



Full wwPDB EM Validation Report ⓘ

Sep 17, 2026 – 05:59 AM EDT

PDB ID : 8URM / pdb_00008urm
EMDB ID : EMD-42495
Title : E. coli 70S ribosome with unmodified tRNA^{Pro}(GGG) bound to slippery P-site CCC-C codon and tRNA^{Val}(UAC) in the A site
Authors : Kimbrough, E.M.; Dunham, C.M.; Nguyen, H.A.
Deposited on : 2023-10-26
Resolution : 3.00 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:

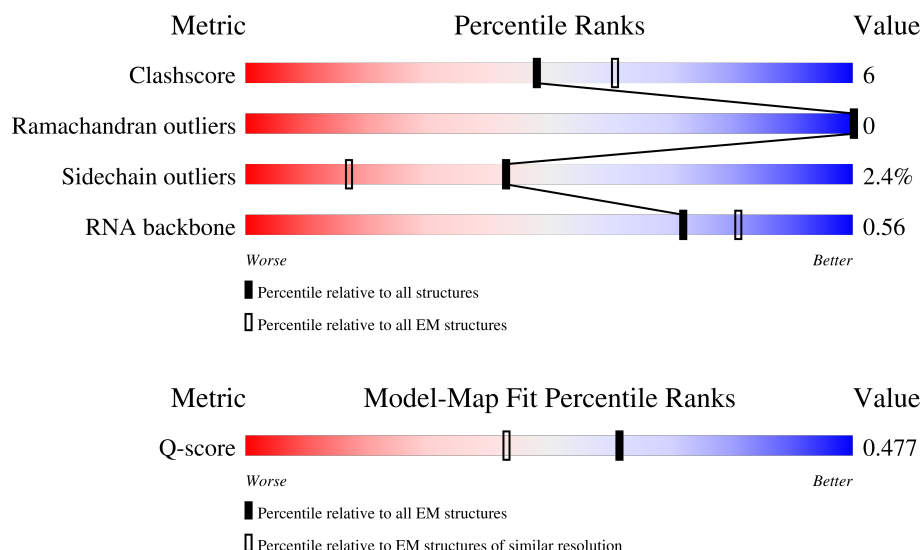
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.00 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.



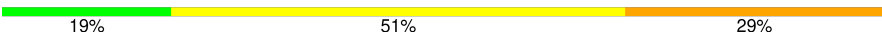
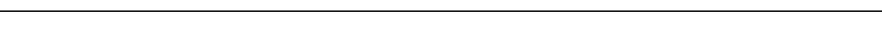
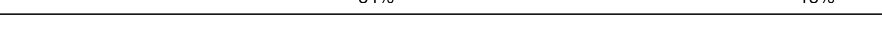
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	

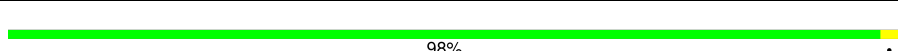
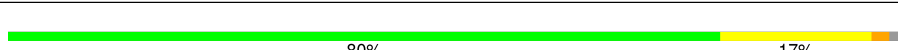
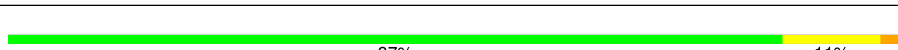
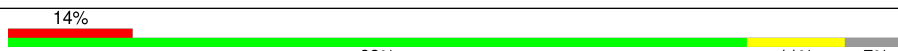
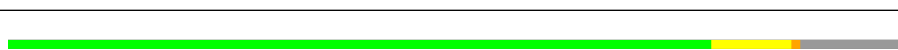
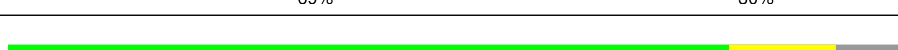
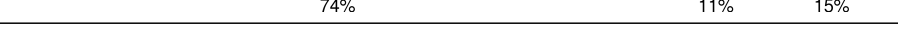
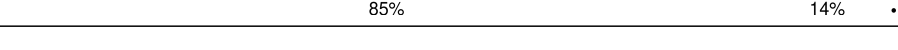
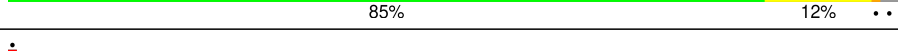
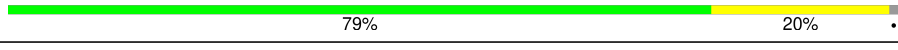
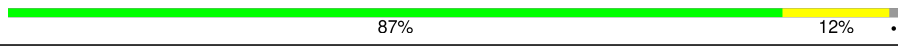
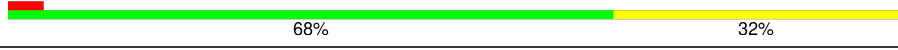
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Mol	Chain	Length	Quality of chain
4	4	18	
5	5	77	
6	6	76	
7	B	273	
8	C	209	
9	D	201	
10	E	179	
11	F	177	
12	G	149	
13	J	142	
14	K	123	
15	L	144	
16	M	136	
17	N	127	
18	O	117	
19	P	115	
20	Q	118	
21	R	103	
22	S	110	
23	T	100	
24	U	104	
25	V	94	
26	W	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	178	
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	90% 9%
55	z	71	85% 14%

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 148557 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 13S 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	1540	Total	C	N	O	P	0	0
			33049	14747	6057	10705	1540		

- 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	12	Total	C	N	O	P	0	0
			252	113	43	84	12		

- Molecule 5 is a RNA chain called tRNA ProL.

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 RNA chain called tRNA Val.

Mol	Chain	Residues	Atoms					AltConf	Trace	
6	6	76	Total	C	N	O	P	S	0	0
			1627	728	292	531	75	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	34	CM0	U	conflict	GB 1847302804

- 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	S	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	S	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	84	Total	C	N	O	S	0	0
			634	391	129	113	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 Small ribosomal subunit protein uS7.

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 Small ribosomal subunit protein uS15.

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).

Mol	Chain	Residues	Atoms		AltConf
56	1	287	Total	Mg	0
			287	287	
56	2	97	Total	Mg	0
			97	97	
56	3	7	Total	Mg	0
			7	7	
56	B	1	Total	Mg	0
			1	1	
56	Q	1	Total	Mg	0
			1	1	
56	S	1	Total	Mg	0
			1	1	
56	m	1	Total	Mg	0
			1	1	

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		AltConf
57	1	1328	Total	O	0
			1328	1328	
57	2	518	Total	O	0
			518	518	
57	3	13	Total	O	0
			13	13	
57	4	1	Total	O	0
			1	1	
57	5	1	Total	O	0
			1	1	
57	6	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
57	B	10	Total 10	O 10	0
57	C	3	Total 3	O 3	0
57	D	5	Total 5	O 5	0
57	E	4	Total 4	O 4	0
57	G	1	Total 1	O 1	0
57	J	1	Total 1	O 1	0
57	K	2	Total 2	O 2	0
57	L	5	Total 5	O 5	0
57	M	2	Total 2	O 2	0
57	N	5	Total 5	O 5	0
57	Q	2	Total 2	O 2	0
57	R	3	Total 3	O 3	0
57	S	2	Total 2	O 2	0
57	U	1	Total 1	O 1	0
57	W	3	Total 3	O 3	0
57	Y	1	Total 1	O 1	0
57	a	1	Total 1	O 1	0
57	b	4	Total 4	O 4	0
57	d	1	Total 1	O 1	0
57	e	2	Total 2	O 2	0
57	f	1	Total 1	O 1	0

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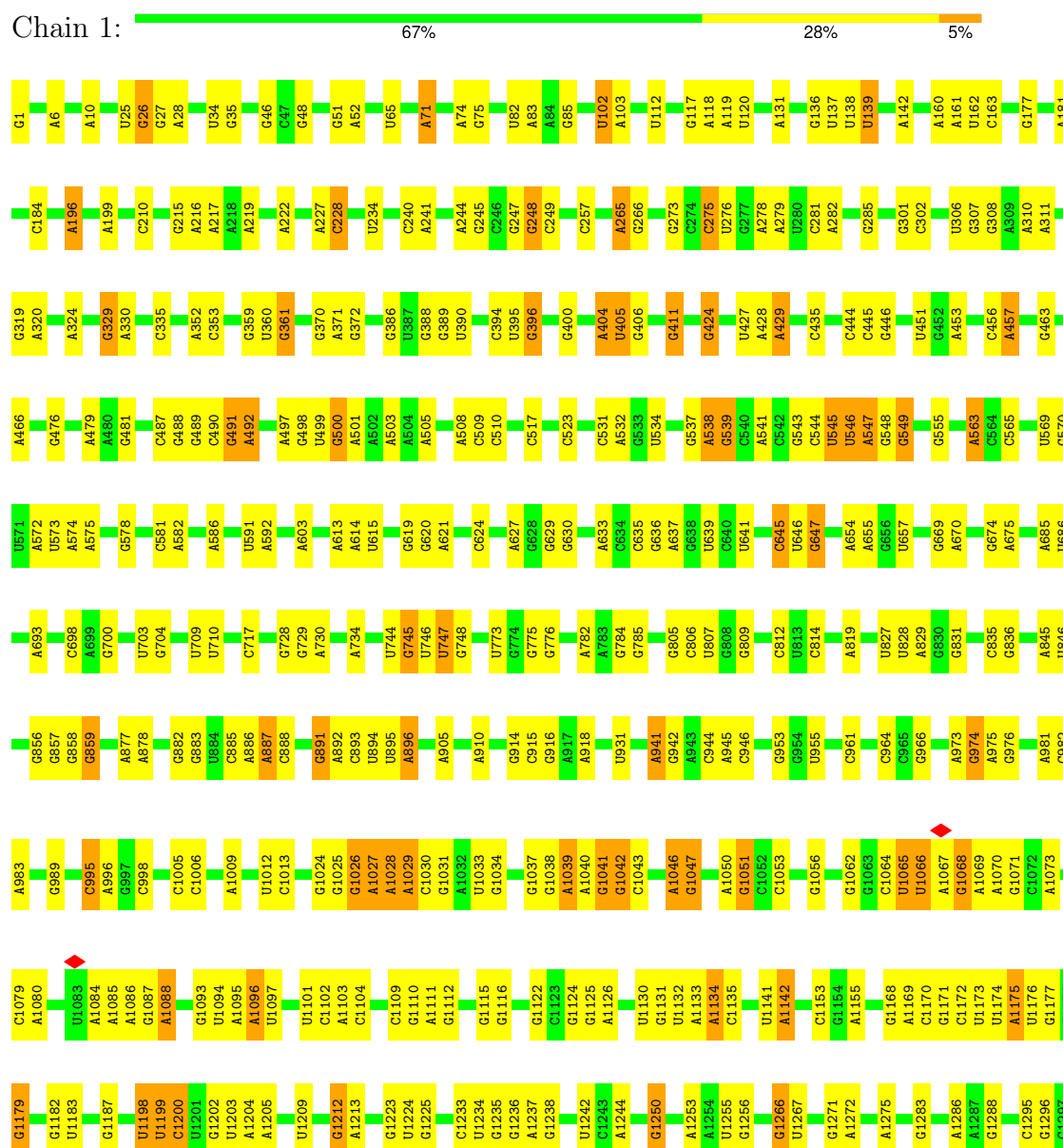
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Mol	Chain	Residues	Atoms		AltConf
57	g	6	Total 6	O 6	0
57	h	2	Total 2	O 2	0
57	i	19	Total 19	O 19	0
57	j	1	Total 1	O 1	0
57	l	3	Total 3	O 3	0
57	m	1	Total 1	O 1	0
57	n	1	Total 1	O 1	0
57	o	2	Total 2	O 2	0
57	q	5	Total 5	O 5	0
57	r	1	Total 1	O 1	0
57	s	2	Total 2	O 2	0
57	t	2	Total 2	O 2	0
57	u	2	Total 2	O 2	0
57	x	1	Total 1	O 1	0
57	y	1	Total 1	O 1	0
57	z	1	Total 1	O 1	0

3 Residue-property plots

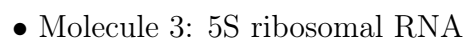
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 13S ribosomal RNA

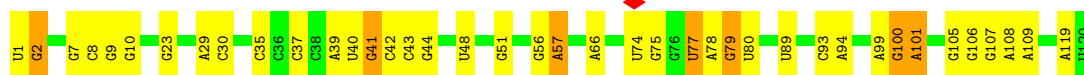


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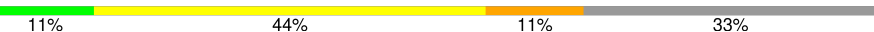
• Molecule 2: 16S ribosomal RNA



Chain 3:  67% 28% 6%

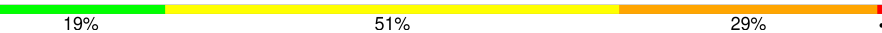


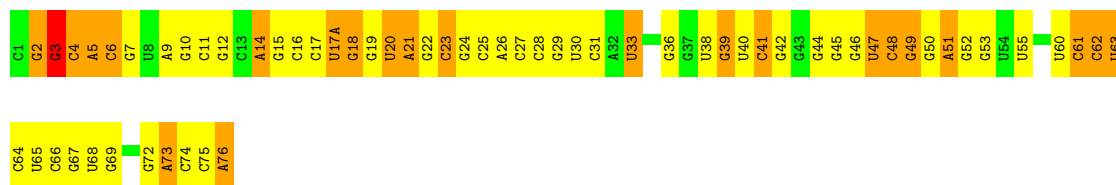
- Molecule 4: mRNA

Chain 4:  11% 44% 11% 33%

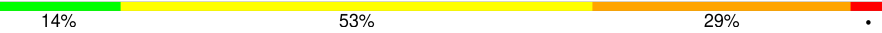


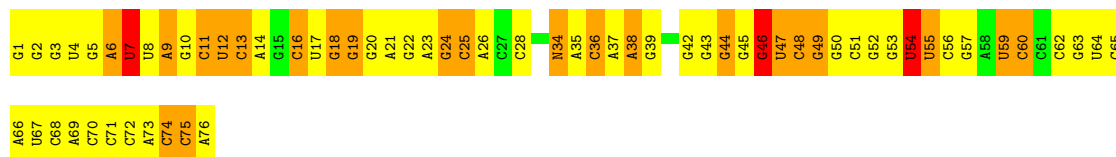
- Molecule 5: tRNA ProL

Chain 5:  19% 51% 29%



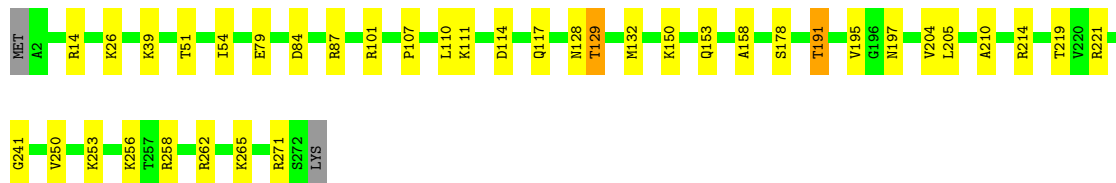
- Molecule 6: tRNA Val

Chain 6:  14% 53% 29%



- Molecule 7: 50S ribosomal protein L2

Chain B:  85% 13%



- Molecule 8: 50S ribosomal protein L3

Chain C:  86% 14%



- Molecule 9: 50S ribosomal protein L4

Chain D:  91% 9%



- Molecule 10: 50S ribosomal protein L5

Chain E:  78% 20% ..



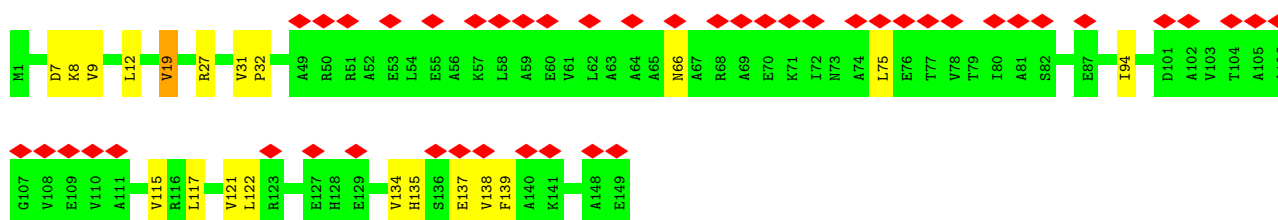
- Molecule 11: 50S ribosomal protein L6

Chain F:  87% 12% .



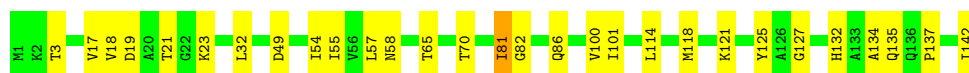
- Molecule 12: 50S ribosomal protein L9

Chain G:  31% 87% 13% .



- Molecule 13: Large ribosomal subunit protein uL13

Chain J:  80% 20% .

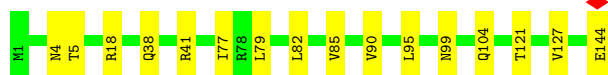
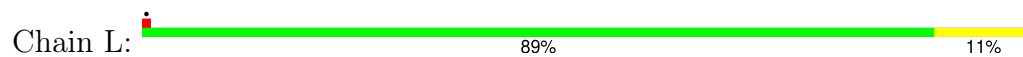


- Molecule 14: 50S ribosomal protein L14

Chain K:  90% 9% .



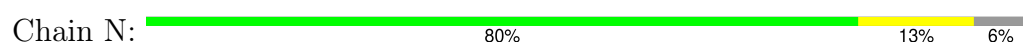
- Molecule 15: 50S ribosomal protein L15



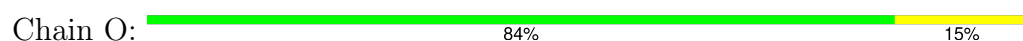
- Molecule 16: 50S ribosomal protein L16



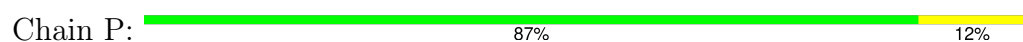
- Molecule 17: 50S ribosomal protein L17



- Molecule 18: Large ribosomal subunit protein uL18



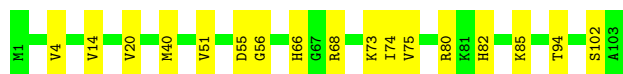
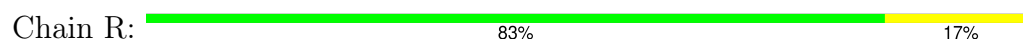
- Molecule 19: Large ribosomal subunit protein bL19



- Molecule 20: 50S ribosomal protein L20



- Molecule 21: Ribosomal protein L21



- Molecule 22: 50S ribosomal protein L22

Chain S:  88% 11% .



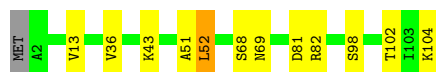
- Molecule 23: 50S ribosomal protein L23

Chain T:  90% 6% .



- Molecule 24: 50S ribosomal protein L24

Chain U:  88% 11% ..

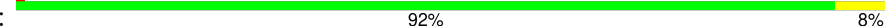


- Molecule 25: Large ribosomal subunit protein bL25

Chain V:  91% 9%



- Molecule 26: Large ribosomal subunit protein bL27

Chain W:  92% 8%



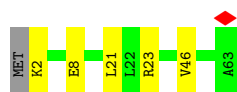
- Molecule 27: 50S ribosomal protein L28

Chain X:  79% 19% .



- Molecule 28: Large ribosomal subunit protein uL29

Chain Y:  90% 8% .



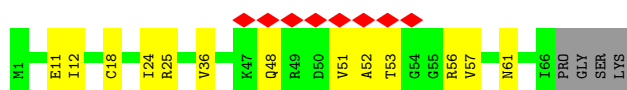
- Molecule 29: 50S ribosomal protein L30

Chain Z:  90% 8%



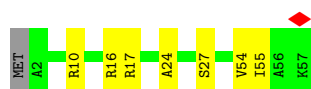
- Molecule 30: 50S ribosomal protein L31

Chain a:  11% 76% 19% 6%



- Molecule 31: 50S ribosomal protein L32

Chain b:  86% 12%

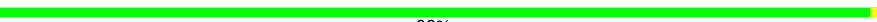


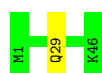
- Molecule 32: 50S ribosomal protein L33

Chain c:  82% 13% 5%



- Molecule 33: 50S ribosomal protein L34

Chain d:  98%



- Molecule 34: 50S ribosomal protein L35

Chain e:  80% 17%

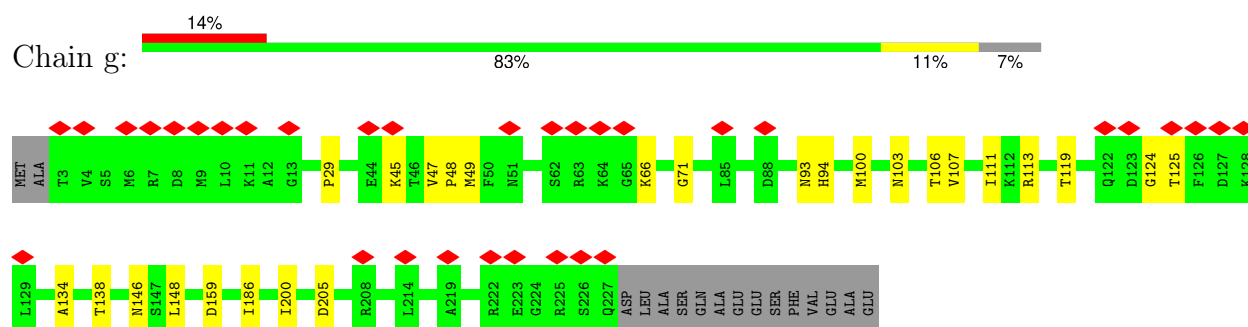


- Molecule 35: 50S ribosomal protein L36

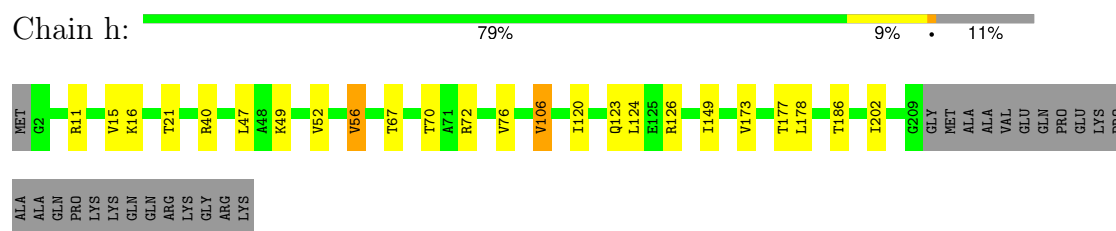
Chain f:  87% 11%



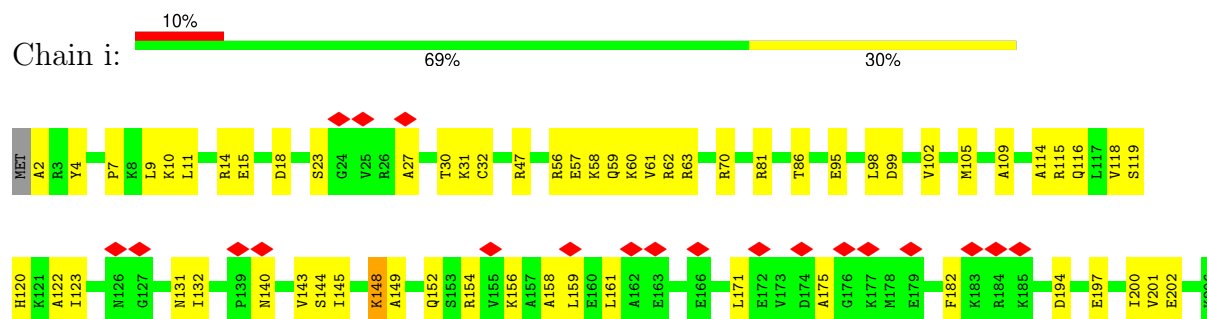
- Molecule 36: 30S ribosomal protein S2



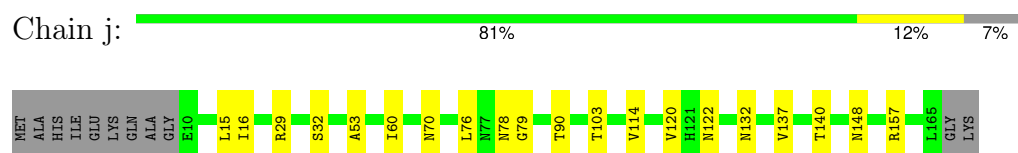
- Molecule 37: 30S ribosomal protein S3



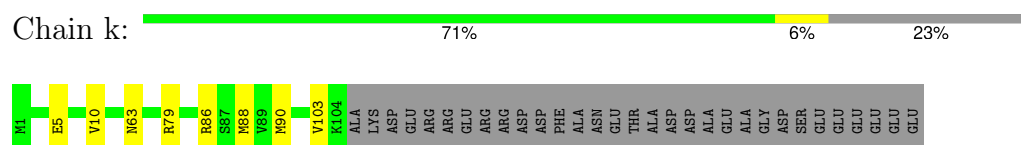
- Molecule 38: 30S ribosomal protein S4



- Molecule 39: 30S ribosomal protein S5

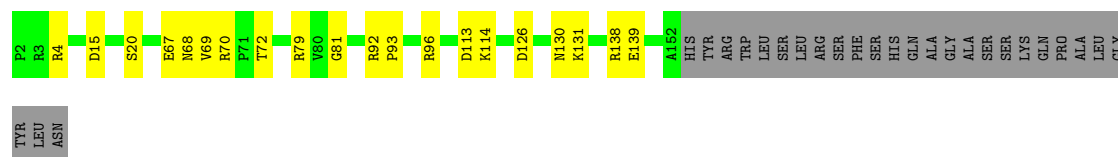


- Molecule 40: 30S ribosomal protein S6



- Molecule 41: Small ribosomal subunit protein uS7





- Molecule 42: Small ribosomal subunit protein uS8

Chain m: 85% 14%



- Molecule 43: Small ribosomal subunit protein uS9

Chain n: 85% 12%



- Molecule 44: Small ribosomal subunit protein uS10

Chain o: 76% 17%



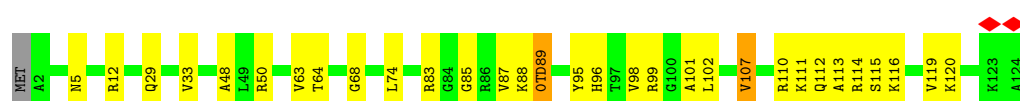
- Molecule 45: 30S ribosomal protein S11

Chain p: 79% 12% 9%



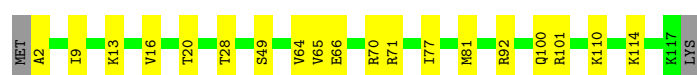
- Molecule 46: Small ribosomal subunit protein uS12

Chain q: 74% 23%



- Molecule 47: 30S ribosomal protein S13

Chain r: 82% 16%



- Molecule 48: Small ribosomal subunit protein uS14

Chain s:  79% 20%



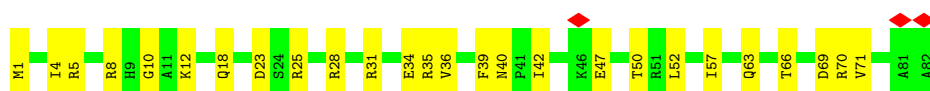
- Molecule 49: Small ribosomal subunit protein uS15

Chain t:  87% 12%



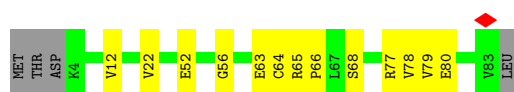
- Molecule 50: 30S ribosomal protein S16

Chain u:  68% 32%



- Molecule 51: Small ribosomal subunit protein uS17

Chain v:  80% 15% 5%



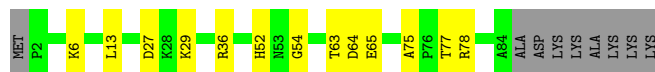
- Molecule 52: 30S ribosomal protein S18

Chain w:  72% 16% 12%



- Molecule 53: Small ribosomal subunit protein uS19

Chain x:  76% 14% 10%

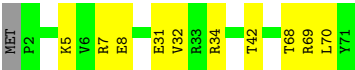
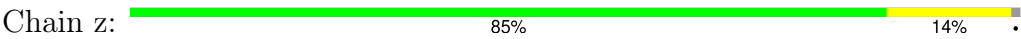


- Molecule 54: 30S ribosomal protein S20

Chain y:  90% 9%



- 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	173856	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	0.050	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	427.6, 427.6, 427.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.069, 1.069, 1.069	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, PSU, 5MC, 4OC, 0TD, 1MG, 4SU, 2MA, OMU, 7MG, OMG, 5MU, UR3, MG, 2MG, MA6, CM0, OMC, 6MZ

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	0.14	0/69335	0.25	0/108168
2	2	0.12	0/36722	0.23	0/57278
3	3	0.11	0/2872	0.22	0/4478
4	4	0.44	0/280	1.09	4/433 (0.9%)
5	5	0.34	0/1841	0.59	5/2870 (0.2%)
6	6	0.44	0/1668	0.52	1/2595 (0.0%)
7	B	0.21	0/2121	0.35	0/2852
8	C	0.21	0/1586	0.34	0/2134
9	D	0.19	0/1571	0.32	0/2113
10	E	0.15	0/1434	0.37	0/1926
11	F	0.14	0/1333	0.32	0/1805
12	G	0.15	0/1122	0.33	0/1515
13	J	0.19	0/1152	0.31	0/1551
14	K	0.20	0/955	0.33	0/1279
15	L	0.20	0/1062	0.34	0/1413
16	M	0.20	0/1093	0.35	0/1460
17	N	0.21	0/964	0.39	0/1289
18	O	0.15	0/902	0.34	0/1209
19	P	0.18	0/929	0.34	0/1242
20	Q	0.20	0/960	0.32	0/1278
21	R	0.21	0/829	0.37	0/1107
22	S	0.21	0/864	0.34	0/1156
23	T	0.19	0/752	0.27	0/1005
24	U	0.16	0/796	0.32	0/1062
25	V	0.18	0/766	0.33	0/1025
26	W	0.18	0/642	0.31	0/848
27	X	0.20	0/635	0.36	0/848
28	Y	0.15	0/502	0.32	0/667
29	Z	0.19	0/452	0.36	0/605
30	a	0.15	0/531	0.31	0/709
31	b	0.19	0/450	0.36	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.18	0/433	0.33	0/576
33	d	0.22	0/380	0.39	0/498
34	e	0.20	0/513	0.42	0/676
35	f	0.21	0/303	0.32	0/397
36	g	0.14	0/1791	0.33	0/2413
37	h	0.18	0/1663	0.35	0/2241
38	i	0.16	0/1665	0.38	0/2227
39	j	0.18	0/1165	0.34	0/1568
40	k	0.18	0/867	0.34	0/1171
41	l	0.14	0/1195	0.32	0/1602
42	m	0.16	0/989	0.31	0/1326
43	n	0.16	0/1034	0.33	0/1375
44	o	0.16	0/800	0.35	0/1082
45	p	0.16	0/893	0.33	0/1205
46	q	0.19	0/960	0.42	0/1286
47	r	0.14	0/909	0.33	0/1215
48	s	0.14	0/817	0.32	0/1088
49	t	0.15	0/722	0.29	0/964
50	u	0.22	0/659	0.44	0/884
51	v	0.15	0/657	0.37	0/881
52	w	0.15	0/553	0.28	0/743
53	x	0.14	0/680	0.28	0/915
54	y	0.15	0/675	0.30	0/895
55	z	0.13	0/597	0.32	0/792
All	All	0.16	0/158041	0.28	10/236539 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	12	A	C2'-C3'-O3'	9.67	124.01	109.50
5	5	3	G	C4'-C3'-O3'	7.79	121.09	109.40
4	4	11	A	C4'-C3'-O3'	-6.91	102.64	113.00
5	5	41	C	C2'-C3'-O3'	6.83	123.94	113.70
5	5	2	G	C4'-C3'-O3'	6.66	119.38	109.40
4	4	12	A	C3'-C2'-O2'	6.20	123.90	114.60
5	5	39	G	C2'-C3'-O3'	5.69	122.23	113.70
6	6	36	C	C2'-C3'-O3'	5.68	122.22	113.70
4	4	12	A	C4'-C3'-O3'	5.65	117.87	109.40
5	5	73	A	C4'-C3'-O3'	-5.45	104.82	113.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62334	0	31367	515	0
2	2	33049	0	16652	357	0
3	3	2569	0	1301	27	0
4	4	252	0	130	3	0
5	5	1648	0	834	46	0
6	6	1627	0	832	66	0
7	B	2082	0	2154	25	0
8	C	1565	0	1616	22	0
9	D	1552	0	1619	10	0
10	E	1410	0	1444	28	0
11	F	1313	0	1358	9	0
12	G	1111	0	1148	12	0
13	J	1129	0	1162	19	0
14	K	946	0	1023	9	0
15	L	1053	0	1129	13	0
16	M	1074	0	1157	11	0
17	N	951	0	994	10	0
18	O	892	0	923	12	0
19	P	917	0	962	9	0
20	Q	947	0	1019	9	0
21	R	816	0	839	14	0
22	S	857	0	922	8	0
23	T	746	0	811	3	0
24	U	788	0	844	7	0
25	V	753	0	780	7	0
26	W	634	0	653	5	0
27	X	625	0	652	10	0
28	Y	501	0	531	6	0
29	Z	448	0	488	4	0
30	a	522	0	524	7	0
31	b	444	0	458	6	0
32	c	426	0	464	7	0
33	d	377	0	418	1	0
34	e	504	0	572	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	f	302	0	343	4	0
36	g	1760	0	1787	14	0
37	h	1636	0	1710	11	0
38	i	1643	0	1707	64	0
39	j	1152	0	1196	14	0
40	k	848	0	846	5	0
41	l	1181	0	1238	12	0
42	m	979	0	1031	13	0
43	n	1022	0	1070	15	0
44	o	790	0	831	16	0
45	p	877	0	887	9	0
46	q	957	0	1017	27	0
47	r	900	0	965	12	0
48	s	805	0	844	18	0
49	t	714	0	734	6	0
50	u	649	0	666	19	0
51	v	648	0	691	11	0
52	w	544	0	560	10	0
53	x	663	0	688	10	0
54	y	669	0	719	5	0
55	z	589	0	629	9	0
56	1	287	0	0	0	0
56	2	97	0	0	0	0
56	3	7	0	0	0	0
56	B	1	0	0	0	0
56	Q	1	0	0	0	0
56	S	1	0	0	0	0
56	m	1	0	0	0	0
57	1	1328	0	0	43	0
57	2	518	0	0	20	0
57	3	13	0	0	0	0
57	4	1	0	0	0	0
57	5	1	0	0	0	0
57	6	2	0	0	0	0
57	B	10	0	0	2	0
57	C	3	0	0	0	0
57	D	5	0	0	1	0
57	E	4	0	0	0	0
57	G	1	0	0	0	0
57	J	1	0	0	0	0
57	K	2	0	0	0	0
57	L	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	M	2	0	0	0	0
57	N	5	0	0	1	0
57	Q	2	0	0	0	0
57	R	3	0	0	2	0
57	S	2	0	0	0	0
57	U	1	0	0	0	0
57	W	3	0	0	0	0
57	Y	1	0	0	0	0
57	a	1	0	0	1	0
57	b	4	0	0	0	0
57	d	1	0	0	0	0
57	e	2	0	0	1	0
57	f	1	0	0	0	0
57	g	6	0	0	1	0
57	h	2	0	0	0	0
57	i	19	0	0	4	0
57	j	1	0	0	0	0
57	l	3	0	0	0	0
57	m	1	0	0	0	0
57	n	1	0	0	0	0
57	o	2	0	0	1	0
57	q	5	0	0	1	0
57	r	1	0	0	0	0
57	s	2	0	0	1	0
57	t	2	0	0	0	0
57	u	2	0	0	1	0
57	x	1	0	0	0	0
57	y	1	0	0	0	0
57	z	1	0	0	0	0
All	All	148557	0	97939	1377	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 6.

All (1377) 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)
2:2:542:G:OP1	38:i:10:LYS:NZ	2.02	0.91
1:1:1065:U:O4	1:1:1069:A:O2'	1.88	0.90
1:1:1174:U:O2'	1:1:1175:A:O4'	1.91	0.89
38:i:148:LYS:O	38:i:152:GLN:NE2	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:572:A:OP2	21:R:80:ARG:NH2	2.06	0.88
5:5:18:G:H1	5:5:55:U:H6	1.19	0.88
1:1:2286:G:O6	32:c:23:THR:OG1	1.92	0.87
1:1:1582:C:O2'	1:1:1583:A:O4'	1.92	0.87
12:G:66:ASN:ND2	12:G:134:VAL:O	2.08	0.86
16:M:110:GLU:OE2	16:M:114:ARG:NH2	2.09	0.86
2:2:403:C:OP1	38:i:115:ARG:NH2	2.11	0.84
1:1:1125:G:OP2	1:1:1126:A:O2'	1.96	0.83
6:6:7:4SU:S4	6:6:66:A:N6	2.48	0.83
2:2:1005:A:O2'	2:2:1037:C:O2'	1.97	0.83
1:1:1869:G:O6	1:1:1873:G:N1	2.11	0.83
1:1:2646:C:OP2	1:1:2732:G:O2'	1.96	0.83
2:2:662:U:O2'	2:2:836:G:OP1	1.96	0.83
2:2:1493:A:O2'	2:2:1494:G:OP1	1.95	0.83
1:1:1288:G:N2	1:1:1288:G:OP2	2.12	0.83
1:1:2052:A:O2'	8:C:148:GLN:O	1.97	0.82
6:6:50:G:H1	6:6:64:U:H3	0.83	0.82
1:1:2171:A:O2'	1:1:2173:A:OP1	1.96	0.82
1:1:2645:G:OP2	1:1:2645:G:N2	2.10	0.82
2:2:685:G:N2	2:2:705:G:O6	2.13	0.82
1:1:324:A:OP2	1:1:1205:A:N6	2.13	0.82
1:1:2285:C:OP2	32:c:6:ARG:NH1	2.12	0.82
39:j:157:ARG:NH1	42:m:99:LEU:O	2.13	0.82
2:2:71:A:N6	2:2:99:C:O2	2.13	0.82
1:1:1779:U:OP2	1:1:1784:A:N6	2.12	0.81
14:K:9:ASN:OD1	14:K:18:ARG:NH1	2.13	0.81
1:1:1801:A:OP2	7:B:150:LYS:NZ	2.14	0.81
1:1:1341:G:OP2	1:1:1394:U:O2'	1.97	0.81
2:2:1266:G:N2	2:2:1269:A:OP2	2.13	0.81
48:s:2:ALA:N	48:s:67:THR:O	2.14	0.80
1:1:1450:G:N2	1:1:1452:G:O6	2.12	0.80
1:1:2848:G:O2'	1:1:2867:G:N2	2.15	0.80
2:2:979:C:O2	48:s:59:ARG:NE	2.15	0.80
2:2:126:G:OP1	2:2:605:U:O2'	1.99	0.80
10:E:33:LYS:NZ	10:E:35:THR:OG1	2.15	0.80
2:2:544:G:OP1	38:i:56:ARG:NH2	2.14	0.80
2:2:1321:U:O3'	53:x:78:ARG:NH2	2.15	0.79
2:2:413:G:N2	38:i:31:LYS:O	2.15	0.79
47:r:110:LYS:O	47:r:114:LYS:NZ	2.15	0.79
1:1:2261:C:OP1	26:W:19:LYS:NZ	2.16	0.79
1:1:2166:U:O4	1:1:2171:A:N6	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:138:U:O2'	1:1:139:U:O2	2.00	0.78
1:1:2139:U:O2	1:1:2152:G:O6	2.00	0.78
48:s:66:GLN:NE2	57:s:201:HOH:O	2.15	0.78
1:1:1416:G:O2'	1:1:1417:C:O5'	2.01	0.78
1:1:1660:G:N2	1:1:2689:U:O4	2.15	0.78
2:2:626:G:OP1	50:u:35:ARG:NH2	2.17	0.78
1:1:2312:U:O2	10:E:37:ASN:ND2	2.16	0.78
1:1:219:A:N3	1:1:234:U:O2'	2.16	0.78
1:1:517:C:OP2	31:b:10:ARG:NH2	2.17	0.78
9:D:125:SER:O	9:D:137:LYS:NZ	2.15	0.77
2:2:507:C:OP2	2:2:508:U:O2'	1.99	0.77
1:1:2144:G:O2'	1:1:2145:C:O5'	2.03	0.77
3:3:79:G:N7	25:V:14:LYS:NZ	2.32	0.77
1:1:2116:G:N7	1:1:2165:C:N4	2.33	0.77
2:2:120:A:O2'	2:2:122:G:N7	2.17	0.77
2:2:790:A:OP1	5:5:38:U:O2'	2.03	0.77
1:1:2182:U:O2'	1:1:2183:A:N7	2.15	0.77
46:q:120:LYS:O	57:q:201:HOH:O	2.03	0.76
2:2:33:A:N3	46:q:29:GLN:NE2	2.33	0.76
1:1:1992:G:N2	1:1:1996:C:O2'	2.18	0.76
3:3:77:U:O2'	25:V:78:GLN:OE1	2.02	0.76
2:2:339:C:OP2	14:K:98:ARG:NH1	2.18	0.76
2:2:401:C:O2'	2:2:621:A:N3	2.19	0.76
2:2:438:U:OP1	57:2:1703:HOH:O	2.03	0.76
1:1:1250:G:N7	15:L:18:ARG:NH2	2.34	0.76
6:6:5:G:H2'	6:6:6:A:H8	1.50	0.76
2:2:620:C:O2'	57:2:1702:HOH:O	2.03	0.76
38:i:122:ALA:HB1	38:i:149:ALA:HB2	1.65	0.75
2:2:39:G:OP1	57:2:1701:HOH:O	2.03	0.75
3:3:7:G:OP1	18:O:4:LYS:NZ	2.19	0.75
1:1:887:A:OP2	57:1:3301:HOH:O	2.03	0.75
2:2:152:A:N6	2:2:169:C:O2	2.20	0.75
1:1:1187:G:OP1	21:R:85:LYS:NZ	2.13	0.75
2:2:451:A:O5'	50:u:70:ARG:NH2	2.19	0.75
11:F:29:LYS:NZ	11:F:80:THR:O	2.19	0.75
2:2:82:G:O6	2:2:86:G:N2	2.18	0.74
44:o:48:ARG:NH1	57:o:201:HOH:O	2.20	0.74
1:1:989:G:OP2	29:Z:12:SER:OG	2.01	0.74
1:1:177:G:OP2	1:1:177:G:N2	2.13	0.74
17:N:30:ARG:NH1	17:N:74:GLU:OE1	2.20	0.74
36:g:29:PRO:O	36:g:45:LYS:NZ	2.14	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:621:A:OP2	15:L:99:ASN:ND2	2.20	0.74
1:1:2258:C:O2'	1:1:2427:C:OP2	2.05	0.74
5:5:9:A:O2'	5:5:10:G:N7	2.19	0.74
1:1:2528:U:O2'	1:1:2530:A:OP1	2.05	0.74
2:2:1060:U:O2'	44:o:58:ASN:OD1	2.04	0.74
1:1:1085:A:O2'	1:1:1086:A:O4'	2.05	0.74
1:1:2287:A:OP1	32:c:30:LYS:NZ	2.21	0.74
2:2:552:U:O2'	46:q:83:ARG:O	2.04	0.74
38:i:60:LYS:NZ	38:i:194:ASP:O	2.20	0.74
1:1:1447:C:O2'	1:1:1544:A:N3	2.19	0.73
1:1:2200:C:OP2	27:X:37:ARG:NH2	2.20	0.73
2:2:1145:A:O2'	2:2:1146:A:O5'	2.06	0.73
1:1:1131:G:HO2'	1:1:2025:C:HO2'	1.33	0.73
1:1:1528:A:OP2	1:1:1543:G:N2	2.21	0.73
2:2:1152:A:OP1	44:o:72:ARG:NH1	2.21	0.73
1:1:546:U:O2'	1:1:547:A:OP2	2.07	0.73
2:2:1534:A:OP1	57:2:1704:HOH:O	2.05	0.73
1:1:301:G:OP2	24:U:82:ARG:NH1	2.21	0.72
2:2:1003:G:N2	2:2:1005:A:O5'	2.21	0.72
1:1:1754:A:N1	1:1:2716:C:O2'	2.21	0.72
1:1:2530:A:N7	11:F:172:LYS:NZ	2.38	0.72
2:2:78:A:N3	57:2:1715:HOH:O	2.21	0.72
2:2:701:U:OP1	2:2:702:A:O2'	2.03	0.72
2:2:1377:A:OP1	41:l:92:ARG:NH1	2.22	0.72
6:6:62:C:H2'	6:6:63:G:H8	1.54	0.72
7:B:84:ASP:OD2	7:B:87:ARG:NE	2.22	0.72
2:2:1124:G:O2'	2:2:1145:A:N6	2.21	0.72
1:1:641:U:O2'	1:1:2350:C:OP1	2.08	0.72
1:1:2176:A:OP1	57:1:3306:HOH:O	2.08	0.72
2:2:410:G:OP2	38:i:31:LYS:NZ	2.23	0.72
1:1:1730:C:O2	1:1:1731:G:N1	2.23	0.72
1:1:1789:A:OP2	7:B:221:ARG:NH1	2.22	0.72
1:1:2857:G:N2	1:1:2860:A:OP2	2.16	0.72
1:1:905:A:O2'	57:1:3305:HOH:O	2.07	0.72
1:1:2122:U:OP1	57:1:3304:HOH:O	2.07	0.72
2:2:1222:G:OP2	2:2:1322:C:N4	2.23	0.72
18:O:33:ARG:O	18:O:65:THR:OG1	2.03	0.72
1:1:257:C:O2	15:L:104:GLN:NE2	2.23	0.72
1:1:1266:G:OP1	31:b:16:ARG:NE	2.22	0.71
1:1:2033:A:O2'	1:1:2035:G:OP1	2.04	0.71
1:1:807:U:OP2	15:L:41:ARG:NH1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:829:A:OP2	57:1:3307:HOH:O	2.08	0.71
2:2:470:C:OP1	57:2:1706:HOH:O	2.08	0.71
2:2:564:C:OP2	46:q:12:ARG:NH1	2.23	0.71
1:1:1919:A:N1	2:2:1495:U:O2'	2.22	0.71
2:2:517:G:OP1	57:2:1705:HOH:O	2.08	0.71
48:s:41:ARG:NH2	53:x:6:LYS:O	2.24	0.70
6:6:26:A:H61	6:6:44:G:H1	1.37	0.70
1:1:639:U:O4	57:1:3309:HOH:O	2.09	0.70
2:2:1531:A:OP1	57:2:1707:HOH:O	2.10	0.70
42:m:15:ARG:NH1	42:m:75:ILE:O	2.25	0.70
1:1:411:G:OP2	1:1:2406:A:O2'	2.07	0.70
2:2:157:U:O2	2:2:164:G:O6	2.09	0.70
1:1:1379:U:O2'	1:1:1380:G:OP1	2.10	0.70
2:2:671:G:O2'	40:k:79:ARG:NH1	2.23	0.70
2:2:746:A:O2'	2:2:747:A:O5'	2.08	0.70
1:1:1681:G:OP1	57:1:3310:HOH:O	2.10	0.70
1:1:1712:U:OP2	1:1:1713:A:O2'	2.03	0.70
43:n:84:THR:HG21	43:n:103:PHE:HB3	1.74	0.70
1:1:745:1MG:HO2'	1:1:748:G:HO2'	1.37	0.69
38:i:144:SER:O	38:i:145:ILE:HD13	1.92	0.69
1:1:549:G:OP1	57:1:3312:HOH:O	2.11	0.69
38:i:114:ALA:O	38:i:118:VAL:HG23	1.91	0.69
2:2:405:U:O4	38:i:2:ALA:N	2.24	0.69
2:2:542:G:O3'	38:i:14:ARG:NH2	2.25	0.69
1:1:1942:C:OP2	1:1:1943:U:O2'	2.04	0.69
1:1:2327:A:OP1	57:1:3311:HOH:O	2.10	0.69
51:v:79:VAL:HG12	51:v:80:GLU:H	1.57	0.69
2:2:297:G:N2	2:2:300:A:OP2	2.23	0.69
41:l:79:ARG:NH2	41:l:81:GLY:O	2.25	0.69
7:B:26:LYS:NZ	57:B:402:HOH:O	2.26	0.69
10:E:80:ARG:NH1	10:E:81:GLN:O	2.26	0.69
13:J:49:ASP:OD2	13:J:121:LYS:NZ	2.22	0.69
35:f:11:CYS:SG	35:f:12:ARG:N	2.65	0.69
1:1:65:U:OP2	57:1:3315:HOH:O	2.11	0.69
41:l:68:ASN:O	41:l:138:ARG:NH1	2.25	0.69
1:1:27:G:O2'	1:1:28:A:OP2	2.10	0.69
1:1:499:U:H2'	1:1:500:G:H5''	1.74	0.69
2:2:1493:A:HO2'	2:2:1494:G:P	2.16	0.69
45:p:88:GLY:H	45:p:114:THR:HG22	1.57	0.69
38:i:119:SER:OG	57:i:301:HOH:O	2.09	0.68
1:1:2140:G:O6	1:1:2151:U:C4	2.45	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:35:G:H21	46:q:115:SER:HB2	1.58	0.68
2:2:1492:A:O2'	2:2:1493:A:O4'	2.09	0.68
20:Q:97:ASP:OD1	20:Q:98:ILE:N	2.26	0.68
18:O:111:ARG:NH2	18:O:117:PHE:OXT	2.26	0.68
37:h:123:GLN:OE1	37:h:126:ARG:NH2	2.26	0.68
1:1:2637:U:OP2	57:1:3313:HOH:O	2.11	0.68
1:1:1435:G:OP2	57:1:3317:HOH:O	2.12	0.68
55:z:31:GLU:OE2	55:z:34:ARG:NH1	2.27	0.68
2:2:1254:A:OP1	44:o:45:ARG:NH1	2.26	0.68
1:1:882:G:O2'	6:6:20:G:O6	2.11	0.68
1:1:1997:C:OP2	57:1:3314:HOH:O	2.11	0.67
2:2:8:A:N6	38:i:202:GLU:O	2.26	0.67
2:2:1396:A:OP2	57:2:1708:HOH:O	2.12	0.67
1:1:1094:U:N3	1:1:1097:U:OP2	2.27	0.67
2:2:362:G:N2	2:2:365:U:OP2	2.25	0.67
3:3:8:C:O3'	18:O:25:ARG:NH1	2.28	0.67
8:C:46:ARG:NH2	8:C:89:GLU:OE2	2.26	0.67
2:2:811:C:OP2	57:2:1710:HOH:O	2.13	0.67
5:5:5:A:O2'	5:5:6:C:O5'	2.12	0.67
2:2:1270:G:HO2'	2:2:1313:U:HO2'	1.42	0.67
1:1:2388:A:OP1	57:1:3316:HOH:O	2.11	0.67
2:2:18:C:OP1	39:j:132:ASN:ND2	2.27	0.67
2:2:411:A:O2'	2:2:413:G:OP2	2.09	0.67
2:2:1537:U:OP1	57:2:1709:HOH:O	2.12	0.67
21:R:82:HIS:O	57:R:201:HOH:O	2.11	0.67
1:1:2306:C:OP2	1:1:2307:G:O2'	2.06	0.67
1:1:498:G:O3'	24:U:43:LYS:NZ	2.27	0.67
1:1:1028:A:N3	57:1:3357:HOH:O	2.28	0.67
1:1:2477:U:O2	35:f:4:ARG:NH2	2.27	0.67
2:2:1100:C:OP1	55:z:69:ARG:NH1	2.26	0.67
1:1:2831:G:N2	1:1:2884:U:OP2	2.27	0.67
2:2:1157:A:N7	2:2:1180:A:N6	2.42	0.67
2:2:1297:G:O2'	41:l:114:LYS:NZ	2.27	0.67
1:1:489:G:N2	1:1:491:G:OP2	2.27	0.67
2:2:970:C:N4	43:n:130:ARG:O	2.28	0.67
1:1:944:C:OP2	57:1:3318:HOH:O	2.13	0.66
2:2:1516:2MG:N2	2:2:1519:MA6:OP2	2.27	0.66
1:1:282:A:N6	1:1:359:G:O6	2.28	0.66
2:2:187:G:O2'	2:2:190:A:N6	2.28	0.66
6:6:48:C:H2'	6:6:59:U:H1'	1.77	0.66
1:1:388:G:O2'	57:1:3303:HOH:O	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:42:C:N3	10:E:90:THR:OG1	2.27	0.66
1:1:745:IMG:O2'	1:1:748:G:O2'	2.11	0.66
1:1:1792:G:OP2	57:1:3320:HOH:O	2.13	0.66
2:2:1527:U:OP2	55:z:42:THR:OG1	2.09	0.66
1:1:2149:U:O4'	57:1:3319:HOH:O	2.13	0.66
37:h:40:ARG:NH1	48:s:92:GLU:OE1	2.28	0.66
2:2:1137:C:O2	2:2:1138:G:N2	2.27	0.66
1:1:2112:G:O6	57:1:3308:HOH:O	2.09	0.66
1:1:2161:C:O2'	1:1:2173:A:O5'	2.12	0.66
2:2:1317:C:OP2	48:s:28:LYS:NZ	2.28	0.66
1:1:1141:U:OP2	13:J:65:THR:OG1	2.13	0.66
17:N:4:ARG:NH1	57:N:201:HOH:O	2.28	0.66
50:u:47:GLU:OE1	57:u:101:HOH:O	2.14	0.66
6:6:11:C:H2'	6:6:12:U:C6	2.31	0.65
6:6:24:G:C2'	6:6:25:C:H5'	2.26	0.65
5:5:4:C:HO2'	5:5:5:A:H8	1.43	0.65
2:2:28:A:O2'	2:2:296:U:OP1	2.13	0.65
5:5:33:U:OP2	43:n:130:ARG:NH1	2.26	0.65
38:i:47:ARG:O	38:i:47:ARG:NH1	2.30	0.65
6:6:26:A:N6	6:6:44:G:H1	1.95	0.65
54:y:17:ALA:O	54:y:21:ASN:ND2	2.30	0.65
1:1:244:A:OP2	34:e:8:ARG:NH2	2.28	0.65
1:1:1869:G:N2	1:1:1872:A:C5	2.65	0.65
7:B:262:ARG:O	7:B:265:LYS:NZ	2.30	0.65
23:T:5:GLU:OE1	23:T:5:GLU:N	2.29	0.65
1:1:1202:G:H21	15:L:4:ASN:HB3	1.61	0.65
2:2:1063:C:OP2	2:2:1064:G:O2'	2.13	0.65
1:1:2591:C:N4	1:1:2592:G:O6	2.30	0.65
13:J:32:LEU:HD22	13:J:54:ILE:HG21	1.79	0.65
1:1:2129:C:O2'	57:1:3322:HOH:O	2.15	0.65
9:D:168:ASP:OD2	9:D:170:ARG:NH1	2.30	0.65
1:1:2079:U:O2'	27:X:23:ASN:OD1	2.14	0.64
1:1:2751:G:OP1	1:1:2751:G:N2	2.29	0.64
1:1:981:A:OP2	1:1:982:C:N4	2.27	0.64
1:1:1062:G:N7	1:1:1088:A:O2'	2.27	0.64
1:1:2266:A:N6	1:1:2273:A:OP2	2.28	0.64
2:2:826:C:O2	42:m:16:ASN:ND2	2.30	0.64
6:6:68:C:H2'	6:6:69:A:C8	2.32	0.64
38:i:152:GLN:O	57:i:302:HOH:O	2.14	0.64
2:2:1315:U:O2'	2:2:1360:A:N3	2.26	0.64
3:3:43:C:O2	10:E:92:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:248:G:O2'	1:1:2432:A:OP1	2.16	0.64
1:1:974:G:O2'	1:1:975:A:OP2	2.16	0.64
1:1:1869:G:O2'	1:1:1870:C:OP1	2.11	0.64
1:1:2796:U:O2'	1:1:2797:U:O5'	2.16	0.64
2:2:1255:G:O2'	2:2:1258:G:N3	2.27	0.64
6:6:24:G:H2'	6:6:25:C:O4'	1.98	0.64
1:1:831:G:O2'	15:L:38:GLN:OE1	2.15	0.63
2:2:451:A:OP1	2:2:481:G:N1	2.32	0.63
47:r:100:GLN:N	47:r:100:GLN:OE1	2.31	0.63
6:6:10:G:N2	6:6:26:A:H1'	2.13	0.63
2:2:397:A:N7	2:2:547:A:O2'	2.32	0.63
2:2:203:G:O2'	2:2:204:G:O4'	2.16	0.63
2:2:980:C:O2'	2:2:981:U:OP1	2.16	0.63
50:u:40:ASN:ND2	50:u:42:ILE:O	2.32	0.63
12:G:12:LEU:HD21	12:G:19:VAL:HG21	1.79	0.63
22:S:31:GLN:N	22:S:31:GLN:OE1	2.31	0.63
44:o:47:GLU:OE1	48:s:76:LYS:NZ	2.31	0.63
2:2:1183:U:O2'	2:2:1185:G:OP2	2.17	0.63
6:6:62:C:H2'	6:6:63:G:C8	2.33	0.63
1:1:1534:U:O2'	1:1:1537:G:O6	2.08	0.63
1:1:1848:A:OP1	57:1:3326:HOH:O	2.16	0.63
2:2:261:U:OP2	54:y:74:ARG:NH2	2.31	0.63
1:1:1437:C:HO2'	1:1:1516:G:HO2'	1.45	0.62
1:1:698:C:O2'	1:1:734:A:N6	2.32	0.62
46:q:68:GLY:O	46:q:99:ARG:NH1	2.32	0.62
10:E:153:ASP:N	10:E:153:ASP:OD1	2.30	0.62
41:l:15:ASP:OD1	41:l:20:SER:N	2.32	0.62
1:1:2126:A:O2'	1:1:2162:G:N2	2.33	0.62
2:2:501:C:OP1	46:q:114:ARG:NH2	2.31	0.62
2:2:689:C:OP1	45:p:29:ASN:ND2	2.31	0.62
2:2:346:G:OP1	19:P:39:ARG:NH1	2.33	0.62
42:m:10:MET:HG3	42:m:27:MET:HE3	1.81	0.62
1:1:918:A:N3	3:3:80:U:O2'	2.32	0.62
2:2:1396:A:O2'	39:j:29:ARG:NH2	2.33	0.62
1:1:1:G:C2	1:1:2903:U:C2	2.87	0.62
1:1:1031:G:H22	1:1:1122:G:H22	1.46	0.62
1:1:2595:G:N2	1:1:2598:A:OP2	2.30	0.62
49:t:64:ARG:NH1	49:t:67:LEU:HD11	2.15	0.62
1:1:1:G:N1	1:1:2903:U:C2	2.68	0.62
30:a:56:ARG:NH1	57:a:101:HOH:O	2.32	0.62
10:E:135:GLN:OE1	10:E:135:GLN:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:137:ASP:O	11:F:141:ILE:HG23	2.00	0.61
1:1:160:A:N3	1:1:2208:C:O2'	2.31	0.61
1:1:1818:U:O2'	7:B:153:GLN:O	2.14	0.61
2:2:510:A:O2'	2:2:541:G:N2	2.34	0.61
1:1:487:C:H42	1:1:492:A:H61	1.47	0.61
5:5:52:G:H2'	5:5:53:G:C8	2.36	0.61
14:K:71:ARG:NH2	14:K:123:LEU:O	2.33	0.61
2:2:530:G:O2'	2:2:531:U:OP1	2.17	0.61
2:2:229:U:O2'	50:u:23:ASP:OD1	2.17	0.61
2:2:677:U:O2	2:2:777:A:O2'	2.17	0.61
2:2:966:2MG:H2'	2:2:967:5MC:C6	2.35	0.61
5:5:11:C:H2'	5:5:12:G:C8	2.36	0.61
1:1:2137:U:O2	57:1:3321:HOH:O	2.14	0.61
2:2:543:U:OP1	38:i:14:ARG:NE	2.33	0.61
1:1:389:G:N2	57:1:3336:HOH:O	2.20	0.60
2:2:591:U:OP2	42:m:31:LYS:NZ	2.30	0.60
2:2:811:C:O2'	2:2:901:A:N1	2.33	0.60
40:k:5:GLU:OE2	52:w:24:LYS:NZ	2.33	0.60
1:1:394:C:OP1	57:1:3324:HOH:O	2.15	0.60
41:l:67:GLU:OE1	41:l:70:ARG:NH1	2.34	0.60
1:1:591:U:HO2'	34:e:2:PRO:N	1.98	0.60
1:1:1202:G:H22	1:1:1242:U:H3	1.49	0.60
1:1:1693:U:O2'	7:B:14:ARG:NH2	2.34	0.60
1:1:2522:U:O2'	1:1:2647:U:OP1	2.14	0.60
3:3:51:G:OP1	18:O:63:LYS:NZ	2.29	0.60
1:1:1682:G:OP2	1:1:1699:G:N2	2.29	0.60
2:2:1005:A:N7	2:2:1024:G:O2'	2.35	0.60
27:X:43:GLU:OE1	27:X:45:ARG:NH1	2.35	0.60
2:2:264:C:O2'	51:v:66:PRO:O	2.18	0.60
1:1:227:A:O2'	1:1:228:C:OP2	2.19	0.60
1:1:629:G:N3	1:1:639:U:O2'	2.35	0.60
1:1:1668:A:O2'	1:1:1674:G:N7	2.23	0.60
38:i:98:LEU:O	38:i:102:VAL:HG23	2.02	0.60
1:1:1:G:C2	1:1:2903:U:O2	2.55	0.60
2:2:440:C:H42	2:2:494:G:H22	1.49	0.60
2:2:673:A:H2'	2:2:674:G:C8	2.37	0.60
16:M:17:ASN:O	16:M:38:ARG:NH1	2.34	0.60
38:i:9:LEU:HD12	38:i:10:LYS:N	2.17	0.60
6:6:4:U:H2'	6:6:5:G:C8	2.37	0.59
39:j:32:SER:OG	39:j:53:ALA:O	2.15	0.59
20:Q:86:ALA:O	20:Q:87:SER:OG	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:612:C:OP1	38:i:81:ARG:NH1	2.34	0.59
8:C:136:ASN:ND2	8:C:139:SER:O	2.35	0.59
5:5:61:C:H2'	5:5:62:C:C6	2.37	0.59
5:5:63:U:H2'	5:5:64:C:C6	2.37	0.59
1:1:2635:A:O2'	8:C:81:GLU:OE1	2.20	0.59
2:2:94:G:N2	2:2:97:G:O6	2.33	0.59
2:2:1261:A:N6	2:2:1274:A:O2'	2.34	0.59
38:i:145:ILE:HG22	38:i:149:ALA:HB3	1.83	0.59
1:1:675:A:N3	1:1:2443:C:O2'	2.30	0.59
1:1:1068:G:O2'	1:1:1096:A:N3	2.36	0.59
6:6:6:A:H2'	6:6:7:4SU:H6	1.84	0.59
30:a:57:VAL:O	30:a:61:ASN:ND2	2.36	0.59
44:o:32:THR:OG1	44:o:83:THR:HG22	2.01	0.59
5:5:63:U:H2'	5:5:64:C:H6	1.68	0.59
6:6:11:C:H2'	6:6:12:U:H6	1.68	0.59
47:r:16:VAL:O	47:r:20:THR:HG23	2.03	0.59
1:1:1922:G:OP2	57:1:3327:HOH:O	2.17	0.58
29:Z:47:MET:O	29:Z:51:VAL:HG22	2.03	0.58
42:m:5:ASP:OD1	42:m:77:ARG:NH1	2.33	0.58
1:1:2144:G:HO2'	1:1:2145:C:P	2.25	0.58
2:2:1073:U:O2	36:g:103:ASN:ND2	2.37	0.58
1:1:1030:C:OP2	57:1:3328:HOH:O	2.17	0.58
1:1:1315:C:O2'	1:1:1392:A:N3	2.29	0.58
1:1:2899:A:N1	1:1:2900:A:N6	2.52	0.58
2:2:1372:U:OP1	43:n:73:SER:OG	2.18	0.58
3:3:40:U:N3	3:3:44:G:OP2	2.36	0.58
38:i:99:ASP:OD1	38:i:115:ARG:NH1	2.36	0.58
43:n:59:GLU:OE1	43:n:59:GLU:N	2.36	0.58
16:M:27:SER:O	16:M:133:LYS:NZ	2.37	0.58
6:6:9:A:H5'	6:6:46:7MG:H1'	1.85	0.58
1:1:1483:G:O6	1:1:1507:C:N4	2.35	0.58
1:1:2705:A:O2'	1:1:2852:G:OP1	2.14	0.58
38:i:47:ARG:NH2	57:i:304:HOH:O	2.34	0.58
1:1:578:G:OP1	1:1:1255:U:O2'	2.22	0.58
1:1:2092:U:OP1	1:1:2199:A:O2'	2.21	0.58
38:i:123:ILE:CD1	38:i:145:ILE:HD12	2.33	0.58
41:l:138:ARG:NH2	41:l:139:GLU:OE2	2.37	0.58
1:1:2499:C:OP2	57:1:3329:HOH:O	2.17	0.58
1:1:1363:C:O2'	1:1:1809:A:N3	2.33	0.57
1:1:2161:C:HO2'	1:1:2173:A:P	2.26	0.57
2:2:2:A:N3	2:2:613:C:O2'	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:944:G:N1	2:2:1338:G:OP2	2.35	0.57
6:6:38:A:H3'	6:6:39:G:H8	1.68	0.57
18:O:35:ILE:HD11	18:O:71:ALA:HA	1.86	0.57
1:1:249:C:O2	34:e:12:LYS:NZ	2.36	0.57
2:2:374:A:O3'	50:u:70:ARG:NH1	2.35	0.57
21:R:73:LYS:NZ	57:R:202:HOH:O	2.36	0.57
1:1:463:G:N2	1:1:466:A:OP2	2.33	0.57
1:1:48:G:N2	1:1:177:G:OP2	2.37	0.57
1:1:2250:G:O2'	1:1:2496:C:OP1	2.21	0.57
2:2:674:G:H21	45:p:118:HIS:HB2	1.68	0.57
1:1:1064:C:O2'	1:1:1065:U:O5'	2.22	0.57
2:2:429:U:H5'	38:i:9:LEU:HD11	1.86	0.57
7:B:129:THR:HG22	7:B:191:THR:HG22	1.86	0.57
22:S:25:ARG:NH1	22:S:74:ILE:O	2.34	0.57
13:J:23:LYS:NZ	13:J:142:ILE:O	2.32	0.57
1:1:102:U:O4	28:Y:2:LYS:N	2.37	0.57
1:1:534:U:O2'	20:Q:49:ASP:OD2	2.20	0.57
2:2:1005:A:N1	57:2:1725:HOH:O	2.31	0.57
6:6:5:G:H2'	6:6:6:A:C8	2.34	0.57
1:1:2619:C:OP1	8:C:157:LYS:NZ	2.33	0.57
2:2:1532:U:O2'	2:2:1534:A:N7	2.34	0.57
6:6:26:A:N1	6:6:44:G:N2	2.52	0.57
18:O:69:ASP:OD1	18:O:70:ALA:N	2.38	0.57
1:1:2117:A:O2'	1:1:2118:U:OP2	2.17	0.57
1:1:2839:G:O2'	17:N:49:GLU:OE1	2.13	0.57
13:J:32:LEU:CD2	13:J:54:ILE:HG21	2.34	0.57
1:1:1671:U:O2	57:1:3323:HOH:O	2.15	0.56
2:2:264:C:O3'	51:v:65:ARG:NH2	2.37	0.56
6:6:47:U:H3'	6:6:48:C:C5'	2.34	0.56
6:6:65:C:H2'	6:6:66:A:H8	1.68	0.56
1:1:976:G:HO2'	1:1:1155:A:HO2'	1.48	0.56
1:1:1901:A:OP2	7:B:253:LYS:NZ	2.33	0.56
1:1:2261:C:N4	26:W:14:ARG:O	2.38	0.56
1:1:2286:G:H4'	1:1:2287:A:O5'	2.04	0.56
2:2:185:U:O4'	54:y:69:LYS:NZ	2.38	0.56
12:G:75:LEU:HD23	12:G:75:LEU:H	1.69	0.56
1:1:499:U:H6	1:1:499:U:O5'	1.88	0.56
1:1:1056:G:N1	1:1:1102:C:OP2	2.36	0.56
27:X:31:PRO:HG2	27:X:33:LEU:HD13	1.87	0.56
44:o:51:VAL:HG13	48:s:81:ARG:HB2	1.88	0.56
49:t:2:SER:OG	49:t:3:LEU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1222:G:OP1	2:2:1321:U:O2'	2.15	0.56
9:D:170:ARG:NH2	9:D:176:ASP:OD1	2.39	0.56
1:1:2620:C:O2'	8:C:162:ALA:O	2.16	0.56
9:D:145:ASP:OD1	9:D:145:ASP:N	2.38	0.56
50:u:4:ILE:O	50:u:71:VAL:HG21	2.06	0.56
1:1:1130:U:N3	1:1:2025:C:OP1	2.36	0.56
13:J:17:VAL:HG12	13:J:55:ILE:HB	1.88	0.56
48:s:42:TRP:O	48:s:46:LEU:HD23	2.06	0.56
2:2:180:U:O2	2:2:196:A:N6	2.38	0.56
2:2:880:C:OP1	46:q:5:ASN:ND2	2.39	0.56
39:j:148:ASN:ND2	42:m:73:GLU:OE1	2.38	0.56
1:1:1:G:N1	1:1:2903:U:N3	2.54	0.56
1:1:26:G:O2'	1:1:27:G:O4'	2.24	0.56
10:E:66:LEU:HD23	10:E:67:ILE:N	2.21	0.56
23:T:52:GLU:OE1	23:T:52:GLU:N	2.39	0.56
1:1:2898:U:O2'	13:J:134:ALA:O	2.17	0.56
1:1:620:G:OP2	57:1:3330:HOH:O	2.18	0.55
7:B:79:GLU:OE2	7:B:101:ARG:NE	2.37	0.55
1:1:1153:C:OP1	20:Q:92:ARG:NH2	2.38	0.55
1:1:1853:A:N3	1:1:2233:U:O2'	2.37	0.55
1:1:1856:U:H2'	1:1:1857:G:O4'	2.07	0.55
2:2:977:A:OP1	48:s:61:ARG:NH2	2.37	0.55
6:6:50:G:N2	6:6:64:U:O2	2.24	0.55
2:2:410:G:O2'	2:2:432:A:N6	2.38	0.55
38:i:145:ILE:CG2	38:i:149:ALA:HB3	2.36	0.55
1:1:498:G:H2'	1:1:499:U:N1	2.21	0.55
2:2:768:A:N3	2:2:1512:U:O2'	2.39	0.55
5:5:49:G:H1	5:5:65:U:H3	1.52	0.55
37:h:70:THR:O	37:h:106:VAL:HG12	2.07	0.55
2:2:1261:A:N6	2:2:1274:A:HO2'	2.04	0.55
43:n:63:LEU:HD12	43:n:63:LEU:O	2.07	0.55
1:1:1296:G:OP1	1:1:2709:G:O2'	2.15	0.55
36:g:119:THR:O	36:g:124:GLY:N	2.39	0.55
39:j:70:ASN:O	39:j:70:ASN:ND2	2.38	0.55
2:2:324:G:N1	2:2:327:A:OP2	2.40	0.55
6:6:12:U:H2'	6:6:13:C:C6	2.42	0.55
3:3:93:C:OP2	25:V:18:ARG:NH1	2.39	0.55
5:5:67:G:H2'	5:5:68:U:C6	2.42	0.55
36:g:186:ILE:HD13	36:g:200:ILE:HB	1.88	0.55
1:1:1799:G:OP1	7:B:258:ARG:NH1	2.40	0.55
1:1:2193:G:O2'	1:1:2194:U:P	2.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1077:G:N2	2:2:1080:A:OP2	2.35	0.55
2:2:1083:U:O2'	2:2:1102:A:OP2	2.25	0.55
28:Y:8:GLU:OE1	28:Y:8:GLU:N	2.31	0.55
1:1:370:G:O2'	1:1:424:G:OP1	2.23	0.54
1:1:2140:G:N1	1:1:2151:U:N3	2.55	0.54
2:2:393:A:OP1	50:u:12:LYS:NZ	2.39	0.54
2:2:1013:G:N2	2:2:1016:A:OP2	2.27	0.54
38:i:159:LEU:HD13	38:i:175:ALA:HB1	1.88	0.54
1:1:2450:A:OP1	1:1:2497:A:O2'	2.10	0.54
34:e:7:VAL:HG23	34:e:10:ALA:HB3	1.89	0.54
36:g:100:MET:HA	36:g:107:VAL:HG21	1.88	0.54
2:2:565:U:OP2	2:2:566:G:O2'	2.18	0.54
6:6:16:C:O2	6:6:18:G:H5'	2.07	0.54
8:C:13:ARG:NH1	19:P:75:GLN:OE1	2.36	0.54
1:1:2564:A:OP1	1:1:2648:G:O2'	2.14	0.54
2:2:201:G:H21	2:2:469:C:H1'	1.73	0.54
2:2:373:A:C2	2:2:374:A:C8	2.95	0.54
1:1:1038:G:H2'	1:1:1039:A:C1'	2.38	0.54
1:1:2140:G:N1	1:1:2151:U:C2	2.76	0.54
21:R:4:VAL:HG22	21:R:40:MET:HB3	1.88	0.54
1:1:2523:G:HO2'	1:1:2764:A:HO2'	1.45	0.54
36:g:134:ALA:O	36:g:138:THR:HG23	2.08	0.54
1:1:995:C:O2	13:J:3:THR:OG1	2.23	0.54
2:2:1147:C:O2'	43:n:7:TYR:OH	2.16	0.54
7:B:117:GLN:N	7:B:128:ASN:OD1	2.38	0.54
38:i:118:VAL:HG22	38:i:123:ILE:HG13	1.88	0.54
1:1:240:C:OP2	1:1:241:A:O2'	2.20	0.53
2:2:620:C:C5	38:i:132:ILE:HD11	2.43	0.53
1:1:2118:U:H5	1:1:2148:G:H21	1.57	0.53
5:5:27:C:O2	5:5:44:G:N2	2.40	0.53
39:j:76:LEU:HD11	39:j:120:VAL:HG12	1.90	0.53
1:1:117:G:OP2	1:1:119:A:O2'	2.24	0.53
1:1:1235:G:O2'	1:1:1236:G:O4'	2.25	0.53
1:1:1275:A:N1	1:1:1295:C:O2'	2.32	0.53
2:2:390:U:O2'	50:u:28:ARG:NH2	2.42	0.53
3:3:48:U:OP2	18:O:30:ARG:NH2	2.38	0.53
6:6:51:C:H2'	6:6:52:G:H8	1.73	0.53
10:E:113:ASP:OD1	47:r:71:ARG:NH2	2.41	0.53
21:R:14:VAL:CG1	21:R:20:VAL:HG11	2.38	0.53
39:j:103:THR:N	39:j:122:ASN:OD1	2.41	0.53
1:1:1102:C:N3	1:1:1103:A:N6	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:q:107:VAL:O	46:q:119:VAL:HG21	2.09	0.53
1:1:1024:G:OP2	1:1:1025:G:O2'	2.21	0.53
1:1:1475:G:O2'	1:1:1514:G:O6	2.24	0.53
1:1:1715:G:O2'	1:1:1743:G:O6	2.24	0.53
1:1:2376:A:N3	18:O:111:ARG:NH1	2.56	0.53
2:2:439:U:O2	38:i:120:HIS:ND1	2.41	0.53
2:2:1383:C:O2'	2:2:1384:C:OP1	2.24	0.53
1:1:1085:A:H2'	1:1:1086:A:C4	2.43	0.53
1:1:2618:G:H21	8:C:155:VAL:HG21	1.74	0.53
3:3:66:A:O4'	3:3:108:A:N6	2.39	0.53
45:p:113:VAL:HG12	52:w:73:ARG:HD2	1.90	0.53
2:2:526:C:OP1	46:q:88:LYS:NZ	2.31	0.53
2:2:1328:C:OP1	47:r:28:THR:HG21	2.09	0.53
5:5:20:U:H2'	5:5:21:A:H4'	1.90	0.53
1:1:245:G:O6	34:e:8:ARG:NH1	2.41	0.53
1:1:491:G:H22	22:S:7:HIS:CE1	2.26	0.53
3:3:39:A:O2'	3:3:40:U:O4'	2.21	0.53
53:x:36:ARG:NH2	53:x:75:ALA:O	2.40	0.53
2:2:890:G:O2'	2:2:906:A:N6	2.41	0.53
1:1:1199:U:O2'	1:1:1200:C:OP2	2.24	0.53
6:6:75:C:H2'	6:6:76:A:C8	2.44	0.53
1:1:1980:G:O2'	1:1:1982:U:OP2	2.22	0.52
1:1:2506:U:N3	1:1:2585:U:O4	2.42	0.52
2:2:974:A:OP1	48:s:69:ARG:NH1	2.42	0.52
1:1:974:G:OP1	1:1:1187:G:O2'	2.20	0.52
1:1:1697:G:OP2	1:1:1698:A:O2'	2.24	0.52
1:1:2720:U:OP1	19:P:53:ARG:NH2	2.41	0.52
5:5:28:C:H2'	5:5:29:G:H8	1.74	0.52
11:F:121:ILE:HD12	11:F:141:ILE:HG22	1.90	0.52
1:1:445:C:H2'	1:1:446:G:O4'	2.09	0.52
1:1:1199:U:H2'	1:1:1199:U:O2	2.09	0.52
1:1:2244:U:O2'	57:1:3331:HOH:O	2.19	0.52
2:2:482:A:HO2'	2:2:483:C:C1'	2.22	0.52
2:2:501:C:O2'	2:2:549:C:O2'	2.05	0.52
38:i:105:MET:HE3	38:i:171:LEU:HD11	1.91	0.52
1:1:896:A:OP1	57:1:3333:HOH:O	2.19	0.52
1:1:1328:A:O2'	1:1:1329:U:O5'	2.23	0.52
2:2:867:G:O2'	2:2:873:A:N1	2.37	0.52
8:C:25:THR:HG21	8:C:193:VAL:HG22	1.90	0.52
9:D:40:ARG:NH2	57:D:301:HOH:O	2.43	0.52
1:1:1328:A:HO2'	1:1:1329:U:P	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2050:C:H2'	1:1:2051:A:O4'	2.08	0.52
2:2:1129:C:O2'	2:2:1139:G:N7	2.34	0.52
1:1:565:C:OP2	21:R:80:ARG:N	2.42	0.52
2:2:436:C:H2'	2:2:437:U:C6	2.45	0.52
2:2:499:A:H1'	2:2:500:G:C8	2.45	0.52
2:2:1125:U:O2'	2:2:1126:U:O5'	2.26	0.52
17:N:56:LYS:NZ	17:N:90:ARG:O	2.41	0.52
1:1:48:G:H22	1:1:177:G:P	2.32	0.52
1:1:1385:A:O2'	1:1:1396:U:O2	2.27	0.52
1:1:2126:A:N6	1:1:2163:A:O4'	2.43	0.52
2:2:1399:C:O2	2:2:1502:A:N6	2.43	0.52
6:6:16:C:H1'	6:6:18:G:OP2	2.10	0.52
1:1:728:G:H3'	1:1:729:G:H5'	1.92	0.52
1:1:1212:G:O2'	1:1:1213:A:OP2	2.28	0.52
5:5:66:C:N4	5:5:67:G:O6	2.43	0.52
13:J:17:VAL:HG13	13:J:137:PRO:HB2	1.91	0.52
38:i:144:SER:C	38:i:145:ILE:HD13	2.34	0.52
1:1:395:U:O2'	1:1:396:G:N7	2.39	0.52
1:1:1170:C:N4	1:1:1179:G:O6	2.41	0.52
2:2:519:C:H2'	2:2:520:A:O4'	2.09	0.52
2:2:993:G:O2'	2:2:994:A:N7	2.41	0.52
3:3:41:G:O6	10:E:69:LYS:NZ	2.39	0.52
10:E:144:ASP:OD1	10:E:145:LYS:N	2.43	0.52
1:1:71:A:OP2	1:1:112:U:O2'	2.24	0.51
1:1:2311:A:HO2'	1:1:2312:U:H6	1.58	0.51
2:2:86:G:O2'	2:2:87:C:O5'	2.27	0.51
38:i:140:ASN:N	38:i:182:PHE:O	2.43	0.51
1:1:265:A:N1	1:1:427:U:O2'	2.41	0.51
1:1:2474:U:O2'	1:1:2475:C:OP1	2.26	0.51
1:1:2822:G:OP1	8:C:164:GLN:NE2	2.43	0.51
2:2:311:C:OP1	50:u:31:ARG:NH2	2.43	0.51
2:2:373:A:C2	2:2:482:A:C6	2.99	0.51
2:2:747:A:O2'	2:2:748:G:O4'	2.26	0.51
2:2:1317:C:O5'	48:s:24:ARG:NH1	2.44	0.51
8:C:176:ASP:OD1	8:C:176:ASP:N	2.39	0.51
37:h:11:ARG:NH1	37:h:177:THR:O	2.42	0.51
1:1:1844:C:O3'	7:B:256:LYS:NZ	2.42	0.51
38:i:123:ILE:HD13	38:i:145:ILE:HD12	1.93	0.51
1:1:2489:U:H2'	1:1:2490:G:O4'	2.11	0.51
2:2:511:C:C2	2:2:512:U:C5	2.98	0.51
1:1:1828:G:OP1	57:1:3334:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2250:G:OP1	16:M:84:LYS:NZ	2.38	0.51
1:1:2304:G:H22	1:1:2312:U:H3	1.56	0.51
6:6:47:U:H3'	6:6:48:C:H5'	1.92	0.51
32:c:23:THR:OG1	32:c:24:THR:N	2.41	0.51
5:5:9:A:H2'	5:5:11:C:H41	1.75	0.51
41:l:68:ASN:ND2	41:l:130:ASN:OD1	2.44	0.51
41:l:126:ASP:O	41:l:131:LYS:N	2.42	0.51
1:1:1041:G:H2'	1:1:1042:G:C8	2.46	0.51
1:1:1587:G:C2	1:1:1588:G:C8	2.98	0.51
2:2:899:C:O2	57:2:1711:HOH:O	2.19	0.51
1:1:2177:C:H2'	1:1:2178:C:N1	2.26	0.51
1:1:2667:C:N3	11:F:110:SER:OG	2.37	0.51
2:2:642:A:N3	42:m:105:SER:OG	2.38	0.51
2:2:713:G:H2'	2:2:714:G:C8	2.46	0.51
2:2:766:A:OP2	2:2:812:G:N2	2.44	0.51
2:2:1383:C:HO2'	2:2:1384:C:P	2.33	0.51
10:E:140:GLU:OE1	10:E:140:GLU:N	2.43	0.51
48:s:88:ALA:HB2	48:s:96:LEU:HD23	1.92	0.51
1:1:400:G:N7	27:X:57:ARG:NH1	2.55	0.51
1:1:1370:C:H2'	1:1:1371:G:O4'	2.11	0.51
2:2:390:U:H2'	2:2:391:G:H8	1.77	0.50
6:6:42:G:H2'	6:6:43:G:O4'	2.11	0.50
1:1:2743:U:OP2	1:1:2755:C:N4	2.43	0.50
55:z:8:GLU:N	55:z:8:GLU:OE1	2.43	0.50
1:1:1790:C:H2'	1:1:1791:A:C8	2.46	0.50
1:1:1869:G:C2	1:1:1872:A:C6	2.99	0.50
2:2:456:A:H61	2:2:476:U:H3	1.59	0.50
5:5:15:G:H22	5:5:48:C:N4	2.09	0.50
6:6:50:G:O6	6:6:64:U:O4	2.29	0.50
31:b:54:VAL:HG23	31:b:55:ILE:HG23	1.94	0.50
45:p:87:LYS:HB2	45:p:113:VAL:HG23	1.92	0.50
2:2:1027:C:H4'	2:2:1028:C:OP1	2.11	0.50
15:L:79:LEU:HA	15:L:82:LEU:HD23	1.94	0.50
41:l:69:VAL:HG12	41:l:69:VAL:O	2.11	0.50
46:q:110:ARG:NE	46:q:112:GLN:O	2.44	0.50
6:6:68:C:H2'	6:6:69:A:H8	1.75	0.50
1:1:674:G:O2'	9:D:62:GLN:NE2	2.44	0.50
1:1:1065:U:O2'	1:1:1066:U:P	2.70	0.50
6:6:51:C:H2'	6:6:52:G:C8	2.47	0.50
7:B:51:THR:HG23	7:B:54:ILE:HD12	1.94	0.50
39:j:15:LEU:HD13	39:j:60:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:110:C:O2'	50:u:25:ARG:O	2.25	0.50
2:2:551:U:O2'	46:q:116:LYS:NZ	2.45	0.50
2:2:898:G:N2	2:2:901:A:OP2	2.44	0.50
2:2:1099:G:O3'	55:z:69:ARG:NH2	2.44	0.50
1:1:404:A:H1'	1:1:405:U:OP2	2.11	0.50
1:1:488:G:N2	1:1:491:G:OP1	2.44	0.50
1:1:964:C:O2'	1:1:2273:A:N3	2.38	0.50
1:1:1:G:C6	1:1:2903:U:N3	2.80	0.50
1:1:2140:G:C6	1:1:2151:U:N3	2.80	0.50
1:1:2744:G:N2	11:F:143:GLN:OE1	2.42	0.50
15:L:4:ASN:OD1	15:L:5:THR:N	2.45	0.50
34:e:28:ASN:O	34:e:36:LYS:NZ	2.44	0.50
36:g:94:HIS:NE2	36:g:146:ASN:OD1	2.45	0.50
1:1:1141:U:H4'	1:1:1142:A:O4'	2.12	0.49
2:2:945:G:C2	2:2:946:A:C8	3.00	0.49
2:2:1316:G:N1	2:2:1319:A:OP2	2.45	0.49
3:3:39:A:C2	3:3:44:G:C2	3.00	0.49
32:c:8:LYS:NZ	57:e:101:HOH:O	2.40	0.49
1:1:2110:G:N1	1:1:2180:U:O4	2.46	0.49
2:2:746:A:H2'	2:2:747:A:C8	2.47	0.49
36:g:113:ARG:NH2	57:g:301:HOH:O	2.40	0.49
37:h:56:VAL:HG22	37:h:67:THR:HB	1.93	0.49
46:q:112:GLN:O	46:q:113:ALA:HB3	2.12	0.49
1:1:2140:G:C6	1:1:2151:U:C4	3.00	0.49
1:1:2821:A:OP2	8:C:115:GLY:N	2.42	0.49
2:2:253:A:N6	2:2:274:A:N1	2.60	0.49
5:5:62:C:H2'	5:5:63:U:C6	2.47	0.49
28:Y:21:LEU:HD13	28:Y:46:VAL:HG23	1.94	0.49
52:w:72:ASP:OD1	52:w:73:ARG:N	2.45	0.49
1:1:161:A:OP2	1:1:162:U:O2'	2.14	0.49
1:1:1244:A:O2'	9:D:29:HIS:NE2	2.42	0.49
5:5:21:A:N6	5:5:47:U:O2'	2.45	0.49
10:E:17:MET:HE1	10:E:25:VAL:HA	1.92	0.49
24:U:102:THR:O	24:U:104:LYS:NZ	2.45	0.49
43:n:88:MET:HE1	43:n:95:ARG:HA	1.94	0.49
1:1:2053:G:N7	57:1:3372:HOH:O	2.34	0.49
2:2:424:G:N2	2:2:425:G:C2	2.80	0.49
2:2:482:A:O2'	2:2:483:C:O4'	2.29	0.49
2:2:1496:C:H2'	2:2:1497:G:O4'	2.11	0.49
13:J:18:VAL:O	13:J:57:LEU:HD23	2.13	0.49
1:1:2347:C:O2'	32:c:21:TYR:OH	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:476:G:N1	1:1:479:A:OP2	2.41	0.49
1:1:685:A:O2'	1:1:773:U:O4	2.26	0.49
1:1:1364:G:OP2	27:X:50:ARG:NH2	2.43	0.49
1:1:2687:U:H2'	1:1:2688:G:O4'	2.12	0.49
1:1:2865:U:OP2	1:1:2866:U:O2'	2.16	0.49
2:2:545:C:OP2	38:i:62:ARG:NH1	2.46	0.49
2:2:1518:MA6:O5'	2:2:1518:MA6:H8	2.13	0.49
15:L:144:GLU:N	15:L:144:GLU:OE1	2.46	0.49
18:O:39:VAL:O	18:O:48:LEU:N	2.46	0.49
38:i:118:VAL:O	38:i:131:ASN:OD1	2.30	0.49
45:p:37:ARG:NH2	45:p:83:GLU:OE2	2.45	0.49
1:1:703:U:H2'	1:1:704:G:O4'	2.13	0.49
1:1:1029:A:N6	1:1:1124:G:H1	2.11	0.49
1:1:1029:A:N6	1:1:1124:G:N1	2.60	0.49
1:1:1109:C:O2'	1:1:1110:G:O4'	2.31	0.49
2:2:77:A:H2'	2:2:78:A:O4'	2.12	0.49
2:2:1141:C:O2'	2:2:1142:G:O5'	2.29	0.49
25:V:6:ALA:HB2	25:V:42:LEU:HD23	1.95	0.49
51:v:78:VAL:HG22	51:v:79:VAL:H	1.77	0.49
1:1:545:U:HO2'	1:1:548:G:H1	1.60	0.49
2:2:91:U:O2'	2:2:92:U:O5'	2.27	0.49
2:2:159:G:N7	57:2:1734:HOH:O	2.35	0.49
2:2:1072:G:H21	36:g:106:THR:HG21	1.77	0.49
5:5:17(A):U:O2'	5:5:18:G:H5''	2.13	0.49
8:C:46:ARG:NH2	8:C:88:GLU:O	2.40	0.49
13:J:125:TYR:OH	13:J:132:HIS:NE2	2.42	0.49
45:p:88:GLY:N	45:p:114:THR:HG22	2.26	0.49
1:1:1527:G:N1	1:1:1544:A:OP2	2.39	0.49
1:1:1604:C:O2'	1:1:1610:A:N1	2.38	0.49
1:1:1695:G:N7	7:B:14:ARG:NH2	2.61	0.49
1:1:1870:C:H2'	1:1:1871:A:C8	2.48	0.48
1:1:2584:U:H3'	1:1:2585:U:H5''	1.95	0.48
2:2:434:U:O2	2:2:435:A:N7	2.46	0.48
6:6:67:U:H2'	6:6:68:C:C6	2.48	0.48
8:C:105:LYS:O	8:C:177:VAL:HG12	2.13	0.48
16:M:28:PHE:N	16:M:104:GLU:OE2	2.46	0.48
38:i:109:ALA:N	38:i:158:ALA:HB1	2.28	0.48
2:2:486:U:C2	2:2:487:A:C8	3.01	0.48
2:2:543:U:H2'	2:2:544:G:O4'	2.12	0.48
2:2:980:C:HO2'	2:2:981:U:P	2.36	0.48
38:i:197:GLU:O	38:i:201:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:34:CM0:H2'	6:6:35:A:O4'	2.13	0.48
13:J:114:LEU:HG	13:J:118:MET:HE3	1.95	0.48
1:1:500:G:N1	1:1:503:A:OP2	2.47	0.48
3:3:40:U:O2'	3:3:43:C:OP2	2.29	0.48
38:i:9:LEU:HD13	38:i:32:CYS:SG	2.54	0.48
53:x:63:THR:OG1	53:x:65:GLU:OE1	2.27	0.48
1:1:1027:A:O2'	57:1:3332:HOH:O	2.19	0.48
1:1:1558:C:O4'	1:1:1560:G:C8	2.66	0.48
1:1:1814:G:OP2	1:1:1815:A:O2'	2.16	0.48
1:1:1882:U:C2	1:1:1883:U:C5	3.02	0.48
2:2:1140:C:O2'	2:2:1141:C:O5'	2.31	0.48
6:6:24:G:O2'	6:6:25:C:H5'	2.12	0.48
44:o:40:ILE:HD11	44:o:73:LEU:HD23	1.95	0.48
1:1:2174:C:N4	57:1:3416:HOH:O	2.45	0.48
1:1:2286:G:H5''	1:1:2287:A:OP1	2.14	0.48
2:2:420:U:O2	2:2:424:G:C6	2.67	0.48
6:6:4:U:H2'	6:6:5:G:H8	1.77	0.48
6:6:64:U:H2'	6:6:65:C:C6	2.48	0.48
2:2:527:7MG:OP1	57:2:1713:HOH:O	2.20	0.48
3:3:1:U:O2'	3:3:2:G:N7	2.43	0.48
38:i:11:LEU:HD13	38:i:63:ARG:HG2	1.95	0.48
50:u:66:THR:HG23	50:u:66:THR:O	2.13	0.48
1:1:499:U:O4	1:1:500:G:N7	2.47	0.48
1:1:1283:G:N1	1:1:1286:A:OP2	2.46	0.48
2:2:541:G:H2'	2:2:542:G:O4'	2.14	0.48
1:1:974:G:HO2'	1:1:975:A:P	2.36	0.48
1:1:2051:A:O2'	1:1:2614:A:N6	2.45	0.48
1:1:2756:U:OP2	35:f:19:ARG:NE	2.30	0.48
2:2:842:U:H3'	2:2:843:U:C5'	2.44	0.48
6:6:53:G:H2'	6:6:54:5MU:C6	2.48	0.48
30:a:48:GLN:HA	30:a:51:VAL:HG22	1.96	0.48
38:i:11:LEU:O	38:i:15:GLU:HG2	2.14	0.48
1:1:388:G:O6	1:1:390:U:O2'	2.10	0.48
1:1:2899:A:C2	1:1:2900:A:N7	2.82	0.48
2:2:558:G:OP2	2:2:559:A:O2'	2.31	0.48
6:6:1:G:C6	6:6:73:A:C6	3.02	0.48
12:G:8:LYS:NZ	12:G:9:VAL:O	2.36	0.48
18:O:62:LEU:HD13	18:O:70:ALA:CB	2.43	0.48
1:1:320:A:N3	9:D:163:ASN:ND2	2.59	0.47
1:1:1037:G:H2'	1:1:1038:G:C8	2.49	0.47
2:2:1151:A:O2'	2:2:1152:A:O4'	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:51:VAL:HG12	21:R:51:VAL:O	2.14	0.47
38:i:4:TYR:CD1	38:i:11:LEU:HD11	2.49	0.47
46:q:63:VAL:HG21	46:q:95:TYR:CE2	2.48	0.47
1:1:1029:A:N6	1:1:1124:G:C6	2.80	0.47
1:1:1798:U:OP2	7:B:271:ARG:NH1	2.38	0.47
1:1:2362:C:OP1	34:e:40:ARG:NE	2.44	0.47
1:1:2768:U:O2	57:1:3325:HOH:O	2.15	0.47
5:5:46:G:H2'	5:5:47:U:H4'	1.97	0.47
50:u:34:GLU:OE1	50:u:36:VAL:N	2.47	0.47
1:1:2353:G:N2	26:W:34:GLY:O	2.37	0.47
2:2:78:A:H2'	2:2:79:G:O4'	2.15	0.47
6:6:1:G:O6	6:6:73:A:N6	2.47	0.47
7:B:111:LYS:N	7:B:114:ASP:OD2	2.44	0.47
1:1:360:U:O3'	1:1:361:G:O4'	2.32	0.47
1:1:586:A:N1	1:1:809:G:O2'	2.37	0.47
2:2:976:G:OP2	2:2:1358:U:O2'	2.32	0.47
2:2:1179:A:H2'	2:2:1180:A:O4'	2.14	0.47
7:B:129:THR:CG2	7:B:191:THR:HG22	2.44	0.47
12:G:27:ARG:NH1	27:X:60:ASP:OD1	2.47	0.47
1:1:1379:U:O2'	1:1:1380:G:P	2.73	0.47
6:6:49:G:C6	6:6:66:A:C6	3.02	0.47
46:q:85:GLY:O	46:q:96:HIS:ND1	2.47	0.47
1:1:1720:U:H2'	1:1:1721:G:O4'	2.14	0.47
2:2:186:C:H2'	2:2:187:G:O4'	2.14	0.47
2:2:470:C:H2'	2:2:471:U:C6	2.49	0.47
5:5:24:G:H2'	5:5:25:C:O4'	2.14	0.47
6:6:1:G:C6	6:6:2:G:C5	3.02	0.47
1:1:882:G:N2	57:1:3352:HOH:O	2.46	0.47
1:1:1462:C:O2'	1:1:2702:G:O2'	2.05	0.47
2:2:197:A:N1	2:2:220:G:O2'	2.48	0.47
5:5:14:A:N6	5:5:21:A:C2	2.83	0.47
13:J:81:ILE:HG23	13:J:82:GLY:N	2.29	0.47
44:o:32:THR:O	44:o:82:LYS:NZ	2.48	0.47
53:x:65:GLU:OE1	53:x:65:GLU:N	2.43	0.47
1:1:1068:G:N2	1:1:1095:A:O3'	2.48	0.47
1:1:2452:C:H2'	1:1:2453:A:O4'	2.13	0.47
2:2:167:A:N6	2:2:168:G:O6	2.48	0.47
2:2:452:A:H62	2:2:480:U:H3	1.63	0.47
2:2:576:C:O2'	57:2:1712:HOH:O	2.19	0.47
5:5:11:C:H2'	5:5:12:G:H8	1.80	0.47
6:6:66:A:H2'	6:6:67:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:n:84:THR:O	43:n:88:MET:HG2	2.15	0.47
1:1:569:U:H2'	1:1:570:G:O4'	2.15	0.47
1:1:630:G:N2	1:1:633:A:OP2	2.39	0.47
1:1:1509:A:O2'	1:1:1510:G:OP2	2.32	0.47
1:1:1521:G:OP2	1:1:1522:A:O2'	2.20	0.47
1:1:1827:U:OP2	7:B:221:ARG:NE	2.48	0.47
2:2:820:U:H4'	2:2:821:G:OP2	2.14	0.47
2:2:1086:U:H3	2:2:1099:G:H22	1.63	0.47
6:6:1:G:C6	6:6:73:A:N6	2.83	0.47
38:i:58:LYS:HA	38:i:200:ILE:HD12	1.96	0.47
1:1:1638:C:O2	1:1:2698:U:O2'	2.33	0.47
1:1:2703:C:C2	1:1:2704:C:C5	3.02	0.47
2:2:991:U:O2'	2:2:992:U:OP2	2.31	0.47
2:2:1315:U:H2'	2:2:1316:G:O4'	2.15	0.47
2:2:1402:4OC:H6	2:2:1402:4OC:O5'	2.15	0.47
52:w:37:GLY:O	52:w:63:ARG:NH2	2.42	0.47
1:1:306:U:H2'	1:1:307:G:O4'	2.14	0.46
1:1:1009:A:N3	1:1:1153:C:O2'	2.41	0.46
13:J:81:ILE:HG23	13:J:82:GLY:H	1.80	0.46
52:w:22:ASP:OD2	52:w:24:LYS:N	2.48	0.46
1:1:1858:A:H2'	1:1:1859:U:O4'	2.15	0.46
29:Z:24:LEU:HD11	29:Z:54:MET:SD	2.55	0.46
53:x:52:HIS:NE2	53:x:54:GLY:O	2.48	0.46
1:1:1417:C:HO2'	1:1:1587:G:HO2'	1.49	0.46
1:1:2070:A:H2'	1:1:2071:A:O4'	2.16	0.46
1:1:2898:U:O4	1:1:2899:A:N6	2.49	0.46
2:2:401:C:H2'	2:2:402:G:C8	2.50	0.46
2:2:527:7MG:CM7	46:q:89:0TD:H5	2.45	0.46
38:i:156:LYS:NZ	57:i:305:HOH:O	2.48	0.46
1:1:1668:A:N3	1:1:1670:C:N4	2.63	0.46
1:1:2887:A:N3	31:b:27:SER:OG	2.39	0.46
2:2:1230:C:H5'	5:5:30:U:H5''	1.97	0.46
43:n:7:TYR:OH	43:n:9:THR:OG1	2.33	0.46
1:1:394:C:H2'	1:1:395:U:O4'	2.16	0.46
1:1:538:A:N6	1:1:555:G:N3	2.63	0.46
2:2:580:C:H2'	2:2:581:G:O4'	2.15	0.46
2:2:978:A:C4	2:2:1319:A:C2	3.03	0.46
2:2:1322:C:N4	57:2:1744:HOH:O	2.44	0.46
20:Q:97:ASP:OD1	20:Q:97:ASP:C	2.59	0.46
1:1:2139:U:C2	1:1:2152:G:O6	2.68	0.46
1:1:2483:C:N3	16:M:123:LYS:NZ	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:482:A:H2'	2:2:483:C:C5	2.51	0.46
2:2:488:C:H4'	2:2:619:U:OP2	2.15	0.46
5:5:3:G:H4'	5:5:4:C:OP1	2.16	0.46
6:6:49:G:O6	6:6:66:A:N6	2.48	0.46
1:1:1040:A:C4	1:1:1041:G:C8	3.04	0.46
1:1:1236:G:OP1	57:1:3337:HOH:O	2.20	0.46
2:2:36:C:O3'	46:q:120:LYS:HA	2.15	0.46
7:B:107:PRO:HD2	7:B:110:LEU:HD22	1.96	0.46
1:1:1038:G:H2'	1:1:1039:A:O4'	2.16	0.46
1:1:1727:C:H2'	1:1:1728:C:C1'	2.46	0.46
2:2:1130:A:H61	2:2:1144:G:H1'	1.81	0.46
5:5:62:C:H2'	5:5:63:U:H6	1.81	0.46
6:6:3:G:C2	6:6:71:C:C2	3.04	0.46
38:i:171:LEU:HD12	38:i:182:PHE:HA	1.98	0.46
44:o:85:ASP:OD1	44:o:85:ASP:N	2.46	0.46
50:u:39:PHE:HD1	50:u:50:THR:HG1	1.62	0.46
1:1:1298:C:H2'	1:1:1299:G:O4'	2.15	0.46
2:2:950:U:OP2	47:r:101:ARG:NH1	2.44	0.46
2:2:981:U:OP2	48:s:9:ARG:NH1	2.48	0.46
2:2:1062:U:H2'	2:2:1063:C:C6	2.51	0.46
17:N:9:GLN:O	17:N:17:ARG:NH2	2.48	0.46
50:u:18:GLN:OE1	50:u:18:GLN:N	2.49	0.46
1:1:275:C:H3'	1:1:276:U:H5'	1.97	0.46
1:1:278:A:OP2	1:1:361:G:N1	2.49	0.46
1:1:1233:C:N3	1:1:1234:U:C5	2.85	0.46
2:2:673:A:H2'	2:2:674:G:H8	1.81	0.46
3:3:94:A:OP1	25:V:19:ARG:NE	2.48	0.46
10:E:25:VAL:O	10:E:28:VAL:HG22	2.16	0.46
36:g:47:VAL:HG23	36:g:48:PRO:HD3	1.97	0.46
37:h:173:VAL:HG13	37:h:173:VAL:O	2.16	0.46
38:i:9:LEU:HD12	38:i:9:LEU:C	2.41	0.46
1:1:1922:G:O2'	1:1:1923:U:H5'	2.17	0.45
2:2:544:G:OP1	38:i:59:GLN:HG3	2.16	0.45
5:5:29:G:H2'	5:5:30:U:H6	1.81	0.45
6:6:52:G:C6	6:6:63:G:C6	3.04	0.45
26:W:71:VAL:HG13	26:W:71:VAL:O	2.15	0.45
45:p:89:PRO:HG3	55:z:32:VAL:HG11	1.98	0.45
1:1:1198:U:O2'	20:Q:4:VAL:HG23	2.16	0.45
1:1:1930:G:O2'	1:1:1968:G:O6	2.26	0.45
1:1:2029:G:N1	1:1:2033:A:OP2	2.41	0.45
1:1:2446:G:N2	1:1:2449:U:O2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:868:C:H2'	2:2:869:G:O4'	2.16	0.45
2:2:1145:A:HO2'	2:2:1146:A:P	2.39	0.45
25:V:61:LEU:HD12	25:V:61:LEU:N	2.31	0.45
38:i:23:SER:HB3	38:i:161:LEU:HD13	1.97	0.45
51:v:79:VAL:HG12	51:v:80:GLU:N	2.29	0.45
1:1:1799:G:N7	7:B:178:SER:OG	2.45	0.45
2:2:408:A:N6	2:2:435:A:C6	2.85	0.45
2:2:424:G:H2'	2:2:425:G:C8	2.51	0.45
2:2:501:C:HO2'	2:2:549:C:C2'	2.20	0.45
2:2:620:C:C6	38:i:132:ILE:HG13	2.52	0.45
36:g:111:ILE:HD11	36:g:148:LEU:HB3	1.97	0.45
1:1:498:G:H2'	1:1:499:U:C1'	2.47	0.45
1:1:835:C:C2	1:1:836:G:C8	3.05	0.45
1:1:1093:G:N2	1:1:1097:U:OP2	2.50	0.45
1:1:1590:A:H2'	1:1:1591:A:C8	2.52	0.45
6:6:13:C:H2'	6:6:14:A:H8	1.81	0.45
15:L:90:VAL:HG23	15:L:90:VAL:O	2.17	0.45
22:S:108:SER:OG	22:S:110:ARG:OXT	2.33	0.45
1:1:814:C:H1'	1:1:1225:G:H21	1.82	0.45
1:1:1026:G:OP1	1:1:1134:A:O2'	2.22	0.45
1:1:1199:U:HO2'	1:1:1200:C:P	2.39	0.45
9:D:24:ASN:CG	9:D:27:LEU:HD23	2.41	0.45
14:K:121:GLU:OE2	19:P:65:SER:OG	2.27	0.45
19:P:24:ASP:OD1	19:P:90:GLY:N	2.50	0.45
2:2:1166:G:N1	2:2:1169:A:OP2	2.50	0.45
13:J:100:VAL:HG23	13:J:101:ILE:N	2.32	0.45
14:K:24:VAL:HG13	14:K:33:ALA:HB2	1.98	0.45
44:o:15:HIS:O	44:o:18:ILE:HG22	2.16	0.45
2:2:1124:G:N2	2:2:1125:U:O4	2.40	0.45
6:6:24:G:C5	6:6:25:C:C5	3.04	0.45
8:C:46:ARG:NH1	8:C:85:ALA:O	2.48	0.45
37:h:120:ILE:O	37:h:124:LEU:HG	2.17	0.45
42:m:9:ASP:OD2	42:m:13:ARG:NH1	2.50	0.45
1:1:1176:U:O2'	1:1:1177:G:N7	2.50	0.45
1:1:2298:A:OP1	10:E:71:ARG:NH2	2.47	0.45
2:2:151:A:N7	2:2:171:A:N6	2.65	0.45
5:5:50:G:H2'	5:5:51:A:H8	1.81	0.45
13:J:58:ASN:N	13:J:127:GLY:O	2.44	0.45
17:N:13:ASN:OD1	17:N:13:ASN:N	2.47	0.45
1:1:2831:G:H21	1:1:2884:U:P	2.39	0.45
2:2:40:C:H42	2:2:402:G:H1	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:417:G:H2'	2:2:418:C:O4'	2.17	0.45
2:2:1357:A:H2'	2:2:1358:U:O4'	2.17	0.45
2:2:1369:C:H2'	2:2:1370:G:O4'	2.16	0.45
7:B:39:LYS:O	57:B:401:HOH:O	2.21	0.45
16:M:73:ILE:HG21	16:M:91:TYR:CZ	2.51	0.45
37:h:49:LYS:O	37:h:72:ARG:NH1	2.49	0.45
1:1:1954:G:O2'	1:1:1956:U:O4	2.33	0.45
1:1:2419:U:H4'	32:c:22:THR:HG21	1.99	0.45
2:2:410:G:O3'	2:2:412:A:N6	2.50	0.45
2:2:1302:C:OP1	47:r:13:LYS:NZ	2.45	0.45
1:1:563:A:OP1	20:Q:41:LYS:NZ	2.50	0.44
1:1:1040:A:H2	1:1:1115:G:H22	1.65	0.44
1:1:1359:A:OP2	1:1:1371:G:N2	2.45	0.44
1:1:1737:G:O3'	1:1:1738:G:O4'	2.34	0.44
1:1:2756:U:H4'	1:1:2757:A:OP1	2.17	0.44
1:1:2847:U:H2'	1:1:2848:G:O4'	2.17	0.44
12:G:31:VAL:HG22	12:G:32:PRO:HD3	1.98	0.44
29:Z:24:LEU:HD21	29:Z:54:MET:SD	2.56	0.44
51:v:52:GLU:OE1	51:v:52:GLU:N	2.38	0.44
2:2:90:C:H2'	2:2:91:U:C6	2.52	0.44
2:2:323:U:O2'	57:2:1714:HOH:O	2.21	0.44
2:2:520:A:OP2	46:q:48:ALA:HB1	2.18	0.44
10:E:33:LYS:HZ2	10:E:35:THR:HG1	1.62	0.44
10:E:98:GLU:OE2	30:a:25:ARG:NH2	2.49	0.44
12:G:31:VAL:N	12:G:32:PRO:CD	2.81	0.44
36:g:71:GLY:O	36:g:93:ASN:HA	2.17	0.44
1:1:619:G:P	1:1:620:G:H22	2.40	0.44
1:1:806:C:O2	1:1:2444:G:O2'	2.36	0.44
1:1:1084:A:O2'	1:1:1085:A:O4'	2.35	0.44
2:2:978:A:C2	2:2:1319:A:C4	3.06	0.44
2:2:1304:G:O3'	2:2:1305:G:O4'	2.34	0.44
3:3:106:G:H2'	3:3:107:G:O4'	2.18	0.44
6:6:69:A:H2'	6:6:70:C:C6	2.52	0.44
8:C:39:ASP:OD1	8:C:39:ASP:N	2.50	0.44
9:D:143:LEU:HD23	9:D:146:VAL:HG11	1.99	0.44
10:E:108:VAL:HG13	10:E:109:PRO:HD3	1.98	0.44
17:N:86:ARG:NH1	17:N:117:ASP:O	2.49	0.44
1:1:2119:A:H62	1:1:2167:U:H2'	1.83	0.44
1:1:2331:G:O2'	1:1:2336:A:N1	2.49	0.44
2:2:513:C:H2'	2:2:514:C:C6	2.53	0.44
3:3:29:A:H2'	3:3:30:C:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:176:PRO:O	10:E:177:PHE:C	2.60	0.44
36:g:66:LYS:N	36:g:159:ASP:OD1	2.50	0.44
51:v:78:VAL:HG22	51:v:79:VAL:N	2.33	0.44
1:1:247:G:O6	34:e:12:LYS:NZ	2.38	0.44
1:1:249:C:OP2	1:1:2394:C:O2'	2.24	0.44
1:1:329:G:OP2	24:U:69:ASN:ND2	2.45	0.44
1:1:1320:C:H2'	1:1:1329:U:OP1	2.17	0.44
2:2:1144:G:N2	2:2:1146:A:H62	2.16	0.44
5:5:21:A:C8	5:5:47:U:O2	2.71	0.44
1:1:592:A:C2	34:e:4:ILE:HD11	2.53	0.44
1:1:728:G:H3'	1:1:729:G:C5'	2.47	0.44
1:1:1041:G:O2'	1:1:1042:G:H5'	2.17	0.44
1:1:1065:U:O2'	1:1:1066:U:OP2	2.36	0.44
1:1:1103:A:H2'	1:1:1104:C:O4'	2.18	0.44
1:1:2797:U:N3	57:1:3373:HOH:O	2.34	0.44
2:2:36:C:H4'	46:q:119:VAL:O	2.18	0.44
2:2:624:C:H4'	50:u:10:GLY:HA2	1.98	0.44
2:2:1184:G:C2	2:2:1185:G:C8	3.06	0.44
8:C:21:SER:O	8:C:21:SER:OG	2.35	0.44
10:E:132:VAL:HG12	10:E:152:LEU:HG	2.00	0.44
43:n:26:GLY:N	43:n:62:ASP:OD1	2.36	0.44
46:q:33:VAL:HG13	46:q:33:VAL:O	2.17	0.44
1:1:693:A:O2'	1:1:1353:A:N3	2.38	0.44
1:1:2249:U:N3	1:1:2253:G:OP2	2.43	0.44
2:2:86:G:HO2'	2:2:87:C:C4'	2.31	0.44
2:2:1008:U:H4'	2:2:1009:U:OP1	2.16	0.44
6:6:19:G:H5'	6:6:57:G:H21	1.83	0.44
24:U:51:ALA:O	24:U:52:LEU:HG	2.17	0.44
42:m:10:MET:CG	42:m:27:MET:HE3	2.46	0.44
49:t:33:THR:HG22	49:t:63:ARG:HH11	1.83	0.44
1:1:2113:U:O2'	1:1:2114:A:O5'	2.35	0.44
1:1:2250:G:N2	1:1:2276:G:OP1	2.50	0.44
2:2:323:U:H2'	2:2:324:G:O4'	2.18	0.44
2:2:418:C:H2'	2:2:419:C:C6	2.53	0.44
2:2:1047:G:HO2'	2:2:1215:G:HO2'	1.64	0.44
2:2:1316:G:P	48:s:28:LYS:HZ1	2.41	0.44
3:3:9:G:C2	3:3:10:G:C8	3.06	0.44
5:5:21:A:N7	5:5:47:U:H1'	2.32	0.44
27:X:72:ARG:NH1	27:X:78:TYR:OH	2.51	0.44
28:Y:8:GLU:O	28:Y:8:GLU:HG2	2.17	0.44
1:1:624:C:O2'	1:1:657:U:OP1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:891:G:C6	1:1:892:A:C5	3.06	0.44
1:1:966:G:O4'	1:1:2267:A:N6	2.51	0.44
1:1:2175:C:N3	1:1:2176:A:N6	2.66	0.44
1:1:2261:C:C2	1:1:2262:U:C5	3.06	0.44
2:2:1028:C:O2	2:2:1034:G:N1	2.51	0.44
2:2:1383:C:O2'	2:2:1384:C:P	2.75	0.44
16:M:70:ASP:OD1	16:M:70:ASP:N	2.47	0.44
1:1:308:G:O2'	1:1:329:G:N2	2.51	0.43
1:1:2291:U:O2'	1:1:2374:C:O2	2.35	0.43
2:2:687:A:C2	2:2:704:A:C5	3.06	0.43
5:5:28:C:H2'	5:5:29:G:C8	2.51	0.43
5:5:64:C:H2'	5:5:65:U:C6	2.53	0.43
7:B:210:ALA:O	7:B:214:ARG:HG2	2.18	0.43
20:Q:43:GLY:HA3	21:R:75:VAL:CG1	2.48	0.43
46:q:110:ARG:HE	46:q:110:ARG:HA	1.83	0.43
50:u:69:ASP:OD1	50:u:69:ASP:N	2.51	0.43
1:1:856:G:H2'	1:1:857:G:C8	2.53	0.43
10:E:37:ASN:O	10:E:153:ASP:OD1	2.36	0.43
12:G:121:VAL:HG13	12:G:122:LEU:N	2.34	0.43
39:j:114:VAL:HG11	39:j:140:THR:HG21	2.00	0.43
46:q:63:VAL:HG22	46:q:64:THR:H	1.82	0.43
46:q:98:VAL:HG23	46:q:101:ALA:HB3	2.00	0.43
1:1:859:G:O2'	1:1:916:G:O6	2.30	0.43
1:1:1040:A:N3	1:1:1041:G:C8	2.86	0.43
1:1:2547:A:H2'	1:1:2548:U:C6	2.54	0.43
1:1:2578:G:H21	8:C:130:GLN:NE2	2.16	0.43
2:2:594:U:H2'	2:2:595:A:O4'	2.19	0.43
2:2:1130:A:O2'	43:n:5:GLN:OE1	2.25	0.43
52:w:33:ILE:HG22	52:w:34:THR:O	2.17	0.43
1:1:523:C:H4'	1:1:539:G:N2	2.33	0.43
1:1:941:A:H2'	1:1:942:G:O4'	2.19	0.43
1:1:1534:U:N3	1:1:1536:C:N3	2.67	0.43
1:1:1666:G:H4'	14:K:6:THR:HG23	1.99	0.43
2:2:367:U:HO2'	2:2:368:U:H4'	1.83	0.43
2:2:399:G:H2'	2:2:400:C:C6	2.53	0.43
3:3:44:G:N2	3:3:48:U:C2	2.85	0.43
16:M:66:ARG:NH1	16:M:104:GLU:OE1	2.45	0.43
48:s:46:LEU:HD12	53:x:13:LEU:HD13	1.99	0.43
1:1:886:A:C2'	1:1:887:A:O5'	2.66	0.43
1:1:976:G:O2'	1:1:1155:A:O2'	2.24	0.43
1:1:1433:A:H2'	1:1:1434:A:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1652:A:H2'	1:1:1653:G:O4'	2.19	0.43
1:1:2484:G:OP1	16:M:44:ARG:NH1	2.52	0.43
2:2:227:G:N2	50:u:63:GLN:O	2.41	0.43
2:2:1486:G:H2'	2:2:1487:G:O4'	2.18	0.43
5:5:23:C:H2'	5:5:24:G:C8	2.53	0.43
6:6:25:C:C2	6:6:26:A:C8	3.06	0.43
22:S:27:LYS:O	22:S:71:VAL:HG22	2.19	0.43
55:z:68:THR:OG1	55:z:69:ARG:N	2.51	0.43
1:1:499:U:H2'	1:1:500:G:C5'	2.46	0.43
27:X:41:GLU:OE2	27:X:44:LYS:NZ	2.36	0.43
38:i:57:GLU:O	38:i:61:VAL:HG23	2.18	0.43
55:z:5:LYS:O	55:z:7:ARG:NH1	2.50	0.43
1:1:453:A:N3	1:1:457:A:O2'	2.51	0.43
1:1:1209:U:O2'	1:1:1237:A:N1	2.49	0.43
38:i:123:ILE:HD12	38:i:145:ILE:HD12	2.00	0.43
1:1:1182:G:H2'	1:1:1183:U:O4'	2.18	0.43
1:1:1870:C:O2'	1:1:1871:A:O4'	2.35	0.43
2:2:375:U:C2	2:2:376:G:C8	3.07	0.43
2:2:546:A:OP1	38:i:70:ARG:HG2	2.18	0.43
2:2:958:A:N3	2:2:985:C:O2'	2.46	0.43
14:K:76:VAL:HG22	19:P:73:VAL:HG22	2.01	0.43
47:r:81:MET:O	47:r:92:ARG:NH2	2.44	0.43
1:1:700:G:O2'	1:1:1632:A:N3	2.40	0.43
1:1:1295:C:C2	1:1:1296:G:C8	3.07	0.43
1:1:2576:G:O2'	1:1:2579:C:OP2	2.33	0.43
1:1:2657:A:O2'	11:F:160:LYS:NZ	2.49	0.43
2:2:779:C:H2'	2:2:780:A:O4'	2.18	0.43
2:2:918:A:H2'	2:2:919:A:O4'	2.18	0.43
2:2:1031:C:O3'	2:2:1032:G:N2	2.52	0.43
2:2:1159:U:O4'	2:2:1182:G:N2	2.52	0.43
2:2:1494:G:H2'	2:2:1494:G:N3	2.33	0.43
4:4:14:G:H4'	4:4:14:G:OP1	2.18	0.43
5:5:68:U:H2'	5:5:69:G:C8	2.53	0.43
47:r:2:ALA:O	47:r:9:ILE:N	2.52	0.43
1:1:2193:G:O2'	1:1:2194:U:OP1	2.33	0.43
1:1:2585:U:H3	5:5:76:A:HO3'	1.64	0.43
1:1:2596:U:O2'	7:B:241:GLY:O	2.37	0.43
3:3:30:C:H1'	3:3:57:A:H61	1.84	0.43
6:6:3:G:H2'	6:6:4:U:C6	2.54	0.43
42:m:11:LEU:HD22	42:m:75:ILE:HD11	2.00	0.43
43:n:12:ARG:O	43:n:13:LYS:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:o:82:LYS:O	44:o:85:ASP:OD1	2.36	0.43
47:r:66:GLU:O	47:r:70:ARG:HG2	2.19	0.43
51:v:63:GLU:OE1	51:v:64:CYS:N	2.52	0.43
1:1:2100:G:C6	1:1:2190:G:C6	3.07	0.42
1:1:2555:U:C6	6:6:74:C:N4	2.87	0.42
5:5:64:C:H2'	5:5:65:U:H6	1.84	0.42
21:R:66:HIS:ND1	21:R:94:THR:HG22	2.33	0.42
22:S:65:ASP:OD1	22:S:66:ILE:N	2.52	0.42
38:i:4:TYR:CE1	38:i:11:LEU:HD11	2.54	0.42
49:t:44:ALA:O	49:t:47:LYS:NZ	2.46	0.42
54:y:27:MET:O	54:y:30:THR:HG22	2.19	0.42
55:z:70:LEU:HD23	55:z:70:LEU:H	1.83	0.42
1:1:886:A:H2'	1:1:887:A:O4'	2.20	0.42
1:1:1040:A:C2	1:1:1041:G:C8	3.06	0.42
2:2:1071:C:H2'	2:2:1072:G:H8	1.84	0.42
6:6:26:A:H2'	6:6:26:A:N3	2.33	0.42
6:6:66:A:C6	6:6:67:U:C4	3.08	0.42
30:a:11:GLU:OE1	30:a:12:ILE:N	2.52	0.42
40:k:90:MET:HE1	52:w:23:TYR:CZ	2.54	0.42
42:m:54:ASP:OD2	42:m:54:ASP:N	2.52	0.42
1:1:26:G:C2'	1:1:27:G:O4'	2.68	0.42
1:1:281:C:N4	1:1:282:A:H62	2.17	0.42
1:1:428:A:C2'	1:1:429:A:O5'	2.67	0.42
1:1:1202:G:H21	15:L:4:ASN:CB	2.29	0.42
1:1:1998:A:O2'	1:1:2724:U:O2'	2.30	0.42
14:K:80:ASP:OD2	19:P:62:ARG:NH1	2.42	0.42
40:k:88:MET:HE1	52:w:61:ARG:HG3	2.01	0.42
1:1:26:G:H2'	1:1:27:G:O4'	2.19	0.42
1:1:1936:A:C8	1:1:1940:U:C2	3.08	0.42
1:1:2683:C:O2	14:K:70:ARG:NH2	2.48	0.42
2:2:501:C:H2'	2:2:502:A:H8	1.84	0.42
2:2:544:G:O5'	38:i:59:GLN:NE2	2.52	0.42
2:2:1108:G:N3	2:2:1108:G:H2'	2.35	0.42
38:i:15:GLU:HG3	38:i:60:LYS:HA	2.00	0.42
38:i:27:ALA:HB3	38:i:30:THR:HG22	2.01	0.42
39:j:78:ASN:OD1	39:j:79:GLY:N	2.48	0.42
1:1:744:U:H2'	1:1:745:1MG:O4'	2.19	0.42
1:1:2412:A:H2'	1:1:2413:G:O4'	2.19	0.42
1:1:2899:A:C2	1:1:2900:A:C5	3.07	0.42
2:2:130:A:N6	2:2:233:C:O2	2.52	0.42
2:2:320:A:H2'	2:2:321:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:546:A:H4'	2:2:548:G:H4'	2.01	0.42
2:2:684:U:O2	45:p:41:ALA:HB3	2.20	0.42
2:2:714:G:H2'	2:2:715:A:C8	2.54	0.42
2:2:746:A:C2'	2:2:747:A:O5'	2.67	0.42
6:6:13:C:H6	6:6:13:C:OP2	2.03	0.42
6:6:75:C:H2'	6:6:76:A:N9	2.34	0.42
19:P:47:VAL:HG11	19:P:50:ILE:HD11	2.02	0.42
24:U:81:ASP:OD2	24:U:98:SER:OG	2.22	0.42
1:1:249:C:P	1:1:2394:C:HO2'	2.41	0.42
1:1:1050:A:C2'	1:1:1051:G:O5'	2.67	0.42
1:1:1168:G:O2'	57:1:3302:HOH:O	2.03	0.42
1:1:1360:G:N7	1:1:1361:G:C8	2.88	0.42
1:1:2181:U:H2'	1:1:2182:U:O4'	2.20	0.42
1:1:2756:U:C4	1:1:2759:G:O6	2.73	0.42
2:2:142:G:H2'	2:2:143:A:O4'	2.19	0.42
2:2:145:G:OP2	57:2:1716:HOH:O	2.21	0.42
2:2:254:G:P	51:v:68:SER:HG	2.42	0.42
2:2:530:G:O6	4:4:21:U:H1'	2.20	0.42
2:2:604:G:H2'	2:2:605:U:O4'	2.19	0.42
2:2:721:G:H4'	2:2:722:G:O4'	2.20	0.42
2:2:991:U:HO2'	2:2:992:U:P	2.43	0.42
12:G:7:ASP:OD2	12:G:8:LYS:N	2.52	0.42
54:y:60:ARG:O	54:y:64:LYS:HG2	2.20	0.42
1:1:52:A:OP2	1:1:119:A:N6	2.47	0.42
1:1:210:C:OP1	33:d:29:GLN:NE2	2.51	0.42
1:1:1037:G:H2'	1:1:1038:G:H8	1.85	0.42
1:1:1416:G:O2'	1:1:1417:C:P	2.77	0.42
1:1:2031:A:OP2	57:1:3338:HOH:O	2.21	0.42
1:1:2467:C:O2	16:M:123:LYS:NZ	2.49	0.42
1:1:2792:A:H3'	1:1:2793:C:H5''	2.02	0.42
2:2:40:C:C2	2:2:41:G:C8	3.08	0.42
2:2:206:C:N4	57:2:1773:HOH:O	2.52	0.42
2:2:1130:A:C2	2:2:1131:G:C8	3.07	0.42
2:2:1157:A:C2	2:2:1181:G:C4	3.07	0.42
2:2:1397:C:OP2	39:j:29:ARG:NH2	2.53	0.42
10:E:108:VAL:HA	10:E:111:ILE:HD12	2.01	0.42
10:E:117:LEU:HD12	10:E:176:PRO:HD2	2.01	0.42
12:G:134:VAL:HG23	12:G:138:VAL:HG13	2.02	0.42
38:i:102:VAL:CG1	38:i:114:ALA:HB1	2.50	0.42
44:o:66:GLU:HB3	48:s:99:ALA:HB2	2.02	0.42
49:t:47:LYS:O	49:t:53:ARG:NH2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:307:G:N1	1:1:310:A:OP2	2.34	0.42
1:1:635:C:H2'	1:1:636:G:O4'	2.20	0.42
1:1:1235:G:H2'	1:1:1236:G:N9	2.35	0.42
1:1:1542:U:H2'	1:1:1543:G:O4'	2.19	0.42
1:1:2111:U:OP2	1:1:2145:C:N4	2.53	0.42
1:1:2838:G:C4	1:1:2839:G:C8	3.07	0.42
2:2:123:U:C2	2:2:124:C:C5	3.08	0.42
2:2:435:A:H2'	2:2:436:C:C6	2.55	0.42
2:2:438:U:O2'	2:2:440:C:N4	2.51	0.42
2:2:747:A:H2'	2:2:748:G:C8	2.55	0.42
3:3:37:C:O2	18:O:100:HIS:NE2	2.45	0.42
6:6:72:C:H2'	6:6:73:A:C8	2.55	0.42
11:F:132:VAL:O	11:F:132:VAL:HG23	2.20	0.42
15:L:82:LEU:HD13	15:L:90:VAL:HG11	2.02	0.42
30:a:11:GLU:OE1	30:a:24:ILE:N	2.53	0.42
37:h:70:THR:C	37:h:106:VAL:HG12	2.45	0.42
46:q:87:VAL:O	46:q:87:VAL:HG23	2.19	0.42
1:1:497:A:H2'	1:1:498:G:C8	2.55	0.42
1:1:1266:G:O2'	1:1:1267:U:OP2	2.36	0.42
2:2:391:G:H2'	2:2:392:C:O4'	2.20	0.42
2:2:436:C:O2	38:i:154:ARG:NH1	2.53	0.42
2:2:1494:G:C2	2:2:1495:U:C5	3.08	0.42
10:E:13:VAL:HG23	10:E:14:LYS:N	2.35	0.42
21:R:74:ILE:HD12	21:R:74:ILE:H	1.85	0.42
38:i:11:LEU:HD13	38:i:63:ARG:HE	1.85	0.42
47:r:64:VAL:HG12	47:r:65:VAL:N	2.35	0.42
1:1:319:G:H2'	1:1:320:A:O4'	2.20	0.42
1:1:335:C:O2	24:U:68:SER:OG	2.37	0.42
1:1:2602:A:H4'	1:1:2603:G:H5'	2.02	0.42
1:1:2820:A:N6	8:C:197:THR:O	2.53	0.42
2:2:539:A:H2'	2:2:540:G:O4'	2.19	0.42
2:2:662:U:H2'	2:2:663:A:C8	2.55	0.42
5:5:25:C:H2'	5:5:26:A:O4'	2.20	0.42
5:5:49:G:H2'	5:5:50:G:C8	2.55	0.42
38:i:7:PRO:O	38:i:11:LEU:HG	2.20	0.42
39:j:90:THR:HG22	39:j:90:THR:O	2.18	0.42
1:1:645:C:H2'	1:1:647:G:N7	2.34	0.41
1:1:1079:C:C2	1:1:1080:A:C8	3.08	0.41
1:1:2140:G:N1	1:1:2152:G:N7	2.68	0.41
2:2:381:C:H2'	2:2:382:A:O4'	2.20	0.41
2:2:401:C:OP2	38:i:70:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:982:U:H4'	2:2:983:A:O4'	2.20	0.41
2:2:1125:U:C2	2:2:1127:G:C8	3.08	0.41
2:2:1493:A:O2'	2:2:1494:G:P	2.73	0.41
43:n:106:ARG:NH1	43:n:107:ASP:O	2.50	0.41
1:1:196:A:H61	1:1:831:G:H21	1.67	0.41
1:1:2420:C:OP1	34:e:34:THR:HG23	2.19	0.41
1:1:2820:A:N1	17:N:4:ARG:NH2	2.68	0.41
2:2:73:C:C2'	2:2:74:A:H5'	2.50	0.41
2:2:747:A:H2'	2:2:748:G:O4'	2.20	0.41
3:3:39:A:H2'	3:3:40:U:C6	2.55	0.41
6:6:50:G:H2'	6:6:51:C:C6	2.56	0.41
10:E:66:LEU:HD23	10:E:67:ILE:C	2.45	0.41
13:J:57:LEU:HD23	13:J:57:LEU:H	1.85	0.41
25:V:6:ALA:HB2	25:V:42:LEU:CD2	2.50	0.41
53:x:64:ASP:OD1	53:x:64:ASP:N	2.48	0.41
1:1:265:A:O2'	1:1:428:A:N6	2.53	0.41
1:1:2821:A:H2'	1:1:2822:G:O4'	2.20	0.41
1:1:2889:C:H2'	1:1:2890:G:O4'	2.21	0.41
2:2:20:U:H2'	2:2:21:G:O4'	2.20	0.41
2:2:54:C:H2'	2:2:352:C:H41	1.84	0.41
2:2:422:C:H1'	2:2:423:G:N2	2.36	0.41
2:2:619:U:H5'	2:2:620:C:P	2.60	0.41
2:2:1141:C:O2'	2:2:1142:G:P	2.79	0.41
2:2:1347:G:O2'	2:2:1373:G:O6	2.31	0.41
2:2:1370:G:C2	2:2:1371:G:C8	3.09	0.41
5:5:7:G:C6	5:5:67:G:N1	2.88	0.41
23:T:4:GLU:OE2	28:Y:23:ARG:NH1	2.54	0.41
49:t:55:GLY:O	49:t:59:MET:HG3	2.20	0.41
1:1:301:G:C4	1:1:302:C:C5	3.09	0.41
1:1:998:C:OP1	20:Q:84:LYS:NZ	2.46	0.41
1:1:1030:C:O2	35:f:37:GLN:NE2	2.54	0.41
1:1:1039:A:C6	1:1:1040:A:C5	3.08	0.41
1:1:1395:A:O2'	1:1:1397:U:C6	2.73	0.41
2:2:5:U:O2	2:2:5:U:O4'	2.36	0.41
2:2:747:A:C2'	2:2:748:G:O4'	2.68	0.41
2:2:1126:U:O4	44:o:9:ARG:NH1	2.53	0.41
5:5:25:C:C2	5:5:26:A:C8	3.09	0.41
5:5:30:U:H2'	5:5:31:C:C6	2.55	0.41
26:W:33:ALA:N	26:W:64:ASP:OD1	2.53	0.41
43:n:12:ARG:HG3	43:n:13:LYS:H	1.85	0.41
46:q:110:ARG:CZ	46:q:112:GLN:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:184:C:O2'	1:1:217:A:N3	2.50	0.41
1:1:444:C:O2'	1:1:445:C:H5'	2.20	0.41
1:1:1614:A:N6	22:S:92:ARG:O	2.50	0.41
1:1:1869:G:N2	1:1:1871:A:C8	2.88	0.41
2:2:435:A:C5	2:2:436:C:C4	3.08	0.41
2:2:1027:C:C4'	2:2:1028:C:OP1	2.68	0.41
2:2:1356:G:H2'	2:2:1357:A:C8	2.54	0.41
10:E:163:ASP:OD1	10:E:164:GLU:N	2.53	0.41
44:o:10:LEU:HD22	44:o:10:LEU:N	2.35	0.41
52:w:33:ILE:HD13	52:w:39:ILE:HA	2.01	0.41
1:1:1202:G:N2	1:1:1242:U:H3	2.16	0.41
1:1:1990:C:H2'	1:1:1991:U:C1'	2.51	0.41
1:1:2286:G:C5'	1:1:2287:A:O4'	2.69	0.41
2:2:1221:G:H4'	53:x:77:THR:HG21	2.01	0.41
2:2:1251:A:H2'	2:2:1252:A:O4'	2.21	0.41
5:5:49:G:H2'	5:5:50:G:H8	1.86	0.41
17:N:24:MET:HB3	17:N:44:LEU:HD13	2.03	0.41
28:Y:21:LEU:CD1	28:Y:46:VAL:HG23	2.50	0.41
37:h:149:ILE:HD12	37:h:202:ILE:CD1	2.50	0.41
1:1:498:G:C5	1:1:499:U:C4	3.08	0.41
1:1:565:C:P	21:R:80:ARG:H	2.44	0.41
1:1:685:A:C8	1:1:773:U:C4	3.09	0.41
1:1:1874:C:H2'	1:1:1875:G:O4'	2.21	0.41
2:2:429:U:OP1	38:i:9:LEU:HD11	2.20	0.41
2:2:502:A:H61	2:2:543:U:H3	1.68	0.41
2:2:628:G:H2'	2:2:629:A:C8	2.56	0.41
2:2:653:U:OP1	42:m:56:LYS:NZ	2.45	0.41
2:2:1008:U:O3'	2:2:1009:U:O4'	2.38	0.41
4:4:15:C:H2'	4:4:16:C:C6	2.56	0.41
6:6:74:C:O2'	6:6:75:C:P	2.79	0.41
15:L:77:ILE:HD11	15:L:95:LEU:HD13	2.02	0.41
17:N:37:THR:HG22	17:N:39:PRO:HD2	2.02	0.41
36:g:47:VAL:CG2	36:g:48:PRO:HD3	2.51	0.41
41:l:93:PRO:O	41:l:96:ARG:HG2	2.20	0.41
46:q:111:LYS:O	46:q:114:ARG:NH1	2.54	0.41
51:v:77:ARG:NH1	51:v:78:VAL:O	2.54	0.41
1:1:645:C:H2'	1:1:647:G:C8	2.56	0.41
1:1:1224:U:OP2	21:R:68:ARG:NH1	2.54	0.41
1:1:1589:U:O2'	1:1:1590:A:H8	2.03	0.41
1:1:1770:G:C6	1:1:1983:G:C6	3.09	0.41
1:1:2328:A:H2'	1:1:2329:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2586:U:H2'	1:1:2587:A:O4'	2.21	0.41
2:2:544:G:N2	2:2:545:C:H1'	2.35	0.41
2:2:932:C:O3'	41:l:4:ARG:NH1	2.54	0.41
2:2:979:C:O2	2:2:979:C:H2'	2.20	0.41
12:G:135:HIS:HB3	12:G:138:VAL:HG12	2.03	0.41
30:a:51:VAL:HG23	30:a:52:ALA:N	2.36	0.41
1:1:6:A:N3	13:J:135:GLN:NE2	2.66	0.41
1:1:497:A:C3'	1:1:498:G:C8	3.04	0.41
1:1:1038:G:H22	1:1:1116:G:H22	1.67	0.41
1:1:1223:G:C4	1:1:1225:G:OP2	2.74	0.41
1:1:2028:U:H2'	1:1:2029:G:O4'	2.21	0.41
1:1:2297:A:O2'	57:1:3339:HOH:O	2.22	0.41
1:1:2467:C:H2'	1:1:2468:A:O4'	2.21	0.41
1:1:2496:C:H2'	1:1:2497:A:O4'	2.21	0.41
1:1:2799:A:O2'	1:1:2800:A:H5''	2.21	0.41
2:2:6:G:HO2'	2:2:7:A:C5'	2.34	0.41
2:2:246:A:C2	2:2:282:A:C5	3.08	0.41
2:2:371:A:O2'	2:2:372:C:O4'	2.38	0.41
2:2:413:G:H4'	2:2:428:G:H21	1.86	0.41
2:2:502:A:O2'	2:2:550:G:H4'	2.21	0.41
2:2:515:G:C5	2:2:516:PSU:C2	3.09	0.41
2:2:972:C:OP2	44:o:59:LYS:NZ	2.47	0.41
2:2:1120:C:H2'	2:2:1121:U:C6	2.55	0.41
2:2:1181:G:H1'	2:2:1182:G:C4	2.55	0.41
2:2:1317:C:OP1	48:s:56:SER:OG	2.34	0.41
3:3:66:A:H61	3:3:107:G:H2'	1.86	0.41
3:3:100:G:N1	3:3:101:A:C5	2.89	0.41
5:5:10:G:O6	5:5:45:G:N2	2.39	0.41
6:6:16:C:N3	6:6:60:C:H1'	2.36	0.41
8:C:24:VAL:HG12	8:C:178:VAL:HG21	2.02	0.41
12:G:137:GLU:OE2	12:G:137:GLU:N	2.54	0.41
37:h:15:VAL:HG23	37:h:16:LYS:N	2.36	0.41
50:u:5:ARG:NH2	50:u:23:ASP:O	2.53	0.41
1:1:487:C:H42	1:1:492:A:N6	2.15	0.41
1:1:669:G:H2'	1:1:670:A:N7	2.36	0.41
1:1:1005:C:C2	1:1:1006:C:C5	3.08	0.41
1:1:2899:A:N3	1:1:2900:A:N7	2.69	0.41
2:2:1372:U:H2'	2:2:1373:G:O4'	2.21	0.41
2:2:1388:C:C2	2:2:1389:C:C5	3.08	0.41
22:S:23:LEU:HD11	31:b:24:ALA:HB2	2.03	0.41
51:v:12:VAL:O	51:v:56:GLY:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1577:C:H2'	1:1:1578:U:C1'	2.52	0.40
1:1:1590:A:H2'	1:1:1591:A:H8	1.86	0.40
1:1:1736:U:H2'	1:1:1737:G:O4'	2.21	0.40
1:1:2469:A:H2'	1:1:2470:G:O4'	2.21	0.40
2:2:374:A:C5	2:2:375:U:C5	3.09	0.40
2:2:842:U:O3'	2:2:844:G:N2	2.54	0.40
10:E:66:LEU:HD23	10:E:66:LEU:C	2.47	0.40
19:P:88:ARG:NH2	19:P:110:ILE:O	2.46	0.40
1:1:25:U:C2'	1:1:26:G:O5'	2.69	0.40
1:1:581:C:H2'	1:1:582:A:H8	1.85	0.40
1:1:886:A:C6	1:1:891:G:C5	3.09	0.40
1:1:1046:A:H3'	1:1:1047:G:H5'	2.03	0.40
1:1:1344:U:H3'	1:1:1345:C:H5'	2.03	0.40
1:1:1654:A:O2'	8:C:118:PHE:O	2.32	0.40
1:1:1882:U:N3	1:1:1883:U:C5	2.89	0.40
1:1:2717:C:H2'	1:1:2718:G:O4'	2.22	0.40
1:1:2727:A:O2'	1:1:2728:U:H5'	2.21	0.40
2:2:37:U:O2'	2:2:547:A:N1	2.51	0.40
2:2:39:G:H2'	2:2:40:C:H6	1.85	0.40
2:2:402:G:C2	2:2:403:C:N4	2.88	0.40
2:2:475:C:H2'	2:2:476:U:O4'	2.21	0.40
2:2:746:A:HO2'	2:2:747:A:C5'	2.32	0.40
2:2:751:U:H2'	2:2:752:G:O4'	2.21	0.40
2:2:1081:A:C2	2:2:1082:A:C8	3.09	0.40
2:2:1279:G:O2'	2:2:1282:C:N4	2.53	0.40
8:C:178:VAL:N	8:C:188:LEU:O	2.50	0.40
53:x:27:ASP:OD2	53:x:29:LYS:NZ	2.52	0.40
1:1:1587:G:N3	1:1:1588:G:C8	2.90	0.40
1:1:1775:U:O4	1:1:1789:A:H2	2.04	0.40
1:1:2025:C:H2'	1:1:2026:U:C6	2.56	0.40
1:1:2438:U:O2'	1:1:2440:C:OP1	2.33	0.40
1:1:2900:A:C6	1:1:2901:C:C5	3.09	0.40
2:2:404:G:C4	2:2:405:U:C5	3.09	0.40
2:2:1431:A:H2'	2:2:1432:G:O4'	2.22	0.40
6:6:8:U:O2'	6:6:9:A:OP2	2.34	0.40
11:F:9:VAL:O	11:F:49:THR:OG1	2.20	0.40
21:R:55:ASP:OD1	21:R:56:GLY:N	2.52	0.40
27:X:71:LEU:HD23	27:X:76:GLU:O	2.20	0.40
38:i:9:LEU:HD13	38:i:32:CYS:CB	2.51	0.40
1:1:82:U:H2'	1:1:83:A:O4'	2.21	0.40
1:1:1266:G:OP2	31:b:17:ARG:NH2	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1378:A:O2'	1:1:1380:G:N7	2.49	0.40
1:1:1586:A:C2	1:1:1587:G:H1'	2.56	0.40
1:1:2244:U:H2'	1:1:2245:U:O4'	2.22	0.40
2:2:74:A:C4	2:2:75:G:C8	3.09	0.40
2:2:337:G:C2	2:2:338:A:C5	3.09	0.40
2:2:444:G:H2'	2:2:445:G:O4'	2.21	0.40
2:2:1160:G:C6	2:2:1161:C:C4	3.09	0.40
2:2:1238:A:H5'	2:2:1336:C:H41	1.85	0.40
6:6:38:A:H8	6:6:38:A:H5''	1.87	0.40
7:B:158:ALA:HB1	7:B:197:ASN:O	2.21	0.40
10:E:37:ASN:OD1	10:E:38:MET:N	2.55	0.40
38:i:159:LEU:HD13	38:i:175:ALA:CB	2.51	0.40
46:q:48:ALA:HB3	46:q:50:ARG:HE	1.86	0.40
1:1:83:A:O2'	1:1:103:A:N6	2.53	0.40
2:2:179:A:H2'	2:2:180:U:O4'	2.21	0.40
2:2:469:C:C2	2:2:470:C:C6	3.09	0.40
13:J:19:ASP:CG	13:J:21:THR:HG22	2.47	0.40
39:j:137:VAL:HA	39:j:140:THR:HG22	2.03	0.40
40:k:86:ARG:NH1	52:w:64:TYR:O	2.55	0.40
47:r:77:ILE:HG22	47:r:81:MET:HE3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	B	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
8	C	207/209 (99%)	194 (94%)	13 (6%)	0	100	100
9	D	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
10	E	175/179 (98%)	166 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	F	173/177 (98%)	162 (94%)	11 (6%)	0	100	100
12	G	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
13	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
14	K	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
15	L	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
16	M	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	N	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
18	O	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
19	P	112/115 (97%)	111 (99%)	1 (1%)	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%)	106 (98%)	2 (2%)	0	100	100
23	T	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
24	U	101/104 (97%)	95 (94%)	6 (6%)	0	100	100
25	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
26	W	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
27	X	75/78 (96%)	75 (100%)	0	0	100	100
28	Y	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
29	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
30	a	64/70 (91%)	61 (95%)	3 (5%)	0	100	100
31	b	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
32	c	50/55 (91%)	50 (100%)	0	0	100	100
33	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
34	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
35	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
36	g	223/241 (92%)	211 (95%)	12 (5%)	0	100	100
37	h	206/233 (88%)	199 (97%)	7 (3%)	0	100	100
38	i	203/206 (98%)	195 (96%)	8 (4%)	0	100	100
39	j	154/167 (92%)	145 (94%)	9 (6%)	0	100	100
40	k	102/135 (76%)	97 (95%)	5 (5%)	0	100	100
41	l	149/178 (84%)	142 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	m	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
43	n	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
44	o	97/103 (94%)	91 (94%)	6 (6%)	0	100	100
45	p	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
46	q	120/124 (97%)	110 (92%)	10 (8%)	0	100	100
47	r	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
48	s	98/101 (97%)	98 (100%)	0	0	100	100
49	t	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
50	u	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
51	v	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
52	w	64/75 (85%)	64 (100%)	0	0	100	100
53	x	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
54	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
55	z	68/71 (96%)	68 (100%)	0	0	100	100
All	All	5616/5911 (95%)	5403 (96%)	213 (4%)	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	
7	B	216/218 (99%)	208 (96%)	8 (4%)	30	64
8	C	164/164 (100%)	160 (98%)	4 (2%)	43	73
9	D	165/165 (100%)	161 (98%)	4 (2%)	43	73
10	E	148/150 (99%)	143 (97%)	5 (3%)	32	66
11	F	136/138 (99%)	127 (93%)	9 (7%)	15	46
12	G	114/114 (100%)	109 (96%)	5 (4%)	25	60
13	J	116/116 (100%)	113 (97%)	3 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	K	104/104 (100%)	103 (99%)	1 (1%)	68	84
15	L	103/103 (100%)	100 (97%)	3 (3%)	37	70
16	M	109/109 (100%)	107 (98%)	2 (2%)	51	77
17	N	99/103 (96%)	97 (98%)	2 (2%)	48	76
18	O	86/87 (99%)	84 (98%)	2 (2%)	44	74
19	P	99/100 (99%)	97 (98%)	2 (2%)	48	76
20	Q	89/90 (99%)	88 (99%)	1 (1%)	65	83
21	R	84/84 (100%)	83 (99%)	1 (1%)	63	82
22	S	93/93 (100%)	91 (98%)	2 (2%)	45	74
23	T	81/84 (96%)	80 (99%)	1 (1%)	63	82
24	U	84/85 (99%)	81 (96%)	3 (4%)	31	65
25	V	78/78 (100%)	77 (99%)	1 (1%)	61	81
26	W	62/62 (100%)	61 (98%)	1 (2%)	55	79
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%)	56 (95%)	3 (5%)	21	55
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%)	48 (94%)	3 (6%)	18	50
35	f	34/34 (100%)	33 (97%)	1 (3%)	37	70
36	g	187/199 (94%)	184 (98%)	3 (2%)	55	79
37	h	171/190 (90%)	163 (95%)	8 (5%)	23	58
38	i	172/173 (99%)	166 (96%)	6 (4%)	32	65
39	j	119/126 (94%)	118 (99%)	1 (1%)	73	86
40	k	91/116 (78%)	88 (97%)	3 (3%)	33	67
41	l	124/146 (85%)	122 (98%)	2 (2%)	55	79
42	m	104/105 (99%)	102 (98%)	2 (2%)	50	76
43	n	105/107 (98%)	104 (99%)	1 (1%)	68	84
44	o	86/90 (96%)	80 (93%)	6 (7%)	14	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	p	90/99 (91%)	85 (94%)	5 (6%)	19	52
46	q	102/103 (99%)	99 (97%)	3 (3%)	37	70
47	r	94/96 (98%)	93 (99%)	1 (1%)	65	83
48	s	83/84 (99%)	82 (99%)	1 (1%)	63	82
49	t	76/77 (99%)	76 (100%)	0	100	100
50	u	65/65 (100%)	61 (94%)	4 (6%)	16	49
51	v	74/78 (95%)	73 (99%)	1 (1%)	59	80
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	4672/4827 (97%)	4558 (98%)	114 (2%)	43	73

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	B	129	THR
7	B	132	MET
7	B	191	THR
7	B	195	VAL
7	B	204	VAL
7	B	205	LEU
7	B	219	THR
7	B	250	VAL
8	C	73	VAL
8	C	151	THR
8	C	177	VAL
8	C	180	VAL
9	D	107	SER
9	D	120	VAL
9	D	169	VAL
9	D	199	MET
10	E	31	VAL
10	E	108	VAL
10	E	147	ASP
10	E	153	ASP
10	E	157	THR
11	F	10	VAL

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Mol	Chain	Res	Type
11	F	11	VAL
11	F	72	LEU
11	F	89	LEU
11	F	117	LEU
11	F	127	THR
11	F	133	LEU
11	F	140	VAL
11	F	171	THR
12	G	19	VAL
12	G	94	ILE
12	G	115	VAL
12	G	117	LEU
12	G	139	PHE
13	J	70	THR
13	J	81	ILE
13	J	86	GLN
14	K	98	ARG
15	L	85	VAL
15	L	121	THR
15	L	127	VAL
16	M	7	THR
16	M	63	ILE
17	N	28	LEU
17	N	57	THR
18	O	28	VAL
18	O	36	TYR
19	P	30	VAL
19	P	80	VAL
20	Q	18	LEU
21	R	102	SER
22	S	7	HIS
22	S	96	ILE
23	T	61	LEU
24	U	13	VAL
24	U	36	VAL
24	U	52	LEU
25	V	46	LYS
26	W	32	LEU
30	a	18	CYS
30	a	36	VAL
30	a	53	THR
34	e	31	HIS

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Mol	Chain	Res	Type
34	e	33	LEU
34	e	34	THR
35	f	4	ARG
36	g	49	MET
36	g	125	THR
36	g	205	ASP
37	h	21	THR
37	h	47	LEU
37	h	52	VAL
37	h	56	VAL
37	h	76	VAL
37	h	106	VAL
37	h	178	LEU
37	h	186	THR
38	i	18	ASP
38	i	86	THR
38	i	95	GLU
38	i	116	GLN
38	i	143	VAL
38	i	148	LYS
39	j	16	ILE
40	k	10	VAL
40	k	63	ASN
40	k	103	VAL
41	l	72	THR
41	l	113	ASP
42	m	18	GLN
42	m	126	ILE
43	n	63	LEU
44	o	11	LYS
44	o	15	HIS
44	o	17	LEU
44	o	18	ILE
44	o	64	GLN
44	o	66	GLU
45	p	16	VAL
45	p	26	SER
45	p	35	THR
45	p	64	GLN
45	p	74	VAL
46	q	74	LEU
46	q	102	LEU

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Mol	Chain	Res	Type
46	q	107	VAL
47	r	49	SER
48	s	51	LEU
50	u	1	MET
50	u	8	ARG
50	u	52	LEU
50	u	57	ILE
51	v	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
7	B	163	GLN
8	C	134	HIS
8	C	173	GLN
9	D	92	HIS
9	D	136	GLN
9	D	165	HIS
11	F	30	ASN
12	G	66	ASN
15	L	35	HIS
16	M	88	ASN
17	N	11	ASN
17	N	31	HIS
17	N	73	ASN
18	O	29	HIS
18	O	61	GLN
21	R	12	HIS
22	S	9	HIS
24	U	53	ASN
25	V	24	ASN
26	W	3	HIS
26	W	12	ASN
35	f	33	HIS
36	g	168	HIS
36	g	227	GLN
38	i	36	GLN
38	i	40	GLN
38	i	54	GLN
38	i	136	GLN
38	i	152	GLN
39	j	148	ASN

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Mol	Chain	Res	Type
41	l	68	ASN
43	n	4	ASN
43	n	37	GLN
44	o	70	HIS
44	o	99	GLN
45	p	38	GLN
45	p	81	ASN
48	s	66	GLN
49	t	40	GLN
50	u	63	GLN
50	u	79	ASN
53	x	53	ASN
54	y	61	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2904 (99%)	426 (14%)	13 (0%)
2	2	1538/1540 (99%)	251 (16%)	7 (0%)
3	3	119/120 (99%)	18 (15%)	0
4	4	11/18 (61%)	6 (54%)	1 (9%)
5	5	76/77 (98%)	33 (43%)	7 (9%)
6	6	75/76 (98%)	31 (41%)	3 (4%)
All	All	4721/4735 (99%)	765 (16%)	31 (0%)

All (765) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	26	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	51	G
1	1	71	A
1	1	74	A
1	1	75	G
1	1	85	G
1	1	102	U
1	1	118	A
1	1	120	U

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Mol	Chain	Res	Type
1	1	131	A
1	1	136	G
1	1	137	U
1	1	139	U
1	1	142	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A
1	1	222	A
1	1	228	C
1	1	248	G
1	1	265	A
1	1	266	G
1	1	273	G
1	1	275	C
1	1	279	A
1	1	285	G
1	1	311	A
1	1	329	G
1	1	330	A
1	1	352	A
1	1	353	C
1	1	361	G
1	1	371	A
1	1	372	G
1	1	386	G
1	1	396	G
1	1	404	A
1	1	405	U
1	1	406	G
1	1	411	G
1	1	424	G
1	1	429	A
1	1	435	C
1	1	451	U
1	1	456	C
1	1	457	A
1	1	481	G
1	1	490	C

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Mol	Chain	Res	Type
1	1	491	G
1	1	492	A
1	1	500	G
1	1	501	A
1	1	505	A
1	1	508	A
1	1	509	C
1	1	510	C
1	1	531	C
1	1	532	A
1	1	537	G
1	1	538	A
1	1	539	G
1	1	541	A
1	1	543	G
1	1	544	C
1	1	545	U
1	1	546	U
1	1	547	A
1	1	549	G
1	1	563	A
1	1	573	U
1	1	574	A
1	1	575	A
1	1	603	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	627	A
1	1	637	A
1	1	645	C
1	1	646	U
1	1	647	G
1	1	654	A
1	1	655	A
1	1	686	U
1	1	709	U
1	1	710	U
1	1	717	C
1	1	730	A
1	1	747	5MU
1	1	775	G

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Mol	Chain	Res	Type
1	1	776	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	877	A
1	1	878	A
1	1	883	G
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	910	A
1	1	914	G
1	1	915	C
1	1	931	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G
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	1012	U
1	1	1013	C
1	1	1026	G
1	1	1027	A
1	1	1028	A

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Mol	Chain	Res	Type
1	1	1029	A
1	1	1033	U
1	1	1034	G
1	1	1039	A
1	1	1041	G
1	1	1042	G
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1051	G
1	1	1053	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1087	G
1	1	1088	A
1	1	1096	A
1	1	1101	U
1	1	1111	A
1	1	1112	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
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	1179	G
1	1	1198	U
1	1	1199	U
1	1	1200	C
1	1	1203	U
1	1	1204	A
1	1	1212	G
1	1	1238	G

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Mol	Chain	Res	Type
1	1	1250	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1300	G
1	1	1301	A
1	1	1314	C
1	1	1321	A
1	1	1329	U
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1408	G
1	1	1416	G
1	1	1417	C
1	1	1428	C
1	1	1453	A
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1503	A
1	1	1508	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1535	A
1	1	1536	C
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1582	C
1	1	1583	A
1	1	1584	U
1	1	1587	G
1	1	1590	A

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Mol	Chain	Res	Type
1	1	1607	C
1	1	1610	A
1	1	1616	A
1	1	1646	C
1	1	1647	U
1	1	1648	U
1	1	1674	G
1	1	1677	A
1	1	1694	C
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1738	G
1	1	1764	C
1	1	1773	A
1	1	1784	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1816	C
1	1	1829	A
1	1	1858	A
1	1	1867	G
1	1	1868	C
1	1	1869	G
1	1	1870	C
1	1	1872	A
1	1	1873	G
1	1	1906	G
1	1	1913	A
1	1	1914	C
1	1	1916	A
1	1	1919	A
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1931	U
1	1	1937	A
1	1	1955	U
1	1	1964	G
1	1	1967	C
1	1	1970	A

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Mol	Chain	Res	Type
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	2020	A
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2072	C
1	1	2093	G
1	1	2102	G
1	1	2104	C
1	1	2107	G
1	1	2110	G
1	1	2111	U
1	1	2113	U
1	1	2115	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2120	G
1	1	2123	G
1	1	2124	G
1	1	2125	G
1	1	2127	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2145	C
1	1	2146	C

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Mol	Chain	Res	Type
1	1	2147	A
1	1	2148	G
1	1	2157	G
1	1	2158	A
1	1	2159	G
1	1	2161	C
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2168	G
1	1	2169	A
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2182	U
1	1	2185	U
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2194	U
1	1	2198	A
1	1	2199	A
1	1	2204	G
1	1	2211	A
1	1	2225	A
1	1	2238	G
1	1	2239	G
1	1	2250	G
1	1	2251	OMG
1	1	2252	G
1	1	2266	A
1	1	2278	A
1	1	2283	C
1	1	2287	A
1	1	2297	A
1	1	2305	U
1	1	2308	G
1	1	2309	A
1	1	2322	A
1	1	2325	G

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Mol	Chain	Res	Type
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2361	G
1	1	2383	G
1	1	2385	C
1	1	2395	C
1	1	2396	G
1	1	2402	U
1	1	2403	C
1	1	2420	C
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	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	2491	U
1	1	2494	G
1	1	2502	G
1	1	2503	2MA
1	1	2504	PSU
1	1	2506	U
1	1	2512	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2578	G

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Mol	Chain	Res	Type
1	1	2585	U
1	1	2586	U
1	1	2602	A
1	1	2609	U
1	1	2613	U
1	1	2615	U
1	1	2629	U
1	1	2630	G
1	1	2639	A
1	1	2646	C
1	1	2661	G
1	1	2689	U
1	1	2690	U
1	1	2714	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	2798	U
1	1	2818	U
1	1	2820	A
1	1	2849	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
2	2	2	A
2	2	4	U
2	2	5	U
2	2	6	G
2	2	9	G
2	2	22	G
2	2	31	G

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Mol	Chain	Res	Type
2	2	32	A
2	2	37	U
2	2	39	G
2	2	44	A
2	2	47	C
2	2	48	C
2	2	51	A
2	2	57	G
2	2	68	G
2	2	70	U
2	2	72	A
2	2	73	C
2	2	74	A
2	2	81	A
2	2	82	G
2	2	83	C
2	2	84	U
2	2	85	U
2	2	87	C
2	2	88	U
2	2	92	U
2	2	94	G
2	2	95	C
2	2	120	A
2	2	130	A
2	2	131	A
2	2	141	G
2	2	164	G
2	2	173	U
2	2	181	A
2	2	182	A
2	2	183	C
2	2	191	G
2	2	197	A
2	2	199	A
2	2	200	G
2	2	204	G
2	2	210	C
2	2	211	G
2	2	212	G
2	2	226	G
2	2	245	U

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Mol	Chain	Res	Type
2	2	247	G
2	2	251	G
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	328	C
2	2	332	G
2	2	347	G
2	2	352	C
2	2	354	G
2	2	360	G
2	2	367	U
2	2	372	C
2	2	373	A
2	2	392	C
2	2	397	A
2	2	406	G
2	2	409	U
2	2	411	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	423	G
2	2	424	G
2	2	429	U
2	2	436	C
2	2	438	U
2	2	439	U
2	2	440	C
2	2	448	A
2	2	449	G
2	2	451	A
2	2	454	G
2	2	455	G
2	2	463	U
2	2	467	U
2	2	468	A
2	2	469	C

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Mol	Chain	Res	Type
2	2	474	G
2	2	478	A
2	2	479	U
2	2	480	U
2	2	481	G
2	2	482	A
2	2	483	C
2	2	484	G
2	2	485	U
2	2	486	U
2	2	495	A
2	2	496	A
2	2	497	G
2	2	499	A
2	2	502	A
2	2	509	A
2	2	510	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	521	G
2	2	527	7MG
2	2	531	U
2	2	532	A
2	2	536	C
2	2	537	G
2	2	547	A
2	2	559	A
2	2	563	A
2	2	564	C
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	618	C
2	2	619	U
2	2	620	C
2	2	621	A
2	2	632	U
2	2	653	U
2	2	665	A

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Mol	Chain	Res	Type
2	2	687	A
2	2	688	G
2	2	700	G
2	2	721	G
2	2	723	U
2	2	731	G
2	2	747	A
2	2	777	A
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	844	G
2	2	846	G
2	2	902	G
2	2	914	A
2	2	926	G
2	2	934	C
2	2	960	U
2	2	966	2MG
2	2	969	A
2	2	972	C
2	2	975	A
2	2	976	G
2	2	977	A
2	2	981	U
2	2	989	U
2	2	992	U
2	2	993	G
2	2	996	A
2	2	1004	A
2	2	1008	U
2	2	1009	U
2	2	1010	U
2	2	1018	G
2	2	1021	A
2	2	1022	A
2	2	1026	G

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Mol	Chain	Res	Type
2	2	1027	C
2	2	1028	C
2	2	1030	U
2	2	1043	G
2	2	1046	A
2	2	1065	U
2	2	1066	C
2	2	1084	G
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1108	G
2	2	1124	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1138	G
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1142	G
2	2	1145	A
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1176	A
2	2	1196	A
2	2	1197	A
2	2	1213	A
2	2	1227	A
2	2	1241	G
2	2	1260	G
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1285	A
2	2	1286	U
2	2	1287	A

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Mol	Chain	Res	Type
2	2	1300	G
2	2	1305	G
2	2	1317	C
2	2	1320	C
2	2	1322	C
2	2	1336	C
2	2	1353	G
2	2	1363	A
2	2	1364	U
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	1452	C
2	2	1475	G
2	2	1492	A
2	2	1493	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1519	MA6
2	2	1529	G
2	2	1530	G
2	2	1533	C
2	2	1536	C
2	2	1537	U
2	2	1538	C
2	2	1539	C
3	3	2	G
3	3	23	G
3	3	35	C
3	3	41	G
3	3	56	G
3	3	57	A
3	3	74	U
3	3	75	G

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Mol	Chain	Res	Type
3	3	77	U
3	3	78	A
3	3	79	G
3	3	89	U
3	3	99	A
3	3	100	G
3	3	101	A
3	3	105	G
3	3	109	A
3	3	119	A
4	4	12	A
4	4	13	U
4	4	14	G
4	4	18	C
4	4	19	G
4	4	22	A
5	5	2	G
5	5	3	G
5	5	4	C
5	5	5	A
5	5	6	C
5	5	14	A
5	5	16	C
5	5	17	C
5	5	17(A)	U
5	5	18	G
5	5	19	G
5	5	20	U
5	5	21	A
5	5	22	G
5	5	23	C
5	5	33	U
5	5	36	G
5	5	40	U
5	5	41	C
5	5	42	G
5	5	47	U
5	5	48	C
5	5	49	G
5	5	51	A
5	5	60	U
5	5	61	C

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Mol	Chain	Res	Type
5	5	62	C
5	5	63	U
5	5	72	G
5	5	73	A
5	5	74	C
5	5	75	C
5	5	76	A
6	6	6	A
6	6	7	4SU
6	6	9	A
6	6	11	C
6	6	12	U
6	6	13	C
6	6	16	C
6	6	17	U
6	6	18	G
6	6	19	G
6	6	21	A
6	6	22	G
6	6	23	A
6	6	24	G
6	6	25	C
6	6	28	C
6	6	36	C
6	6	38	A
6	6	44	G
6	6	45	G
6	6	46	7MG
6	6	47	U
6	6	48	C
6	6	49	G
6	6	54	5MU
6	6	55	PSU
6	6	56	C
6	6	59	U
6	6	60	C
6	6	74	C
6	6	75	C

All (31) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
1	1	404	A
1	1	784	G
1	1	894	U
1	1	1199	U
1	1	1328	A
1	1	1379	U
1	1	1869	G
1	1	1913	A
1	1	2144	G
1	1	2193	G
1	1	2286	G
1	1	2425	A
1	1	2474	U
2	2	980	C
2	2	1008	U
2	2	1027	C
2	2	1109	C
2	2	1145	A
2	2	1383	C
2	2	1493	A
4	4	12	A
5	5	2	G
5	5	3	G
5	5	19	G
5	5	21	A
5	5	39	G
5	5	41	C
5	5	60	U
6	6	19	G
6	6	46	7MG
6	6	60	C

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

38 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$
6	6MZ	6	37	6	22,25,26	1.56	5 (22%)	29,36,39	2.31	10 (34%)
1	G7M	1	2069	1	23,26,27	2.54	9 (39%)	34,39,42	1.92	10 (29%)
2	2MG	2	966	2	23,26,27	2.92	9 (39%)	33,38,41	2.19	12 (36%)
6	7MG	6	46	6	23,26,27	3.50	10 (43%)	27,39,42	2.03	8 (29%)
2	PSU	2	516	2	18,21,22	1.11	1 (5%)	21,30,33	2.03	5 (23%)
2	MA6	2	1519	2	23,26,27	1.48	5 (21%)	33,38,41	2.90	12 (36%)
1	6MZ	1	1618	1	22,25,26	3.31	4 (18%)	29,36,39	2.26	11 (37%)
6	5MU	6	54	6	19,22,23	4.62	7 (36%)	27,32,35	3.82	9 (33%)
1	PSU	1	1911	1	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
2	7MG	2	527	2	23,26,27	3.91	11 (47%)	27,39,42	2.19	9 (33%)
6	4SU	6	7	6	18,21,22	3.59	8 (44%)	25,30,33	2.50	4 (16%)
2	4OC	2	1402	2	20,23,24	3.17	8 (40%)	25,32,35	0.89	1 (4%)
1	OMU	1	2552	1	19,22,23	3.07	8 (42%)	25,31,34	1.78	5 (20%)
6	PSU	6	55	6	18,21,22	1.44	4 (22%)	21,30,33	2.15	4 (19%)
2	2MG	2	1516	2	23,26,27	2.86	9 (39%)	33,38,41	2.12	9 (27%)
1	2MA	1	2503	1	22,25,26	3.83	9 (40%)	32,37,40	3.78	11 (34%)
1	PSU	1	955	1	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
6	CM0	6	34	6	21,26,27	2.39	7 (33%)	26,37,40	1.81	5 (19%)
1	2MG	1	2445	1	23,26,27	2.84	9 (39%)	33,38,41	2.08	10 (30%)
1	1MG	1	745	1	23,26,27	3.08	8 (34%)	33,39,42	2.00	8 (24%)
1	5MC	1	1962	1	19,22,23	3.84	8 (42%)	26,32,35	1.01	2 (7%)
1	5MU	1	747	1	19,22,23	4.82	7 (36%)	27,32,35	3.59	9 (33%)
2	MA6	2	1518	2	23,26,27	1.47	4 (17%)	33,38,41	2.80	11 (33%)
1	PSU	1	2580	1	18,21,22	1.08	1 (5%)	21,30,33	2.14	6 (28%)
1	PSU	1	2605	1	18,21,22	1.08	1 (5%)	21,30,33	2.07	5 (23%)
1	PSU	1	2504	1	18,21,22	1.05	1 (5%)	21,30,33	1.96	5 (23%)
1	OMG	1	2251	5,1	23,26,27	2.41	9 (39%)	32,38,41	2.48	10 (31%)
1	PSU	1	1917	1	18,21,22	1.10	1 (5%)	21,30,33	1.99	5 (23%)
2	5MC	2	1407	2	19,22,23	3.83	8 (42%)	26,32,35	0.97	2 (7%)
2	5MC	2	967	2	19,22,23	3.89	8 (42%)	26,32,35	0.98	2 (7%)
1	2MG	1	1835	1	23,26,27	2.89	8 (34%)	33,38,41	2.13	9 (27%)
1	PSU	1	2457	1	18,21,22	1.06	1 (5%)	21,30,33	2.03	6 (28%)
46	0TD	q	89	46	8,9,10	1.70	1 (12%)	6,11,13	1.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	1	2498	1	19,22,23	2.96	8 (42%)	25,31,34	0.75	0
1	5MU	1	1939	1	19,22,23	4.82	7 (36%)	27,32,35	3.60	9 (33%)
2	2MG	2	1207	2	23,26,27	2.92	9 (39%)	33,38,41	2.10	10 (30%)
2	UR3	2	1498	2	19,22,23	2.94	8 (42%)	26,32,35	1.53	4 (15%)
1	PSU	1	746	56,1	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)

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
6	6MZ	6	37	6	-	2/9/27/28	0/3/3/3
1	G7M	1	2069	1	-	1/7/25/26	0/3/3/3
2	2MG	2	966	2	-	0/9/27/28	0/3/3/3
6	7MG	6	46	6	-	1/7/37/38	0/3/3/3
2	PSU	2	516	2	-	1/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	2/11/29/30	0/3/3/3
1	6MZ	1	1618	1	-	2/9/27/28	0/3/3/3
6	5MU	6	54	6	-	2/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	7MG	2	527	2	-	3/7/37/38	0/3/3/3
6	4SU	6	7	6	-	0/7/25/26	0/2/2/2
2	4OC	2	1402	2	-	0/9/29/30	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
6	PSU	6	55	6	-	2/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
1	2MA	1	2503	1	-	3/7/25/26	0/3/3/3
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
6	CM0	6	34	6	-	3/12/30/31	0/2/2/2
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
1	1MG	1	745	1	-	0/7/25/26	0/3/3/3
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/11/29/30	0/3/3/3
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	OMG	1	2251	5,1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	0/9/27/28	0/3/3/3
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
46	0TD	q	89	46	-	2/7/12/14	-
1	OMC	1	2498	1	-	0/9/27/28	0/2/2/2
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	0/9/27/28	0/3/3/3
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
1	PSU	1	746	56,1	-	1/7/25/26	0/2/2/2

All (224) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1618	6MZ	C6-N6	14.27	1.50	1.34
1	1	2503	2MA	C4-N3	11.55	1.49	1.34
1	1	747	5MU	C2-N1	11.22	1.56	1.38
1	1	1939	5MU	C2-N1	11.14	1.55	1.38
6	6	54	5MU	C2-N1	10.36	1.54	1.38
1	1	747	5MU	C6-N1	10.28	1.55	1.38
1	1	1939	5MU	C6-N1	10.27	1.55	1.38
1	1	747	5MU	C4-C5	10.21	1.61	1.44
1	1	1939	5MU	C4-C5	10.20	1.61	1.44
2	2	527	7MG	C8-N9	10.06	1.52	1.45
6	6	54	5MU	C6-N1	9.74	1.54	1.38
6	6	54	5MU	C4-C5	9.39	1.60	1.44
2	2	967	5MC	C6-C5	9.14	1.49	1.34
2	2	1407	5MC	C6-C5	9.09	1.49	1.34
1	1	1962	5MC	C6-C5	8.96	1.49	1.34
1	1	745	1MG	C2-N3	8.66	1.47	1.33
6	6	46	7MG	C8-N9	8.40	1.51	1.45
6	6	54	5MU	C4-N3	-8.32	1.23	1.38
2	2	527	7MG	C5-N7	8.10	1.45	1.35
2	2	1498	UR3	C2-N1	7.94	1.49	1.38
1	1	1939	5MU	C4-N3	-7.77	1.24	1.38
6	6	46	7MG	C5-N7	7.70	1.45	1.35
1	1	747	5MU	C4-N3	-7.69	1.24	1.38
2	2	966	2MG	C2-N3	7.55	1.46	1.32
1	1	1835	2MG	C2-N3	7.52	1.46	1.32
2	2	1207	2MG	C2-N3	7.47	1.46	1.32
2	2	1402	4OC	C4-N3	7.40	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	7	4SU	C4-N3	7.38	1.45	1.37
2	2	1516	2MG	C2-N3	7.20	1.45	1.32
1	1	2552	OMU	C2-N1	7.15	1.49	1.38
1	1	2445	2MG	C2-N3	7.13	1.45	1.32
1	1	2503	2MA	C2-N3	7.09	1.46	1.34
1	1	2552	OMU	C2-N3	7.00	1.50	1.38
2	2	967	5MC	C4-N3	6.98	1.45	1.34
1	1	1962	5MC	C4-N3	6.94	1.45	1.34
2	2	527	7MG	C4-N9	6.85	1.46	1.37
2	2	1407	5MC	C4-N3	6.83	1.45	1.34
2	2	967	5MC	C5-C4	6.82	1.49	1.44
2	2	966	2MG	C4-N3	6.68	1.49	1.34
1	1	1962	5MC	C5-C4	6.64	1.49	1.44
2	2	1407	5MC	C5-C4	6.62	1.49	1.44
2	2	1207	2MG	C4-N3	6.61	1.49	1.34
1	1	1835	2MG	C4-N3	6.61	1.49	1.34
1	1	2503	2MA	C6-N1	6.56	1.43	1.35
6	6	7	4SU	C2-N1	6.55	1.48	1.38
1	1	2251	OMG	C4-N3	6.47	1.49	1.34
1	1	2069	G7M	C4-N3	6.44	1.49	1.34
1	1	2445	2MG	C4-N3	6.39	1.48	1.34
2	2	967	5MC	C2-N3	6.39	1.49	1.36
2	2	1516	2MG	C4-N3	6.38	1.48	1.34
1	1	1962	5MC	C2-N3	6.34	1.48	1.36
1	1	2498	OMC	C2-N3	6.34	1.48	1.36
6	6	7	4SU	C2-N3	6.33	1.49	1.38
2	2	527	7MG	C2-N3	6.31	1.48	1.33
2	2	1402	4OC	C2-N3	6.29	1.48	1.36
1	1	2503	2MA	C2-N1	6.28	1.44	1.34
2	2	1407	5MC	C2-N3	6.22	1.48	1.36
2	2	1498	UR3	C6-C5	6.21	1.49	1.35
2	2	1402	4OC	C6-C5	6.13	1.49	1.35
1	1	745	1MG	C4-N3	6.11	1.48	1.34
2	2	1207	2MG	C2-N2	6.02	1.46	1.33
2	2	966	2MG	C2-N2	5.99	1.46	1.33
6	6	46	7MG	C2-N3	5.98	1.47	1.33
2	2	1516	2MG	C2-N2	5.97	1.45	1.33
1	1	2498	OMC	C6-C5	5.95	1.48	1.35
1	1	1835	2MG	C2-N2	5.89	1.45	1.33
6	6	34	CM0	C2-N1	5.89	1.47	1.38
1	1	745	1MG	C2-N2	5.85	1.44	1.34
1	1	2445	2MG	C2-N2	5.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1939	5MU	C6-C5	5.68	1.43	1.34
2	2	527	7MG	C4-N3	5.67	1.47	1.34
1	1	2552	OMU	C6-C5	5.66	1.48	1.35
1	1	747	5MU	C6-C5	5.60	1.43	1.34
6	6	34	CM0	C2-N3	5.56	1.47	1.38
6	6	46	7MG	C4-N9	5.37	1.44	1.37
1	1	2069	G7M	C2-N3	5.36	1.46	1.33
1	1	2251	OMG	C2-N3	5.36	1.46	1.33
6	6	7	4SU	C6-C5	5.33	1.47	1.35
2	2	1498	UR3	C2-N3	5.27	1.49	1.39
6	6	46	7MG	C4-N3	5.25	1.46	1.34
6	6	7	4SU	C4-S4	-5.20	1.59	1.68
6	6	54	5MU	C6-C5	5.18	1.43	1.34
1	1	2498	OMC	C4-N3	5.14	1.44	1.34
6	6	7	4SU	C5-C4	4.91	1.48	1.42
2	2	1207	2MG	C2-N1	4.88	1.44	1.36
2	2	1516	2MG	C2-N1	4.85	1.44	1.36
2	2	966	2MG	C2-N1	4.83	1.44	1.36
1	1	1835	2MG	C2-N1	4.71	1.44	1.36
1	1	2069	G7M	C2-N2	4.69	1.45	1.34
1	1	2498	OMC	C4-N4	4.67	1.45	1.33
1	1	2445	2MG	C2-N1	4.63	1.44	1.36
1	1	2503	2MA	C5-C6	4.61	1.53	1.41
1	1	2251	OMG	C2-N2	4.61	1.45	1.34
1	1	1962	5MC	C6-N1	4.55	1.45	1.38
2	2	1407	5MC	C6-N1	4.53	1.45	1.38
2	2	967	5MC	C6-N1	4.52	1.45	1.38
2	2	1402	4OC	C4-N4	4.50	1.45	1.36
2	2	967	5MC	C4-N4	4.47	1.45	1.34
1	1	2498	OMC	C2-N1	4.36	1.49	1.40
1	1	1962	5MC	C2-N1	4.35	1.49	1.40
1	1	2552	OMU	C4-N3	4.33	1.46	1.38
2	2	1407	5MC	C4-N4	4.32	1.45	1.34
1	1	1962	5MC	C4-N4	4.32	1.45	1.34
1	1	745	1MG	C5-C6	4.29	1.56	1.45
2	2	967	5MC	C2-N1	4.27	1.49	1.40
2	2	1407	5MC	C2-N1	4.26	1.49	1.40
2	2	1402	4OC	C2-N1	4.23	1.48	1.40
6	6	37	6MZ	C5-C4	4.23	1.46	1.39
1	1	745	1MG	O6-C6	-4.06	1.14	1.23
1	1	2069	G7M	C5-N7	-4.01	1.34	1.39
1	1	745	1MG	C2-N1	3.83	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1519	MA6	C6-N6	3.80	1.47	1.36
2	2	1518	MA6	C6-N6	3.75	1.47	1.36
2	2	1402	4OC	C5-C4	3.64	1.49	1.41
1	1	746	PSU	C6-C5	3.60	1.39	1.35
2	2	516	PSU	C6-C5	3.59	1.39	1.35
2	2	527	7MG	C2-N1	3.58	1.46	1.37
6	6	34	CM0	O2-C2	-3.57	1.16	1.23
1	1	1917	PSU	C6-C5	3.56	1.39	1.35
1	1	955	PSU	C6-C5	3.51	1.39	1.35
2	2	527	7MG	C6-N1	3.48	1.45	1.38
1	1	1911	PSU	C6-C5	3.46	1.39	1.35
1	1	2605	PSU	C6-C5	3.37	1.39	1.35
1	1	2069	G7M	C5-C6	3.32	1.52	1.43
2	2	527	7MG	C2-N2	3.32	1.41	1.34
2	2	527	7MG	C5-C6	3.31	1.51	1.43
6	6	46	7MG	C2-N1	3.31	1.45	1.37
1	1	2580	PSU	C6-C5	3.30	1.38	1.35
1	1	2457	PSU	C6-C5	3.29	1.38	1.35
6	6	46	7MG	C2-N2	3.28	1.41	1.34
1	1	2504	PSU	C6-C5	3.27	1.38	1.35
6	6	46	7MG	O6-C6	-3.27	1.17	1.23
1	1	1835	2MG	C5-N7	-3.22	1.32	1.39
6	6	46	7MG	C6-N1	3.22	1.44	1.38
2	2	1207	2MG	C5-N7	-3.18	1.32	1.39
1	1	2503	2MA	C6-N6	-3.17	1.26	1.34
6	6	34	CM0	C4-N3	3.14	1.44	1.38
1	1	2445	2MG	C5-N7	-3.12	1.32	1.39
1	1	2498	OMC	C6-N1	3.12	1.45	1.38
2	2	966	2MG	C5-N7	-3.11	1.32	1.39
2	2	1516	2MG	C5-N7	-3.10	1.32	1.39
6	6	34	CM0	C6-N1	3.09	1.43	1.38
2	2	527	7MG	O6-C6	-3.08	1.17	1.23
2	2	1402	4OC	C6-N1	3.07	1.45	1.38
6	6	54	5MU	O4-C4	-3.04	1.17	1.23
1	1	745	1MG	C5-N7	-3.02	1.33	1.39
1	1	2251	OMG	C5-N7	-3.01	1.33	1.39
46	q	89	0TD	CB-CA	-3.00	1.53	1.54
1	1	2069	G7M	C6-N1	3.00	1.44	1.38
6	6	55	PSU	C4-N3	-2.98	1.33	1.38
1	1	1618	6MZ	C5-C4	-2.96	1.33	1.39
6	6	55	PSU	C6-C5	2.92	1.38	1.35
2	2	1519	MA6	C5-C4	-2.92	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1518	MA6	C5-C4	-2.91	1.33	1.39
1	1	1618	6MZ	C5-N7	-2.91	1.33	1.39
6	6	46	7MG	C5-C6	2.90	1.50	1.43
1	1	2503	2MA	C5-N7	-2.87	1.33	1.39
6	6	54	5MU	O2-C2	-2.87	1.18	1.23
1	1	2552	OMU	O4-C4	-2.86	1.18	1.24
6	6	34	CM0	O4-C4	-2.85	1.18	1.23
6	6	7	4SU	O2-C2	-2.84	1.18	1.23
2	2	1498	UR3	C6-N1	2.82	1.44	1.38
1	1	2251	OMG	C2-N1	2.80	1.44	1.37
1	1	2552	OMU	C6-N1	2.79	1.44	1.38
2	2	1518	MA6	C5-N7	-2.70	1.34	1.39
2	2	1402	4OC	O2-C2	-2.70	1.18	1.23
1	1	2498	OMC	O2-C2	-2.69	1.18	1.23
1	1	1962	5MC	O2-C2	-2.65	1.18	1.23
1	1	2445	2MG	O6-C6	-2.65	1.18	1.23
1	1	747	5MU	O4-C4	-2.64	1.18	1.23
2	2	1498	UR3	O2-C2	-2.63	1.17	1.22
1	1	1835	2MG	O6-C6	-2.62	1.18	1.23
1	1	1939	5MU	O4-C4	-2.62	1.18	1.23
2	2	1407	5MC	O2-C2	-2.62	1.18	1.23
1	1	2069	G7M	C2-N1	2.62	1.44	1.37
2	2	1207	2MG	O6-C6	-2.61	1.18	1.23
6	6	37	6MZ	C5-N7	-2.61	1.34	1.39
2	2	1498	UR3	O4-C4	-2.61	1.18	1.23
2	2	1519	MA6	C5-N7	-2.61	1.34	1.39
2	2	966	2MG	O6-C6	-2.59	1.18	1.23
2	2	967	5MC	O2-C2	-2.59	1.18	1.23
2	2	1516	2MG	O6-C6	-2.56	1.18	1.23
6	6	37	6MZ	C5-C6	2.48	1.47	1.41
6	6	34	CM0	O5-C7	-2.46	1.39	1.44
6	6	7	4SU	C6-N1	2.46	1.44	1.38
2	2	1498	UR3	C5-C4	2.46	1.50	1.43
1	1	2445	2MG	C4-N9	-2.45	1.31	1.38
1	1	1939	5MU	O2-C2	-2.44	1.18	1.23
1	1	747	5MU	O2-C2	-2.43	1.18	1.23
2	2	1516	2MG	C4-N9	-2.42	1.31	1.38
1	1	2251	OMG	C5-C6	2.41	1.53	1.44
1	1	2251	OMG	O6-C6	-2.41	1.19	1.23
2	2	1207	2MG	C5-C6	2.41	1.53	1.44
2	2	1516	2MG	C5-C6	2.41	1.53	1.44
2	2	966	2MG	C5-C6	2.39	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1835	2MG	C5-C6	2.37	1.53	1.44
1	1	2069	G7M	O6-C6	-2.37	1.19	1.23
2	2	1516	2MG	C6-N1	2.36	1.43	1.38
1	1	2503	2MA	C4-N9	-2.36	1.32	1.37
1	1	2552	OMU	O2-C2	-2.36	1.18	1.23
1	1	2552	OMU	C5-C4	2.36	1.48	1.43
1	1	2445	2MG	C5-C6	2.35	1.53	1.44
2	2	1207	2MG	C6-N1	2.33	1.43	1.38
1	1	2251	OMG	C6-N1	2.33	1.43	1.38
1	1	2498	OMC	C5-C4	2.33	1.48	1.42
2	2	1498	UR3	C4-N3	2.32	1.45	1.40
1	1	2445	2MG	C6-N1	2.31	1.43	1.38
1	1	745	1MG	C8-N9	-2.29	1.32	1.37
2	2	966	2MG	C6-N1	2.26	1.43	1.38
1	1	2503	2MA	C8-N7	2.26	1.36	1.31
6	6	37	6MZ	C4-N9	-2.22	1.33	1.37
1	1	1618	6MZ	C8-N9	-2.21	1.33	1.37
1	1	1835	2MG	C6-N1	2.21	1.43	1.38
1	1	2069	G7M	C4-N9	-2.20	1.32	1.38
2	2	1519	MA6	C4-N9	-2.18	1.33	1.37
6	6	55	PSU	C2-N3	-2.17	1.33	1.37
2	2	1207	2MG	C4-N9	-2.15	1.32	1.38
1	1	2251	OMG	C4-N9	-2.13	1.32	1.38
2	2	1518	MA6	C4-N9	-2.07	1.33	1.37
2	2	966	2MG	C4-N9	-2.06	1.32	1.38
6	6	55	PSU	C2-N1	-2.05	1.34	1.36
6	6	37	6MZ	C8-N7	2.04	1.35	1.31
2	2	1519	MA6	C10-N6	2.03	1.50	1.45
2	2	527	7MG	C8-N7	2.00	1.52	1.42

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2503	2MA	C1'-N9-C8	-13.69	96.70	127.09
6	6	54	5MU	C5-C4-N3	12.63	126.30	115.32
1	1	747	5MU	C5-C4-N3	12.06	125.81	115.32
1	1	1939	5MU	C5-C4-N3	12.06	125.81	115.32
1	1	2503	2MA	C4-N9-C1'	11.84	154.32	126.63
6	6	54	5MU	C5-C6-N1	-10.05	112.39	123.31
2	2	1519	MA6	N1-C6-N6	-9.76	104.97	116.86
2	2	1518	MA6	N1-C6-N6	-9.27	105.56	116.86
1	1	1939	5MU	C5-C6-N1	-8.80	113.76	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	747	5MU	C5-C6-N1	-8.60	113.97	123.31
6	6	7	4SU	C4-N3-C2	-8.57	119.10	127.31
1	1	2251	OMG	C1'-N9-C8	-7.16	106.39	126.73
6	6	55	PSU	N1-C2-N3	6.65	122.18	115.17
1	1	2251	OMG	C1'-N9-C4	6.42	145.45	126.49
1	1	1835	2MG	C2-N3-C4	6.37	119.97	112.00
2	2	1207	2MG	C2-N3-C4	6.36	119.96	112.00
2	2	966	2MG	C2-N3-C4	6.33	119.92	112.00
2	2	1516	2MG	C2-N3-C4	6.27	119.85	112.00
1	1	2445	2MG	C2-N3-C4	6.14	119.69	112.00
2	2	1519	MA6	C5-C6-N6	6.12	135.01	125.33
6	6	7	4SU	C5-C4-N3	5.98	120.32	114.75
6	6	37	6MZ	C5-C4-N3	-5.96	118.51	126.72
6	6	34	CM0	C4-N3-C2	-5.96	119.52	127.34
1	1	2503	2MA	C5-C4-N3	-5.74	121.13	127.18
2	2	1518	MA6	C5-C6-N6	5.70	134.35	125.33
2	2	1519	MA6	N1-C2-N3	-5.62	120.07	128.58
6	6	54	5MU	O4-C4-C5	-5.57	118.55	124.92
1	1	1618	6MZ	N1-C2-N3	-5.53	120.22	128.58
1	1	2552	OMU	C4-N3-C2	-5.47	119.83	126.61
2	2	1518	MA6	N1-C2-N3	-5.46	120.32	128.58
1	1	1835	2MG	C5-C4-N3	-5.43	119.75	128.39
2	2	516	PSU	C4-N3-C2	-5.39	118.95	126.37
6	6	54	5MU	C4-N3-C2	-5.33	120.36	127.34
1	1	2580	PSU	N1-C2-N3	5.30	120.75	115.17
2	2	966	2MG	C5-C4-N3	-5.29	119.96	128.39
1	1	1939	5MU	O4-C4-C5	-5.24	118.92	124.92
1	1	745	1MG	C5-C4-N3	-5.21	120.09	128.39
2	2	1498	UR3	C4-N3-C2	-5.18	120.41	124.58
2	2	1207	2MG	C5-C4-N3	-5.18	120.15	128.39
1	1	2605	PSU	N1-C2-N3	5.17	120.62	115.17
1	1	2605	PSU	C4-N3-C2	-5.16	119.26	126.37
1	1	747	5MU	O4-C4-C5	-5.11	119.07	124.92
2	2	516	PSU	N1-C2-N3	5.10	120.55	115.17
1	1	2503	2MA	N9-C8-N7	-5.05	106.78	113.94
2	2	1518	MA6	C5-C4-N3	-5.02	119.80	126.72
1	1	2580	PSU	C4-N3-C2	-5.02	119.45	126.37
1	1	2457	PSU	N1-C2-N3	5.02	120.46	115.17
1	1	1939	5MU	C4-N3-C2	-4.98	120.82	127.34
1	1	2251	OMG	C5-C4-N3	-4.96	120.49	128.39
1	1	1911	PSU	C4-N3-C2	-4.95	119.56	126.37
1	1	1917	PSU	C4-N3-C2	-4.95	119.56	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1917	PSU	N1-C2-N3	4.94	120.38	115.17
1	1	746	PSU	C4-N3-C2	-4.94	119.57	126.37
1	1	1911	PSU	N1-C2-N3	4.92	120.36	115.17
1	1	746	PSU	N1-C2-N3	4.92	120.36	115.17
2	2	1516	2MG	C5-C4-N3	-4.91	120.58	128.39
1	1	2457	PSU	C4-N3-C2	-4.90	119.62	126.37
1	1	2504	PSU	C4-N3-C2	-4.89	119.63	126.37
1	1	1618	6MZ	C5-C4-N3	-4.88	120.00	126.72
1	1	745	1MG	C1'-N9-C4	-4.87	112.10	126.49
1	1	747	5MU	C4-N3-C2	-4.86	120.97	127.34
2	2	527	7MG	C5-C6-N1	4.85	119.48	110.94
2	2	1519	MA6	C5-C4-N3	-4.84	120.06	126.72
1	1	955	PSU	C4-N3-C2	-4.83	119.72	126.37
1	1	955	PSU	N1-C2-N3	4.83	120.26	115.17
1	1	2504	PSU	N1-C2-N3	4.81	120.24	115.17
1	1	2445	2MG	C5-C4-N3	-4.81	120.74	128.39
1	1	1939	5MU	N3-C2-N1	4.79	121.13	114.89
6	6	37	6MZ	N3-C4-N9	4.74	135.24	127.17
6	6	46	7MG	C5-C6-N1	4.72	119.25	110.94
1	1	745	1MG	C1'-N9-C8	4.62	139.85	126.73
1	1	747	5MU	N3-C2-N1	4.61	120.90	114.89
6	6	54	5MU	N3-C2-N1	4.54	120.80	114.89
2	2	527	7MG	C4-C5-N7	4.44	110.62	105.38
6	6	46	7MG	C4-C5-N7	4.36	110.52	105.38
1	1	747	5MU	C5M-C5-C4	4.34	123.41	118.78
6	6	34	CM0	N3-C2-N1	4.32	120.51	114.89
1	1	2251	OMG	C2-N3-C4	4.31	119.73	112.30
6	6	7	4SU	C5-C4-S4	-4.28	119.41	124.31
2	2	527	7MG	C2-N3-C4	4.27	119.65	112.30
1	1	2069	G7M	C2-N3-C4	4.26	119.63	112.30
1	1	1835	2MG	C2-N1-C6	-4.25	119.42	124.55
6	6	55	PSU	C4-N3-C2	-4.23	120.54	126.37
2	2	1519	MA6	N9-C8-N7	-4.21	107.96	113.94
2	2	527	7MG	C5-C4-N3	-4.18	120.29	128.13
2	2	1516	2MG	N1-C2-N2	4.16	120.81	116.56
6	6	37	6MZ	C9-N6-C6	-4.14	119.01	122.85
2	2	1518	MA6	C4-C5-C6	4.10	120.15	115.91
2	2	966	2MG	C2-N1-C6	-4.09	119.60	124.55
1	1	1618	6MZ	N9-C8-N7	-4.08	108.15	113.94
2	2	1516	2MG	C2-N1-C6	-4.07	119.63	124.55
2	2	1207	2MG	C2-N1-C6	-4.06	119.64	124.55
1	1	2445	2MG	N1-C2-N2	4.00	120.64	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2445	2MG	C2-N1-C6	-3.94	119.79	124.55
2	2	1518	MA6	N9-C8-N7	-3.93	108.36	113.94
1	1	1939	5MU	C5M-C5-C4	3.92	122.96	118.78
6	6	46	7MG	C2-N3-C4	3.89	119.00	112.30
6	6	54	5MU	C5M-C5-C6	-3.86	117.63	122.85
1	1	2069	G7M	C5-C6-N1	3.84	119.78	111.84
6	6	7	4SU	N3-C2-N1	3.83	119.88	114.89
1	1	2069	G7M	C5-C4-N3	-3.82	120.93	128.15
6	6	54	5MU	C5M-C5-C4	3.81	122.85	118.78
2	2	1519	MA6	C4-C5-C6	3.81	119.85	115.91
1	1	747	5MU	C5M-C5-C6	-3.78	117.73	122.85
6	6	37	6MZ	C2-N3-C4	3.75	120.98	111.83
6	6	55	PSU	O2-C2-N1	-3.70	118.97	122.79
1	1	2552	OMU	N3-C2-N1	3.69	119.69	114.89
1	1	1618	6MZ	C9-N6-C6	-3.64	119.48	122.85
1	1	1939	5MU	C5M-C5-C6	-3.55	118.04	122.85
1	1	2580	PSU	O2-C2-N1	-3.53	119.15	122.79
1	1	745	1MG	C2-N3-C4	3.51	119.88	111.98
1	1	2069	G7M	O6-C6-C5	-3.50	120.20	128.01
2	2	1498	UR3	C5-C4-N3	3.49	119.64	115.04
1	1	2552	OMU	C5-C4-N3	3.49	119.68	114.80
1	1	1618	6MZ	C4-C5-C6	3.48	119.67	116.78
1	1	2069	G7M	N9-C4-N3	3.42	132.79	125.95
6	6	46	7MG	C5-C4-N3	-3.42	121.72	128.13
1	1	1618	6MZ	C2-N3-C4	3.39	120.11	111.83
2	2	1519	MA6	C2-N3-C4	3.38	120.09	111.83
2	2	1518	MA6	C2-N3-C4	3.35	120.01	111.83
2	2	1207	2MG	N1-C2-N2	3.31	119.94	116.56
2	2	1519	MA6	C2-N1-C6	3.31	119.91	111.83
6	6	37	6MZ	C4-C5-N7	-3.29	106.82	110.58
2	2	1518	MA6	C2-N1-C6	3.19	119.62	111.83
1	1	2503	2MA	C5-N7-C8	3.18	108.44	103.45
1	1	2503	2MA	N3-C2-N1	-3.17	120.18	125.77
1	1	2503	2MA	N3-C4-N9	3.16	131.01	126.99
1	1	2251	OMG	N9-C8-N7	-3.15	107.55	113.40
6	6	37	6MZ	N1-C2-N3	-3.15	123.82	128.58
2	2	966	2MG	N9-C4-N3	3.14	132.24	125.95
1	1	2457	PSU	O2-C2-N1	-3.14	119.55	122.79
1	1	1835	2MG	N9-C4-N3	3.13	132.21	125.95
1	1	2069	G7M	C1'-N9-C4	-3.12	117.26	126.49
6	6	37	6MZ	C6-C5-N7	3.09	135.80	132.43
2	2	527	7MG	O6-C6-C5	-3.09	120.04	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2503	2MA	C4-N9-C8	3.08	108.97	105.74
1	1	2251	OMG	C2-N1-C6	-3.06	119.56	125.11
2	2	1518	MA6	N3-C4-N9	3.05	132.35	127.17
2	2	1407	5MC	C5-C6-N1	-3.03	120.02	123.31
1	1	2605	PSU	O2-C2-N1	-3.00	119.69	122.79
2	2	1207	2MG	N9-C4-N3	2.98	131.91	125.95
1	1	2069	G7M	C2-N1-C6	-2.98	119.71	125.11
1	1	745	1MG	N9-C4-N3	2.98	131.90	125.95
6	6	46	7MG	O6-C6-C5	-2.96	120.36	127.62
2	2	527	7MG	N9-C4-N3	2.96	129.79	125.46
1	1	1835	2MG	N1-C2-N2	2.95	119.58	116.56
2	2	967	5MC	C5-C6-N1	-2.95	120.11	123.31
1	1	2580	PSU	C6-N1-C2	-2.94	119.96	122.69
1	1	2504	PSU	O2-C2-N1	-2.93	119.77	122.79
1	1	1911	PSU	O2-C2-N1	-2.92	119.78	122.79
1	1	2552	OMU	O4-C4-C5	-2.91	120.14	125.16
2	2	527	7MG	C2-N1-C6	-2.90	119.85	125.11
1	1	2445	2MG	N9-C8-N7	-2.89	108.03	113.40
1	1	955	PSU	O2-C2-N1	-2.88	119.82	122.79
2	2	516	PSU	O2-C2-N1	-2.87	119.83	122.79
2	2	1519	MA6	N3-C4-N9	2.87	132.04	127.17
1	1	1618	6MZ	N3-C4-N9	2.87	132.04	127.17
2	2	966	2MG	N1-C2-N2	2.84	119.46	116.56
1	1	1939	5MU	O2-C2-N1	-2.84	119.10	122.80
2	2	1516	2MG	N9-C8-N7	-2.82	108.17	113.40
1	1	1917	PSU	O2-C2-N1	-2.82	119.88	122.79
2	2	966	2MG	N9-C8-N7	-2.81	108.19	113.40
1	1	745	1MG	N9-C8-N7	-2.81	108.19	113.40
2	2	527	7MG	C5-C4-N9	2.80	109.92	106.33
1	1	746	PSU	O2-C2-N1	-2.78	119.92	122.79
1	1	747	5MU	O2-C2-N1	-2.77	119.19	122.80
1	1	2069	G7M	CN7-N7-C5	2.76	130.24	126.80
2	2	1519	MA6	C5-N7-C8	2.76	107.79	103.45
2	2	1207	2MG	N9-C8-N7	-2.76	108.28	113.40
1	1	1618	6MZ	C5-N7-C8	2.73	107.73	103.45
6	6	54	5MU	O2-C2-N1	-2.72	119.26	122.80
1	1	2251	OMG	N9-C4-N3	2.71	131.37	125.95
6	6	37	6MZ	C4-N9-C8	2.69	108.56	105.74
1	1	2503	2MA	CM2-C2-N1	2.69	121.15	117.13
1	1	1835	2MG	N9-C8-N7	-2.68	108.43	113.40
1	1	1962	5MC	C5-C6-N1	-2.68	120.41	123.31
1	1	747	5MU	O4-C4-N3	-2.65	115.12	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1835	2MG	C5-C6-N1	2.64	119.98	113.25
6	6	54	5MU	O4-C4-N3	-2.64	115.15	120.11
1	1	2069	G7M	N9-C8-N7	-2.63	106.09	112.48
2	2	966	2MG	C5-C6-N1	2.63	119.94	113.25
2	2	1207	2MG	C5-C6-N1	2.61	119.90	113.25
1	1	2605	PSU	C6-N1-C2	-2.61	120.27	122.69
1	1	745	1MG	C5-C6-N1	2.61	119.84	115.02
2	2	1518	MA6	C5-N7-C8	2.60	107.53	103.45
1	1	2457	PSU	C6-C5-C4	2.59	119.92	118.17
6	6	34	CM0	O5-C7-C8	-2.59	105.37	110.93
1	1	2251	OMG	C5-C6-N1	2.58	119.83	113.25
1	1	746	PSU	C6-N1-C2	-2.57	120.30	122.69
1	1	1939	5MU	O4-C4-N3	-2.57	115.28	120.11
1	1	2457	PSU	C6-N1-C2	-2.57	120.31	122.69
2	2	1516	2MG	C5-C6-N1	2.57	119.80	113.25
1	1	2445	2MG	C5-C6-N1	2.55	119.75	113.25
6	6	46	7MG	C2-N1-C6	-2.54	120.50	125.11
2	2	1516	2MG	N9-C4-N3	2.54	131.03	125.95
1	1	2445	2MG	N9-C4-N3	2.53	131.01	125.95
6	6	46	7MG	C5-C4-N9	2.53	109.57	106.33
1	1	2504	PSU	C6-C5-C4	2.50	119.86	118.17
1	1	955	PSU	C6-N1-C2	-2.48	120.39	122.69
2	2	966	2MG	O2'-C2'-C3'	2.48	119.77	111.82
2	2	516	PSU	C6-C5-C4	2.48	119.85	118.17
1	1	1911	PSU	C6-C5-C4	2.47	119.84	118.17
1	1	2069	G7M	CN7-N7-C8	-2.47	121.06	124.79
1	1	2251	OMG	O6-C6-C5	-2.45	120.05	126.53
1	1	2580	PSU	C6-C5-C4	2.44	119.82	118.17
2	2	966	2MG	O6-C6-C5	-2.44	120.08	126.53
6	6	37	6MZ	C5-N7-C8	2.44	107.29	103.45
2	2	1516	2MG	O6-C6-C5	-2.44	120.09	126.53
1	1	1835	2MG	O6-C6-C5	-2.43	120.11	126.53
2	2	1207	2MG	O6-C6-C5	-2.43	120.12	126.53
1	1	1917	PSU	C6-N1-C2	-2.43	120.44	122.69
2	2	527	7MG	N9-C8-N7	2.43	106.81	103.37
1	1	1911	PSU	C6-N1-C2	-2.40	120.46	122.69
1	1	2445	2MG	O6-C6-C5	-2.39	120.21	126.53
1	1	2580	PSU	O4'-C1'-C2'	2.39	108.45	105.15
1	1	2605	PSU	C6-C5-C4	2.39	119.78	118.17
1	1	2504	PSU	C6-N1-C2	-2.35	120.51	122.69
1	1	1917	PSU	C6-C5-C4	2.35	119.76	118.17
2	2	1519	MA6	C4-N9-C8	2.33	108.19	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1618	6MZ	C5-C6-N1	2.32	120.64	118.15
2	2	1498	UR3	C1'-N1-C2	2.31	120.83	117.04
6	6	55	PSU	C3'-C2'-C1'	2.31	104.42	101.69
1	1	2503	2MA	C4-C5-N7	-2.30	107.95	110.58
2	2	1402	4OC	C6-C5-C4	2.28	119.75	117.00
1	1	2251	OMG	C8-N7-C5	2.25	108.27	104.26
6	6	34	CM0	O2-C2-N1	-2.24	119.88	122.80
2	2	1498	UR3	C6-N1-C2	-2.22	119.98	121.80
6	6	46	7MG	N9-C4-N3	2.22	128.71	125.46
1	1	1962	5MC	CM5-C5-C6	-2.21	119.86	122.85
6	6	34	CM0	C1'-N1-C2	2.19	121.52	117.59
2	2	967	5MC	CM5-C5-C6	-2.16	119.93	122.85
2	2	1519	MA6	C4-C5-N7	-2.12	108.16	110.58
1	1	2457	PSU	O4'-C1'-C2'	2.11	108.07	105.15
1	1	2445	2MG	CM2-N2-C2	-2.10	119.15	123.65
2	2	1207	2MG	N1-C2-N3	-2.06	120.20	123.68
2	2	966	2MG	C8-N7-C5	2.06	107.92	104.26
1	1	1618	6MZ	C4-N9-C8	2.05	107.89	105.74
1	1	2552	OMU	O2-C2-N1	-2.05	120.13	122.80
2	2	1407	5MC	CM5-C5-C6	-2.05	120.08	122.85
2	2	516	PSU	C6-N1-C2	-2.04	120.80	122.69
1	1	2503	2MA	N6-C6-N1	2.04	119.78	117.03
1	1	1835	2MG	C8-N7-C5	2.03	107.87	104.26
2	2	1518	MA6	C4-N9-C8	2.03	107.87	105.74
1	1	1618	6MZ	C4-C5-N7	-2.02	108.27	110.58
1	1	745	1MG	CM1-N1-C6	2.02	120.77	117.64
6	6	37	6MZ	N9-C8-N7	-2.02	111.08	113.94
2	2	1516	2MG	N1-C2-N3	-2.02	120.28	123.68
2	2	966	2MG	N1-C2-N3	-2.01	120.29	123.68
1	1	2445	2MG	N1-C2-N3	-2.01	120.29	123.68
2	2	1207	2MG	C8-N7-C5	2.00	107.83	104.26
2	2	966	2MG	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (29) 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	2504	PSU	O4'-C4'-C5'-O5'
2	2	516	PSU	O4'-C1'-C5-C6
2	2	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	6	37	6MZ	C5-C6-N6-C9
6	6	37	6MZ	N1-C6-N6-C9
1	1	2445	2MG	C3'-C4'-C5'-O5'
2	2	527	7MG	C3'-C4'-C5'-O5'
6	6	55	PSU	O4'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
6	6	54	5MU	C3'-C4'-C5'-O5'
6	6	54	5MU	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
2	2	527	7MG	O4'-C4'-C5'-O5'
6	6	34	CM0	O5-C7-C8-O8
6	6	55	PSU	C3'-C4'-C5'-O5'
6	6	34	CM0	C8-C7-O5-C5
6	6	34	CM0	O5-C7-C8-O9
46	q	89	0TD	CG-CB-SB-CSB
46	q	89	0TD	SB-CB-CG-OD1
6	6	46	7MG	C4'-C5'-O5'-P
2	2	527	7MG	C4'-C5'-O5'-P
1	1	2069	G7M	O4'-C4'-C5'-O5'
1	1	746	PSU	C2'-C1'-C5-C6
1	1	2503	2MA	O4'-C1'-N9-C8
1	1	2503	2MA	C4'-C5'-O5'-P
1	1	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

14 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	966	2MG	1	0
6	6	46	7MG	1	0
2	2	516	PSU	1	0
2	2	1519	MA6	1	0
6	6	54	5MU	1	0
2	2	527	7MG	2	0
6	6	7	4SU	2	0
2	2	1402	4OC	1	0
2	2	1516	2MG	1	0
6	6	34	CM0	1	0
1	1	745	1MG	3	0
2	2	1518	MA6	1	0
2	2	967	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	q	89	0TD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 395 ligands modelled in this entry, 395 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

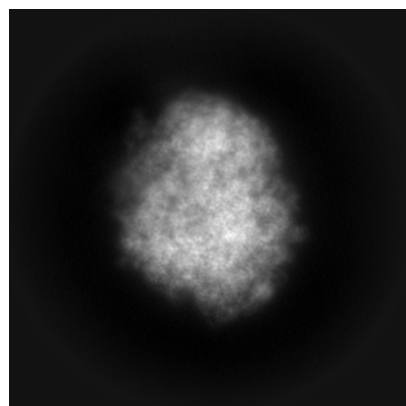
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42495. These allow visual inspection of the internal detail of the map and identification of artifacts.

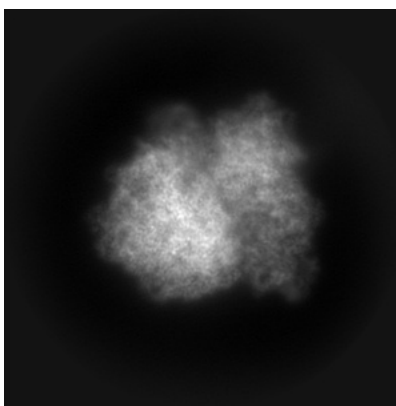
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

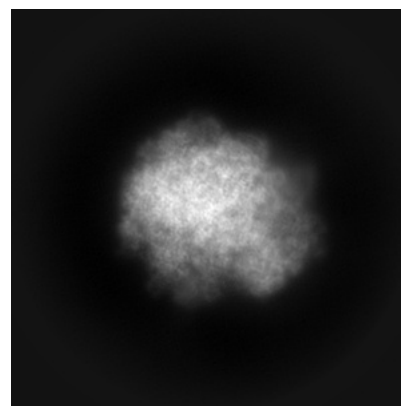
6.1.1 Primary map



X

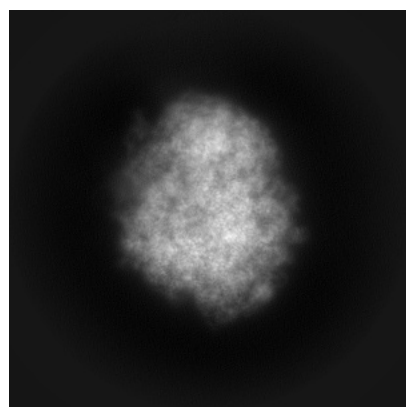


Y

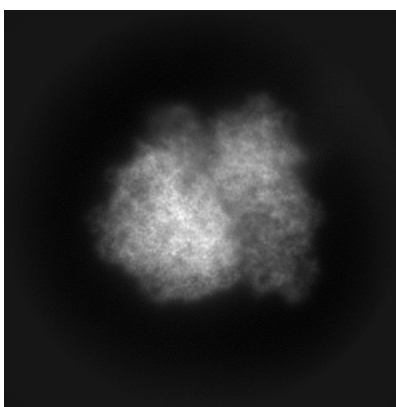


Z

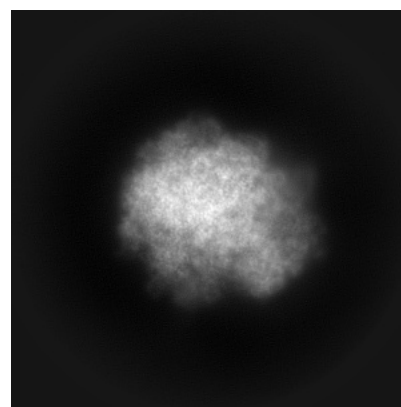
6.1.2 Raw map



X



Y

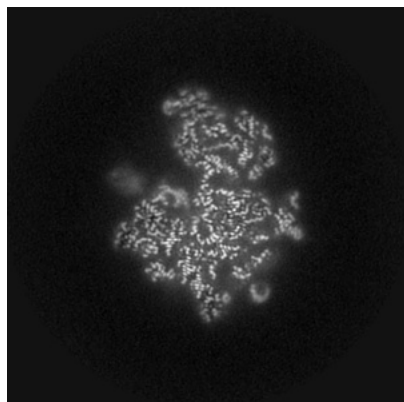


Z

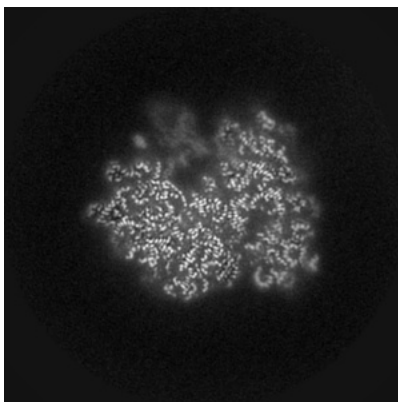
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

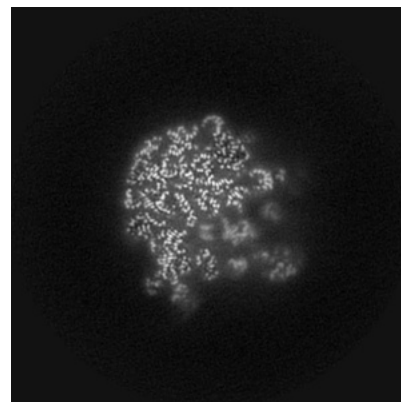
6.2.1 Primary map



X Index: 200

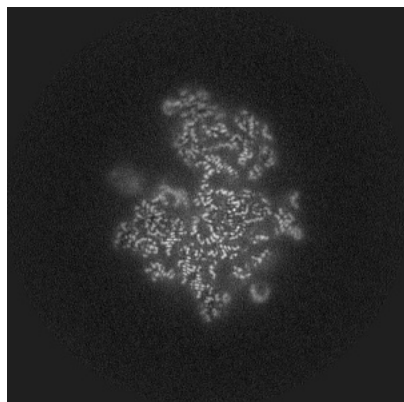


Y Index: 200

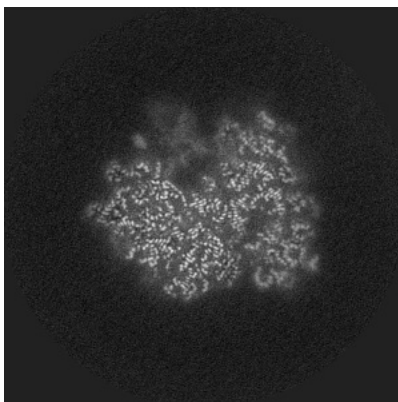


Z Index: 200

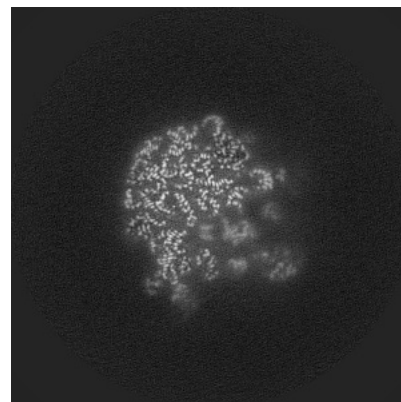
6.2.2 Raw map



X Index: 200



Y Index: 200

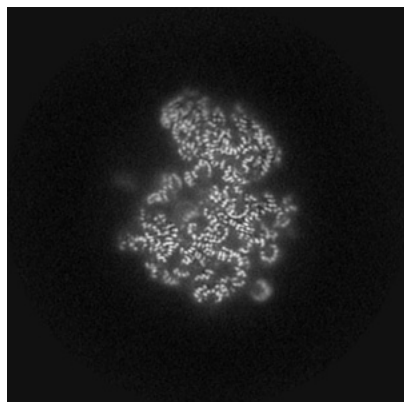


Z Index: 200

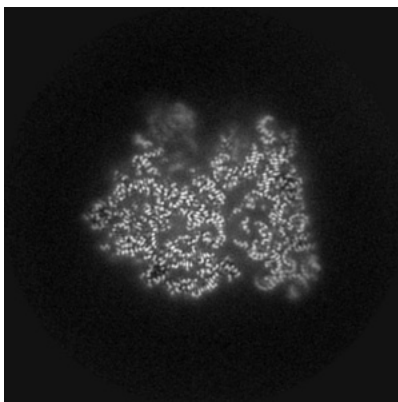
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

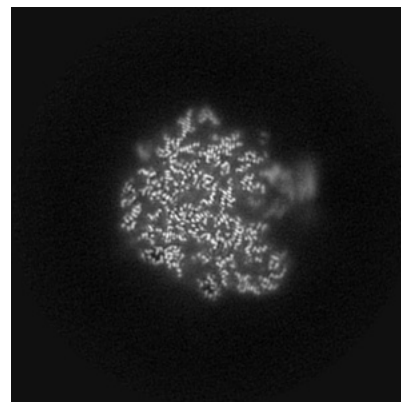
6.3.1 Primary map



X Index: 210

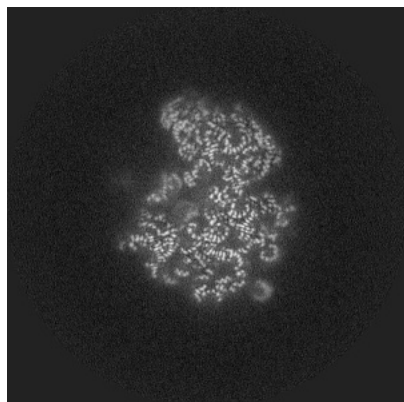


Y Index: 208

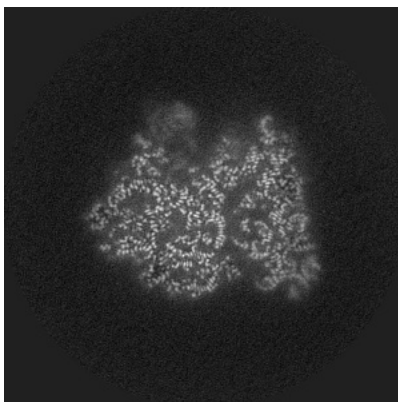


Z Index: 170

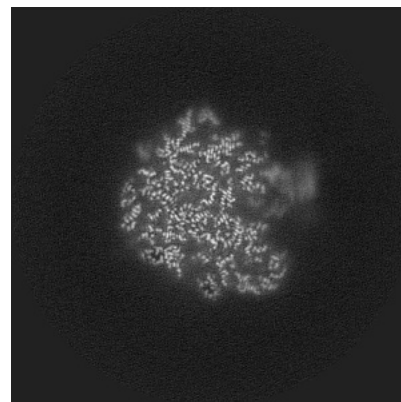
6.3.2 Raw map



X Index: 211



Y Index: 209

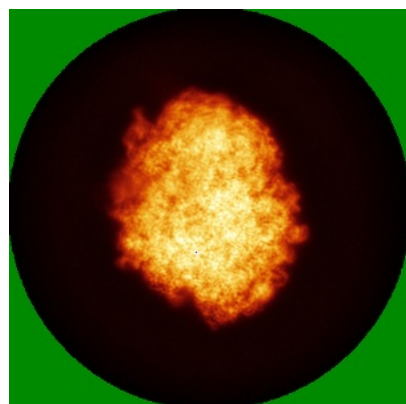


Z Index: 170

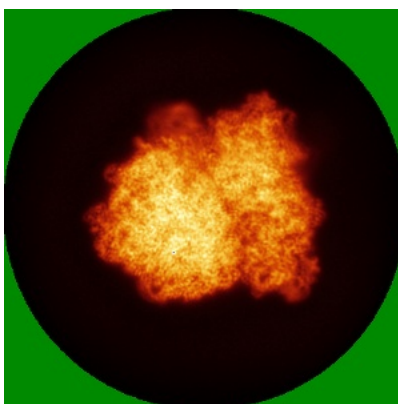
The images above show the largest variance slices of the map in three orthogonal directions.

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

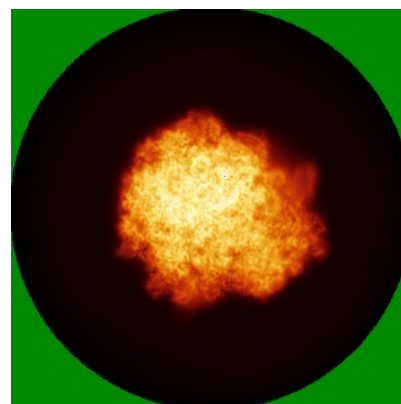
6.4.1 Primary map



X

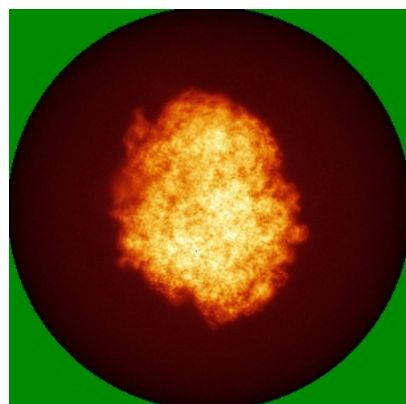


Y

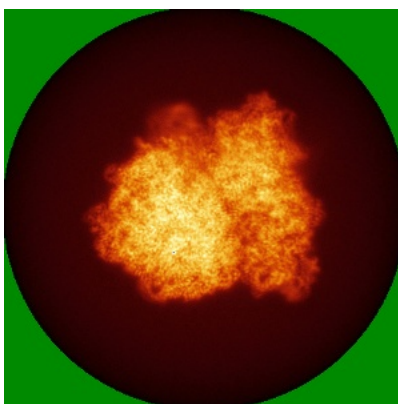


Z

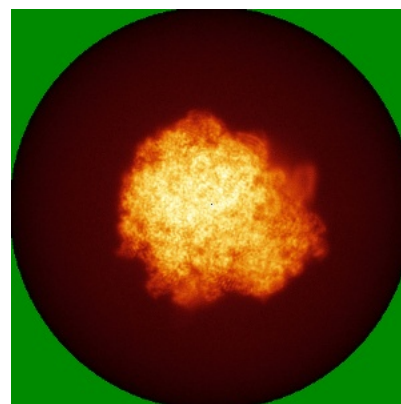
6.4.2 Raw map



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



X



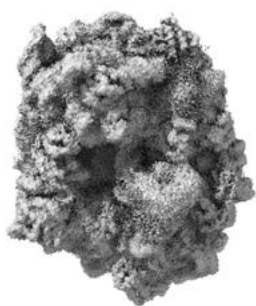
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



X



Y



Z

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.

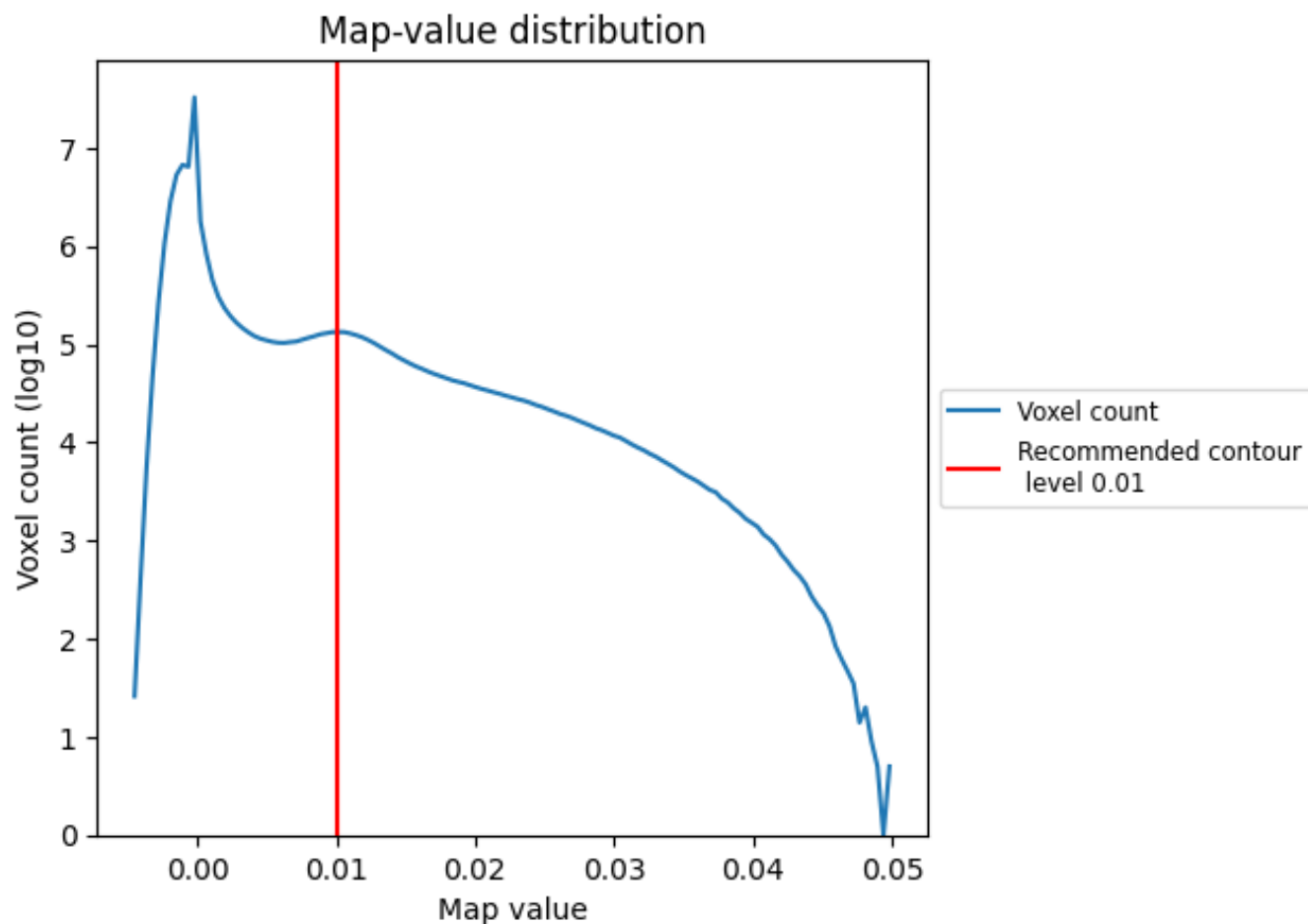
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

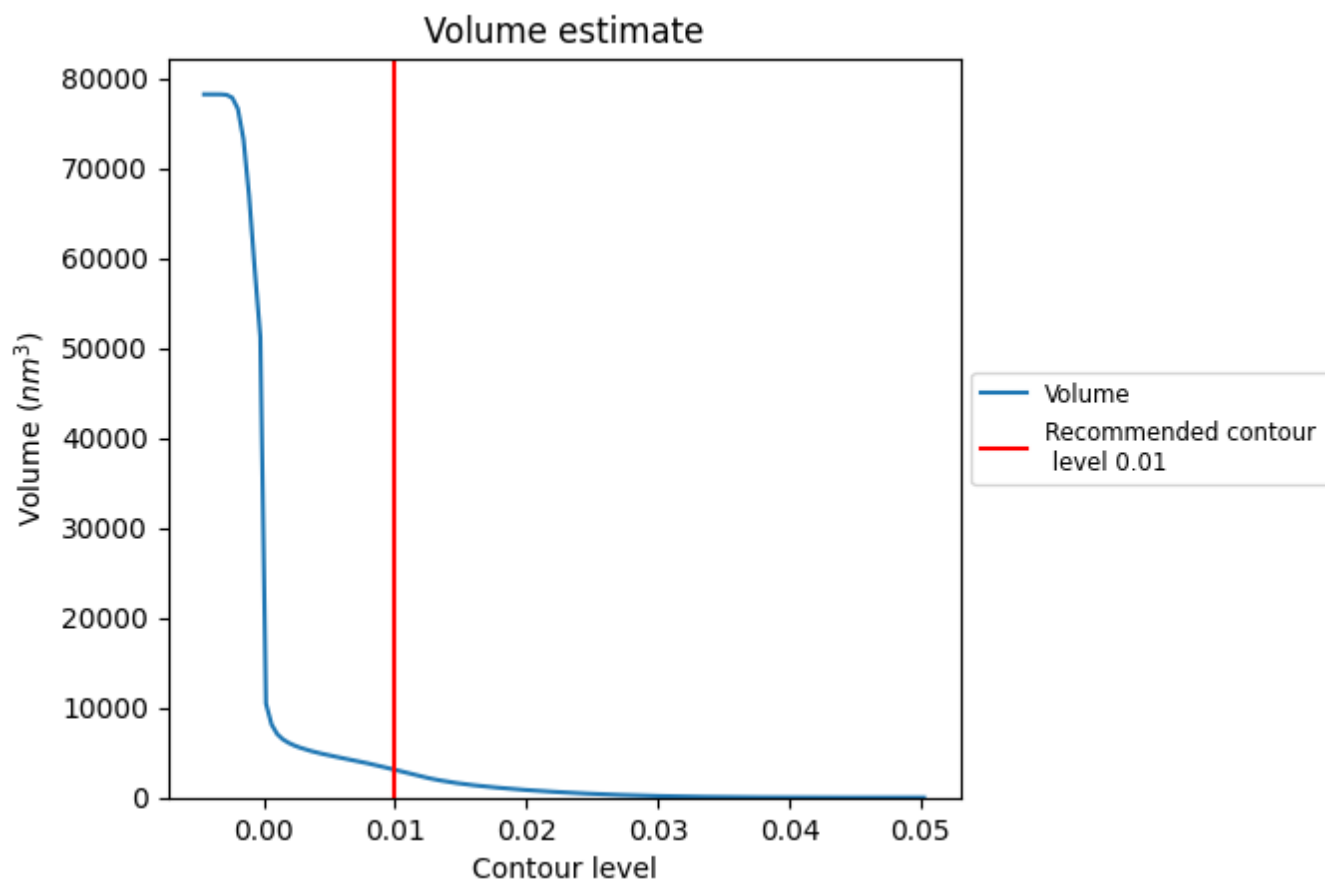
This section contains the results of statistical analysis of the map.

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.

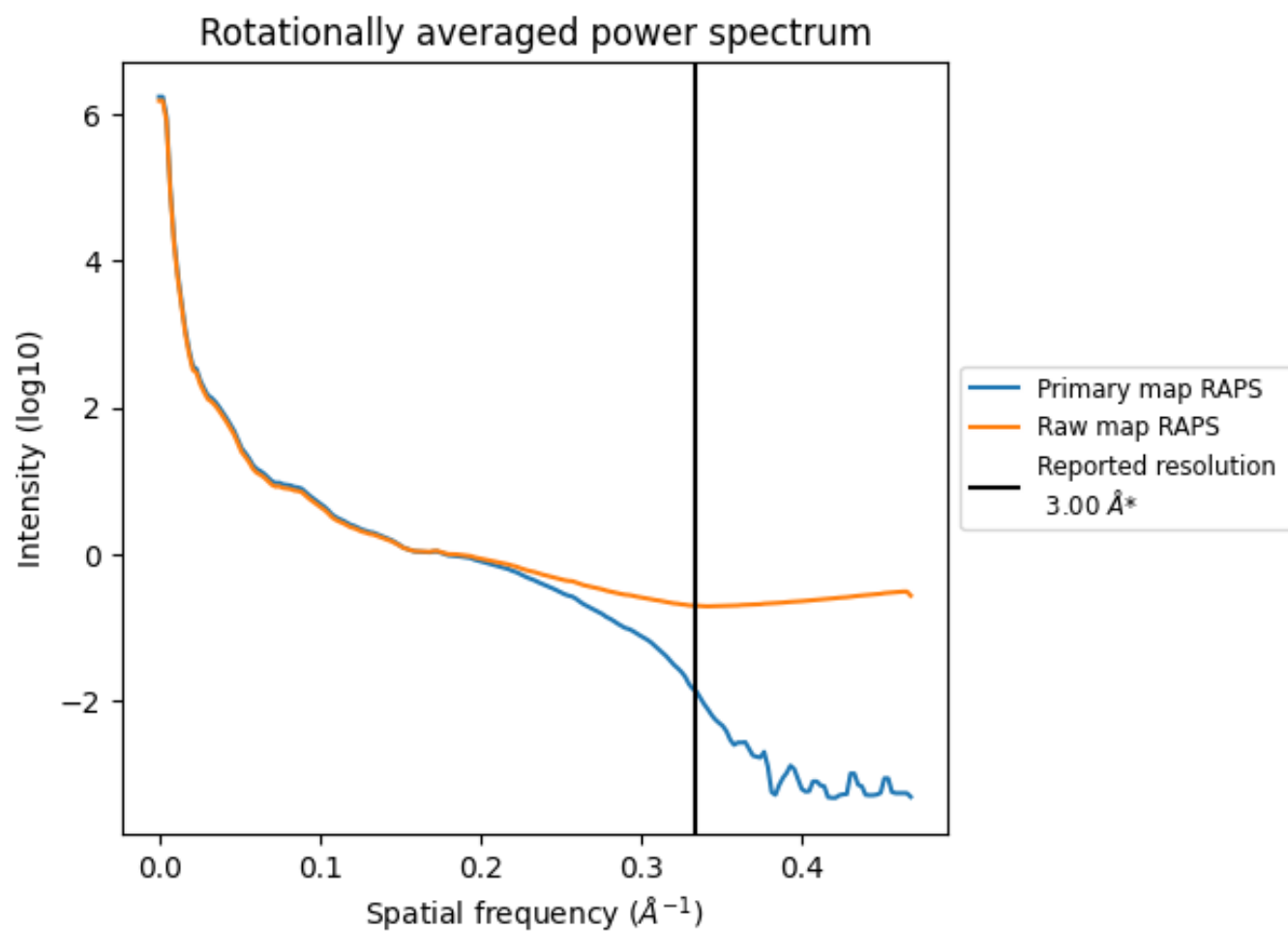
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3079 nm^3 ; this corresponds to an approximate mass of 2781 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 ⓘ

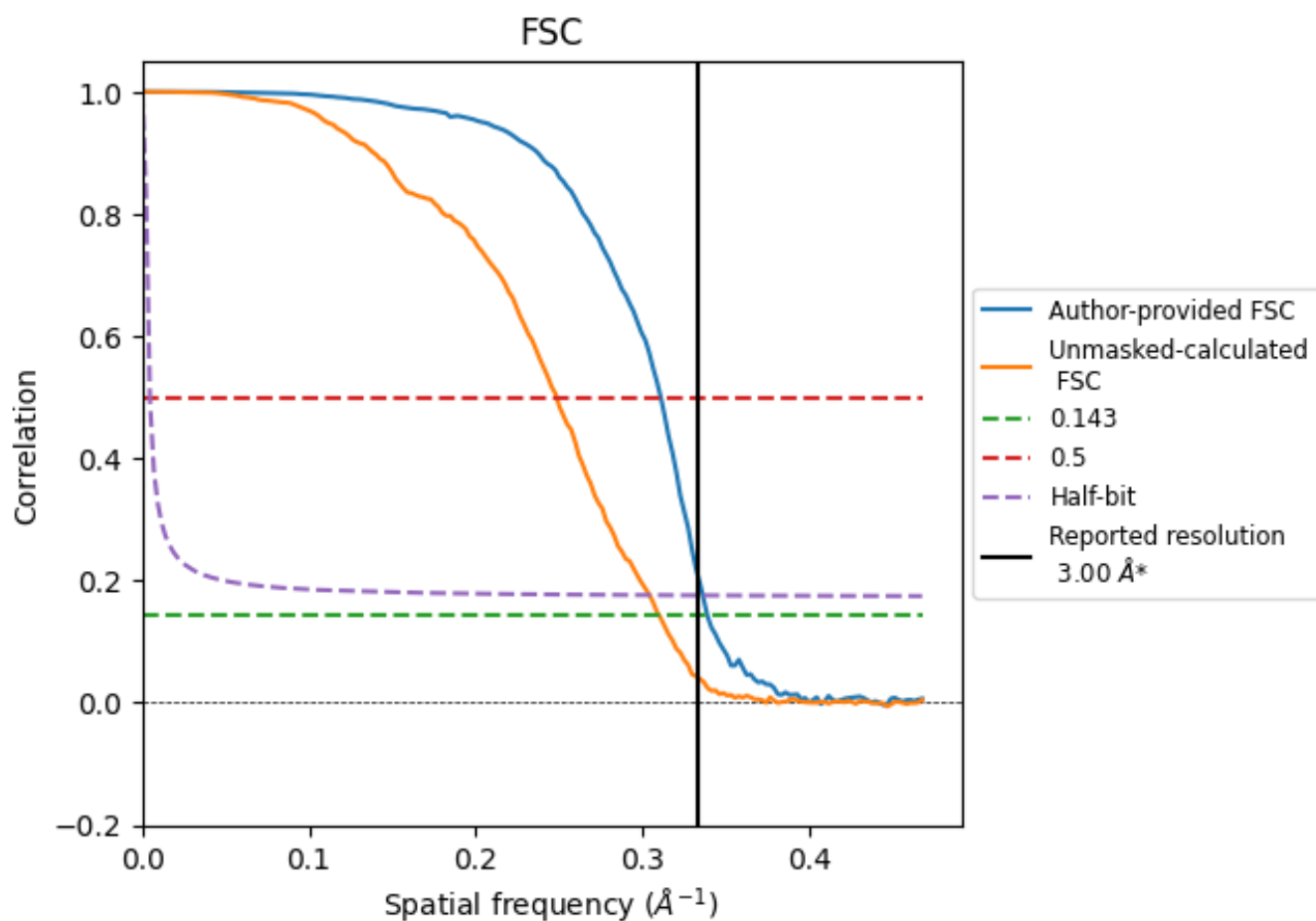


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

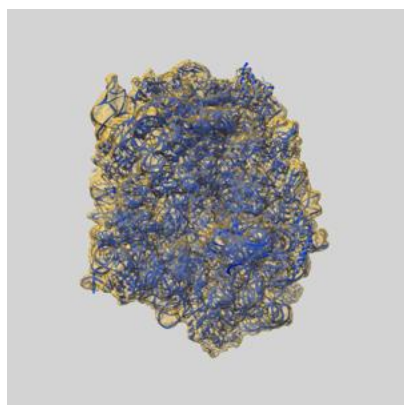
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.95	3.22	2.97
Unmasked-calculated*	3.23	4.02	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

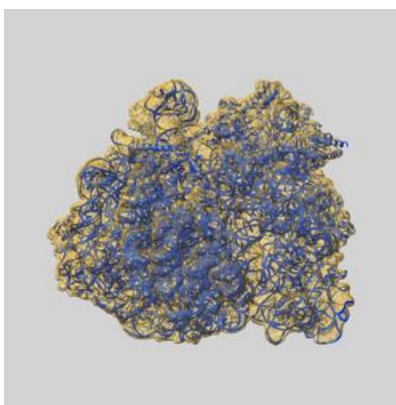
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42495 and PDB model 8URM. Per-residue inclusion information can be found in section [3](#) on page [17](#).

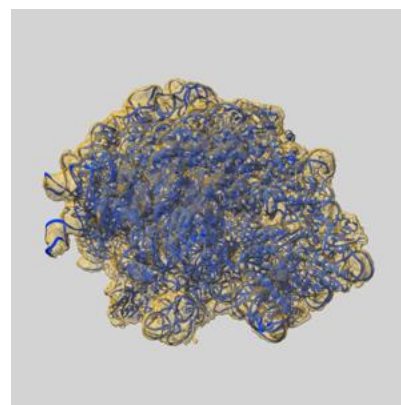
9.1 Map-model overlay [i](#)



X



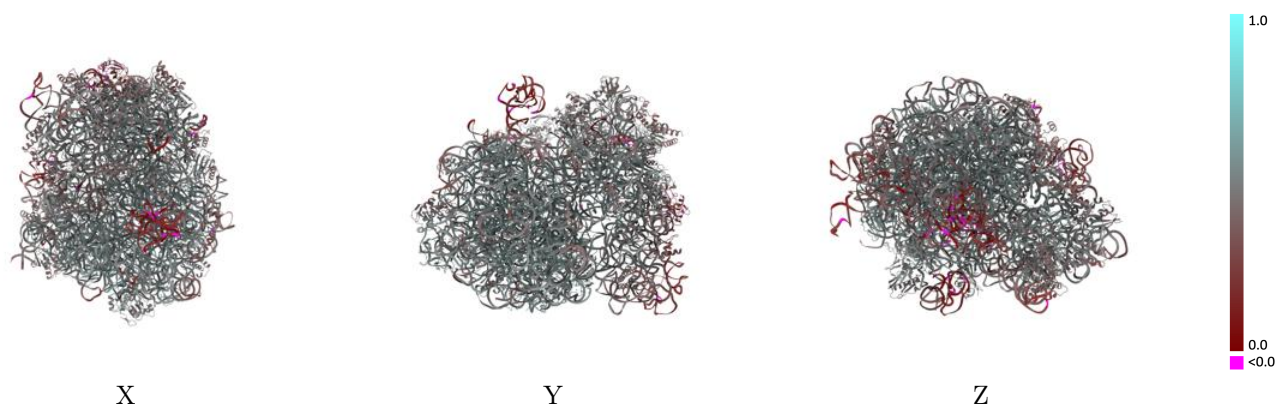
Y



Z

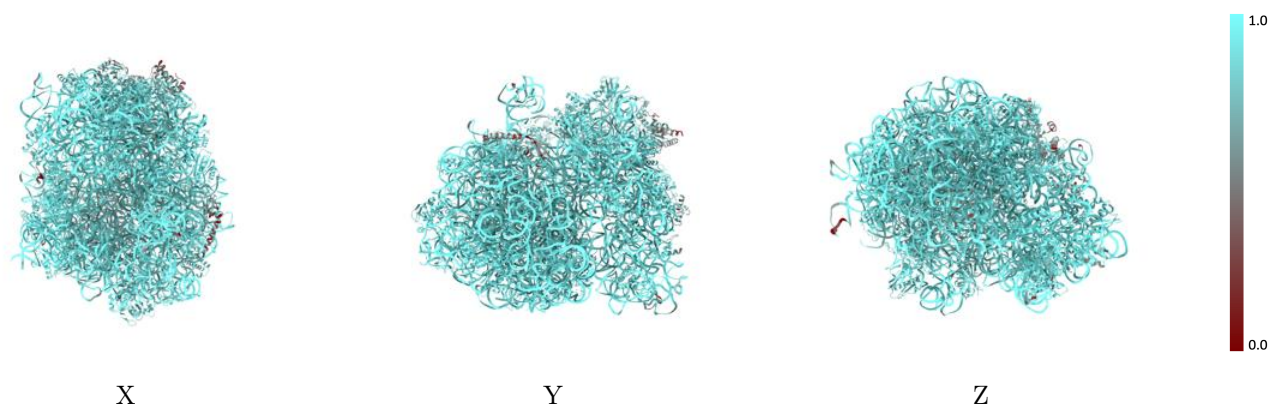
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



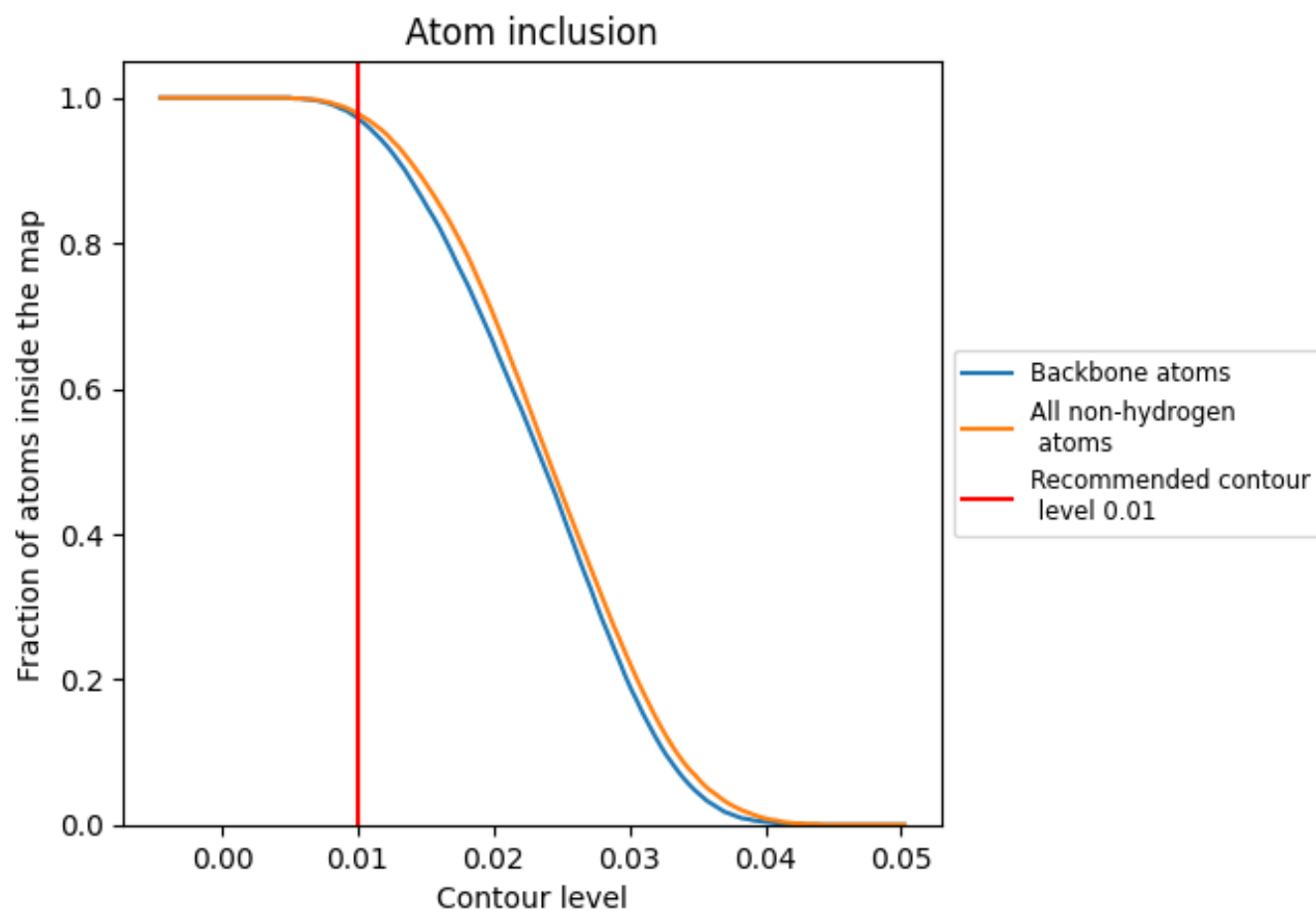
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9780	 0.4770
1	 0.9940	 0.4960
2	 0.9890	 0.4500
3	 0.9900	 0.4650
4	 1.0000	 0.4320
5	 1.0000	 0.4400
6	 0.9980	 0.4250
B	 0.9990	 0.5470
C	 0.9820	 0.5390
D	 0.9490	 0.5030
E	 0.9640	 0.4460
F	 0.9500	 0.4650
G	 0.5800	 0.3770
J	 0.9900	 0.5260
K	 0.9970	 0.5400
L	 0.9730	 0.5220
M	 0.9990	 0.5330
N	 0.9970	 0.5370
O	 0.9540	 0.4720
P	 0.9920	 0.5280
Q	 0.9890	 0.5250
R	 0.9510	 0.5330
S	 0.9870	 0.5270
T	 0.9800	 0.5040
U	 0.9610	 0.5100
V	 0.9430	 0.5020
W	 0.9850	 0.5100
X	 0.9930	 0.5290
Y	 0.9530	 0.4580
Z	 0.9610	 0.5180
a	 0.7910	 0.3930
b	 0.9790	 0.5270
c	 0.9930	 0.5130
d	 1.0000	 0.5440
e	 1.0000	 0.5460



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Chain	Atom inclusion	Q-score
f	 1.0000	 0.5300
g	 0.6850	 0.4190
h	 0.9590	 0.4730
i	 0.8430	 0.2270
j	 0.9860	 0.4950
k	 0.9550	 0.4570
l	 0.9700	 0.4280
m	 0.9660	 0.4960
n	 0.9590	 0.4590
o	 0.9010	 0.4470
p	 0.9890	 0.4850
q	 0.9780	 0.4200
r	 0.9640	 0.4480
s	 0.9820	 0.4750
t	 0.9810	 0.4660
u	 0.9300	 0.3670
v	 0.9760	 0.4520
w	 0.9870	 0.4240
x	 0.9680	 0.4700
y	 0.9740	 0.4180
z	 0.9800	 0.4110