:114:LYS:HG3	2.21	0.40
5:5:44:G:H1'	47:r:117:LYS:CD	2.52	0.40
5:5:62:C:H2'	5:5:63:U:C6	2.56	0.40
10:E:13:VAL:HG23	10:E:14:LYS:N	2.36	0.40
13:J:4:PHE:O	20:Q:64:ARG:NH1	2.51	0.40
18:O:33:ARG:O	18:O:34:HIS:CG	2.74	0.40
18:O:53:THR:OG1	18:O:65:THR:OG1	2.27	0.40
21:R:63:VAL:O	21:R:63:VAL:HG23	2.21	0.40
26:W:19:LYS:HB2	26:W:21:LEU:HD11	2.03	0.40
27:X:65:ASP:OD1	27:X:66:THR:N	2.52	0.40
41:l:47:LEU:HG	41:l:58:GLU:HB2	2.03	0.40
1:1:176:A:O2'	1:1:177:G:H5'	2.21	0.40
1:1:404:A:O2'	1:1:405:U:OP2	2.29	0.40
1:1:825:A:H2'	1:1:826:U:O4'	2.22	0.40
1:1:1050:A:H2'	1:1:1051:G:O5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1410:G:C6	1:1:1593:A:N1	2.90	0.40
1:1:2786:U:O2'	8:C:63:PRO:O	2.39	0.40
1:1:2815:C:C2	1:1:2816:G:C8	3.10	0.40
2:2:151:A:C5	2:2:152:A:C8	3.09	0.40
2:2:380:G:N1	2:2:384:G:O6	2.54	0.40
2:2:522:C:H2'	2:2:523:A:O4'	2.22	0.40
2:2:799:G:H2'	2:2:800:G:O4'	2.21	0.40
2:2:964:A:H2	2:2:969:A:N3	2.19	0.40
2:2:1123:U:H3	2:2:1150:A:H61	1.70	0.40
2:2:1151:A:O2'	2:2:1152:A:H5''	2.21	0.40
2:2:1160:G:C6	2:2:1161:C:C4	3.09	0.40
2:2:1428:A:H2'	2:2:1429:A:O4'	2.21	0.40
3:3:30:C:H2'	3:3:31:C:H5'	2.03	0.40
6:A:160:GLN:OE1	6:A:160:GLN:HA	2.21	0.40
8:C:2:ILE:CD1	8:C:48:ILE:HD11	2.51	0.40
14:K:107:LEU:O	14:K:109:SER:N	2.53	0.40
19:P:54:GLY:N	19:P:57:SER:OG	2.54	0.40
37:h:52:VAL:HG23	37:h:68:ILE:CG2	2.51	0.40
43:n:43:THR:O	43:n:46:MET:HG2	2.21	0.40
47:r:16:VAL:HG23	47:r:17:ILE:HG12	2.03	0.40
52:w:62:ALA:HB3	52:w:68:LEU:HD12	2.04	0.40
1:1:121:G:H4'	1:1:149:A:H5'	2.03	0.40
1:1:393:C:C2	1:1:394:C:C5	3.09	0.40
1:1:684:G:C2	1:1:794:A:C2	3.09	0.40
1:1:896:A:HO2'	1:1:897:C:P	2.37	0.40
1:1:1571:A:H2'	1:1:1572:A:O4'	2.22	0.40
1:1:2028:U:H2'	1:1:2029:G:O4'	2.21	0.40
1:1:2135:A:H2'	1:1:2135:A:N3	2.37	0.40
1:1:2658:C:H2'	1:1:2659:G:O4'	2.21	0.40
1:1:2839:G:N2	17:N:91:ALA:O	2.46	0.40
2:2:881:G:OP2	46:q:9:ARG:NH2	2.48	0.40
2:2:1100:C:H2'	2:2:1102:A:O5'	2.21	0.40
3:3:15:A:O4'	3:3:109:A:C8	2.74	0.40
10:E:52:ASN:HB2	10:E:150:ARG:HH22	1.87	0.40
15:L:27:LEU:HD12	15:L:27:LEU:N	2.37	0.40
16:M:67:VAL:HG12	16:M:68:PHE:N	2.36	0.40
23:T:55:VAL:HG21	23:T:85:VAL:HG13	2.04	0.40
26:W:47:ALA:HB1	26:W:51:VAL:HG23	2.02	0.40
44:o:36:VAL:O	44:o:36:VAL:HG13	2.22	0.40
1:1:219:A:H2'	1:1:220:G:O4'	2.22	0.40
1:1:591:U:O4	1:1:592:A:N6	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:812:C:OP1	20:Q:13:ARG:NH1	2.54	0.40
1:1:1652:A:OP1	17:N:8:ARG:NH1	2.48	0.40
1:1:1723:G:O6	1:1:1737:G:H1'	2.21	0.40
1:1:2644:G:O2'	1:1:2645:G:H5'	2.22	0.40
2:2:516:PSU:H4'	2:2:517:G:OP1	2.20	0.40
2:2:980:C:H2'	2:2:981:U:O4'	2.22	0.40
2:2:1010:U:H2'	2:2:1011:C:C6	2.56	0.40
2:2:1290:G:C5	2:2:1291:U:C5	3.10	0.40
2:2:1356:G:H2'	2:2:1357:A:C8	2.57	0.40
5:5:16:C:H3'	5:5:17:C:C5	2.56	0.40
5:5:52:G:H2'	5:5:53:G:H8	1.87	0.40
8:C:24:VAL:O	8:C:24:VAL:HG23	2.21	0.40
10:E:122:PHE:O	10:E:123:ASP:HB3	2.21	0.40
14:K:76:VAL:H	19:P:73:VAL:HG22	1.87	0.40
36:g:191:SER:OG	36:g:192:ASP:N	2.53	0.40
40:k:36:ILE:HD12	40:k:64:VAL:HG12	2.04	0.40
42:m:113:ASP:OD1	42:m:114:ARG:N	2.54	0.40
44:o:45:ARG:HB3	44:o:69:THR:CG2	2.52	0.40
50:u:4:ILE:HG13	50:u:21:VAL:HG12	2.03	0.40
50:u:20:VAL:HG12	50:u:35:ARG:HA	2.04	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	65/232 (28%)	62 (95%)	3 (5%)	0	100	100
7	B	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
8	C	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
9	D	199/201 (99%)	194 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	E	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
11	F	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
12	G	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
13	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
14	K	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	L	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
16	M	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
17	N	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
18	O	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
19	P	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
20	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
21	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
22	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
23	T	92/100 (92%)	91 (99%)	1 (1%)	0	100	100
24	U	101/104 (97%)	97 (96%)	4 (4%)	0	100	100
25	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
26	W	76/84 (90%)	71 (93%)	5 (7%)	0	100	100
27	X	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	Y	60/63 (95%)	60 (100%)	0	0	100	100
29	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
30	a	64/70 (91%)	59 (92%)	5 (8%)	0	100	100
31	b	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
32	c	50/55 (91%)	47 (94%)	3 (6%)	0	100	100
33	d	44/46 (96%)	44 (100%)	0	0	100	100
34	e	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
35	f	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
36	g	223/241 (92%)	215 (96%)	8 (4%)	0	100	100
37	h	206/233 (88%)	195 (95%)	11 (5%)	0	100	100
38	i	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
39	j	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
40	k	102/135 (76%)	97 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	l	149/179 (83%)	135 (91%)	14 (9%)	0	100	100
42	m	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
43	n	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
44	o	97/103 (94%)	86 (89%)	11 (11%)	0	100	100
45	p	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
46	q	120/124 (97%)	107 (89%)	13 (11%)	0	100	100
47	r	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
48	s	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
49	t	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
50	u	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
51	v	78/84 (93%)	69 (88%)	9 (12%)	0	100	100
52	w	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
53	x	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
54	y	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
55	z	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	5675/6144 (92%)	5407 (95%)	268 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	54/179 (30%)	54 (100%)	0	100	100
7	B	216/218 (99%)	216 (100%)	0	100	100
8	C	164/164 (100%)	164 (100%)	0	100	100
9	D	165/165 (100%)	165 (100%)	0	100	100
10	E	148/150 (99%)	148 (100%)	0	100	100
11	F	136/138 (99%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	G	114/114 (100%)	114 (100%)	0	100	100
13	J	116/116 (100%)	116 (100%)	0	100	100
14	K	104/104 (100%)	104 (100%)	0	100	100
15	L	103/103 (100%)	103 (100%)	0	100	100
16	M	109/109 (100%)	109 (100%)	0	100	100
17	N	99/103 (96%)	99 (100%)	0	100	100
18	O	86/87 (99%)	86 (100%)	0	100	100
19	P	99/100 (99%)	99 (100%)	0	100	100
20	Q	89/90 (99%)	89 (100%)	0	100	100
21	R	84/84 (100%)	84 (100%)	0	100	100
22	S	93/93 (100%)	93 (100%)	0	100	100
23	T	81/84 (96%)	81 (100%)	0	100	100
24	U	84/85 (99%)	84 (100%)	0	100	100
25	V	78/78 (100%)	78 (100%)	0	100	100
26	W	59/62 (95%)	59 (100%)	0	100	100
27	X	67/68 (98%)	67 (100%)	0	100	100
28	Y	54/55 (98%)	54 (100%)	0	100	100
29	Z	48/49 (98%)	48 (100%)	0	100	100
30	a	59/62 (95%)	59 (100%)	0	100	100
31	b	47/48 (98%)	47 (100%)	0	100	100
32	c	47/49 (96%)	47 (100%)	0	100	100
33	d	38/38 (100%)	38 (100%)	0	100	100
34	e	51/52 (98%)	51 (100%)	0	100	100
35	f	34/34 (100%)	34 (100%)	0	100	100
36	g	187/199 (94%)	187 (100%)	0	100	100
37	h	171/190 (90%)	171 (100%)	0	100	100
38	i	172/173 (99%)	172 (100%)	0	100	100
39	j	119/126 (94%)	119 (100%)	0	100	100
40	k	91/116 (78%)	91 (100%)	0	100	100
41	l	124/147 (84%)	124 (100%)	0	100	100
42	m	104/105 (99%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	n	105/107 (98%)	105 (100%)	0	100	100
44	o	86/90 (96%)	86 (100%)	0	100	100
45	p	90/99 (91%)	90 (100%)	0	100	100
46	q	102/103 (99%)	102 (100%)	0	100	100
47	r	94/96 (98%)	94 (100%)	0	100	100
48	s	83/84 (99%)	83 (100%)	0	100	100
49	t	76/77 (99%)	76 (100%)	0	100	100
50	u	65/65 (100%)	65 (100%)	0	100	100
51	v	74/78 (95%)	74 (100%)	0	100	100
52	w	57/65 (88%)	57 (100%)	0	100	100
53	x	72/79 (91%)	72 (100%)	0	100	100
54	y	65/66 (98%)	65 (100%)	0	100	100
55	z	60/61 (98%)	60 (100%)	0	100	100
All	All	4723/5007 (94%)	4723 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
6	A	188	ASN
8	C	49	GLN
8	C	164	GLN
9	D	115	GLN
9	D	136	GLN
12	G	66	ASN
13	J	128	ASN
17	N	81	ASN
18	O	38	GLN
19	P	75	GLN
22	S	9	HIS
24	U	54	GLN
28	Y	36	GLN
31	b	4	GLN
32	c	45	GLN
33	d	16	HIS
33	d	26	ASN

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Mol	Chain	Res	Type
36	g	19	GLN
36	g	109	GLN
36	g	120	GLN
37	h	25	ASN
37	h	176	HIS
38	i	71	GLN
38	i	100	ASN
39	j	148	ASN
40	k	17	GLN
40	k	94	HIS
41	l	86	GLN
43	n	50	GLN
43	n	75	GLN
44	o	99	GLN
47	r	52	GLN
50	u	40	ASN
50	u	59	HIS
52	w	75	GLN
55	z	9	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2904 (99%)	478 (16%)	19 (0%)
2	2	1532/1540 (99%)	236 (15%)	6 (0%)
3	3	119/120 (99%)	23 (19%)	1 (0%)
4	4	7/18 (38%)	4 (57%)	1 (14%)
5	5	76/77 (98%)	27 (35%)	1 (1%)
All	All	4636/4659 (99%)	768 (16%)	28 (0%)

All (768) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	27	G
1	1	34	U
1	1	46	G
1	1	63	A
1	1	74	A
1	1	75	G
1	1	85	G

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Mol	Chain	Res	Type
1	1	96	C
1	1	101	A
1	1	102	U
1	1	103	A
1	1	118	A
1	1	120	U
1	1	126	A
1	1	131	A
1	1	136	G
1	1	139	U
1	1	140	C
1	1	143	C
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	216	A
1	1	222	A
1	1	223	A
1	1	228	C
1	1	248	G
1	1	266	G
1	1	274	C
1	1	275	C
1	1	277	G
1	1	278	A
1	1	279	A
1	1	311	A
1	1	329	G
1	1	330	A
1	1	346	A
1	1	352	A
1	1	353	C
1	1	354	A
1	1	359	G
1	1	360	U
1	1	361	G
1	1	368	A
1	1	371	A
1	1	372	G
1	1	375	G
1	1	386	G

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Mol	Chain	Res	Type
1	1	396	G
1	1	404	A
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	429	A
1	1	451	U
1	1	457	A
1	1	480	A
1	1	481	G
1	1	490	C
1	1	491	G
1	1	492	A
1	1	497	A
1	1	499	U
1	1	501	A
1	1	503	A
1	1	505	A
1	1	509	C
1	1	531	C
1	1	532	A
1	1	540	C
1	1	541	A
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	549	G
1	1	563	A
1	1	572	A
1	1	573	U
1	1	575	A
1	1	603	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	621	A
1	1	627	A
1	1	637	A
1	1	643	A

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Mol	Chain	Res	Type
1	1	645	C
1	1	646	U
1	1	647	G
1	1	653	U
1	1	654	A
1	1	686	U
1	1	708	G
1	1	717	C
1	1	725	G
1	1	730	A
1	1	747	5MU
1	1	775	G
1	1	782	A
1	1	784	G
1	1	785	G
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	869	G
1	1	877	A
1	1	878	A
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	896	A
1	1	897	C
1	1	910	A
1	1	914	G
1	1	915	C
1	1	931	U
1	1	941	A
1	1	946	C

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Mol	Chain	Res	Type
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	995	C
1	1	996	A
1	1	1009	A
1	1	1012	U
1	1	1013	C
1	1	1026	G
1	1	1029	A
1	1	1030	C
1	1	1032	A
1	1	1033	U
1	1	1034	G
1	1	1037	G
1	1	1040	A
1	1	1042	G
1	1	1043	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1048	A
1	1	1051	G
1	1	1057	A
1	1	1062	G
1	1	1065	U
1	1	1066	U
1	1	1068	G
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1081	U
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1089	A
1	1	1096	A
1	1	1097	U
1	1	1100	C
1	1	1101	U
1	1	1107	G

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Mol	Chain	Res	Type
1	1	1111	A
1	1	1112	G
1	1	1114	C
1	1	1115	G
1	1	1120	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1136	G
1	1	1142	A
1	1	1169	A
1	1	1171	G
1	1	1172	C
1	1	1173	U
1	1	1175	A
1	1	1176	U
1	1	1180	U
1	1	1198	U
1	1	1199	U
1	1	1200	C
1	1	1202	G
1	1	1204	A
1	1	1212	G
1	1	1227	G
1	1	1236	G
1	1	1238	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1284	A
1	1	1293	C
1	1	1300	G
1	1	1301	A
1	1	1321	A
1	1	1329	U
1	1	1345	C
1	1	1359	A
1	1	1365	A

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Mol	Chain	Res	Type
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1395	A
1	1	1408	G
1	1	1416	G
1	1	1417	C
1	1	1428	C
1	1	1437	C
1	1	1460	U
1	1	1461	C
1	1	1467	U
1	1	1476	U
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1533	C
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1583	A
1	1	1584	U
1	1	1586	A
1	1	1588	G
1	1	1590	A
1	1	1608	A
1	1	1610	A
1	1	1618	6MZ
1	1	1646	C
1	1	1647	U

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Mol	Chain	Res	Type
1	1	1648	U
1	1	1649	G
1	1	1674	G
1	1	1715	G
1	1	1716	U
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1735	A
1	1	1736	U
1	1	1737	G
1	1	1738	G
1	1	1756	G
1	1	1764	C
1	1	1773	A
1	1	1786	A
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1816	C
1	1	1829	A
1	1	1835	2MG
1	1	1848	A
1	1	1857	G
1	1	1858	A
1	1	1859	U
1	1	1869	G
1	1	1870	C
1	1	1875	G
1	1	1878	G
1	1	1883	U
1	1	1906	G
1	1	1914	C
1	1	1916	A
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1931	U
1	1	1936	A
1	1	1937	A

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Mol	Chain	Res	Type
1	1	1938	A
1	1	1942	C
1	1	1955	U
1	1	1966	A
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	2020	A
1	1	2021	C
1	1	2022	U
1	1	2023	C
1	1	2030	A
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	2069	G7M
1	1	2072	C
1	1	2093	G
1	1	2101	A
1	1	2102	G
1	1	2107	G
1	1	2110	G
1	1	2111	U
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

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Mol	Chain	Res	Type
1	1	2123	G
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2135	A
1	1	2138	G
1	1	2142	A
1	1	2144	G
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2148	G
1	1	2158	A
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2166	U
1	1	2169	A
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2176	A
1	1	2180	U
1	1	2183	A
1	1	2188	U
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	2226	C
1	1	2238	G
1	1	2239	G

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Mol	Chain	Res	Type
1	1	2266	A
1	1	2278	A
1	1	2283	C
1	1	2287	A
1	1	2305	U
1	1	2309	A
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2383	G
1	1	2385	C
1	1	2396	G
1	1	2402	U
1	1	2406	A
1	1	2423	U
1	1	2425	A
1	1	2426	A
1	1	2428	G
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	2475	C
1	1	2476	A
1	1	2478	A
1	1	2480	C
1	1	2491	U
1	1	2492	U
1	1	2494	G
1	1	2502	G
1	1	2503	2MA
1	1	2504	PSU
1	1	2505	G
1	1	2513	A

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Mol	Chain	Res	Type
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2573	C
1	1	2585	U
1	1	2586	U
1	1	2603	G
1	1	2609	U
1	1	2613	U
1	1	2615	U
1	1	2629	U
1	1	2630	G
1	1	2661	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2718	G
1	1	2726	A
1	1	2729	G
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2765	A
1	1	2777	G
1	1	2778	A
1	1	2779	U
1	1	2793	C
1	1	2794	C
1	1	2795	C
1	1	2798	U
1	1	2818	U
1	1	2820	A
1	1	2825	G
1	1	2833	U
1	1	2834	G
1	1	2849	U
1	1	2867	G
1	1	2872	A

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Mol	Chain	Res	Type
1	1	2873	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2893	A
1	1	2897	U
1	1	2900	A
2	2	2	A
2	2	3	A
2	2	4	U
2	2	5	U
2	2	6	G
2	2	7	A
2	2	8	A
2	2	9	G
2	2	31	G
2	2	39	G
2	2	47	C
2	2	48	C
2	2	51	A
2	2	52	C
2	2	69	G
2	2	70	U
2	2	72	A
2	2	73	C
2	2	74	A
2	2	75	G
2	2	76	G
2	2	83	C
2	2	84	U
2	2	85	U
2	2	87	C
2	2	89	U
2	2	90	C
2	2	94	G
2	2	95	C
2	2	108	G
2	2	120	A
2	2	127	G
2	2	131	A
2	2	141	G

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Mol	Chain	Res	Type
2	2	144	G
2	2	164	G
2	2	174	A
2	2	189	A
2	2	192	A
2	2	197	A
2	2	202	G
2	2	209	U
2	2	211	G
2	2	212	G
2	2	226	G
2	2	240	G
2	2	244	U
2	2	247	G
2	2	251	G
2	2	262	A
2	2	266	G
2	2	267	C
2	2	279	A
2	2	280	C
2	2	289	G
2	2	306	A
2	2	321	A
2	2	328	C
2	2	332	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	372	C
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	429	U
2	2	456	A
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U

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Mol	Chain	Res	Type
2	2	468	A
2	2	474	G
2	2	475	C
2	2	478	A
2	2	481	G
2	2	482	A
2	2	484	G
2	2	486	U
2	2	492	C
2	2	493	A
2	2	495	A
2	2	496	A
2	2	509	A
2	2	511	C
2	2	512	U
2	2	517	G
2	2	518	C
2	2	519	C
2	2	521	G
2	2	527	7MG
2	2	531	U
2	2	532	A
2	2	547	A
2	2	559	A
2	2	564	C
2	2	571	U
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	588	G
2	2	595	A
2	2	596	A
2	2	653	U
2	2	665	A
2	2	687	A
2	2	700	G
2	2	702	A
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G

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Mol	Chain	Res	Type
2	2	747	A
2	2	748	G
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
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	846	G
2	2	851	G
2	2	902	G
2	2	914	A
2	2	926	G
2	2	934	C
2	2	935	A
2	2	960	U
2	2	966	2MG
2	2	969	A
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	978	A
2	2	989	U
2	2	992	U
2	2	993	G
2	2	996	A
2	2	999	C
2	2	1000	A
2	2	1004	A
2	2	1005	A
2	2	1014	A
2	2	1017	U
2	2	1018	G
2	2	1020	G
2	2	1023	U
2	2	1025	U
2	2	1028	C

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Mol	Chain	Res	Type
2	2	1029	U
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1035	A
2	2	1046	A
2	2	1048	G
2	2	1053	G
2	2	1065	U
2	2	1079	G
2	2	1085	U
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1103	C
2	2	1108	G
2	2	1124	G
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1142	G
2	2	1145	A
2	2	1158	C
2	2	1159	U
2	2	1167	A
2	2	1168	U
2	2	1169	A
2	2	1176	A
2	2	1196	A
2	2	1197	A
2	2	1210	C
2	2	1213	A
2	2	1227	A
2	2	1228	C
2	2	1236	A
2	2	1238	A
2	2	1241	G
2	2	1258	G
2	2	1260	G
2	2	1268	G

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Mol	Chain	Res	Type
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1299	A
2	2	1302	C
2	2	1305	G
2	2	1317	C
2	2	1320	C
2	2	1323	G
2	2	1353	G
2	2	1363	A
2	2	1379	G
2	2	1384	C
2	2	1398	A
2	2	1419	G
2	2	1432	G
2	2	1441	A
2	2	1446	A
2	2	1448	C
2	2	1452	C
2	2	1453	G
2	2	1492	A
2	2	1493	A
2	2	1494	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	4	C
3	3	15	A
3	3	16	G
3	3	23	G
3	3	35	C
3	3	41	G
3	3	44	G

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Mol	Chain	Res	Type
3	3	66	A
3	3	67	G
3	3	73	A
3	3	76	G
3	3	77	U
3	3	78	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	108	A
3	3	109	A
3	3	115	A
3	3	116	G
3	3	117	G
3	3	119	A
4	4	15	G
4	4	18	C
4	4	19	C
4	4	20	G
5	5	3	G
5	5	4	C
5	5	5	A
5	5	6	C
5	5	8	U
5	5	14	A
5	5	16	C
5	5	17	C
5	5	19	G
5	5	20	U
5	5	21	A
5	5	33	U
5	5	34	G
5	5	35	G
5	5	37	G
5	5	44	G
5	5	46	G
5	5	47	U
5	5	48	C
5	5	53	G
5	5	54	U
5	5	57	A
5	5	68	U

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Mol	Chain	Res	Type
5	5	72	G
5	5	73	A
5	5	75	C
5	5	76	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	278	A
1	1	328	U
1	1	404	A
1	1	491	G
1	1	784	G
1	1	894	U
1	1	1328	A
1	1	1358	G
1	1	1379	U
1	1	1507	C
1	1	1736	U
1	1	1858	A
1	1	2122	U
1	1	2126	A
1	1	2188	U
1	1	2193	G
1	1	2308	G
1	1	2425	A
1	1	2430	A
2	2	4	U
2	2	492	C
2	2	516	PSU
2	2	1109	C
2	2	1383	C
2	2	1493	A
3	3	76	G
4	4	18	C
5	5	72	G

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

32 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	2MA	1	2503	1,56	22,25,26	3.87	9 (40%)	32,37,40	3.78	11 (34%)
1	OMC	1	2498	1	19,22,23	2.99	8 (42%)	25,31,34	0.75	0
2	2MG	2	1516	2	23,26,27	2.90	9 (39%)	33,38,41	2.04	9 (27%)
2	2MG	2	1207	2	23,26,27	2.91	9 (39%)	33,38,41	2.10	8 (24%)
2	5MC	2	1407	2	19,22,23	3.86	8 (42%)	26,32,35	0.96	2 (7%)
2	MA6	2	1518	2	23,26,27	1.46	4 (17%)	33,38,41	2.87	12 (36%)
1	PSU	1	2504	1	18,21,22	1.10	1 (5%)	21,30,33	1.98	5 (23%)
1	6MZ	1	1618	1	22,25,26	3.33	4 (18%)	29,36,39	2.26	12 (41%)
1	PSU	1	2457	1	18,21,22	1.07	1 (5%)	21,30,33	2.07	6 (28%)
1	PSU	1	2605	1	18,21,22	1.07	1 (5%)	21,30,33	2.03	5 (23%)
2	MA6	2	1519	2	23,26,27	1.46	5 (21%)	33,38,41	2.89	11 (33%)
2	PSU	2	516	2,56	18,21,22	1.08	1 (5%)	21,30,33	2.14	6 (28%)
1	5MU	1	1939	1	19,22,23	4.84	7 (36%)	27,32,35	3.59	9 (33%)
1	2MG	1	2445	1	23,26,27	2.87	9 (39%)	33,38,41	2.11	10 (30%)
1	OMU	1	2552	1	19,22,23	3.11	8 (42%)	25,31,34	1.79	5 (20%)
1	1MG	1	745	1	23,26,27	3.09	8 (34%)	33,39,42	2.05	9 (27%)
1	PSU	1	1911	1	18,21,22	1.10	1 (5%)	21,30,33	2.07	5 (23%)
2	UR3	2	1498	2	19,22,23	2.97	8 (42%)	26,32,35	1.52	2 (7%)
1	2MG	1	1835	1	23,26,27	2.88	9 (39%)	33,38,41	2.14	11 (33%)
1	PSU	1	2580	1	18,21,22	1.11	1 (5%)	21,30,33	2.13	6 (28%)
2	7MG	2	527	2	23,26,27	3.94	11 (47%)	27,39,42	2.22	9 (33%)
1	PSU	1	1917	1	18,21,22	1.10	1 (5%)	21,30,33	1.99	5 (23%)
1	PSU	1	955	1	18,21,22	1.09	1 (5%)	21,30,33	2.02	5 (23%)
1	5MC	1	1962	1	19,22,23	3.85	8 (42%)	26,32,35	0.98	2 (7%)
1	PSU	1	746	1,56	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
46	0TD	q	89	46	8,9,10	2.09	2 (25%)	6,11,13	1.32	0
2	2MG	2	966	2	23,26,27	2.87	9 (39%)	33,38,41	2.19	11 (33%)
1	5MU	1	747	1	19,22,23	4.82	7 (36%)	27,32,35	3.60	9 (33%)
2	5MC	2	967	2	19,22,23	3.88	8 (42%)	26,32,35	0.97	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4OC	2	1402	2	20,23,24	3.17	8 (40%)	25,32,35	0.90	1 (4%)
1	G7M	1	2069	1	23,26,27	2.55	9 (39%)	34,39,42	1.90	10 (29%)
1	OMG	1	2251	1,5	23,26,27	2.45	9 (39%)	32,38,41	2.49	10 (31%)

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	2MA	1	2503	1,56	-	1/7/25/26	0/3/3/3
1	OMC	1	2498	1	-	0/9/27/28	0/2/2/2
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
2	2MG	2	1207	2	-	0/9/27/28	0/3/3/3
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	3/11/29/30	0/3/3/3
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	6MZ	1	1618	1	-	4/9/27/28	0/3/3/3
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	6/11/29/30	0/3/3/3
2	PSU	2	516	2,56	-	2/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
1	1MG	1	745	1	-	0/7/25/26	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	2/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/9/27/28	0/3/3/3
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
2	7MG	2	527	2	-	3/7/37/38	0/3/3/3
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	1	746	1,56	-	1/7/25/26	0/2/2/2
46	0TD	q	89	46	-	1/7/12/14	-
2	2MG	2	966	2	-	3/9/27/28	0/3/3/3
1	5MU	1	747	1	-	1/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
2	4OC	2	1402	2	-	0/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	1	2069	1	-	1/7/25/26	0/3/3/3
1	OMG	1	2251	1,5	-	0/9/27/28	0/3/3/3

All (185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1618	6MZ	C6-N6	14.38	1.50	1.34
1	1	2503	2MA	C4-N3	11.64	1.49	1.34
1	1	747	5MU	C2-N1	11.23	1.56	1.38
1	1	1939	5MU	C2-N1	11.18	1.56	1.38
1	1	1939	5MU	C4-C5	10.33	1.61	1.44
1	1	747	5MU	C6-N1	10.30	1.55	1.38
1	1	1939	5MU	C6-N1	10.29	1.55	1.38
1	1	747	5MU	C4-C5	10.26	1.61	1.44
2	2	527	7MG	C8-N9	9.91	1.52	1.45
2	2	967	5MC	C6-C5	9.31	1.49	1.34
2	2	1407	5MC	C6-C5	9.13	1.49	1.34
1	1	1962	5MC	C6-C5	9.06	1.49	1.34
1	1	745	1MG	C2-N3	8.60	1.47	1.33
2	2	527	7MG	C5-N7	8.22	1.46	1.35
2	2	1498	UR3	C2-N1	7.92	1.49	1.38
1	1	1939	5MU	C4-N3	-7.71	1.24	1.38
1	1	747	5MU	C4-N3	-7.64	1.24	1.38
2	2	1207	2MG	C2-N3	7.48	1.46	1.32
1	1	2445	2MG	C2-N3	7.36	1.46	1.32
1	1	1835	2MG	C2-N3	7.34	1.46	1.32
2	2	1516	2MG	C2-N3	7.31	1.45	1.32
2	2	1402	4OC	C4-N3	7.28	1.45	1.32
1	1	2552	OMU	C2-N1	7.26	1.49	1.38
1	1	2503	2MA	C2-N3	7.23	1.46	1.34
2	2	966	2MG	C2-N3	7.17	1.45	1.32
2	2	527	7MG	C4-N9	7.15	1.46	1.37
1	1	2552	OMU	C2-N3	7.02	1.50	1.38
1	1	1962	5MC	C4-N3	6.90	1.45	1.34
2	2	967	5MC	C5-C4	6.89	1.49	1.44
2	2	1407	5MC	C4-N3	6.89	1.45	1.34
2	2	967	5MC	C4-N3	6.80	1.45	1.34
2	2	1407	5MC	C5-C4	6.78	1.49	1.44
1	1	2503	2MA	C6-N1	6.71	1.44	1.35
2	2	1207	2MG	C4-N3	6.62	1.49	1.34
1	1	1962	5MC	C5-C4	6.61	1.49	1.44
1	1	2251	OMG	C4-N3	6.55	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1835	2MG	C4-N3	6.52	1.49	1.34
1	1	2069	G7M	C4-N3	6.51	1.49	1.34
2	2	1516	2MG	C4-N3	6.47	1.49	1.34
1	1	2445	2MG	C4-N3	6.47	1.49	1.34
2	2	966	2MG	C4-N3	6.47	1.49	1.34
1	1	2503	2MA	C2-N1	6.39	1.45	1.34
1	1	2498	OMC	C2-N3	6.38	1.49	1.36
2	2	527	7MG	C2-N3	6.37	1.48	1.33
1	1	1962	5MC	C2-N3	6.32	1.48	1.36
2	2	1498	UR3	C6-C5	6.30	1.49	1.35
2	2	1402	4OC	C6-C5	6.27	1.49	1.35
1	1	745	1MG	C4-N3	6.19	1.48	1.34
2	2	1402	4OC	C2-N3	6.18	1.48	1.36
2	2	1407	5MC	C2-N3	6.17	1.48	1.36
2	2	1516	2MG	C2-N2	6.09	1.46	1.33
1	1	745	1MG	C2-N2	6.03	1.44	1.34
1	1	2498	OMC	C6-C5	6.02	1.49	1.35
2	2	1207	2MG	C2-N2	5.99	1.46	1.33
2	2	967	5MC	C2-N3	5.95	1.48	1.36
1	1	2445	2MG	C2-N2	5.93	1.45	1.33
1	1	1835	2MG	C2-N2	5.92	1.45	1.33
2	2	966	2MG	C2-N2	5.86	1.45	1.33
1	1	1939	5MU	C6-C5	5.81	1.44	1.34
1	1	2552	OMU	C6-C5	5.78	1.48	1.35
2	2	527	7MG	C4-N3	5.70	1.47	1.34
1	1	747	5MU	C6-C5	5.63	1.43	1.34
1	1	2251	OMG	C2-N3	5.42	1.46	1.33
1	1	2069	G7M	C2-N3	5.37	1.46	1.33
2	2	1498	UR3	C2-N3	5.33	1.49	1.39
1	1	2498	OMC	C4-N3	5.22	1.44	1.34
2	2	1516	2MG	C2-N1	4.98	1.44	1.36
2	2	966	2MG	C2-N1	4.91	1.44	1.36
2	2	1207	2MG	C2-N1	4.90	1.44	1.36
1	1	1835	2MG	C2-N1	4.86	1.44	1.36
1	1	2445	2MG	C2-N1	4.82	1.44	1.36
2	2	967	5MC	C6-N1	4.80	1.46	1.38
1	1	2251	OMG	C2-N2	4.79	1.45	1.34
1	1	2069	G7M	C2-N2	4.73	1.45	1.34
1	1	2503	2MA	C5-C6	4.71	1.54	1.41
1	1	2498	OMC	C4-N4	4.67	1.45	1.33
2	2	1407	5MC	C6-N1	4.61	1.45	1.38
1	1	1962	5MC	C6-N1	4.55	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1402	4OC	C4-N4	4.55	1.45	1.36
46	q	89	0TD	CB-CA	-4.50	1.53	1.54
2	2	967	5MC	C4-N4	4.46	1.45	1.34
2	2	1407	5MC	C4-N4	4.44	1.45	1.34
1	1	1962	5MC	C4-N4	4.43	1.45	1.34
1	1	2498	OMC	C2-N1	4.42	1.49	1.40
1	1	1962	5MC	C2-N1	4.35	1.49	1.40
1	1	745	1MG	C5-C6	4.33	1.56	1.45
1	1	2552	OMU	C4-N3	4.29	1.46	1.38
2	2	1407	5MC	C2-N1	4.22	1.48	1.40
2	2	1402	4OC	C2-N1	4.21	1.48	1.40
2	2	967	5MC	C2-N1	4.16	1.48	1.40
1	1	745	1MG	O6-C6	-4.08	1.14	1.23
1	1	2069	G7M	C5-N7	-3.95	1.34	1.39
1	1	745	1MG	C2-N1	3.92	1.44	1.37
2	2	1518	MA6	C6-N6	3.85	1.47	1.36
2	2	1402	4OC	C5-C4	3.75	1.49	1.41
2	2	1519	MA6	C6-N6	3.74	1.47	1.36
2	2	527	7MG	C2-N1	3.65	1.46	1.37
1	1	746	PSU	C6-C5	3.58	1.39	1.35
2	2	527	7MG	C6-N1	3.57	1.45	1.38
2	2	516	PSU	C6-C5	3.55	1.39	1.35
1	1	1911	PSU	C6-C5	3.52	1.39	1.35
1	1	1917	PSU	C6-C5	3.51	1.39	1.35
1	1	2504	PSU	C6-C5	3.51	1.39	1.35
1	1	955	PSU	C6-C5	3.47	1.39	1.35
2	2	527	7MG	C2-N2	3.45	1.42	1.34
1	1	2580	PSU	C6-C5	3.44	1.39	1.35
2	2	527	7MG	C5-C6	3.42	1.52	1.43
1	1	2457	PSU	C6-C5	3.40	1.39	1.35
1	1	2069	G7M	C5-C6	3.36	1.52	1.43
1	1	2605	PSU	C6-C5	3.35	1.39	1.35
1	1	2498	OMC	C6-N1	3.16	1.45	1.38
2	2	1402	4OC	C6-N1	3.13	1.45	1.38
1	1	2503	2MA	C6-N6	-3.11	1.26	1.34
2	2	1207	2MG	C5-N7	-3.10	1.32	1.39
1	1	1835	2MG	C5-N7	-3.10	1.32	1.39
1	1	2069	G7M	C6-N1	3.09	1.44	1.38
2	2	966	2MG	C5-N7	-3.08	1.32	1.39
2	2	527	7MG	O6-C6	-3.06	1.17	1.23
1	1	2445	2MG	C5-N7	-3.06	1.32	1.39
2	2	1516	2MG	C5-N7	-3.05	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2251	OMG	C5-N7	-2.95	1.33	1.39
1	1	1618	6MZ	C5-N7	-2.93	1.33	1.39
2	2	1519	MA6	C5-C4	-2.91	1.33	1.39
1	1	2552	OMU	O4-C4	-2.90	1.18	1.24
1	1	745	1MG	C5-N7	-2.90	1.33	1.39
1	1	2552	OMU	C6-N1	2.87	1.44	1.38
2	2	1518	MA6	C5-C4	-2.85	1.34	1.39
2	2	1498	UR3	C6-N1	2.85	1.44	1.38
1	1	2251	OMG	C2-N1	2.85	1.44	1.37
1	1	2503	2MA	C5-N7	-2.84	1.33	1.39
1	1	1618	6MZ	C5-C4	-2.79	1.34	1.39
1	1	2498	OMC	O2-C2	-2.70	1.18	1.23
2	2	1402	4OC	O2-C2	-2.70	1.18	1.23
2	2	967	5MC	O2-C2	-2.68	1.18	1.23
2	2	1407	5MC	O2-C2	-2.67	1.18	1.23
1	1	2069	G7M	C2-N1	2.63	1.44	1.37
2	2	1518	MA6	C5-N7	-2.63	1.34	1.39
1	1	1835	2MG	O6-C6	-2.63	1.18	1.23
2	2	1498	UR3	O2-C2	-2.62	1.17	1.22
2	2	1498	UR3	O4-C4	-2.62	1.18	1.23
2	2	966	2MG	O6-C6	-2.62	1.18	1.23
2	2	1519	MA6	C5-N7	-2.61	1.34	1.39
1	1	747	5MU	O4-C4	-2.60	1.18	1.23
1	1	1939	5MU	O4-C4	-2.60	1.18	1.23
1	1	1962	5MC	O2-C2	-2.59	1.18	1.23
2	2	1207	2MG	O6-C6	-2.59	1.18	1.23
2	2	1516	2MG	O6-C6	-2.58	1.18	1.23
1	1	2445	2MG	O6-C6	-2.57	1.18	1.23
2	2	1498	UR3	C5-C4	2.53	1.50	1.43
2	2	966	2MG	C6-N1	2.50	1.43	1.38
1	1	1939	5MU	O2-C2	-2.48	1.18	1.23
1	1	2251	OMG	C5-C6	2.47	1.53	1.44
2	2	1207	2MG	C5-C6	2.46	1.53	1.44
1	1	2251	OMG	O6-C6	-2.46	1.18	1.23
1	1	2498	OMC	C5-C4	2.44	1.48	1.42
1	1	2552	OMU	C5-C4	2.43	1.49	1.43
1	1	2251	OMG	C6-N1	2.42	1.43	1.38
1	1	1835	2MG	C5-C6	2.42	1.53	1.44
1	1	747	5MU	O2-C2	-2.41	1.18	1.23
1	1	2445	2MG	C5-C6	2.41	1.53	1.44
2	2	1498	UR3	C4-N3	2.41	1.45	1.40
2	2	966	2MG	C5-C6	2.41	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2503	2MA	C4-N9	-2.40	1.32	1.37
2	2	1516	2MG	C5-C6	2.39	1.53	1.44
2	2	1516	2MG	C6-N1	2.36	1.43	1.38
1	1	2552	OMU	O2-C2	-2.35	1.18	1.23
2	2	1516	2MG	C4-N9	-2.35	1.32	1.38
2	2	966	2MG	C4-N9	-2.33	1.32	1.38
1	1	2069	G7M	O6-C6	-2.31	1.19	1.23
2	2	1207	2MG	C6-N1	2.28	1.43	1.38
1	1	1835	2MG	C6-N1	2.26	1.43	1.38
1	1	2445	2MG	C6-N1	2.25	1.43	1.38
1	1	2503	2MA	C8-N7	2.24	1.36	1.31
1	1	2445	2MG	C4-N9	-2.23	1.32	1.38
1	1	1618	6MZ	C8-N9	-2.19	1.33	1.37
1	1	1835	2MG	C4-N9	-2.18	1.32	1.38
1	1	745	1MG	C8-N9	-2.16	1.32	1.37
1	1	2069	G7M	C4-N9	-2.13	1.32	1.38
2	2	1207	2MG	C4-N9	-2.11	1.32	1.38
46	q	89	0TD	CSB-SB	-2.08	1.75	1.79
2	2	1518	MA6	C4-N9	-2.05	1.33	1.37
1	1	2251	OMG	C4-N9	-2.04	1.32	1.38
2	2	1519	MA6	C4-N9	-2.04	1.33	1.37
2	2	527	7MG	C8-N7	2.03	1.52	1.42
2	2	1519	MA6	C10-N6	2.02	1.50	1.45

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2503	2MA	C1'-N9-C8	-13.66	96.78	127.09
1	1	747	5MU	C5-C4-N3	12.03	125.78	115.32
1	1	1939	5MU	C5-C4-N3	11.94	125.70	115.32
1	1	2503	2MA	C4-N9-C1'	11.75	154.12	126.63
2	2	1519	MA6	N1-C6-N6	-9.72	105.02	116.86
2	2	1518	MA6	N1-C6-N6	-9.71	105.02	116.86
1	1	747	5MU	C5-C6-N1	-8.81	113.74	123.31
1	1	1939	5MU	C5-C6-N1	-8.78	113.77	123.31
1	1	2251	OMG	C1'-N9-C8	-7.12	106.50	126.73
2	2	966	2MG	C2-N3-C4	6.38	119.99	112.00
1	1	1835	2MG	C2-N3-C4	6.36	119.95	112.00
1	1	2251	OMG	C1'-N9-C4	6.33	145.19	126.49
2	2	1207	2MG	C2-N3-C4	6.30	119.88	112.00
1	1	2445	2MG	C2-N3-C4	6.27	119.84	112.00
2	2	1516	2MG	C2-N3-C4	6.18	119.74	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1518	MA6	C5-C6-N6	6.15	135.07	125.33
2	2	1519	MA6	C5-C6-N6	5.97	134.78	125.33
1	1	2503	2MA	C5-C4-N3	-5.69	121.18	127.18
1	1	1618	6MZ	N1-C2-N3	-5.57	120.16	128.58
1	1	2552	OMU	C4-N3-C2	-5.50	119.78	126.61
2	2	1519	MA6	N1-C2-N3	-5.49	120.28	128.58
2	2	1518	MA6	N1-C2-N3	-5.46	120.32	128.58
2	2	1498	UR3	C4-N3-C2	-5.29	120.33	124.58
2	2	1207	2MG	C5-C4-N3	-5.25	120.03	128.39
1	1	2580	PSU	N1-C2-N3	5.25	120.71	115.17
1	1	2580	PSU	C4-N3-C2	-5.20	119.22	126.37
1	1	1911	PSU	C4-N3-C2	-5.19	119.23	126.37
2	2	516	PSU	N1-C2-N3	5.15	120.60	115.17
1	1	745	1MG	C1'-N9-C4	-5.14	111.30	126.49
1	1	1911	PSU	N1-C2-N3	5.13	120.58	115.17
1	1	1835	2MG	C5-C4-N3	-5.12	120.24	128.39
1	1	2457	PSU	N1-C2-N3	5.11	120.56	115.17
1	1	1939	5MU	O4-C4-C5	-5.11	119.08	124.92
1	1	2503	2MA	N9-C8-N7	-5.11	106.69	113.94
1	1	2605	PSU	C4-N3-C2	-5.08	119.37	126.37
2	2	516	PSU	C4-N3-C2	-5.08	119.37	126.37
1	1	2457	PSU	C4-N3-C2	-5.07	119.39	126.37
1	1	745	1MG	C5-C4-N3	-5.07	120.32	128.39
1	1	2605	PSU	N1-C2-N3	5.07	120.51	115.17
1	1	2445	2MG	C5-C4-N3	-5.06	120.33	128.39
1	1	747	5MU	O4-C4-C5	-5.04	119.15	124.92
1	1	955	PSU	N1-C2-N3	5.02	120.46	115.17
1	1	955	PSU	C4-N3-C2	-5.00	119.48	126.37
2	2	966	2MG	C5-C4-N3	-4.99	120.45	128.39
2	2	1519	MA6	C5-C4-N3	-4.98	119.86	126.72
1	1	1939	5MU	C4-N3-C2	-4.98	120.82	127.34
1	1	2504	PSU	C4-N3-C2	-4.97	119.53	126.37
1	1	2251	OMG	C5-C4-N3	-4.97	120.49	128.39
1	1	746	PSU	C4-N3-C2	-4.95	119.56	126.37
2	2	1518	MA6	C5-C4-N3	-4.94	119.92	126.72
1	1	747	5MU	C4-N3-C2	-4.94	120.87	127.34
1	1	1618	6MZ	C5-C4-N3	-4.93	119.93	126.72
2	2	527	7MG	C5-C6-N1	4.92	119.59	110.94
1	1	1917	PSU	N1-C2-N3	4.90	120.33	115.17
1	1	745	1MG	C1'-N9-C8	4.90	140.65	126.73
1	1	1917	PSU	C4-N3-C2	-4.89	119.63	126.37
1	1	2504	PSU	N1-C2-N3	4.89	120.33	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1516	2MG	C5-C4-N3	-4.88	120.62	128.39
1	1	1939	5MU	N3-C2-N1	4.87	121.23	114.89
1	1	746	PSU	N1-C2-N3	4.80	120.23	115.17
1	1	747	5MU	N3-C2-N1	4.62	120.90	114.89
2	2	966	2MG	N1-C2-N2	4.55	121.20	116.56
2	2	527	7MG	C2-N3-C4	4.46	119.98	112.30
1	1	2251	OMG	C2-N3-C4	4.44	119.95	112.30
2	2	527	7MG	C4-C5-N7	4.27	110.42	105.38
1	1	747	5MU	C5M-C5-C4	4.27	123.34	118.78
2	2	527	7MG	C5-C4-N3	-4.27	120.11	128.13
1	1	2069	G7M	C2-N3-C4	4.27	119.66	112.30
2	2	966	2MG	C2-N1-C6	-4.16	119.52	124.55
2	2	1519	MA6	N9-C8-N7	-4.16	108.03	113.94
2	2	1207	2MG	C2-N1-C6	-4.15	119.53	124.55
1	1	2445	2MG	C2-N1-C6	-4.13	119.56	124.55
1	1	1618	6MZ	N9-C8-N7	-4.09	108.13	113.94
1	1	1835	2MG	C2-N1-C6	-4.08	119.61	124.55
2	2	1518	MA6	C4-C5-C6	4.04	120.09	115.91
1	1	1939	5MU	C5M-C5-C4	4.03	123.08	118.78
2	2	1516	2MG	C2-N1-C6	-3.99	119.72	124.55
2	2	1519	MA6	C4-C5-C6	3.98	120.03	115.91
2	2	1518	MA6	N9-C8-N7	-3.96	108.32	113.94
1	1	1835	2MG	N1-C2-N2	3.89	120.53	116.56
1	1	2069	G7M	C5-C4-N3	-3.88	120.81	128.15
1	1	747	5MU	C5M-C5-C6	-3.86	117.62	122.85
1	1	2069	G7M	C5-C6-N1	3.82	119.73	111.84
1	1	2552	OMU	N3-C2-N1	3.80	119.84	114.89
1	1	2445	2MG	N1-C2-N2	3.77	120.41	116.56
1	1	1939	5MU	C5M-C5-C6	-3.66	117.89	122.85
1	1	2069	G7M	O6-C6-C5	-3.62	119.93	128.01
1	1	2552	OMU	C5-C4-N3	3.56	119.79	114.80
2	2	1498	UR3	C5-C4-N3	3.51	119.66	115.04
1	1	745	1MG	C2-N3-C4	3.50	119.85	111.98
1	1	1618	6MZ	C4-C5-C6	3.50	119.69	116.78
1	1	2069	G7M	N9-C4-N3	3.43	132.81	125.95
2	2	1207	2MG	N1-C2-N2	3.43	120.06	116.56
1	1	1618	6MZ	C9-N6-C6	-3.41	119.69	122.85
1	1	1618	6MZ	C2-N3-C4	3.38	120.09	111.83
2	2	1518	MA6	C2-N3-C4	3.37	120.06	111.83
2	2	1519	MA6	C2-N3-C4	3.35	120.01	111.83
2	2	1516	2MG	N1-C2-N2	3.33	119.96	116.56
2	2	967	5MC	C5-C6-N1	-3.26	119.78	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2503	2MA	N3-C2-N1	-3.24	120.05	125.77
1	1	2251	OMG	N9-C8-N7	-3.24	107.40	113.40
2	2	1518	MA6	C2-N1-C6	3.23	119.71	111.83
1	1	2503	2MA	C5-N7-C8	3.22	108.51	103.45
1	1	2503	2MA	C4-N9-C8	3.20	109.10	105.74
2	2	1519	MA6	C2-N1-C6	3.19	119.62	111.83
1	1	2503	2MA	N3-C4-N9	3.18	131.02	126.99
1	1	2580	PSU	O2-C2-N1	-3.14	119.55	122.79
2	2	527	7MG	O6-C6-C5	-3.08	120.06	127.62
2	2	1519	MA6	N3-C4-N9	3.08	132.40	127.17
2	2	1407	5MC	C5-C6-N1	-3.06	119.99	123.31
1	1	2457	PSU	O2-C2-N1	-3.06	119.63	122.79
2	2	516	PSU	O2-C2-N1	-3.02	119.67	122.79
2	2	1207	2MG	N9-C4-N3	3.01	131.97	125.95
2	2	527	7MG	N9-C4-N3	3.01	129.86	125.46
1	1	2069	G7M	C2-N1-C6	-3.00	119.67	125.11
1	1	2251	OMG	C2-N1-C6	-2.99	119.69	125.11
1	1	2069	G7M	C1'-N9-C4	-2.98	117.68	126.49
2	2	527	7MG	C2-N1-C6	-2.94	119.79	125.11
1	1	2552	OMU	O4-C4-C5	-2.92	120.13	125.16
1	1	2605	PSU	O2-C2-N1	-2.90	119.80	122.79
1	1	2504	PSU	O2-C2-N1	-2.89	119.80	122.79
1	1	1917	PSU	O2-C2-N1	-2.89	119.81	122.79
2	2	527	7MG	C5-C4-N9	2.88	110.02	106.33
2	2	966	2MG	N9-C8-N7	-2.88	108.06	113.40
2	2	1516	2MG	N9-C8-N7	-2.88	108.07	113.40
1	1	745	1MG	N9-C8-N7	-2.87	108.07	113.40
1	1	1618	6MZ	N3-C4-N9	2.87	132.04	127.17
1	1	1962	5MC	C5-C6-N1	-2.84	120.23	123.31
1	1	955	PSU	O2-C2-N1	-2.83	119.87	122.79
1	1	1618	6MZ	C5-N7-C8	2.83	107.90	103.45
1	1	745	1MG	N9-C4-N3	2.82	131.60	125.95
2	2	1518	MA6	N3-C4-N9	2.82	131.97	127.17
1	1	2445	2MG	N9-C8-N7	-2.82	108.17	113.40
1	1	746	PSU	O2-C2-N1	-2.82	119.88	122.79
1	1	1911	PSU	O2-C2-N1	-2.80	119.90	122.79
1	1	1835	2MG	N9-C8-N7	-2.80	108.22	113.40
1	1	1835	2MG	N9-C4-N3	2.79	131.52	125.95
1	1	2457	PSU	C6-C5-C4	2.78	120.05	118.17
1	1	1939	5MU	O2-C2-N1	-2.78	119.18	122.80
1	1	2251	OMG	N9-C4-N3	2.76	131.48	125.95
1	1	2445	2MG	N9-C4-N3	2.75	131.46	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	516	PSU	C6-N1-C2	-2.75	120.14	122.69
2	2	1519	MA6	C5-N7-C8	2.73	107.73	103.45
2	2	1518	MA6	C5-N7-C8	2.71	107.70	103.45
2	2	1207	2MG	N9-C8-N7	-2.69	108.40	113.40
1	1	2503	2MA	CM2-C2-N1	2.69	121.16	117.13
1	1	1911	PSU	C6-C5-C4	2.69	119.99	118.17
1	1	2580	PSU	C6-C5-C4	2.69	119.99	118.17
1	1	747	5MU	O4-C4-N3	-2.68	115.07	120.11
1	1	747	5MU	O2-C2-N1	-2.67	119.31	122.80
1	1	955	PSU	C6-C5-C4	2.67	119.97	118.17
1	1	1917	PSU	C6-C5-C4	2.65	119.96	118.17
2	2	1516	2MG	N9-C4-N3	2.63	131.21	125.95
1	1	2605	PSU	C6-N1-C2	-2.62	120.26	122.69
1	1	2445	2MG	C5-C6-N1	2.62	119.91	113.25
1	1	1835	2MG	C5-C6-N1	2.61	119.89	113.25
1	1	1939	5MU	O4-C4-N3	-2.60	115.22	120.11
1	1	745	1MG	C5-C6-N1	2.60	119.82	115.02
2	2	966	2MG	C5-C6-N1	2.60	119.86	113.25
1	1	2251	OMG	C5-C6-N1	2.59	119.86	113.25
2	2	966	2MG	N9-C4-N3	2.59	131.14	125.95
2	2	1207	2MG	C5-C6-N1	2.59	119.84	113.25
1	1	2069	G7M	N9-C8-N7	-2.58	106.21	112.48
2	2	516	PSU	C3'-C2'-C1'	2.58	104.73	101.69
2	2	1516	2MG	C5-C6-N1	2.56	119.77	113.25
1	1	2069	G7M	CN7-N7-C5	2.54	129.97	126.80
1	1	2580	PSU	C6-N1-C2	-2.54	120.33	122.69
1	1	955	PSU	C6-N1-C2	-2.54	120.33	122.69
2	2	966	2MG	O6-C6-C5	-2.53	119.86	126.53
1	1	2504	PSU	C6-C5-C4	2.51	119.86	118.17
1	1	2457	PSU	C6-N1-C2	-2.46	120.41	122.69
2	2	1516	2MG	O6-C6-C5	-2.44	120.10	126.53
2	2	527	7MG	N9-C8-N7	2.43	106.81	103.37
1	1	1917	PSU	C6-N1-C2	-2.42	120.44	122.69
1	1	2605	PSU	C6-C5-C4	2.42	119.81	118.17
1	1	2251	OMG	O6-C6-C5	-2.42	120.15	126.53
1	1	2445	2MG	O6-C6-C5	-2.42	120.15	126.53
1	1	1911	PSU	C6-N1-C2	-2.38	120.48	122.69
2	2	1207	2MG	O6-C6-C5	-2.37	120.28	126.53
1	1	1835	2MG	O6-C6-C5	-2.36	120.30	126.53
1	1	2503	2MA	C4-C5-N7	-2.35	107.90	110.58
1	1	2580	PSU	O4'-C1'-C2'	2.34	108.39	105.15
1	1	746	PSU	C6-N1-C2	-2.33	120.53	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2251	OMG	C8-N7-C5	2.32	108.39	104.26
2	2	1519	MA6	C4-N9-C8	2.31	108.16	105.74
2	2	1402	4OC	C6-C5-C4	2.30	119.77	117.00
2	2	516	PSU	O4'-C1'-C2'	2.30	108.33	105.15
1	1	2069	G7M	CN7-N7-C8	-2.26	121.37	124.79
1	1	2504	PSU	C6-N1-C2	-2.23	120.62	122.69
1	1	2503	2MA	N6-C6-N1	2.22	120.02	117.03
1	1	1618	6MZ	C5-C6-N1	2.21	120.53	118.15
1	1	1835	2MG	CM2-N2-C2	-2.20	118.93	123.65
1	1	1618	6MZ	C4-C5-N7	-2.18	108.09	110.58
2	2	1518	MA6	C4-C5-N7	-2.16	108.11	110.58
2	2	966	2MG	CM2-N2-C2	-2.15	119.03	123.65
1	1	1962	5MC	CM5-C5-C6	-2.13	119.97	122.85
2	2	1518	MA6	C5-C4-N9	2.11	108.11	105.81
1	1	745	1MG	CM1-N1-C6	2.11	120.91	117.64
1	1	2445	2MG	CM2-N2-C2	-2.09	119.16	123.65
1	1	2552	OMU	O2-C2-N1	-2.07	120.10	122.80
1	1	1835	2MG	C8-N7-C5	2.05	107.92	104.26
2	2	1516	2MG	N1-C2-N3	-2.05	120.23	123.68
1	1	2457	PSU	O4'-C1'-C2'	2.04	107.97	105.15
1	1	1835	2MG	N1-C2-N3	-2.03	120.25	123.68
1	1	1618	6MZ	C5-C4-N9	2.03	108.03	105.81
2	2	1407	5MC	CM5-C5-C6	-2.02	120.11	122.85
2	2	966	2MG	N1-C2-N3	-2.02	120.27	123.68
2	2	966	2MG	C8-N7-C5	2.02	107.86	104.26
1	1	1618	6MZ	C4-N9-C8	2.02	107.86	105.74
1	1	2445	2MG	C8-N7-C5	2.02	107.85	104.26
1	1	745	1MG	C8-N7-C5	2.01	107.85	104.26
2	2	967	5MC	CM5-C5-C6	-2.01	120.13	122.85

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	C5-C6-N6-C9
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
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	966	2MG	O4'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
2	2	527	7MG	C3'-C4'-C5'-O5'
2	2	1498	UR3	O4'-C4'-C5'-O5'
2	2	1518	MA6	N1-C6-N6-C10
2	2	1519	MA6	N1-C6-N6-C10
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
2	2	527	7MG	O4'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C9
2	2	1498	UR3	C3'-C4'-C5'-O5'
46	q	89	0TD	CG-CB-SB-CSB
2	2	527	7MG	C4'-C5'-O5'-P
2	2	966	2MG	C4'-C5'-O5'-P
2	2	1519	MA6	C5-C6-N6-C9
1	1	746	PSU	O4'-C1'-C5-C6
2	2	1519	MA6	C4'-C5'-O5'-P
1	1	2503	2MA	O4'-C1'-N9-C8
1	1	747	5MU	C3'-C4'-C5'-O5'
1	1	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

14 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2503	2MA	1	0
2	2	1516	2MG	1	0
2	2	1518	MA6	2	0
1	1	2504	PSU	1	0
2	2	1519	MA6	2	0
2	2	516	PSU	2	0
1	1	2552	OMU	2	0
1	1	745	1MG	1	0
2	2	1498	UR3	1	0
1	1	955	PSU	1	0
1	1	1962	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	q	89	0TD	1	0
2	2	967	5MC	1	0
2	2	1402	4OC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 531 ligands modelled in this entry, 530 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	LYS	5	101	5	7,8,9	0.51	0	3,8,10	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	LYS	5	101	5	-	2/6/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	5	101	LYS	C-CA-CB-CG
57	5	101	LYS	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	5	101	LYS	3	0

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.

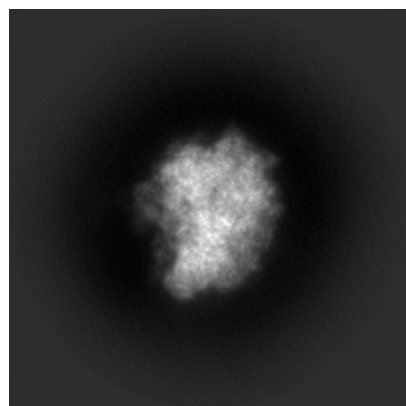
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42541. These allow visual inspection of the internal detail of the map and identification of artifacts.

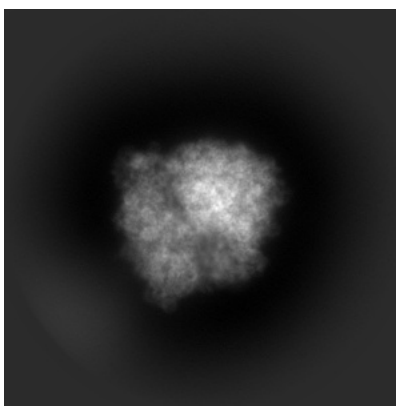
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

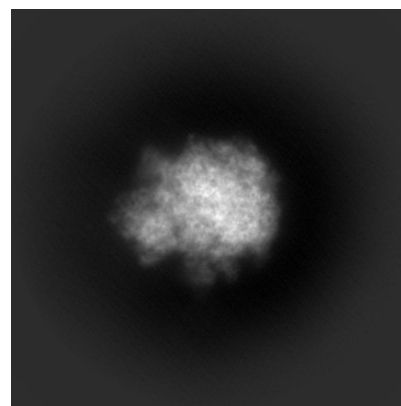
6.1.1 Primary map



X

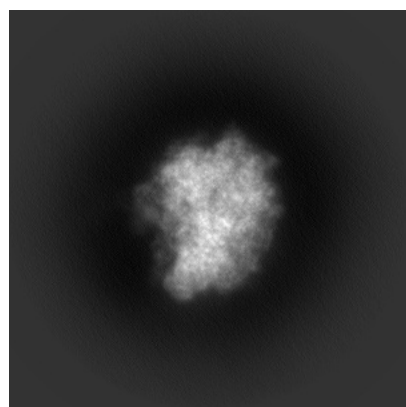


Y

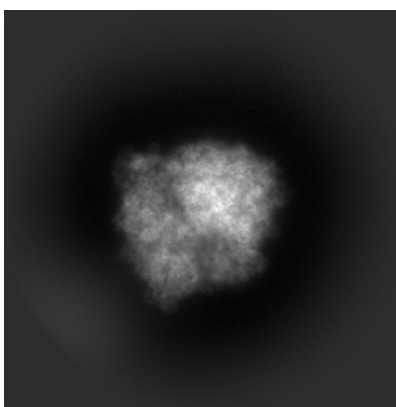


Z

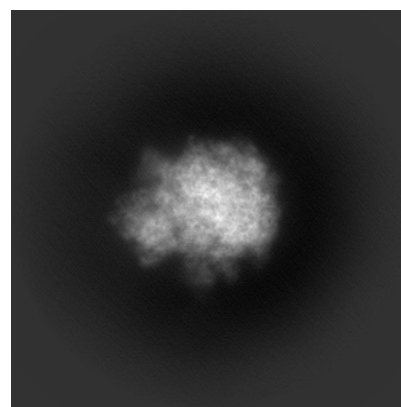
6.1.2 Raw map



X



Y

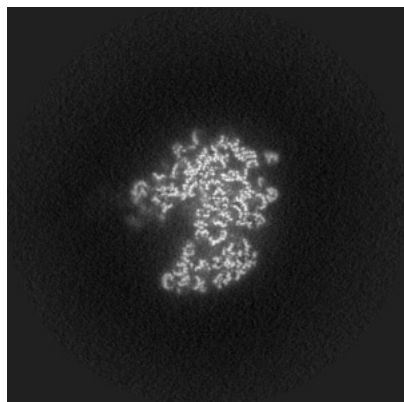


Z

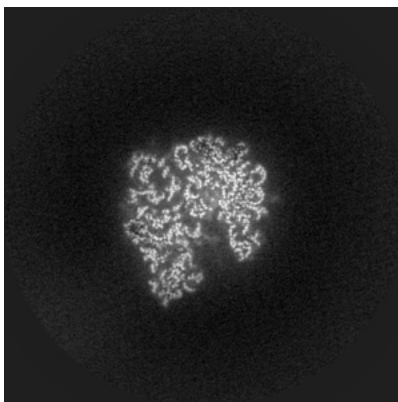
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

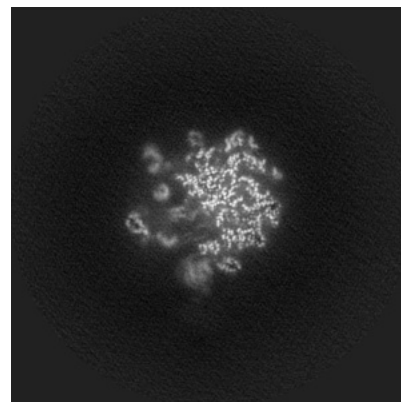
6.2.1 Primary map



X Index: 256

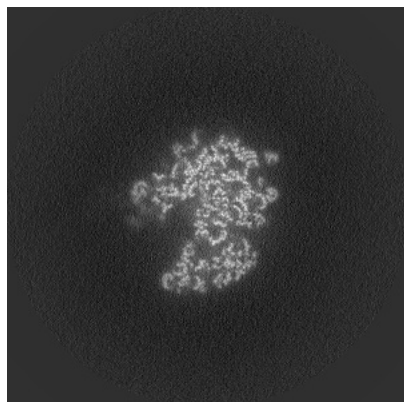


Y Index: 256

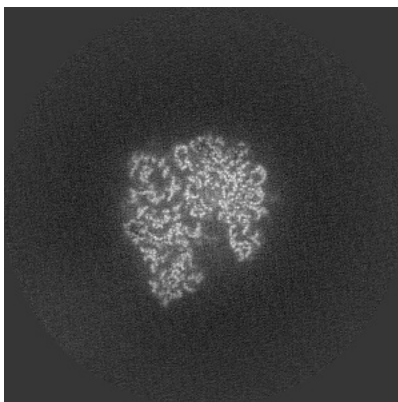


Z Index: 256

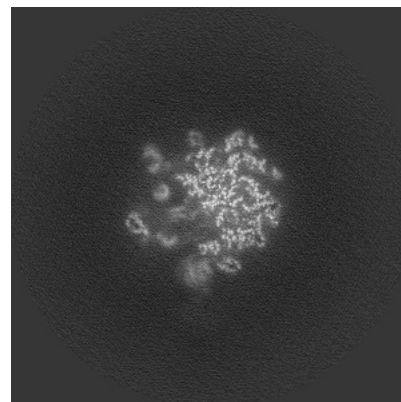
6.2.2 Raw map



X Index: 256



Y Index: 256

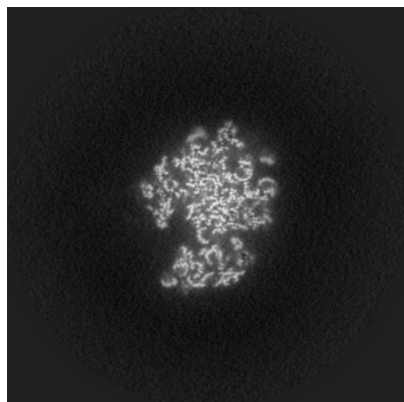


Z Index: 256

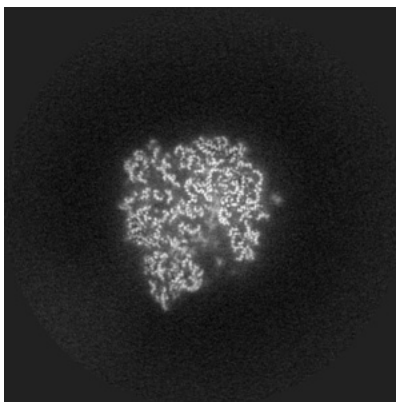
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

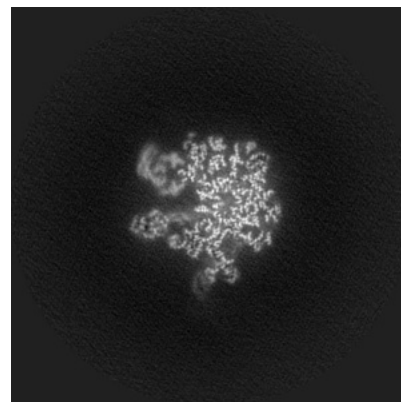
6.3.1 Primary map



X Index: 265

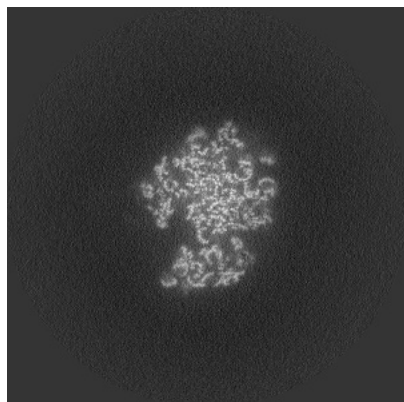


Y Index: 251

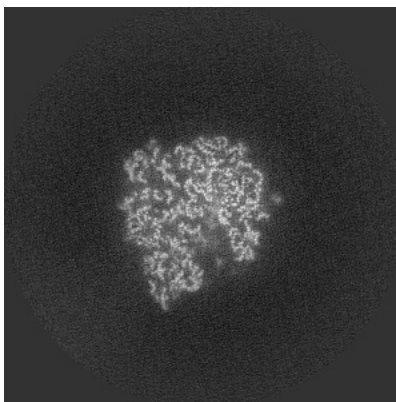


Z Index: 276

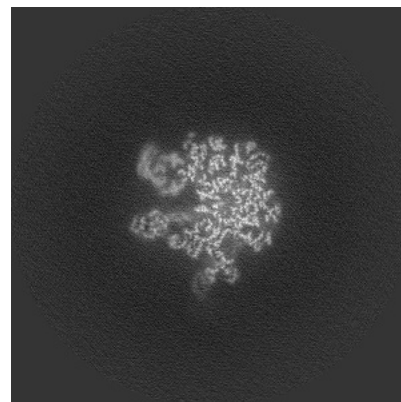
6.3.2 Raw map



X Index: 265



Y Index: 251

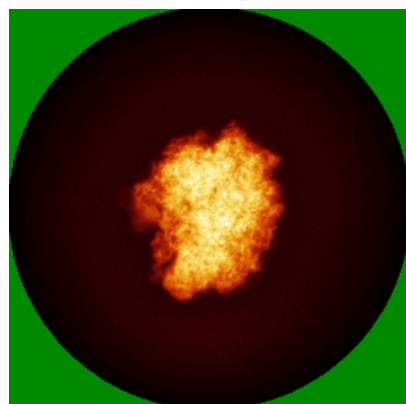


Z Index: 276

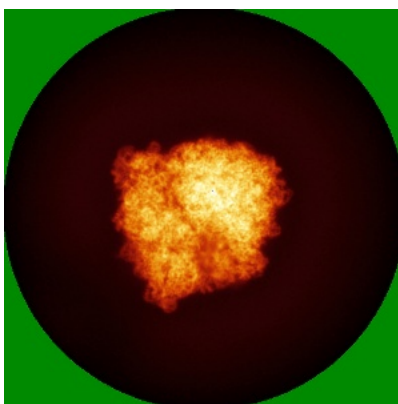
The images above show the largest variance slices of the map in three orthogonal directions.

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

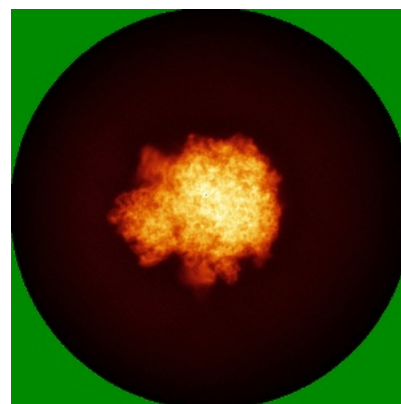
6.4.1 Primary map



X

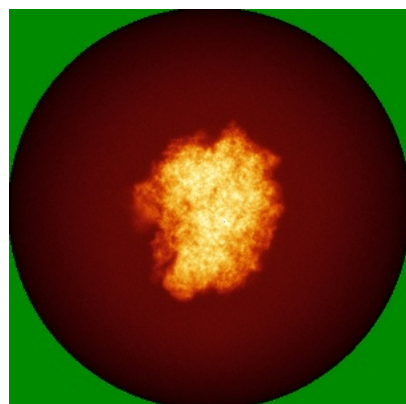


Y

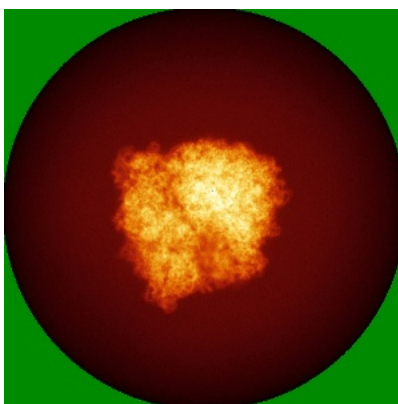


Z

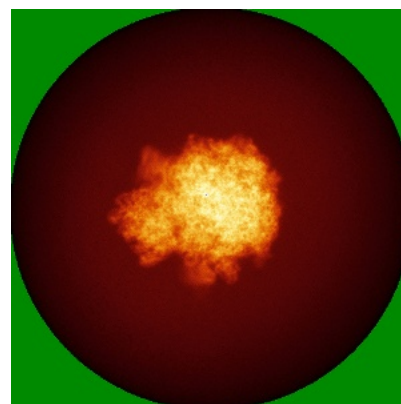
6.4.2 Raw map



X



Y

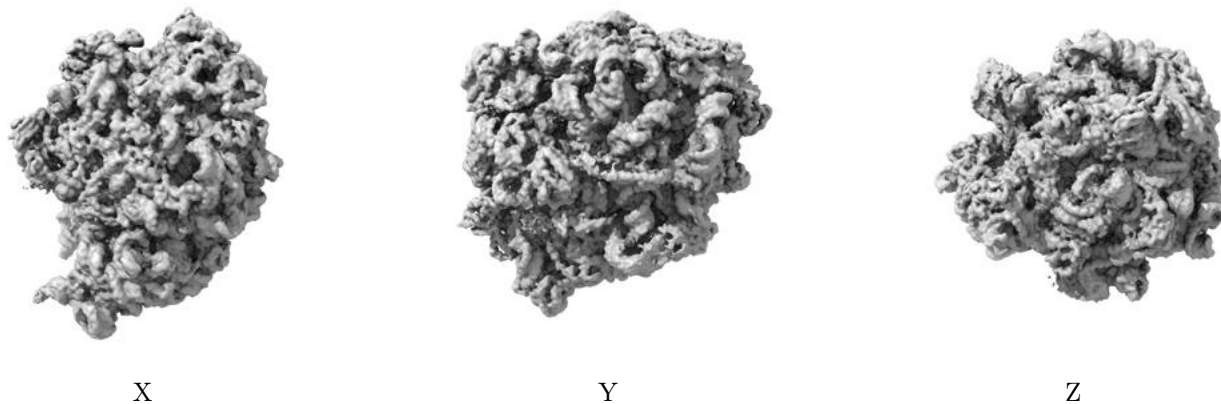


Z

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

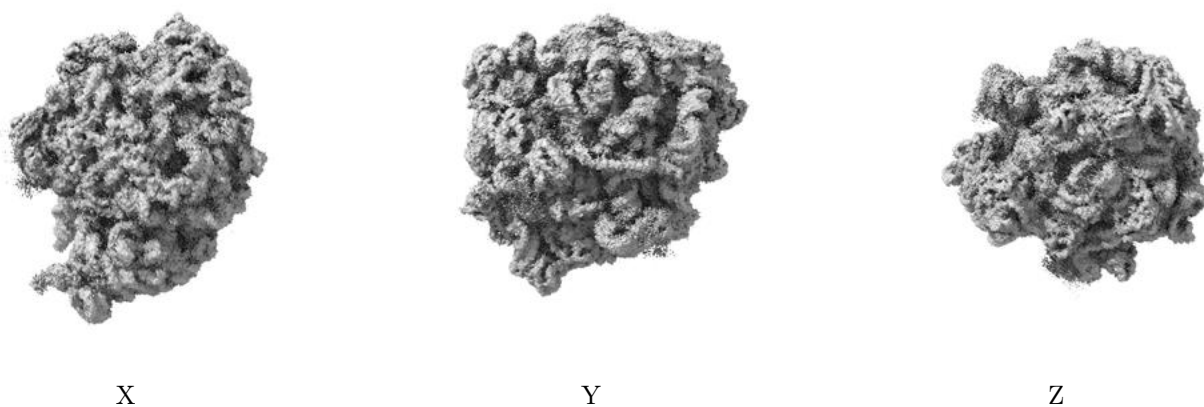
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

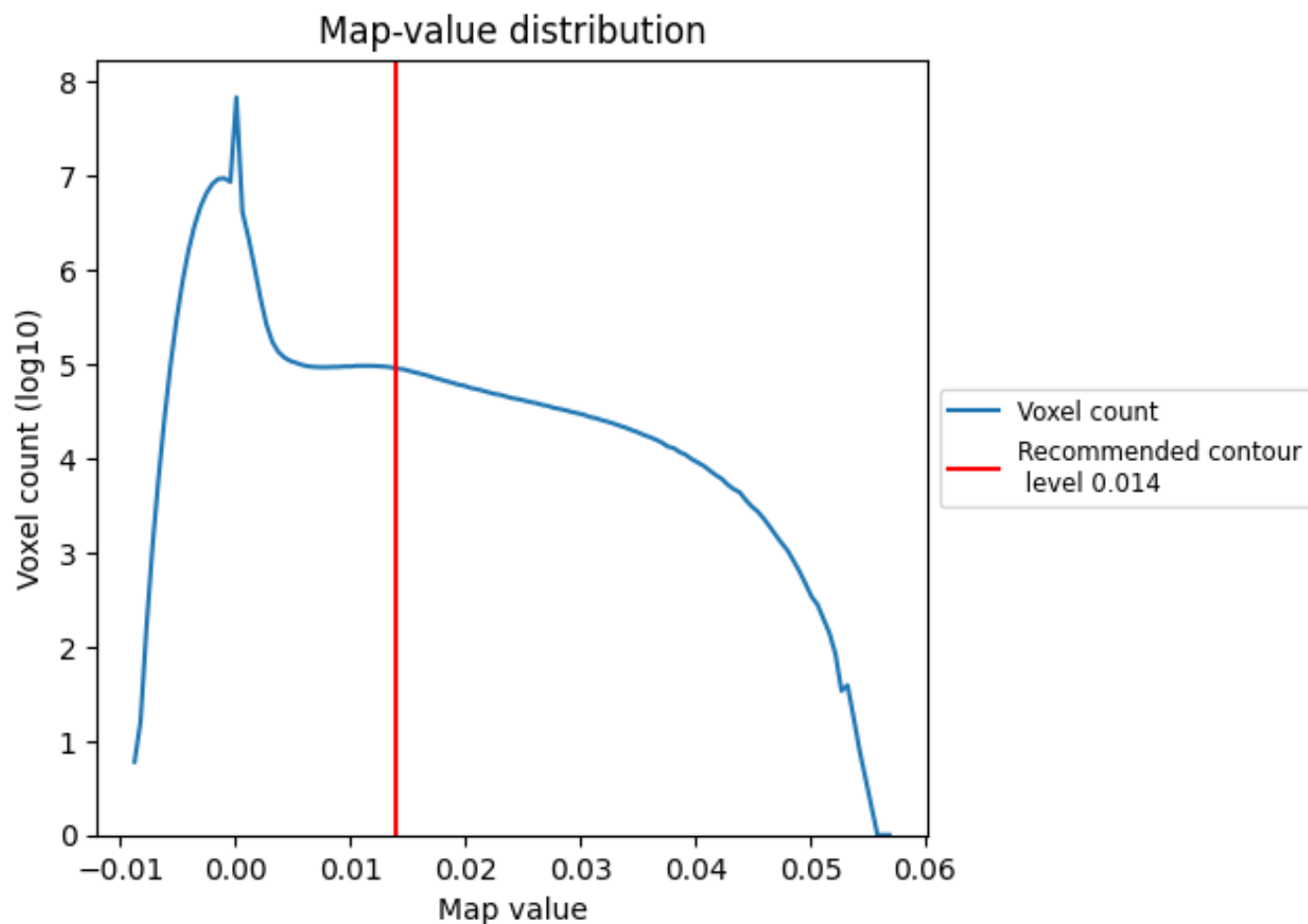
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

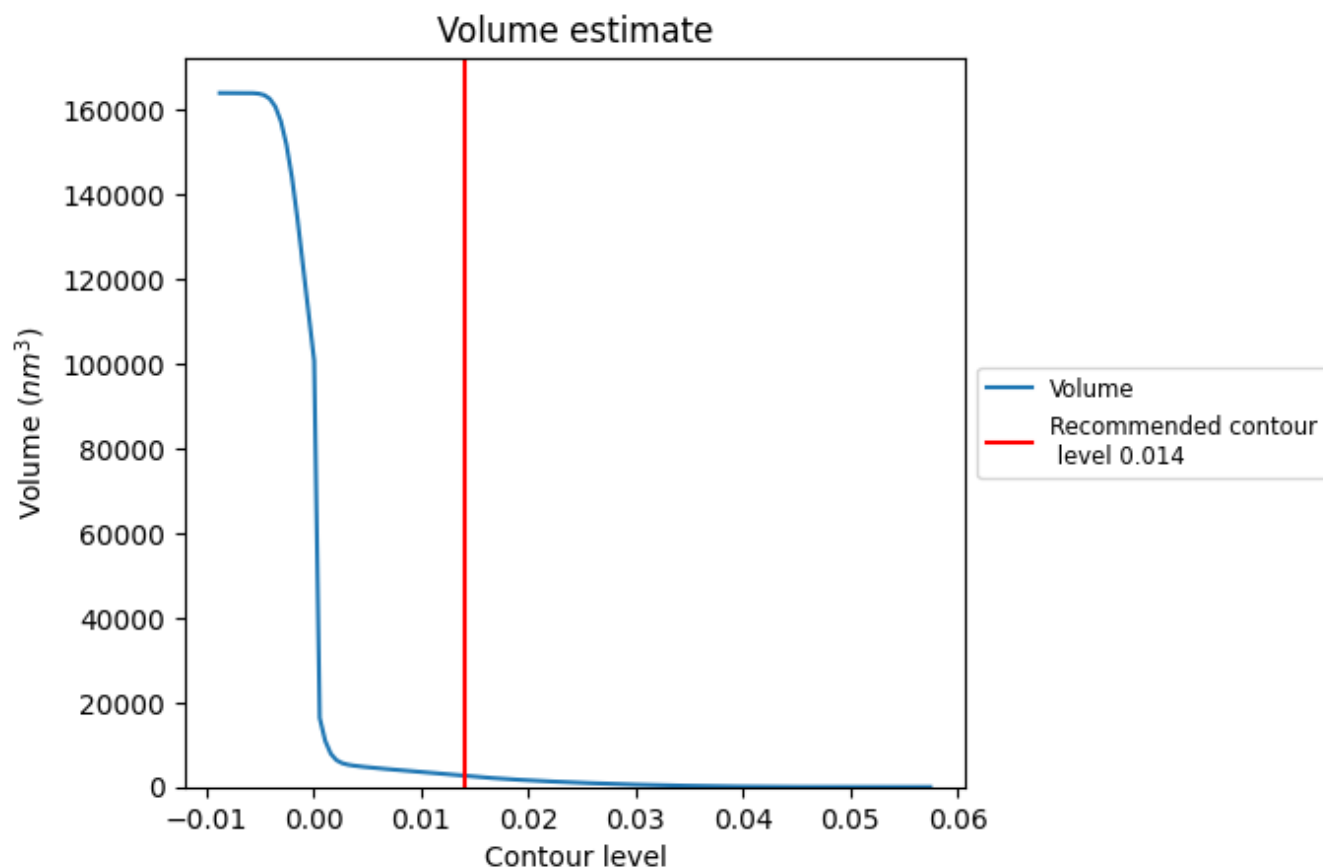
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

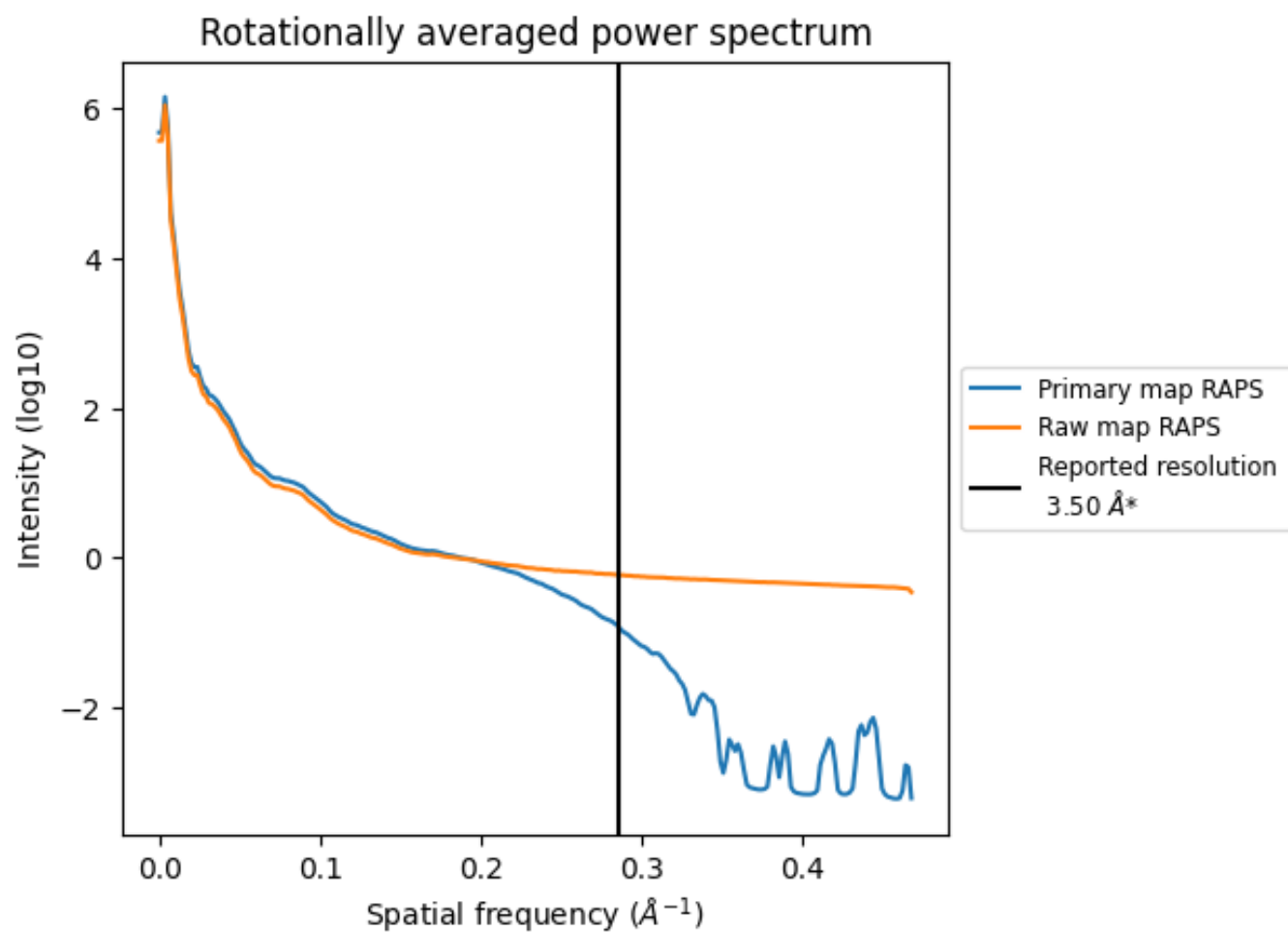
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2637 nm³; this corresponds to an approximate mass of 2382 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 ⓘ

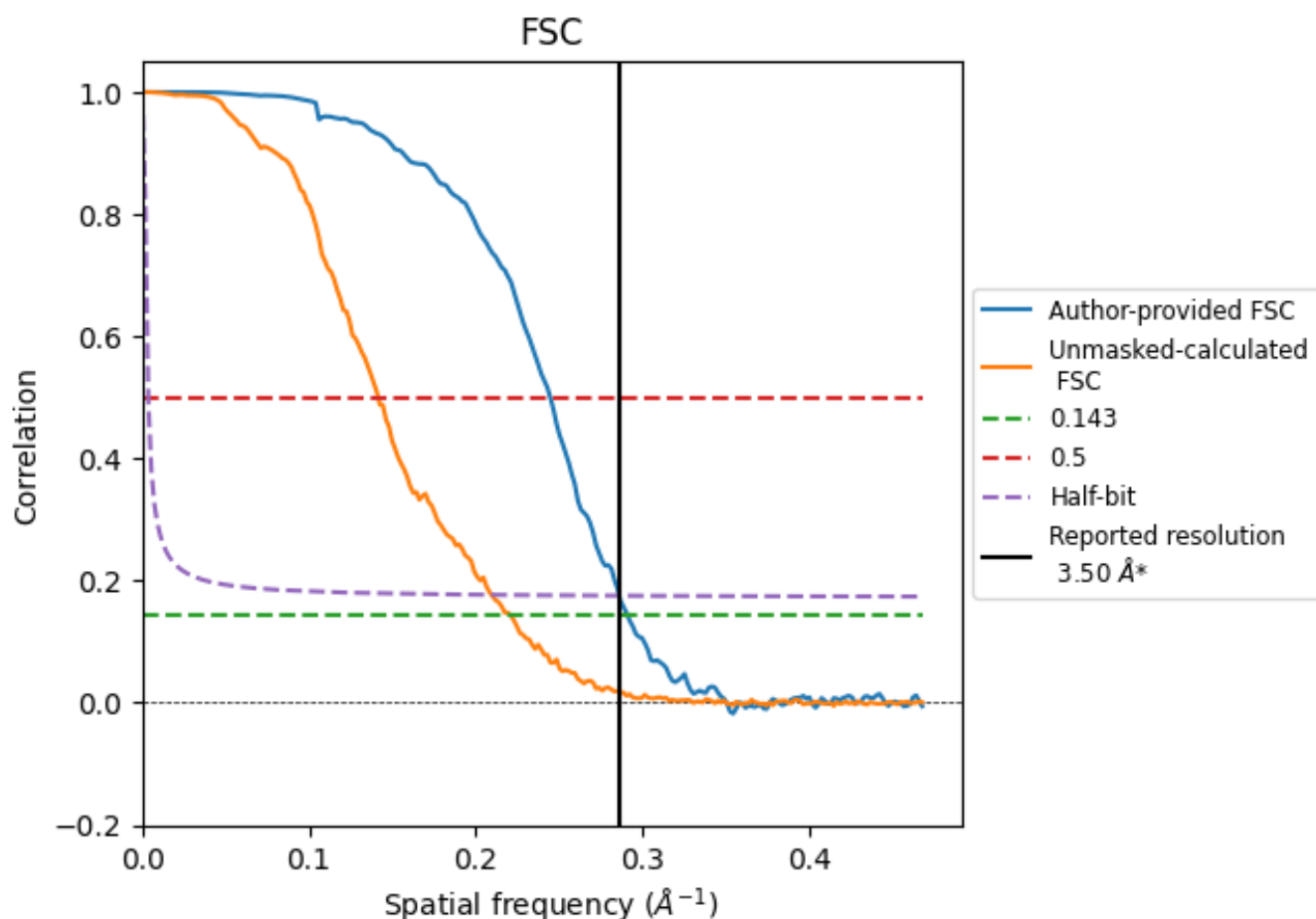


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

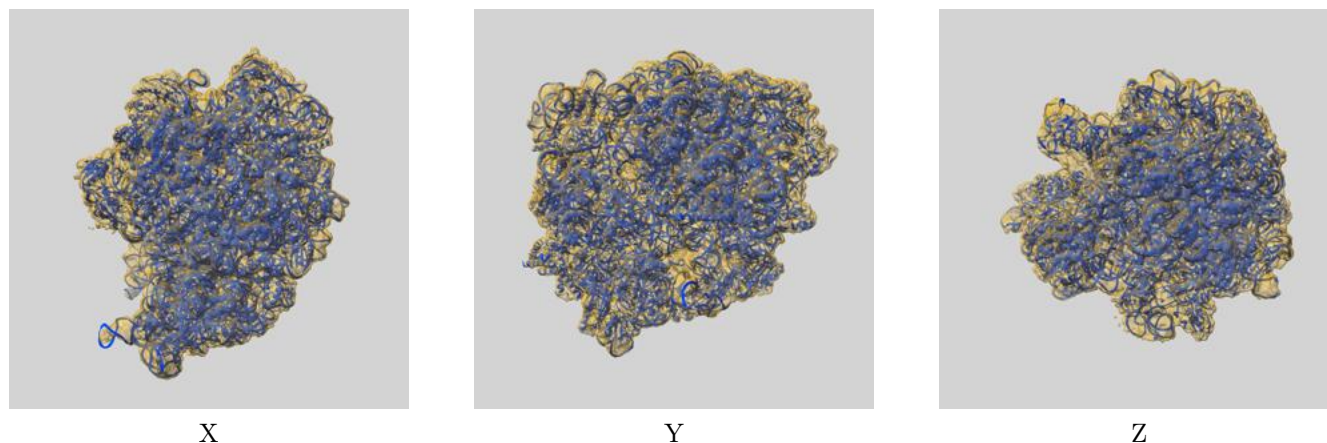
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	4.09	3.50
Unmasked-calculated*	4.52	7.07	4.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.52 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

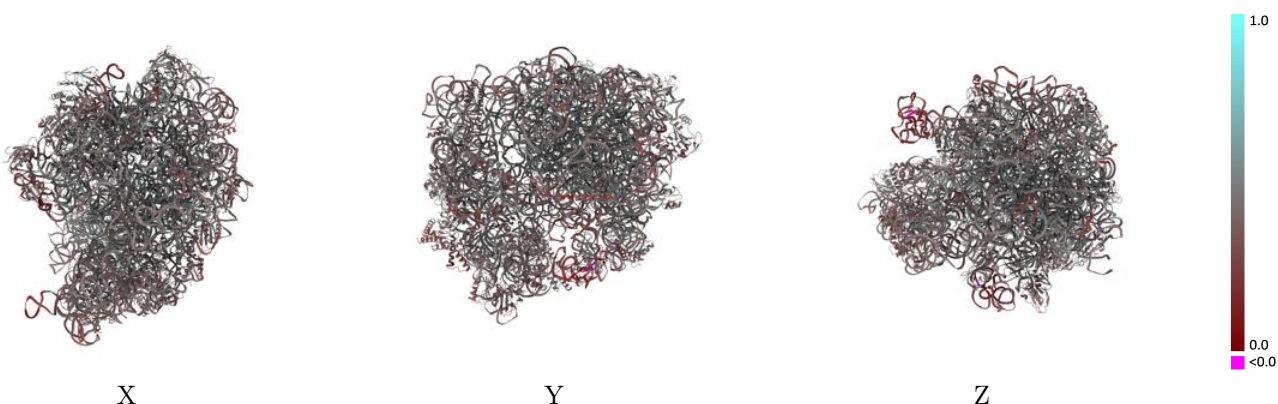
This section contains information regarding the fit between EMDB map EMD-42541 and PDB model 8UTJ. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



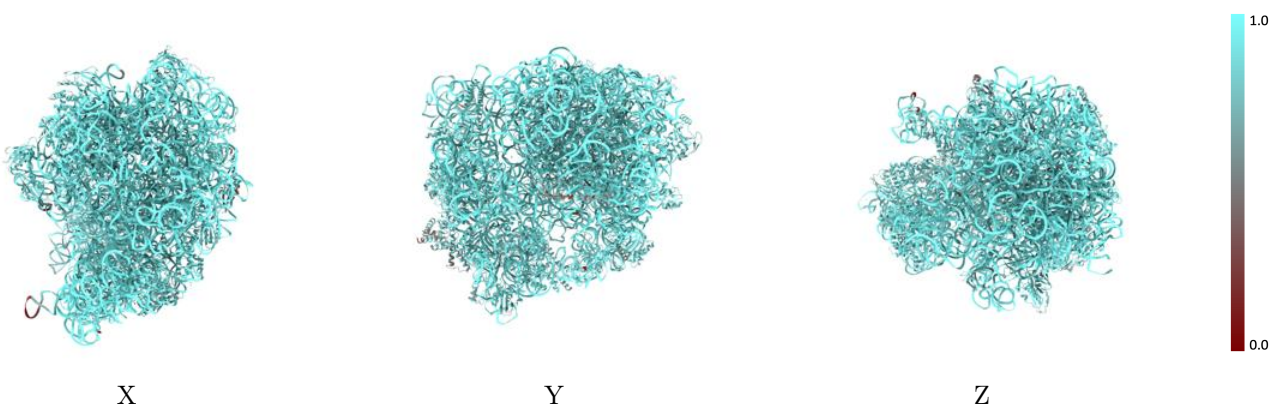
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



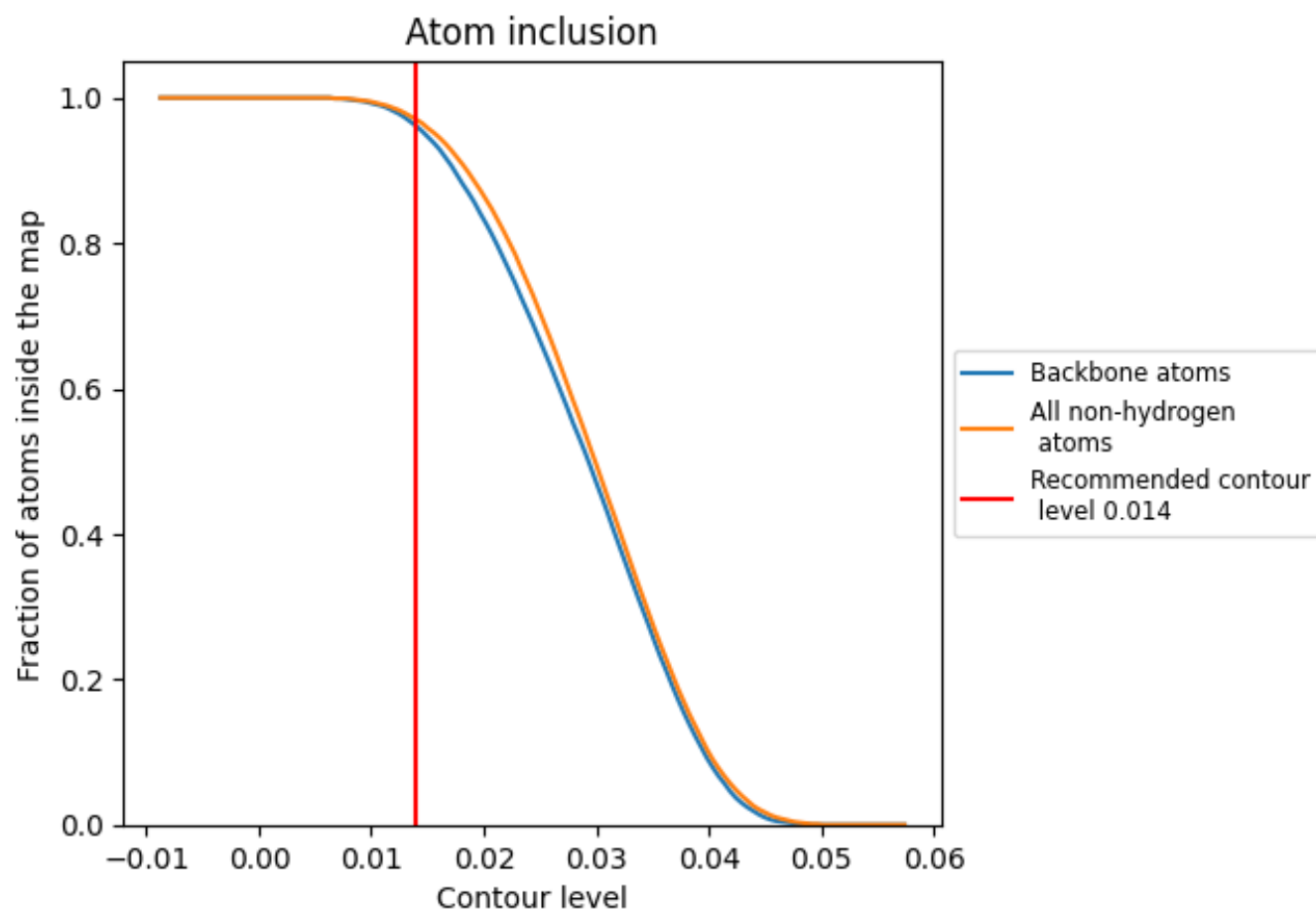
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9700	 0.4300
1	 0.9920	 0.4340
2	 0.9890	 0.4290
3	 0.9920	 0.4260
4	 1.0000	 0.3760
5	 0.9790	 0.3480
A	 0.7920	 0.2380
B	 0.9940	 0.4910
C	 0.9690	 0.4720
D	 0.9220	 0.4460
E	 0.9180	 0.3880
F	 0.8790	 0.4130
G	 0.6690	 0.3360
J	 0.9740	 0.4550
K	 0.9880	 0.4790
L	 0.9400	 0.4650
M	 0.9840	 0.4700
N	 0.9930	 0.4690
O	 0.9240	 0.4190
P	 0.9650	 0.4700
Q	 0.9680	 0.4450
R	 0.9210	 0.4760
S	 0.9700	 0.4590
T	 0.9490	 0.4440
U	 0.9120	 0.4440
V	 0.8970	 0.4350
W	 0.9830	 0.4740
X	 0.9830	 0.4640
Y	 0.8920	 0.3950
Z	 0.9470	 0.4630
a	 0.7750	 0.3550
b	 0.9770	 0.4800
c	 0.9810	 0.4570
d	 1.0000	 0.4790
e	 1.0000	 0.4900



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Chain	Atom inclusion	Q-score
f	 0.9930	 0.4510
g	 0.7050	 0.3620
h	 0.9310	 0.4220
i	 0.9140	 0.4020
j	 0.9640	 0.4440
k	 0.9170	 0.4170
l	 0.9350	 0.3820
m	 0.9410	 0.4420
n	 0.8970	 0.3960
o	 0.8540	 0.3990
p	 0.9480	 0.4290
q	 0.9820	 0.4360
r	 0.9270	 0.3850
s	 0.9550	 0.4110
t	 0.9590	 0.4000
u	 0.9360	 0.4310
v	 0.9680	 0.4260
w	 0.9370	 0.3760
x	 0.9400	 0.4090
y	 0.9680	 0.3940
z	 0.9160	 0.3620