Full wwPDB EM Validation Report

Sep 16, 2026 – 01:31 PM EDT

PDB ID	:	7K00 / pdb_00007k00
EMDB ID	:	EMD-22586
Title	:	Structure of the Bacterial Ribosome at 2 Angstrom Resolution
Authors	:	Watson, Z.L.; Ward, F.R.; Meheust, R.; Ad, O.; Schepartz, A.; Banfield, J.F.; Cate, J.H.D.
Deposited on	:	2020-09-02
Resolution	:	1.98 Å(reported)
Based on initial model	:	4YBB

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 (i) 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 (1)) were used in the production of this report:

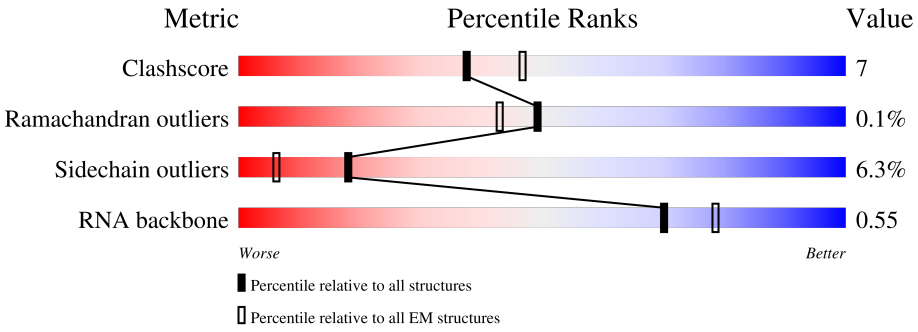
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

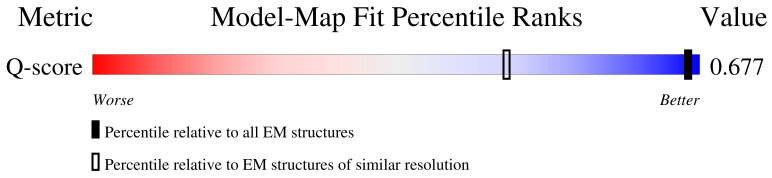
1 Overall quality at a glance

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

The reported resolution of this entry is 1.98 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	1383 (1.50 - 2.48)

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 <=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	A	1542	9% 60% 34% 5% •
2	B	241	44% 71% 19% • 7%
3	C	233	8% 74% 14% • 12%

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Mol	Chain	Length	Quality of chain
4	D	206	42% 69% 25% 5%
5	E	167	72% 20% 7%
6	F	135	12% 50% 26% 24%
7	G	179	20% 61% 21% 15%
8	H	130	78% 22%
9	I	130	8% 81% 16%
10	J	103	41% 67% 26% 5%
11	K	129	7% 66% 21% 9%
12	L	124	11% 77% 19%
13	M	118	7% 75% 20%
14	N	101	5% 84% 15%
15	O	89	7% 81% 17%
16	P	82	26% 78% 21%
17	Q	84	20% 64% 26% 6%
18	R	75	12% 64% 24% 12%
19	S	92	10% 70% 20% 9%
20	T	87	39% 82% 17%
21	U	71	35% 69% 27%
22	a	2904	5% 62% 28% 5% 5%
23	b	120	72% 25%
24	c	273	83% 16%
25	d	209	88% 12%
26	e	201	15% 77% 21%
27	f	179	7% 73% 23%
28	g	177	72% 60% 33% 5%

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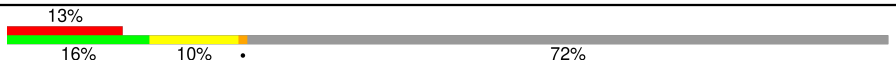
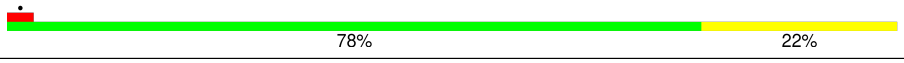
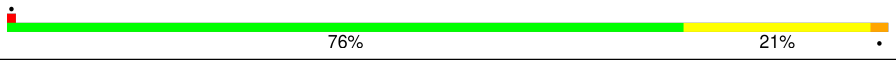
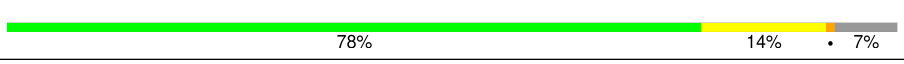
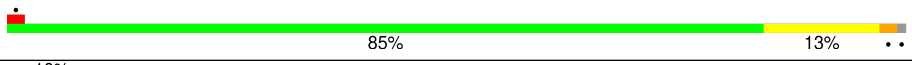
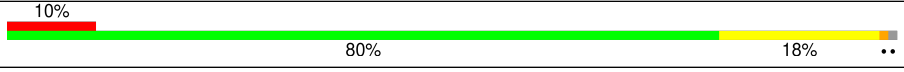
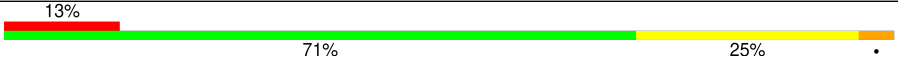
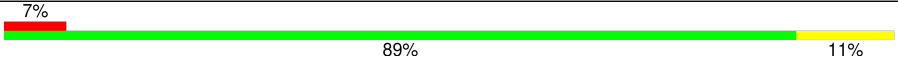
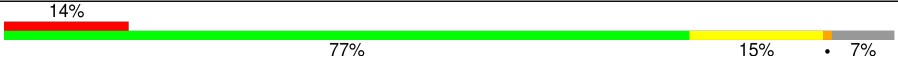
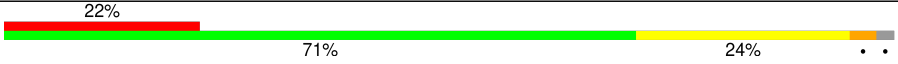
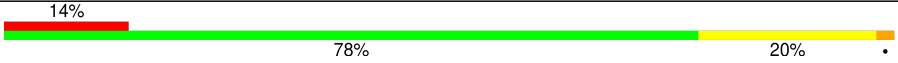
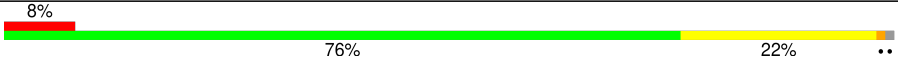
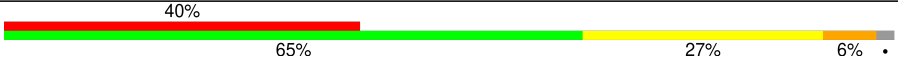
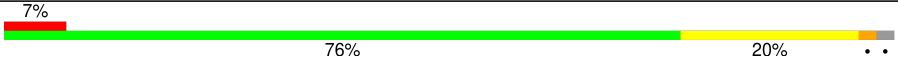
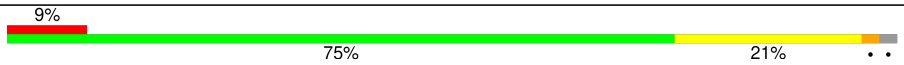
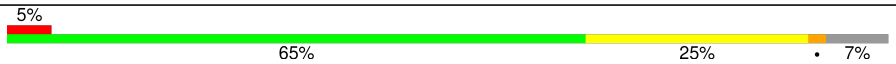
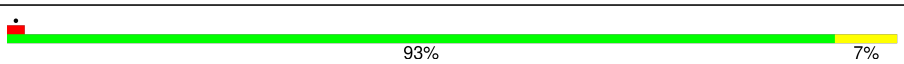
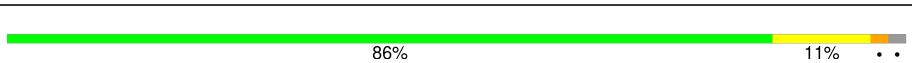
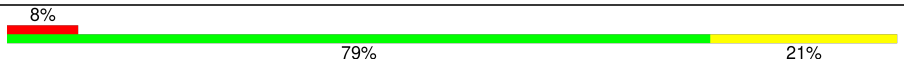
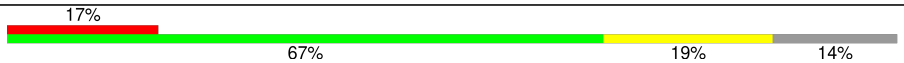
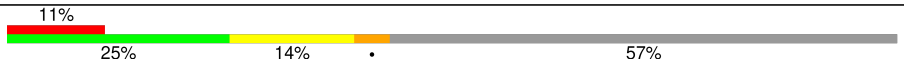
Mol	Chain	Length	Quality of chain
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
46	y	59	
47	z	57	
48	0	55	
49	1	46	
50	2	65	
51	3	38	
52	4	70	
53	X	28	

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Mol	Chain	Length	Quality of chain
54	Y	76	64% 28% 33% 37%
55	Z	76	41% 34% 49% 17%
56	5	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	SPD	a	6210	-	-	X	-
59	SPD	a	6215	-	-	X	-
59	SPD	a	6216	-	-	X	-
60	SPM	a	6223	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 149338 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1519	32612	14552	5986	10555	1519	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1753	1109	315	321	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1624	1028	305	288	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	103	839	530	151	151	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP S1ELC2

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP L4V2J8

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	t	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
48	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	12	Total	C	N	O	P	0	0
			260	117	51	80	12		

- Molecule 54 is a RNA chain called A-site tRNA-val.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Y	74	Total	C	N	O	P	0	0
			1579	705	287	514	73		

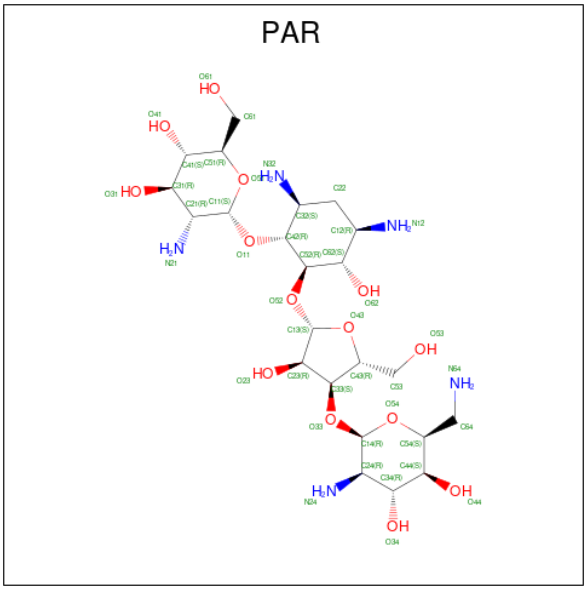
- Molecule 55 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				AltConf
57	A	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	A	93	Total	Mg	0
			93	93	

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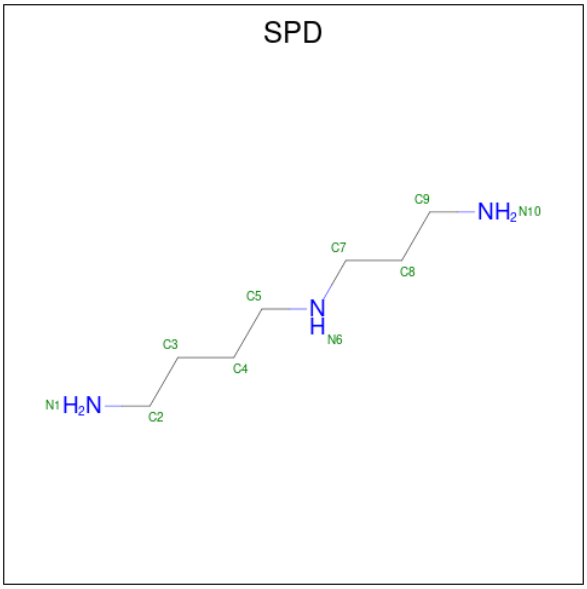
Mol	Chain	Residues	Atoms	AltConf
58	a	208	Total Mg 208 208	0
58	b	5	Total Mg 5 5	0
58	c	1	Total Mg 1 1	0
58	d	1	Total Mg 1 1	0
58	z	1	Total Mg 1 1	0

- Molecule 59 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
59	A	1	Total C N 10 7 3	0
59	A	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0

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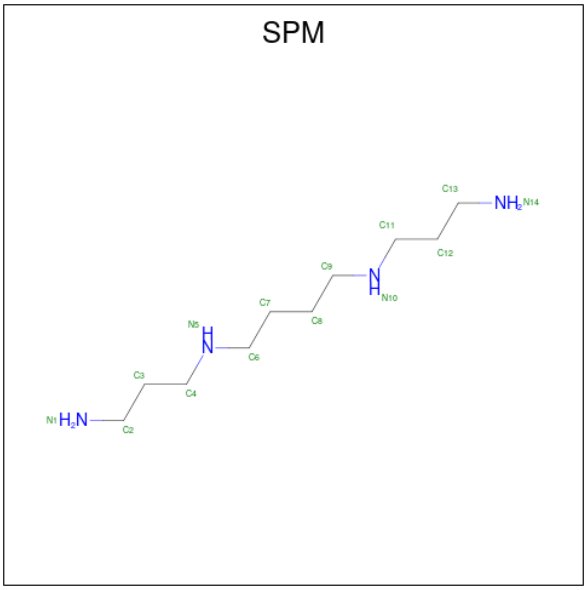
Mol	Chain	Residues	Atoms	AltConf
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0

- Molecule 60 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
60	a	1	Total C N 14 10 4	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
61	3	1	Total Zn 1 1	0
61	4	1	Total Zn 1 1	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	AltConf
62	A	2063	Total O 2063 2063	0
62	B	1	Total O 1 1	0
62	C	46	Total O 46 46	0
62	D	11	Total O 11 11	0
62	E	15	Total O 15 15	0
62	G	5	Total O 5 5	0
62	H	28	Total O 28 28	0
62	I	21	Total O 21 21	0
62	J	15	Total O 15 15	0
62	K	12	Total O 12 12	0
62	L	23	Total O 23 23	0
62	M	18	Total O 18 18	0
62	N	31	Total O 31 31	0
62	O	11	Total O 11 11	0
62	P	10	Total O 10 10	0
62	Q	4	Total O 4 4	0
62	R	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
62	S	24	Total O 24 24	0
62	T	3	Total O 3 3	0
62	U	5	Total O 5 5	0
62	a	4028	Total O 4028 4028	0
62	b	171	Total O 171 171	0
62	c	100	Total O 100 100	0
62	d	38	Total O 38 38	0
62	e	48	Total O 48 48	0
62	f	30	Total O 30 30	0
62	h	6	Total O 6 6	0
62	i	14	Total O 14 14	0
62	j	17	Total O 17 17	0
62	k	50	Total O 50 50	0
62	l	27	Total O 27 27	0
62	m	33	Total O 33 33	0
62	n	42	Total O 42 42	0
62	o	12	Total O 12 12	0
62	p	33	Total O 33 33	0
62	q	20	Total O 20 20	0
62	r	20	Total O 20 20	0
62	s	11	Total O 11 11	0

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Mol	Chain	Residues	Atoms	AltConf
62	t	3	Total O 3 3	0
62	u	4	Total O 4 4	0
62	v	18	Total O 18 18	0
62	w	23	Total O 23 23	0
62	x	2	Total O 2 2	0
62	y	6	Total O 6 6	0
62	z	25	Total O 25 25	0
62	0	7	Total O 7 7	0
62	1	33	Total O 33 33	0
62	2	24	Total O 24 24	0
62	3	3	Total O 3 3	0
62	4	6	Total O 6 6	0
62	X	15	Total O 15 15	0
62	Y	13	Total O 13 13	0
62	Z	19	Total O 19 19	0

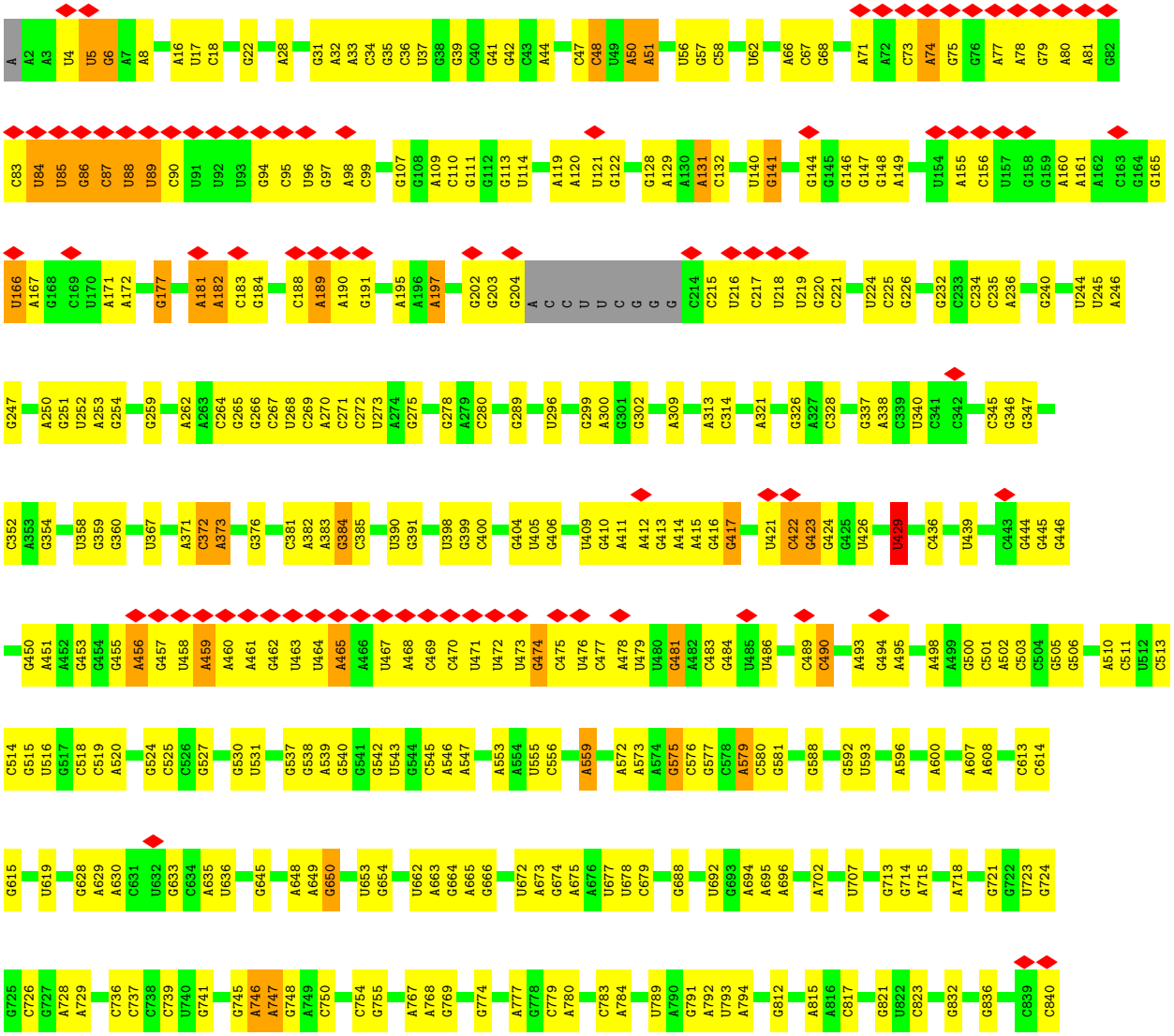
3 Residue-property plots (i)

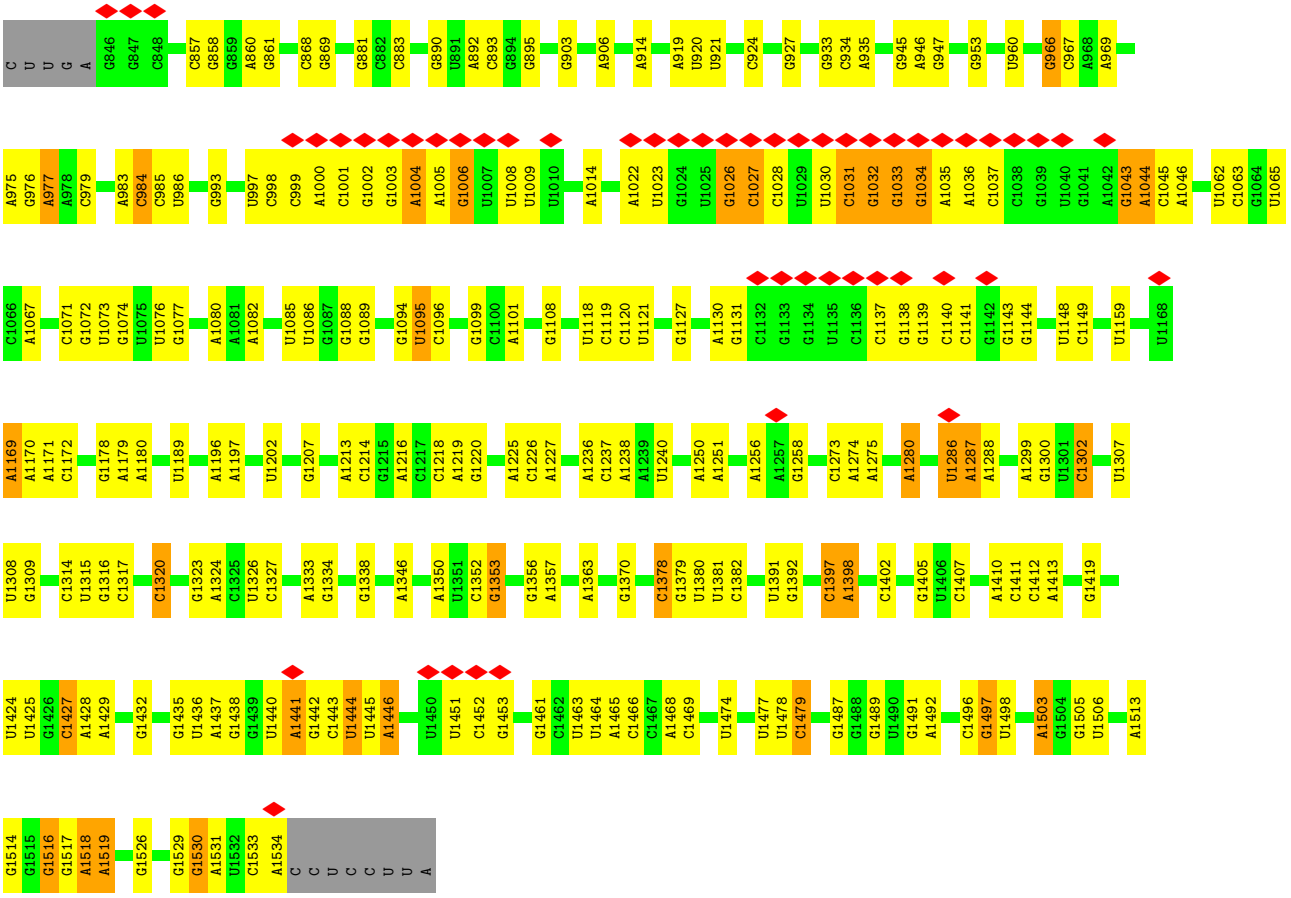
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 16S rRNA

Chain A:



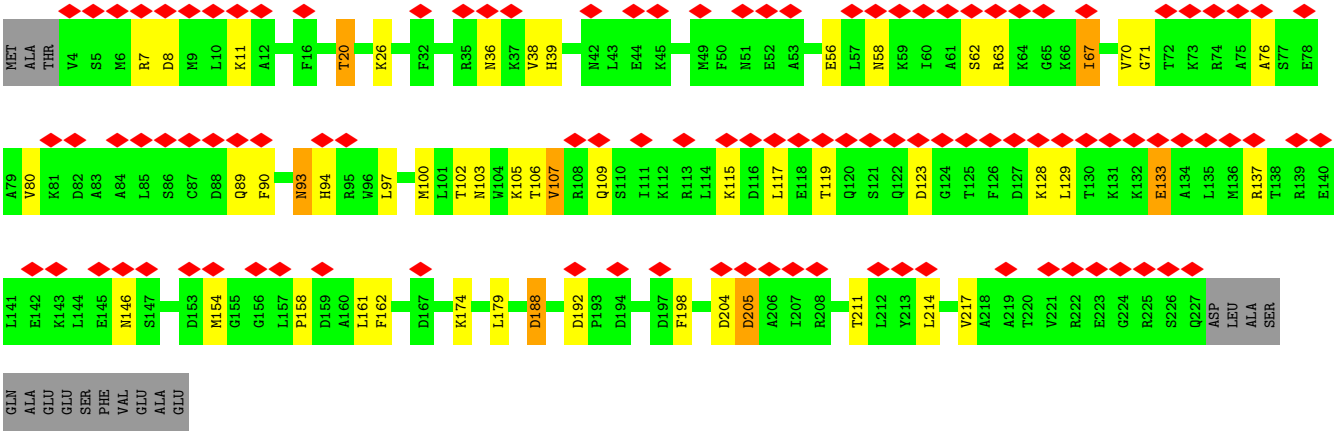




• Molecule 2: 30S ribosomal protein S2

Chain B:

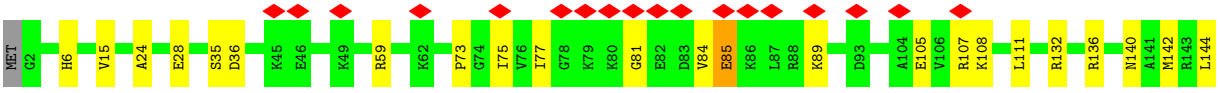


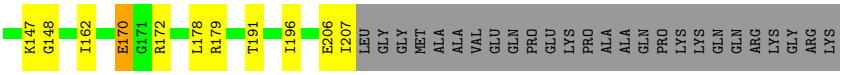


• Molecule 3: 30S ribosomal protein S3

Chain C:



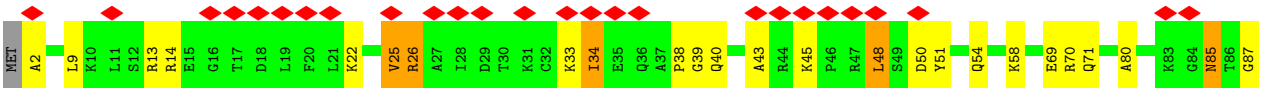


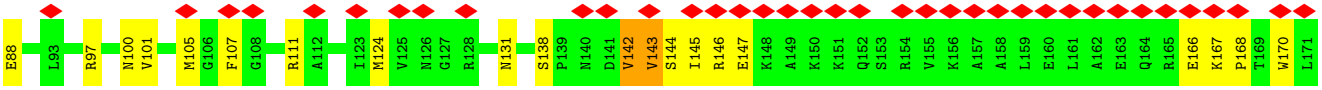


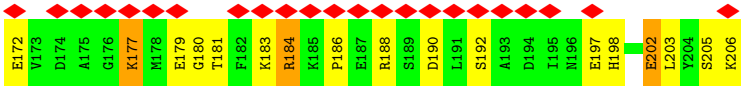
• Molecule 4: 30S ribosomal protein S4

Chain D:





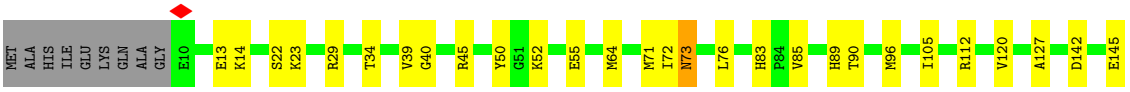


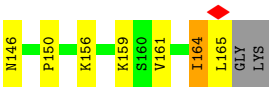


• Molecule 5: 30S ribosomal protein S5

Chain E:



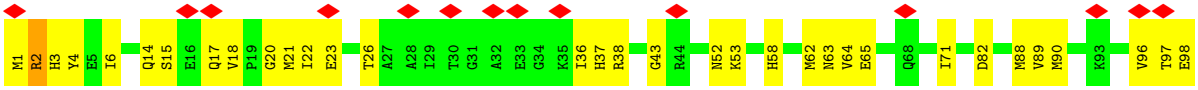


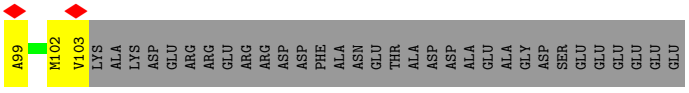


• Molecule 6: 30S ribosomal protein S6

Chain F:



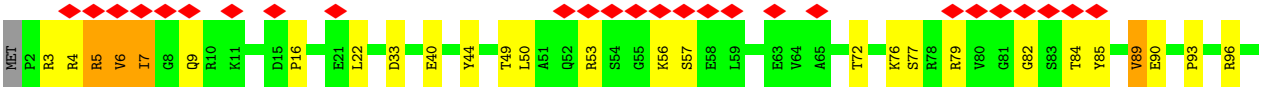


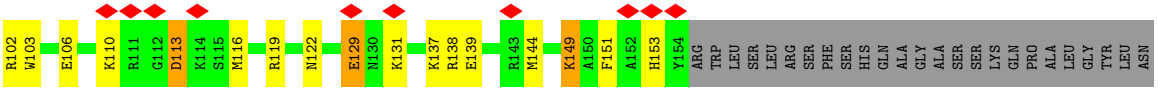


• Molecule 7: 30S ribosomal protein S7

Chain G:



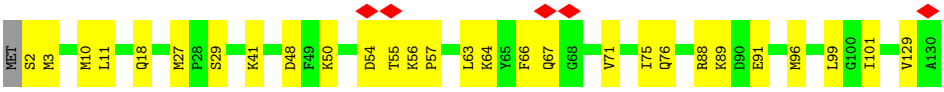




• Molecule 8: 30S ribosomal protein S8

Chain H:

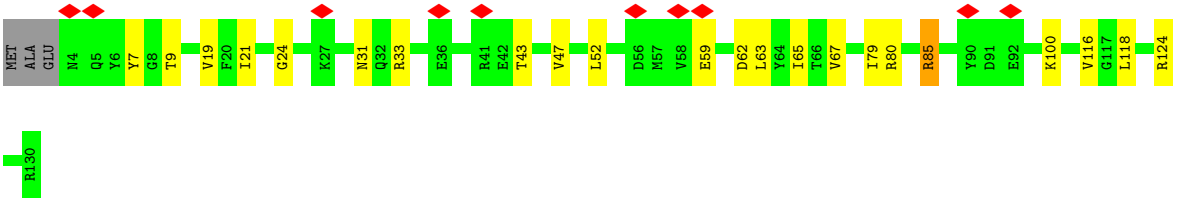




• Molecule 9: 30S ribosomal protein S9

Chain I:

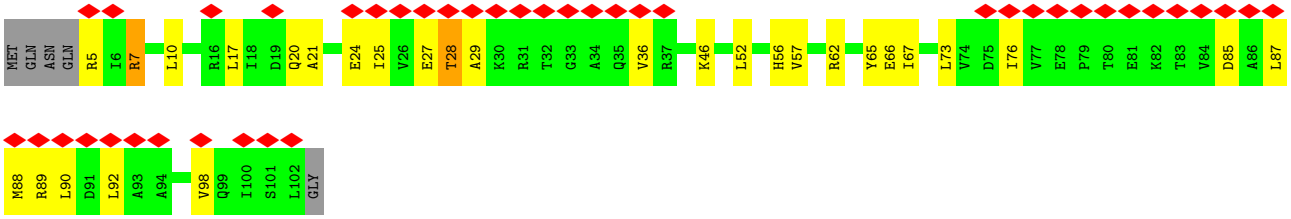




• Molecule 10: 30S ribosomal protein S10

Chain J:

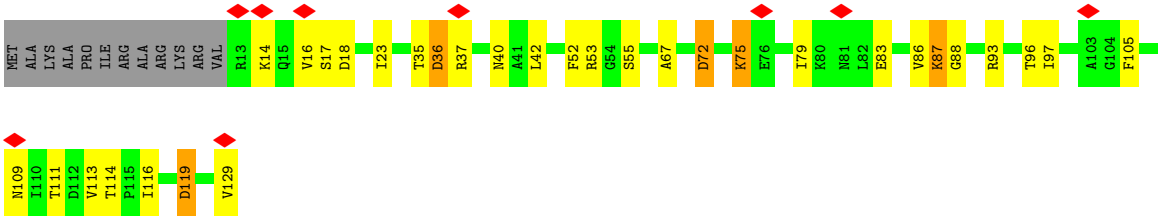




• Molecule 11: 30S ribosomal protein S11

Chain K:

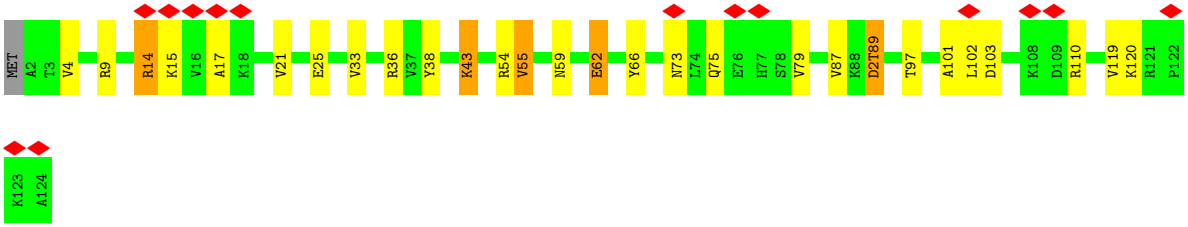




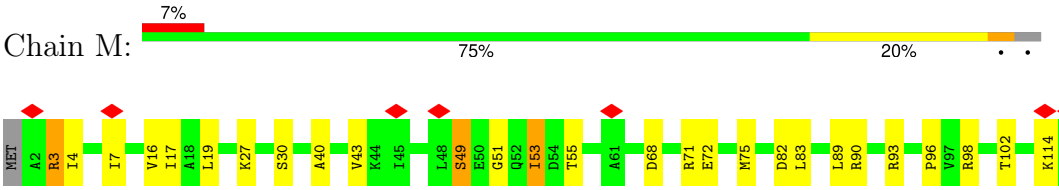
• Molecule 12: 30S ribosomal protein S12

Chain L:

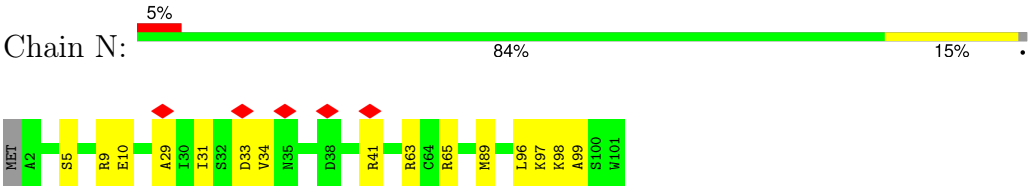




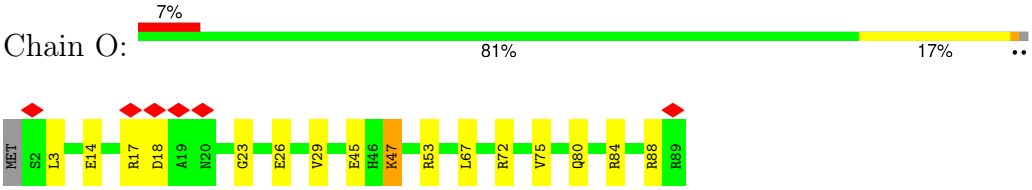
• Molecule 13: 30S ribosomal protein S13



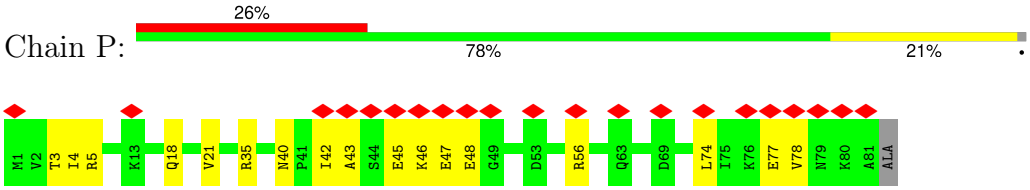
• Molecule 14: 30S ribosomal protein S14



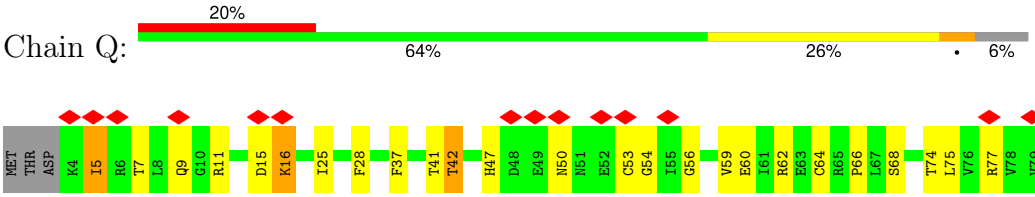
• Molecule 15: 30S ribosomal protein S15



• Molecule 16: 30S ribosomal protein S16

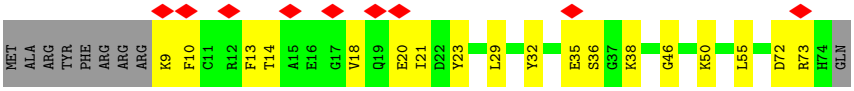


• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

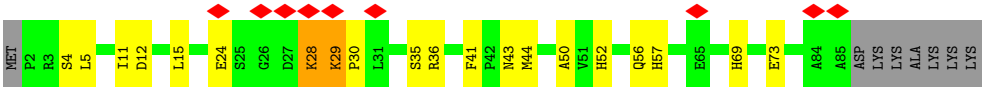




• Molecule 19: 30S ribosomal protein S19

Chain S:

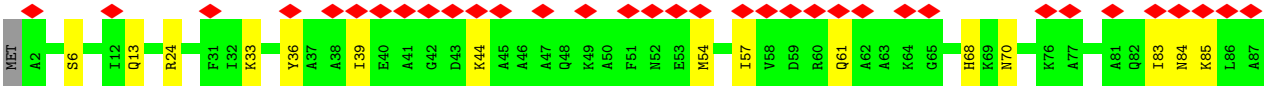




• Molecule 20: 30S ribosomal protein S20

Chain T:

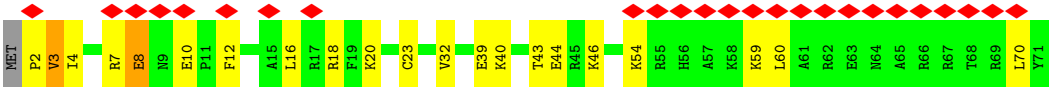




• Molecule 21: 30S ribosomal protein S21

Chain U:

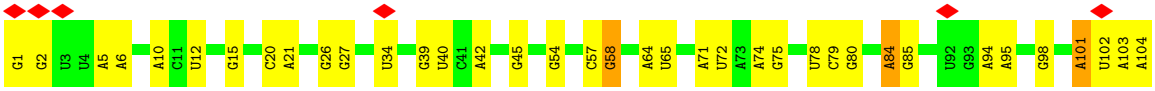


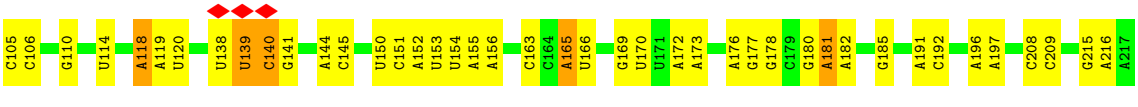


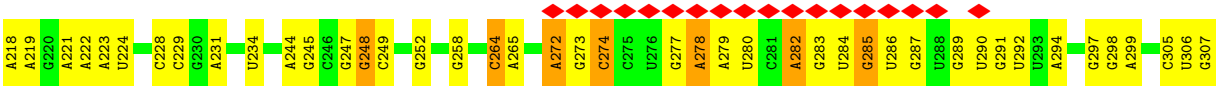
• Molecule 22: 23S rRNA

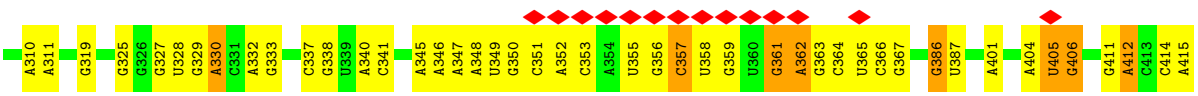
Chain a:

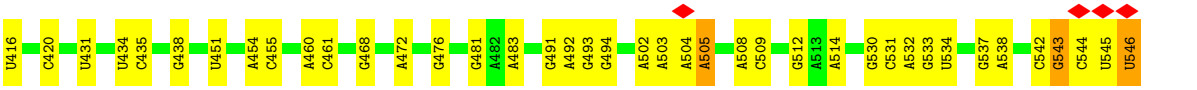


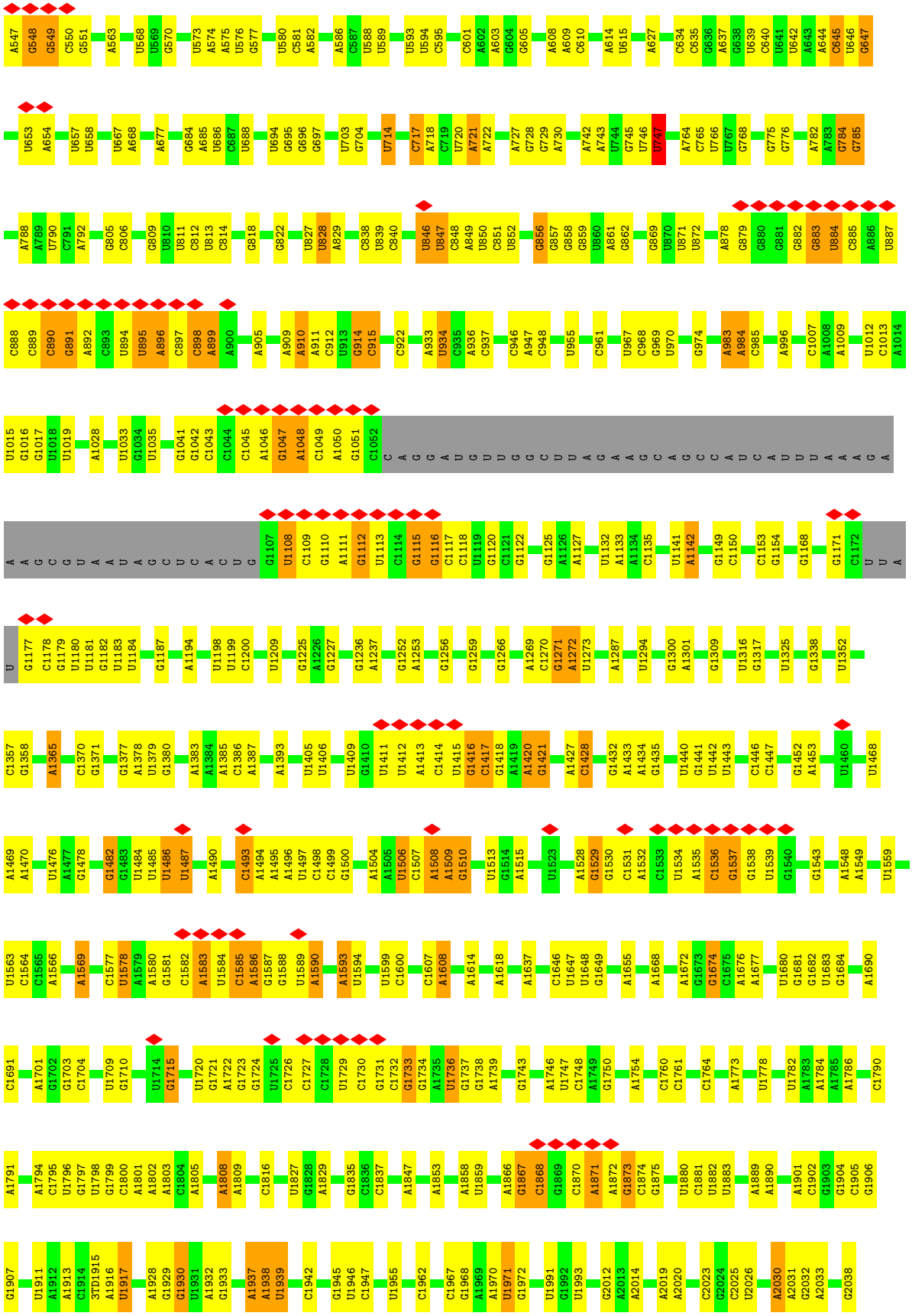


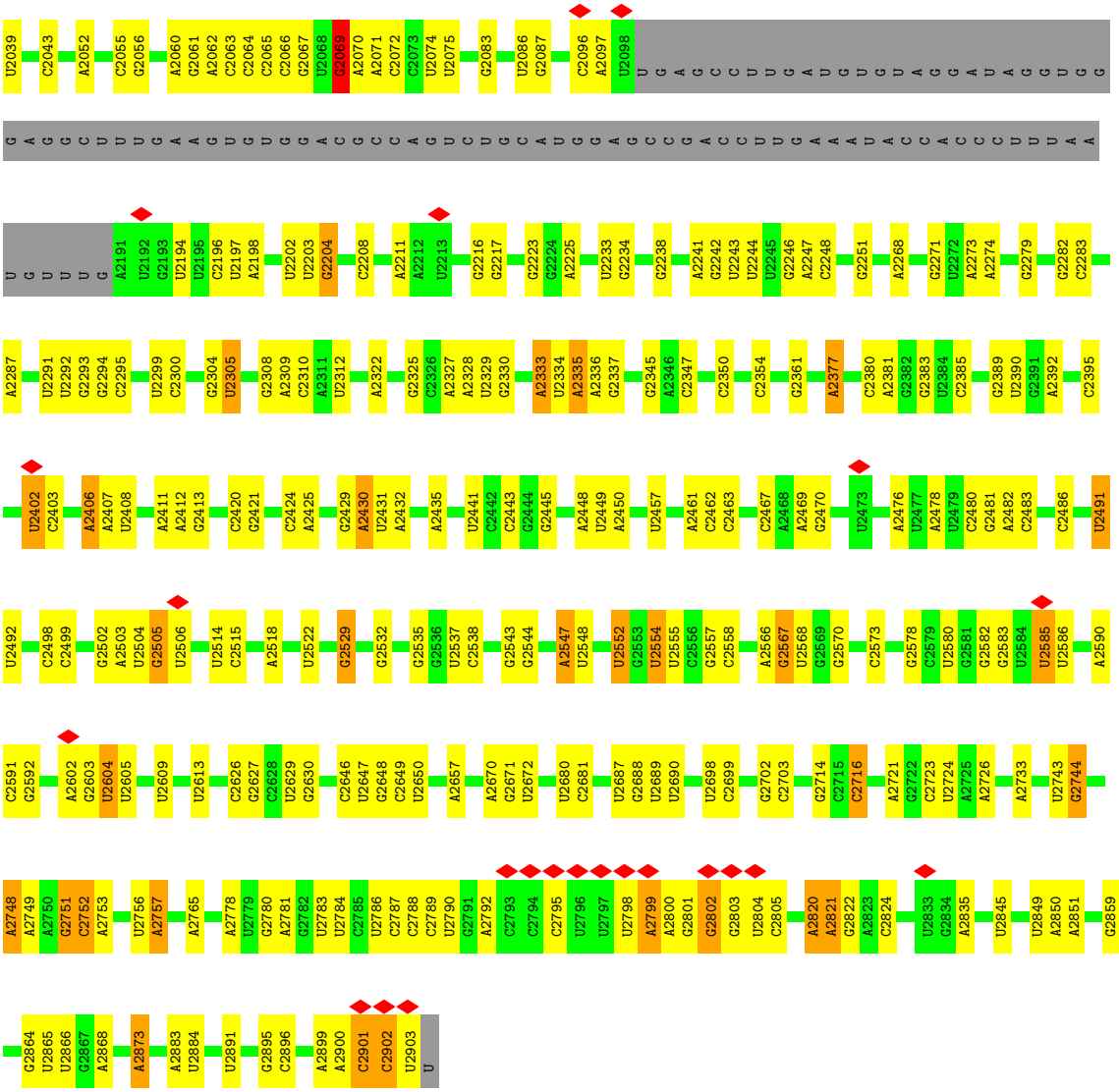












• Molecule 23: 5S rRNA

Chain b:

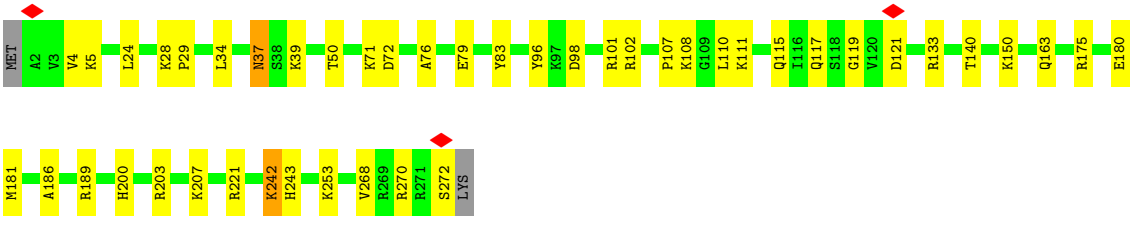




• Molecule 24: 50S ribosomal protein L2

Chain c:

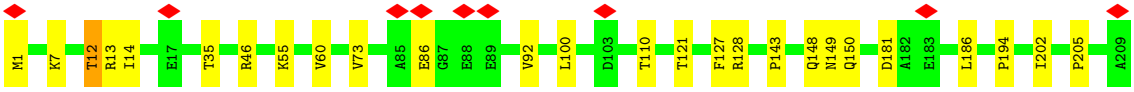




• Molecule 25: 50S ribosomal protein L3

Chain d:

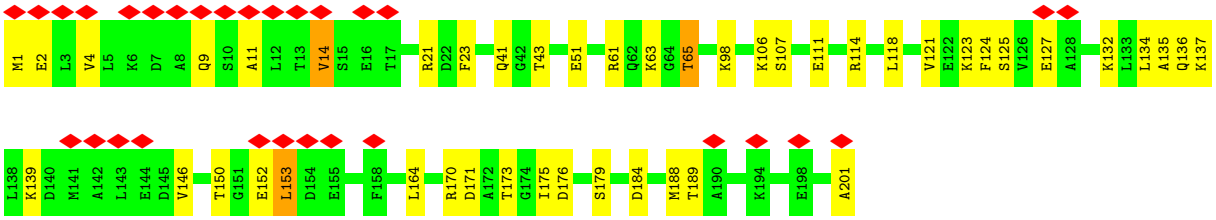




• Molecule 26: 50S ribosomal protein L4

Chain e:

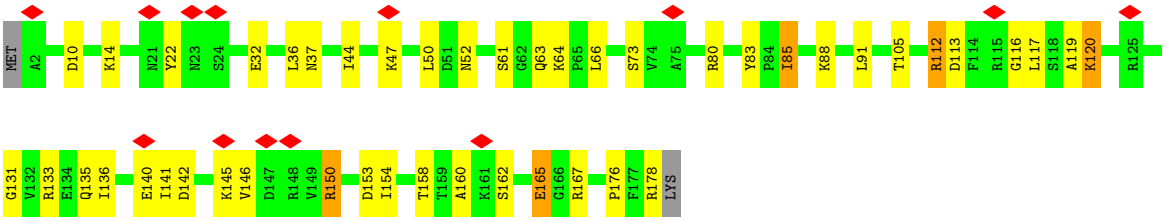




• Molecule 27: 50S ribosomal protein L5

Chain f:

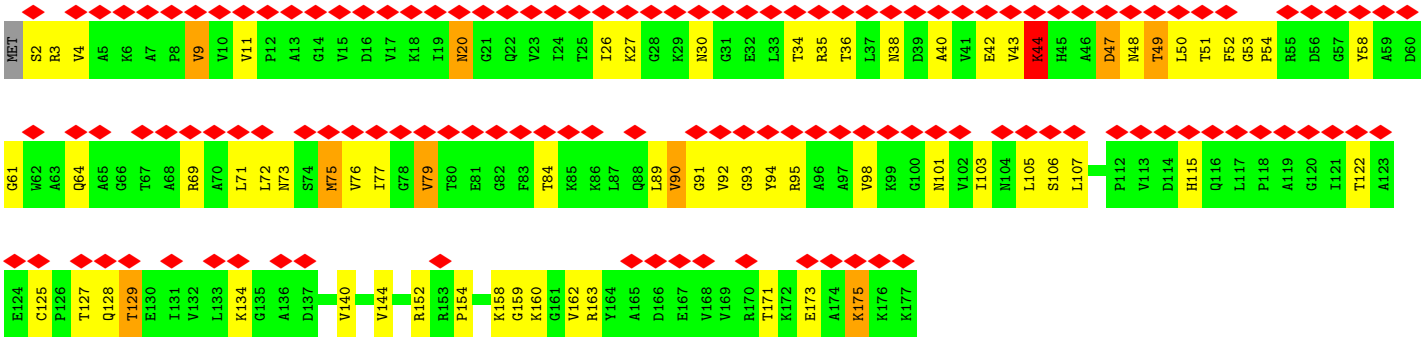




• Molecule 28: 50S ribosomal protein L6

Chain g:

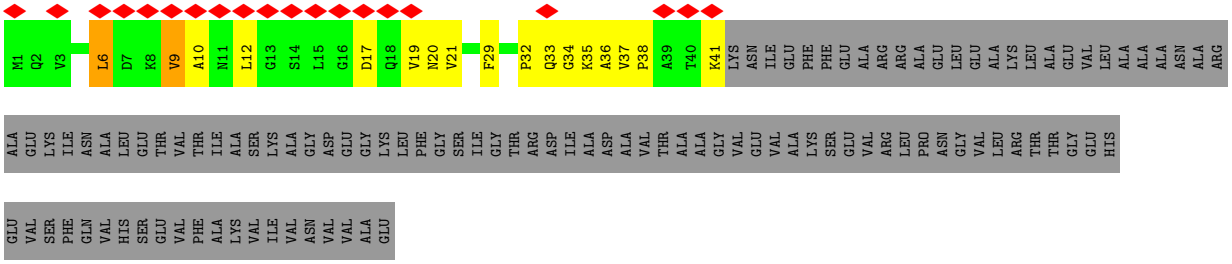




• Molecule 29: 50S ribosomal protein L9

Chain h:

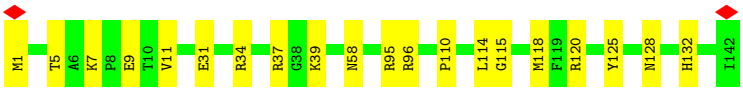




• Molecule 30: 50S ribosomal protein L13

Chain i:

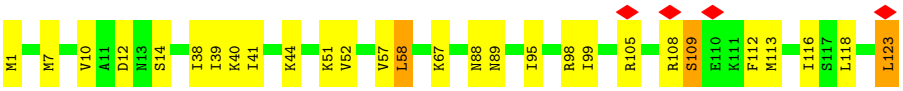




• Molecule 31: 50S ribosomal protein L14

Chain j:

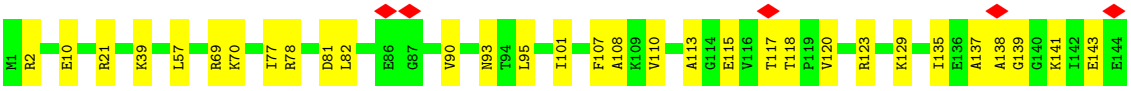




• Molecule 32: 50S ribosomal protein L15

Chain k:

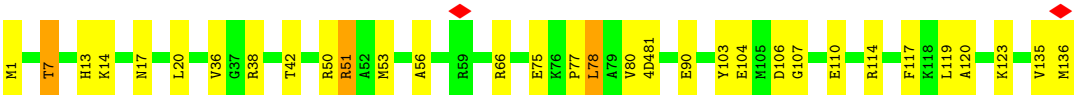




• Molecule 33: 50S ribosomal protein L16

Chain l:





• Molecule 34: 50S ribosomal protein L17

Chain m:





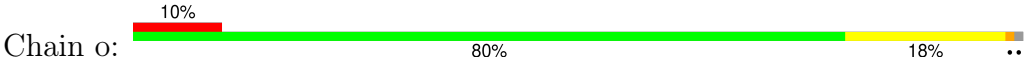
• Molecule 35: 50S ribosomal protein L18

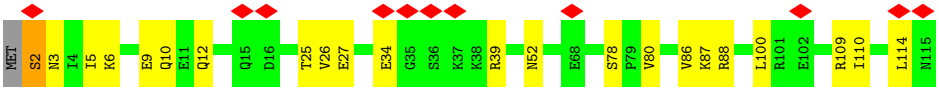
Chain n:



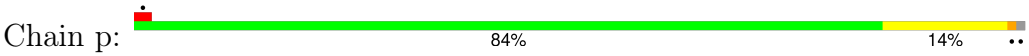


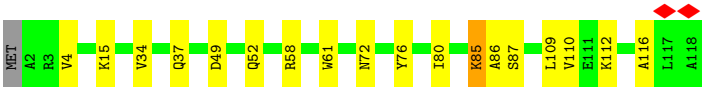
• Molecule 36: 50S ribosomal protein L19





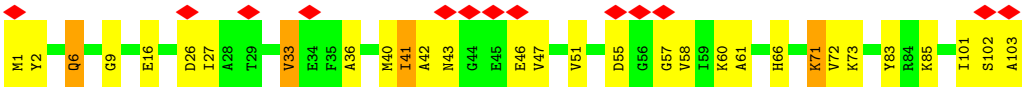
• Molecule 37: 50S ribosomal protein L20



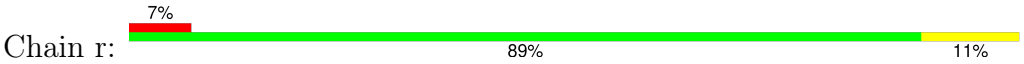


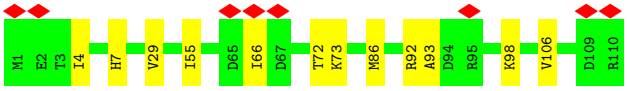
• Molecule 38: 50S ribosomal protein L21





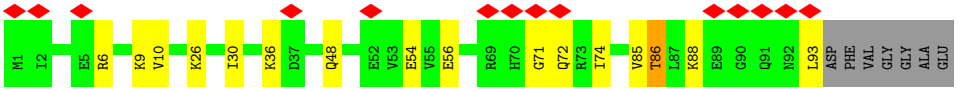
• Molecule 39: 50S ribosomal protein L22





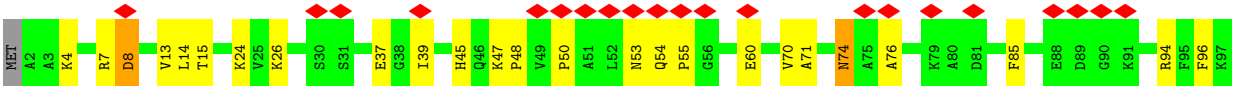
• Molecule 40: 50S ribosomal protein L23

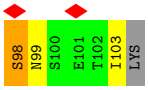




• Molecule 41: 50S ribosomal protein L24



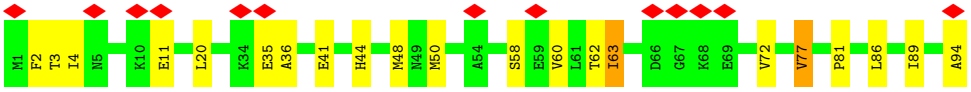




• Molecule 42: 50S ribosomal protein L25

Chain u:

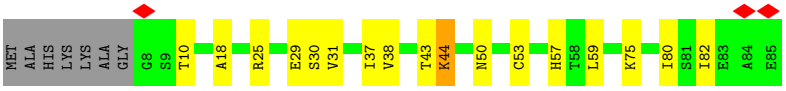




• Molecule 43: 50S ribosomal protein L27

Chain v:

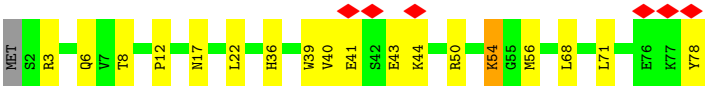




• Molecule 44: 50S ribosomal protein L28

Chain w:

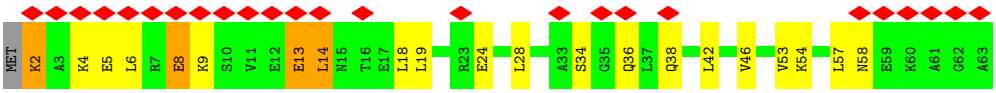




• Molecule 45: 50S ribosomal protein L29

Chain x:

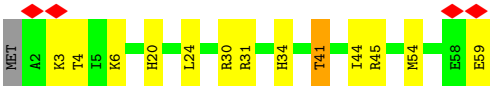




• Molecule 46: 50S ribosomal protein L30

Chain y:

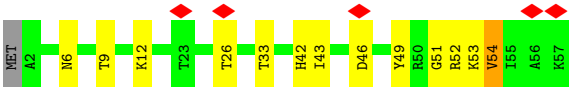




• Molecule 47: 50S ribosomal protein L32

Chain z:

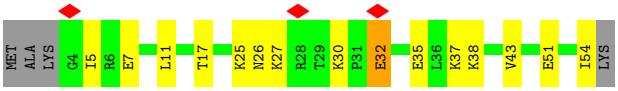




• Molecule 48: 50S ribosomal protein L33

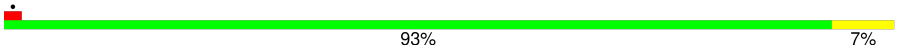
Chain 0:

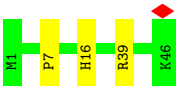




• Molecule 49: 50S ribosomal protein L34

Chain 1:





• Molecule 50: 50S ribosomal protein L35

Chain 2:

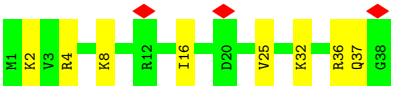




• Molecule 51: 50S ribosomal protein L36

Chain 3:

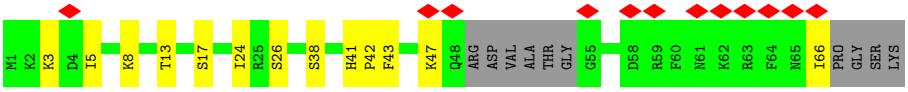




• Molecule 52: 50S ribosomal protein L31

Chain 4:

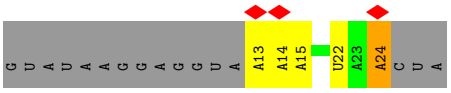




• Molecule 53: mRNA

Chain X:

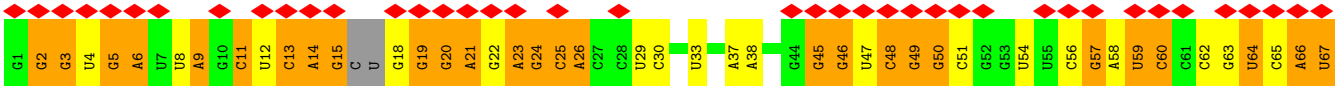


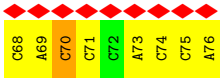


• Molecule 54: A-site tRNA-val

Chain Y:



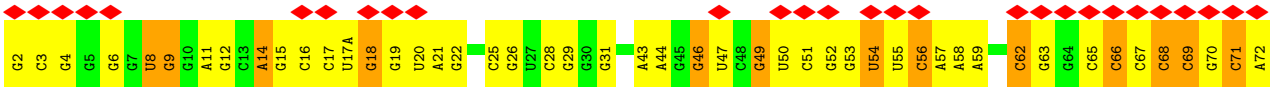




• Molecule 55: P-site tRNA-fMet

Chain Z:

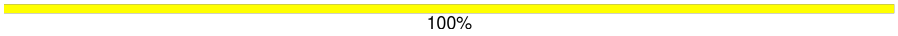






• Molecule 56: E-site tRNA

Chain 5:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	307495	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.341	Depositor
Minimum map value	-0.098	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	353.0528, 353.0528, 353.0528	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7118, 0.7118, 0.7118	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D2T, 4OC, IAS, MEQ, MA6, 1MG, G7M, PSU, SPD, OMG, 4D4, 5MC, ZN, OMU, MS6, 2MA, 3TD, 6MZ, SPM, MG, 5MU, PAR, UR3, OMC, 2MG, H2U

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	A	0.26	0/36236	0.42	1/56520 (0.0%)
2	B	0.29	0/1784	0.52	0/2403
3	C	0.24	0/1651	0.44	0/2225
4	D	0.33	0/1665	0.52	0/2227
5	E	0.32	0/1165	0.57	0/1568
6	F	0.39	0/858	0.65	0/1160
7	G	0.36	0/1219	0.56	0/1635
8	H	0.26	0/989	0.47	0/1326
9	I	0.31	0/1034	0.47	0/1375
10	J	0.36	0/796	0.61	0/1077
11	K	0.34	0/884	0.51	0/1191
12	L	0.32	0/960	0.58	1/1286 (0.1%)
13	M	0.53	0/900	0.75	0/1204
14	N	0.30	0/817	0.50	0/1088
15	O	0.42	0/722	0.63	0/964
16	P	0.26	0/653	0.55	0/877
17	Q	0.34	0/650	0.61	0/871
18	R	0.41	0/553	0.62	0/742
19	S	0.43	0/685	0.63	0/922
20	T	0.29	0/676	0.49	0/895
21	U	0.30	0/597	0.50	0/792
22	a	0.33	1/65651 (0.0%)	0.50	3/102413 (0.0%)
23	b	0.30	0/2850	0.44	2/4444 (0.0%)
24	c	0.38	0/2121	0.62	0/2852
25	d	0.28	0/1576	0.50	0/2119
26	e	0.32	0/1571	0.55	0/2113
27	f	0.32	0/1434	0.53	0/1926
28	g	0.29	0/1343	0.65	2/1816 (0.1%)
29	h	0.41	0/306	0.66	0/413
30	i	0.29	0/1152	0.48	0/1551
31	j	0.29	0/955	0.54	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	k	0.40	0/1062	0.65	0/1413
33	l	0.40	0/1073	0.69	1/1433 (0.1%)
34	m	0.34	0/958	0.58	0/1281
35	n	0.30	0/902	0.58	0/1209
36	o	0.30	0/929	0.56	0/1242
37	p	0.36	0/960	0.56	0/1278
38	q	0.35	0/829	0.62	0/1107
39	r	0.29	0/864	0.50	0/1156
40	s	0.33	0/744	0.60	0/994
41	t	0.32	0/787	0.62	0/1051
42	u	0.32	0/766	0.55	0/1025
43	v	0.41	0/593	0.77	2/785 (0.3%)
44	w	0.49	0/635	0.78	1/848 (0.1%)
45	x	0.31	0/502	0.59	0/667
46	y	0.34	0/453	0.53	0/605
47	z	0.29	0/450	0.51	0/599
48	0	0.36	0/424	0.61	0/565
49	1	0.32	0/380	0.52	0/498
50	2	0.46	0/513	0.67	0/676
51	3	0.31	0/303	0.57	0/397
52	4	0.23	0/488	0.45	0/649
53	X	0.27	0/292	0.38	0/453
54	Y	0.42	0/1764	0.68	1/2747 (0.0%)
55	Z	0.35	0/1813	0.57	0/2825
56	5	0.33	0/46	0.49	0/69
All	All	0.32	1/152983 (0.0%)	0.50	14/228846 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
28	g	0	1
41	t	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2069	G7M	O3'-P	5.57	1.61	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	v	44	LYS	N-CA-C	-7.25	103.31	111.07
12	L	17	ALA	N-CA-C	6.66	118.70	110.91
22	a	1905	C	C4'-C3'-O3'	-6.34	103.48	113.00
22	a	512	G	O4'-C1'-N9	6.15	117.42	108.20
23	b	2	G	O3'-P-O5'	-6.00	95.00	104.00
43	v	43	THR	CB-CA-C	5.99	121.10	112.12
54	Y	45	G	C4'-C3'-O3'	5.88	118.22	109.40
1	A	429	U	C2'-C3'-O3'	-5.50	101.26	109.50
44	w	17	ASN	N-CA-C	-5.46	101.09	109.76
33	l	36	VAL	N-CA-C	-5.45	107.51	112.96
22	a	677	A	C4'-C3'-O3'	-5.24	105.13	113.00
28	g	44	LYS	CA-C-N	5.23	131.53	121.54
28	g	44	LYS	C-N-CA	5.23	131.53	121.54
23	b	2	G	OP2-P-O3'	5.01	123.05	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	101	ALA	Peptide
28	g	47	ASP	Peptide
41	t	99	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32612	0	16432	347	0
2	B	1753	0	1780	33	0
3	C	1624	0	1696	17	0
4	D	1643	0	1707	46	0
5	E	1152	0	1196	21	0
6	F	839	0	833	19	0
7	G	1203	0	1254	34	0
8	H	979	0	1031	22	0
9	I	1022	0	1070	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	786	0	828	18	0
11	K	877	0	884	20	0
12	L	957	0	1017	19	0
13	M	891	0	952	18	0
14	N	805	0	844	12	0
15	O	714	0	734	10	0
16	P	643	0	661	8	0
17	Q	641	0	682	14	0
18	R	544	0	565	10	0
19	S	668	0	693	13	0
20	T	670	0	719	9	0
21	U	589	0	629	13	0
22	a	59130	0	29767	611	0
23	b	2549	0	1291	26	0
24	c	2082	0	2154	33	0
25	d	1566	0	1618	19	0
26	e	1552	0	1619	29	0
27	f	1410	0	1444	33	0
28	g	1323	0	1371	43	0
29	h	303	0	327	17	0
30	i	1129	0	1162	13	0
31	j	946	0	1023	18	0
32	k	1053	0	1129	25	0
33	l	1075	0	1146	29	0
34	m	945	0	989	12	0
35	n	892	0	923	11	0
36	o	917	0	962	16	0
37	p	947	0	1019	12	0
38	q	816	0	839	20	0
39	r	857	0	922	10	0
40	s	738	0	807	8	0
41	t	779	0	831	17	0
42	u	753	0	780	10	0
43	v	586	0	596	11	0
44	w	625	0	652	20	0
45	x	501	0	531	18	0
46	y	449	0	488	8	0
47	z	444	0	458	9	0
48	0	417	0	451	7	0
49	1	377	0	418	3	0
50	2	504	0	572	7	0
51	3	302	0	340	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	4	480	0	478	5	0
53	X	260	0	130	5	0
54	Y	1579	0	804	57	0
55	Z	1623	0	825	29	0
56	5	42	0	23	1	0
57	A	42	0	45	1	0
58	A	93	0	0	0	0
58	a	208	0	0	0	0
58	b	5	0	0	0	0
58	c	1	0	0	0	0
58	d	1	0	0	0	0
58	z	1	0	0	0	0
59	A	20	0	38	2	0
59	a	140	0	266	55	0
60	a	14	0	26	10	0
61	3	1	0	0	0	0
61	4	1	0	0	0	0
62	0	7	0	0	0	0
62	1	33	0	0	0	0
62	2	24	0	0	1	0
62	3	3	0	0	0	0
62	4	6	0	0	0	0
62	A	2063	0	0	36	0
62	B	1	0	0	0	0
62	C	46	0	0	2	0
62	D	11	0	0	3	0
62	E	15	0	0	1	0
62	G	5	0	0	1	0
62	H	28	0	0	3	0
62	I	21	0	0	0	0
62	J	15	0	0	0	0
62	K	12	0	0	0	0
62	L	23	0	0	2	0
62	M	18	0	0	0	0
62	N	31	0	0	0	0
62	O	11	0	0	0	0
62	P	10	0	0	0	0
62	Q	4	0	0	0	0
62	R	1	0	0	0	0
62	S	24	0	0	1	0
62	T	3	0	0	0	0
62	U	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	X	15	0	0	2	0
62	Y	13	0	0	1	0
62	Z	19	0	0	0	0
62	a	4028	0	0	110	0
62	b	171	0	0	9	0
62	c	100	0	0	3	0
62	d	38	0	0	0	0
62	e	48	0	0	3	0
62	f	30	0	0	1	0
62	h	6	0	0	8	0
62	i	14	0	0	0	0
62	j	17	0	0	0	0
62	k	50	0	0	8	0
62	l	27	0	0	3	0
62	m	33	0	0	2	0
62	n	42	0	0	1	0
62	o	12	0	0	0	0
62	p	33	0	0	0	0
62	q	20	0	0	0	0
62	r	20	0	0	3	0
62	s	11	0	0	0	0
62	t	3	0	0	0	0
62	u	4	0	0	0	0
62	v	18	0	0	1	0
62	w	23	0	0	2	0
62	x	2	0	0	6	0
62	y	6	0	0	2	0
62	z	25	0	0	0	0
All	All	149338	0	95471	1756	0

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

All (1756) 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)
13:M:71:ARG:NH2	27:f:113:ASP:CG	1.87	1.33
32:k:143:GLU:HG2	62:k:202:HOH:O	1.30	1.29
45:x:14:LEU:HD22	62:x:101:HOH:O	1.27	1.28
22:a:846:U:H1'	62:a:6326:HOH:O	1.10	1.26
13:M:71:ARG:NH2	27:f:113:ASP:OD1	1.67	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2310:C:C6	62:a:6335:HOH:O	1.67	1.26
27:f:64:LYS:HE2	62:f:219:HOH:O	1.37	1.23
32:k:143:GLU:CG	62:k:202:HOH:O	1.81	1.23
45:x:14:LEU:HB2	62:x:101:HOH:O	1.39	1.22
22:a:2491:U:H6	62:a:8432:HOH:O	1.22	1.22
13:M:71:ARG:NH2	27:f:113:ASP:OD2	1.71	1.20
22:a:2309:A:H2'	62:a:6335:HOH:O	0.99	1.16
45:x:14:LEU:CD2	62:x:101:HOH:O	1.86	1.16
59:a:6215:SPD:H51	62:a:9858:HOH:O	1.48	1.13
22:a:2310:C:H6	62:a:6335:HOH:O	1.08	1.12
45:x:14:LEU:CB	62:x:101:HOH:O	1.98	1.07
1:A:1076:U:OP1	2:B:174:LYS:NZ	1.87	1.07
22:a:332:A:O2'	59:a:6216:SPD:H72	1.54	1.06
59:a:6212:SPD:H22	62:a:6746:HOH:O	1.59	1.00
59:a:6219:SPD:H31	39:r:86:MET:SD	2.02	0.99
22:a:284:U:H5'	62:a:6340:HOH:O	0.82	0.98
2:B:119:THR:O	2:B:123:ASP:HB2	1.64	0.96
53:X:22:U:O2	62:X:101:HOH:O	1.82	0.96
22:a:1252:G:H1	37:p:37:GLN:HE21	1.07	0.96
22:a:338:G:N1	59:a:6216:SPD:H21	1.81	0.94
22:a:2850:A:OP2	59:a:6210:SPD:H91	1.68	0.94
22:a:1043:C:O2	22:a:1112:G:N2	2.00	0.93
22:a:1272:A:N3	62:a:6305:HOH:O	2.03	0.92
26:e:65:THR:HG23	62:e:307:HOH:O	1.70	0.90
53:X:24:A:N7	62:X:102:HOH:O	2.06	0.89
55:Z:18:G:N1	55:Z:55:U:O2	2.06	0.89
22:a:2865:U:O4	59:a:6210:SPD:H52	1.73	0.89
26:e:51:GLU:CD	62:e:302:HOH:O	2.14	0.89
40:s:54:GLU:HG2	40:s:88:LYS:HD2	1.55	0.88
23:b:89:U:N1	62:b:301:HOH:O	2.06	0.87
24:c:270:ARG:NH1	62:c:401:HOH:O	2.05	0.87
1:A:664:G:H22	1:A:741:G:H1	1.20	0.87
22:a:505:A:OP2	59:a:6213:SPD:N1	2.07	0.86
29:h:9:VAL:C	62:h:202:HOH:O	2.17	0.86
22:a:2850:A:OP2	59:a:6210:SPD:C9	2.24	0.85
54:Y:13:C:O2	54:Y:22:G:N1	2.08	0.85
22:a:2554:U:O2	54:Y:74:C:N4	2.10	0.85
32:k:143:GLU:CD	62:k:202:HOH:O	2.08	0.85
54:Y:23:A:H2'	54:Y:24:G:H8	1.42	0.84
3:C:73:PRO:HG3	3:C:105:GLU:HG2	1.58	0.84
22:a:1047:G:HO2'	22:a:1110:G:H1	1.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Z:62:C:H2'	55:Z:63:G:C8	2.12	0.84
13:M:71:ARG:HH22	27:f:113:ASP:CG	1.62	0.84
11:K:23:ILE:HG12	11:K:96:THR:HG21	1.60	0.83
22:a:287:G:N1	22:a:353:C:N3	2.26	0.82
22:a:1478:G:H1	22:a:1513:U:H3	1.22	0.82
55:Z:62:C:H2'	55:Z:63:G:H8	1.40	0.82
22:a:310:A:N3	62:a:6312:HOH:O	2.12	0.82
54:Y:23:A:H2'	54:Y:24:G:C8	2.15	0.82
22:a:2866:U:O4	59:a:6210:SPD:N10	2.12	0.81
62:a:9793:HOH:O	24:c:253:LYS:HB3	1.78	0.81
22:a:911:A:OP1	59:a:6220:SPD:H51	1.79	0.81
1:A:1073:U:O2'	2:B:103:ASN:ND2	2.13	0.81
22:a:332:A:O2'	59:a:6216:SPD:C7	2.28	0.81
22:a:2402:U:H1'	62:a:6572:HOH:O	1.80	0.81
28:g:89:LEU:HB2	28:g:129:THR:HG22	1.62	0.81
22:a:338:G:H1	59:a:6216:SPD:H21	1.46	0.80
29:h:12:LEU:HD13	29:h:19:VAL:HG21	1.64	0.80
62:a:9374:HOH:O	24:c:242:LYS:HE3	1.81	0.80
27:f:158:THR:HG22	27:f:160:ALA:H	1.44	0.80
54:Y:58:A:O2'	54:Y:60:C:OP2	2.00	0.80
13:M:71:ARG:HH21	27:f:113:ASP:CG	1.63	0.79
22:a:1582:C:O2'	22:a:1585:C:N3	2.14	0.79
45:x:14:LEU:CG	62:x:101:HOH:O	2.03	0.79
22:a:2582:G:OP2	62:a:6303:HOH:O	2.01	0.79
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.65	0.79
22:a:228:C:OP2	62:a:6302:HOH:O	2.01	0.78
29:h:9:VAL:CG2	62:h:202:HOH:O	2.32	0.78
29:h:9:VAL:HG23	62:h:202:HOH:O	1.83	0.78
22:a:1434:A:H2'	22:a:1435:G:H8	1.48	0.78
1:A:1086:U:H3	1:A:1099:G:H22	1.31	0.77
62:a:8578:HOH:O	33:l:78:LEU:HD13	1.83	0.77
7:G:113:ASP:OD2	7:G:122:ASN:ND2	2.17	0.76
44:w:8:THR:HG21	44:w:54:LYS:HE3	1.66	0.76
8:H:18:GLN:HG2	8:H:63:LEU:HD13	1.67	0.76
24:c:180:GLU:OE1	62:c:401:HOH:O	2.04	0.76
20:T:68:HIS:HD2	20:T:70:ASN:H	1.32	0.76
22:a:896:A:H2'	54:Y:56:C:O2	1.85	0.76
31:j:38:ILE:HD11	31:j:112:PHE:HZ	1.49	0.76
22:a:846:U:C1'	62:a:6326:HOH:O	1.89	0.76
22:a:1434:A:H2'	22:a:1435:G:C8	2.21	0.76
2:B:205:ASP:OD1	2:B:205:ASP:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:b:354:HOH:O	46:y:20:HIS:HD2	1.67	0.75
59:a:6215:SPD:H102	44:w:22:LEU:CD2	2.00	0.75
1:A:37:U:OP2	12:L:120:LYS:NZ	2.19	0.74
22:a:983:A:OP1	62:a:6306:HOH:O	2.03	0.74
22:a:431:U:OP2	62:a:6304:HOH:O	2.03	0.74
22:a:1418:G:N7	62:a:6333:HOH:O	2.19	0.74
22:a:2648:G:N7	62:a:6336:HOH:O	2.20	0.74
1:A:81:A:N6	1:A:88:U:O4	2.19	0.74
11:K:17:SER:HA	11:K:79:ILE:HA	1.69	0.74
29:h:10:ALA:N	62:h:202:HOH:O	2.19	0.74
22:a:84:A:N1	22:a:98:G:O2'	2.20	0.74
1:A:677:U:H3	1:A:713:G:H22	1.35	0.74
22:a:1971:U:C6	62:a:8102:HOH:O	2.41	0.74
62:a:8913:HOH:O	43:v:57:HIS:HD2	1.70	0.73
1:A:673:A:H2'	1:A:674:G:C8	2.24	0.73
22:a:5:A:H2'	22:a:6:A:C8	2.24	0.73
1:A:688:G:OP1	62:A:1701:HOH:O	2.06	0.73
28:g:158:LYS:HE3	28:g:160:LYS:HD2	1.69	0.73
7:G:113:ASP:OD1	7:G:113:ASP:N	2.17	0.73
1:A:1119:C:OP1	9:I:85:ARG:NH2	2.20	0.73
9:I:52:LEU:HD11	9:I:63:LEU:HD11	1.70	0.73
23:b:89:U:H1'	62:b:301:HOH:O	1.88	0.73
22:a:438:G:N7	62:a:6339:HOH:O	2.20	0.73
27:f:105:THR:HA	52:4:38:SER:HB2	1.71	0.73
59:a:6216:SPD:H22	62:a:8233:HOH:O	1.88	0.72
22:a:172:A:H2'	22:a:173:A:C8	2.23	0.72
22:a:1971:U:C5	62:a:8102:HOH:O	2.40	0.72
41:t:74:ASN:HD22	41:t:76:ALA:H	1.36	0.72
22:a:697:G:O6	60:a:6223:SPM:H42	1.89	0.72
22:a:1236:G:N7	59:a:6213:SPD:H71	2.03	0.72
54:Y:49:G:H2'	54:Y:50:G:H8	1.53	0.72
1:A:530:G:N7	62:A:1719:HOH:O	2.21	0.72
1:A:933:G:O6	7:G:3:ARG:NH2	2.21	0.72
1:A:946:A:H2'	1:A:947:G:C8	2.25	0.72
10:J:29:ALA:HB2	10:J:87:LEU:HD21	1.71	0.71
22:a:333:G:O6	62:a:6308:HOH:O	2.09	0.71
10:J:66:GLU:HB2	14:N:99:ALA:HB2	1.71	0.71
22:a:2851:A:N7	59:a:6210:SPD:N10	2.39	0.71
39:r:92:ARG:HD2	62:r:207:HOH:O	1.90	0.71
22:a:2491:U:H2'	62:a:8432:HOH:O	1.91	0.70
33:l:66:ARG:NH1	33:l:104:GLU:OE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1945:G:OP2	62:a:6307:HOH:O	2.08	0.70
1:A:1189:U:OP1	14:N:98:LYS:NZ	2.24	0.70
22:a:492:A:N1	62:a:6349:HOH:O	2.23	0.70
1:A:754:C:OP1	15:O:72:ARG:NH2	2.25	0.70
29:h:9:VAL:CA	62:h:202:HOH:O	2.36	0.70
4:D:184:ARG:NH2	4:D:190:ASP:OD2	2.24	0.70
22:a:2864:G:O6	59:a:6210:SPD:H51	1.91	0.70
4:D:177:LYS:HB2	4:D:179:GLU:HG2	1.74	0.69
23:b:89:U:C2	62:b:301:HOH:O	2.44	0.69
22:a:287:G:O6	22:a:353:C:N4	2.19	0.69
22:a:172:A:H2'	22:a:173:A:H8	1.57	0.69
22:a:2751:G:H4'	28:g:4:VAL:HG23	1.74	0.69
1:A:493:A:H2'	1:A:494:G:C8	2.26	0.69
22:a:549:G:H2'	22:a:550:C:C6	2.28	0.69
31:j:7:MET:HE1	31:j:44:LYS:HG3	1.75	0.69
7:G:82:GLY:HA3	53:X:13:A:C8	2.28	0.69
23:b:79:G:OP1	62:b:302:HOH:O	2.10	0.69
1:A:1518:MA6:H103	1:A:1519:MA6:H102	1.74	0.69
36:o:100:LEU:HD11	36:o:110:ILE:HD11	1.75	0.69
54:Y:33:U:OP1	62:Y:101:HOH:O	2.11	0.69
62:a:8583:HOH:O	34:m:31:HIS:HE1	1.75	0.69
7:G:5:ARG:O	7:G:6:VAL:HG23	1.92	0.68
22:a:330:A:OP1	62:a:6311:HOH:O	2.11	0.68
7:G:40:GLU:OE2	62:G:201:HOH:O	2.10	0.68
17:Q:25:ILE:HB	17:Q:42:THR:HG23	1.75	0.68
20:T:68:HIS:CD2	20:T:70:ASN:H	2.11	0.68
22:a:538:A:H5"	30:i:7:LYS:HE3	1.73	0.68
28:g:72:LEU:HA	28:g:75:MET:HB2	1.76	0.68
32:k:143:GLU:N	62:k:202:HOH:O	2.25	0.68
22:a:2430:A:OP1	62:a:6313:HOH:O	2.12	0.68
54:Y:14:A:C2	54:Y:22:G:H1'	2.29	0.68
22:a:273:G:N7	62:a:6355:HOH:O	2.26	0.68
22:a:728:G:OP2	59:a:6217:SPD:H22	1.94	0.67
22:a:1720:U:H2'	22:a:1721:G:O4'	1.94	0.67
7:G:53:ARG:NH2	7:G:122:ASN:OD1	2.25	0.67
22:a:1469:A:H2'	22:a:1470:A:C8	2.29	0.67
38:q:43:ASN:HB2	38:q:46:GLU:HB3	1.75	0.67
22:a:1181:U:H2'	22:a:1182:G:C8	2.29	0.67
16:P:74:LEU:O	16:P:78:VAL:HG23	1.95	0.67
22:a:2083:G:OP2	62:a:6315:HOH:O	2.13	0.67
22:a:1200:C:OP1	62:a:6310:HOH:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2354:C:OP1	62:a:6314:HOH:O	2.12	0.67
50:2:45:ARG:O	62:2:101:HOH:O	2.12	0.67
1:A:346:G:OP1	36:o:39:ARG:NH2	2.24	0.67
3:C:77:ILE:HA	3:C:84:VAL:HG13	1.74	0.67
22:a:1042:G:N2	22:a:1113:U:O2	2.24	0.67
27:f:73:SER:HB3	55:Z:56:C:H1'	1.75	0.67
29:h:20:ASN:OD1	62:h:201:HOH:O	2.11	0.67
22:a:2547:A:H2'	22:a:2548:U:C6	2.30	0.66
3:C:35:SER:OG	3:C:59:ARG:NH2	2.29	0.66
1:A:524:G:OP1	62:A:1702:HOH:O	2.12	0.66
22:a:1115:G:O2'	22:a:1116:G:O5'	2.12	0.66
22:a:1194:A:N3	62:a:6365:HOH:O	2.28	0.66
6:F:1:MET:HE3	6:F:65:GLU:HG2	1.77	0.66
22:a:252:G:N7	62:a:6362:HOH:O	2.28	0.66
22:a:688:U:OP2	62:a:6317:HOH:O	2.14	0.66
1:A:216:U:H2'	1:A:217:C:C6	2.30	0.66
4:D:101:VAL:HG12	4:D:105:MET:HE2	1.77	0.66
22:a:1047:G:O2'	22:a:1109:C:N4	2.28	0.66
23:b:2:G:H2'	23:b:3:C:H6	1.60	0.66
44:w:39:TRP:HE1	44:w:41:GLU:HG2	1.60	0.66
25:d:1:MET:HB3	25:d:205:PRO:HG2	1.78	0.66
1:A:812:G:N7	62:A:1749:HOH:O	2.29	0.66
10:J:85:ASP:HA	10:J:88:MET:HB2	1.78	0.66
22:a:273:G:H2'	22:a:274:C:C6	2.31	0.66
4:D:87:GLY:HA3	4:D:197:GLU:HG3	1.78	0.65
41:t:50:PRO:HA	41:t:54:GLN:HB3	1.77	0.65
1:A:422:C:O2	1:A:423:G:N1	2.29	0.65
22:a:2748:A:H5'	28:g:4:VAL:HG21	1.78	0.65
22:a:2337:G:OP2	62:a:6321:HOH:O	2.15	0.65
22:a:2486:C:OP1	62:a:6316:HOH:O	2.14	0.65
7:G:129:GLU:HG3	7:G:131:LYS:HE2	1.79	0.65
27:f:112:ARG:HH12	27:f:133:ARG:HH22	1.43	0.65
1:A:1391:U:H2'	1:A:1392:G:C8	2.31	0.65
28:g:30:ASN:HB3	28:g:79:VAL:HA	1.77	0.65
22:a:258:G:N7	62:a:6373:HOH:O	2.29	0.65
1:A:883:C:OP1	62:A:1704:HOH:O	2.14	0.65
2:B:128:LYS:H	2:B:128:LYS:HD2	1.61	0.65
23:b:2:G:H2'	23:b:3:C:C6	2.31	0.65
26:e:21:ARG:HD3	26:e:106:LYS:HB3	1.79	0.65
22:a:2309:A:C2'	62:a:6335:HOH:O	1.82	0.64
28:g:2:SER:OG	28:g:3:ARG:N	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2087:G:OP1	62:a:6318:HOH:O	2.15	0.64
1:A:44:A:N3	62:A:1757:HOH:O	2.30	0.64
22:a:333:G:H4'	59:a:6216:SPD:H42	1.79	0.64
22:a:828:U:OP1	62:a:6319:HOH:O	2.15	0.64
59:a:6219:SPD:C3	39:r:86:MET:SD	2.84	0.64
54:Y:49:G:H2'	54:Y:50:G:C8	2.32	0.64
1:A:405:U:O4	4:D:2:ALA:N	2.31	0.64
1:A:31:G:O2'	1:A:48:C:N4	2.30	0.64
7:G:5:ARG:O	7:G:6:VAL:CG2	2.46	0.64
22:a:287:G:N2	22:a:353:C:O2	2.29	0.64
59:a:6221:SPD:H52	62:a:7767:HOH:O	1.97	0.64
10:J:52:LEU:HD12	10:J:62:ARG:HD3	1.78	0.64
1:A:269:C:H2'	1:A:270:A:C8	2.33	0.64
55:Z:66:C:H2'	55:Z:67:C:C6	2.33	0.64
1:A:953:G:OP2	62:A:1705:HOH:O	2.15	0.64
1:A:1356:G:H2'	1:A:1357:A:C8	2.33	0.64
1:A:1378:C:O2	7:G:76:LYS:NZ	2.32	0.63
22:a:1048:A:H62	22:a:1110:G:H21	1.45	0.63
1:A:823:C:HO2'	8:H:2:SER:N	1.97	0.63
7:G:6:VAL:O	7:G:6:VAL:HG12	1.97	0.63
22:a:878:A:N7	22:a:899:A:H2	1.94	0.63
44:w:6:GLN:HE21	44:w:50:ARG:H	1.44	0.63
46:y:41:THR:HG21	62:y:101:HOH:O	1.99	0.63
1:A:1004:A:H2'	1:A:1005:A:O4'	1.98	0.63
22:a:1236:G:OP2	59:a:6213:SPD:H21	1.97	0.63
22:a:2392:A:OP2	50:2:31:HIS:HE1	1.82	0.63
28:g:91:GLY:HA2	28:g:160:LYS:HG2	1.79	0.63
4:D:80:ALA:O	62:D:301:HOH:O	2.15	0.63
22:a:290:U:O2	22:a:350:G:N2	2.31	0.63
32:k:10:GLU:CD	32:k:10:GLU:H	2.05	0.63
1:A:510:A:N7	62:A:1758:HOH:O	2.30	0.63
4:D:172:GLU:HG3	4:D:183:LYS:HD2	1.81	0.63
22:a:846:U:C2'	62:a:6326:HOH:O	2.32	0.63
31:j:99:ILE:HD13	31:j:118:LEU:HB2	1.79	0.63
33:l:136:MET:HG2	42:u:77:VAL:HG12	1.81	0.63
36:o:6:LYS:O	36:o:10:GLN:HG2	1.98	0.63
43:v:38:VAL:HG12	43:v:59:LEU:HB2	1.79	0.63
22:a:1047:G:H4'	22:a:1048:A:H5'	1.80	0.63
62:a:8578:HOH:O	33:l:78:LEU:CD1	2.44	0.63
1:A:1350:A:O2'	7:G:33:ASP:OD1	2.16	0.62
22:a:2335:A:OP1	62:a:6322:HOH:O	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:a:9861:HOH:O	33:l:13:HIS:HD2	1.82	0.62
54:Y:62:C:H2'	54:Y:63:G:C8	2.34	0.62
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.80	0.62
1:A:337:G:H2'	1:A:338:A:C8	2.35	0.62
11:K:18:ASP:OD1	11:K:37:ARG:NH1	2.32	0.62
22:a:2327:A:H2'	22:a:2328:A:C8	2.34	0.62
24:c:200:HIS:HE1	24:c:203:ARG:HH11	1.47	0.62
44:w:54:LYS:HD2	44:w:54:LYS:C	2.24	0.62
1:A:783:C:OP2	62:A:1706:HOH:O	2.16	0.62
42:u:2:PHE:HB3	42:u:50:MET:HE3	1.81	0.62
22:a:5:A:H2'	22:a:6:A:H8	1.63	0.62
1:A:390:U:H2'	1:A:391:G:C8	2.35	0.62
1:A:662:U:H2'	1:A:663:A:C8	2.33	0.62
54:Y:49:G:O2'	54:Y:50:G:H5'	1.99	0.62
19:S:69:HIS:ND1	19:S:73:GLU:OE1	2.33	0.61
9:I:116:VAL:HG11	10:J:62:ARG:HG3	1.81	0.61
1:A:131:A:H2'	1:A:132:C:C6	2.35	0.61
1:A:459:A:H2'	1:A:460:A:C8	2.35	0.61
28:g:159:GLY:O	28:g:163:ARG:NH1	2.32	0.61
4:D:184:ARG:HH21	4:D:186:PRO:HA	1.66	0.61
10:J:24:GLU:O	10:J:28:THR:HG22	2.00	0.61
22:a:2432:A:H1'	56:5:75:C:O4'	2.00	0.61
22:a:2482:A:H4'	54:Y:63:G:O2'	1.99	0.61
62:a:6784:HOH:O	24:c:39:LYS:HD2	2.00	0.61
45:x:9:LYS:HB3	45:x:13:GLU:HB2	1.82	0.61
55:Z:43:A:H2'	55:Z:44:A:C8	2.35	0.61
1:A:340:U:OP2	31:j:98:ARG:NH2	2.34	0.61
8:H:41:LYS:NZ	8:H:48:ASP:OD1	2.32	0.61
22:a:1042:G:H1	22:a:1113:U:H3	1.47	0.61
1:A:87:C:H2'	1:A:88:U:C6	2.35	0.61
1:A:1031:C:O2'	1:A:1032:G:N2	2.32	0.61
8:H:89:LYS:HE2	62:H:221:HOH:O	2.00	0.61
23:b:48:U:H2'	23:b:49:C:C6	2.35	0.61
32:k:143:GLU:CA	62:k:202:HOH:O	2.47	0.61
11:K:83:GLU:HG2	11:K:109:ASN:HB2	1.83	0.61
24:c:107:PRO:HD2	24:c:110:LEU:HD22	1.82	0.61
15:O:14:GLU:OE2	15:O:84:ARG:NH2	2.33	0.61
22:a:2243:U:H2'	22:a:2244:U:C6	2.36	0.61
27:f:37:ASN:HB3	27:f:153:ASP:OD1	2.01	0.61
54:Y:65:C:H2'	54:Y:66:A:C8	2.36	0.61
2:B:7:ARG:NH2	2:B:11:LYS:HE2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:695:G:O6	60:a:6223:SPM:C12	2.48	0.60
22:a:1495:A:N3	22:a:1578:U:O2'	2.34	0.60
28:g:40:ALA:HB2	28:g:58:TYR:CD1	2.36	0.60
22:a:2069:G7M:OP2	62:a:6323:HOH:O	2.16	0.60
22:a:2408:U:OP1	62:a:6324:HOH:O	2.16	0.60
12:L:73:ASN:O	12:L:75:GLN:NE2	2.34	0.60
22:a:2537:U:H2'	22:a:2538:C:C6	2.36	0.60
22:a:1794:A:N7	62:a:6392:HOH:O	2.32	0.60
24:c:181:MET:HB3	24:c:268:VAL:HB	1.82	0.60
35:n:2:ASP:N	35:n:2:ASP:OD1	2.32	0.60
22:a:153:U:H2'	22:a:154:U:C6	2.36	0.60
31:j:108:ARG:HH21	36:o:34:GLU:HB3	1.65	0.60
22:a:223:A:OP2	62:a:6325:HOH:O	2.16	0.60
33:l:20:LEU:HD13	42:u:81:PRO:HG2	1.83	0.60
9:I:21:ILE:HG12	9:I:63:LEU:HD22	1.83	0.59
22:a:639:U:H2'	22:a:640:C:C6	2.37	0.59
22:a:1405:U:H2'	22:a:1406:U:C6	2.37	0.59
59:a:6212:SPD:C2	62:a:6746:HOH:O	2.33	0.59
22:a:218:A:N7	62:a:6390:HOH:O	2.31	0.59
22:a:2532:G:O2'	22:a:2657:A:N1	2.35	0.59
45:x:14:LEU:HB3	45:x:57:LEU:HD21	1.84	0.59
55:Z:66:C:H2'	55:Z:67:C:H6	1.67	0.59
22:a:851:C:H2'	22:a:852:U:C6	2.37	0.59
44:w:43:GLU:OE1	62:w:101:HOH:O	2.17	0.59
22:a:1325:U:H3'	62:a:9838:HOH:O	2.02	0.59
32:k:57:LEU:HD22	50:2:54:ASP:HB3	1.84	0.59
42:u:4:ILE:HB	42:u:63:ILE:HG12	1.83	0.59
1:A:895:G:N7	62:A:1766:HOH:O	2.32	0.59
25:d:1:MET:HE2	25:d:205:PRO:HG3	1.84	0.59
54:Y:50:G:H2'	54:Y:51:C:O4'	2.03	0.59
1:A:1526:G:N7	21:U:40:LYS:NZ	2.51	0.59
22:a:1494:A:H2'	22:a:1495:A:C8	2.37	0.59
43:v:59:LEU:HD12	43:v:80:ILE:HD12	1.84	0.59
10:J:24:GLU:HB2	10:J:90:LEU:HD11	1.85	0.59
35:n:39:VAL:HB	35:n:49:VAL:HG22	1.84	0.59
18:R:23:TYR:HA	18:R:29:LEU:HD11	1.85	0.59
22:a:64:A:H2'	22:a:65:U:C6	2.38	0.59
1:A:147:G:H2'	1:A:148:G:C8	2.38	0.59
33:l:42:THR:HB	62:l:219:HOH:O	2.02	0.59
1:A:1382:C:H4'	7:G:79:ARG:HH21	1.67	0.59
25:d:12:THR:HG22	25:d:13:ARG:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:h:33:GLN:NE2	62:h:203:HOH:O	2.36	0.59
10:J:36:VAL:HG12	10:J:76:ILE:HD13	1.85	0.58
22:a:1482:G:H1'	22:a:1509:A:H61	1.67	0.58
22:a:2491:U:C6	62:a:8432:HOH:O	2.13	0.58
26:e:61:ARG:NH2	26:e:63:LYS:O	2.35	0.58
1:A:56:U:H2'	1:A:57:G:C8	2.36	0.58
5:E:13:GLU:HG2	5:E:39:VAL:HG12	1.85	0.58
1:A:542:G:H5'	4:D:39:GLY:HA3	1.85	0.58
3:C:142:MET:HG3	3:C:170:GLU:HG2	1.85	0.58
22:a:2483:C:N3	33:l:123:LYS:NZ	2.50	0.58
26:e:121:VAL:HG21	26:e:124:PHE:HB2	1.84	0.58
30:i:58:ASN:HD21	30:i:128:ASN:ND2	2.01	0.58
47:z:43:ILE:HG22	47:z:49:TYR:HB2	1.85	0.58
1:A:472:U:H2'	1:A:473:U:C6	2.38	0.58
22:a:2273:A:H2'	22:a:2274:A:C8	2.39	0.58
2:B:67:ILE:H	2:B:89:GLN:NE2	2.01	0.58
37:p:86:ALA:HB2	37:p:116:ALA:HB2	1.84	0.58
1:A:71:A:N1	1:A:99:C:O2'	2.37	0.58
1:A:1178:G:O6	62:A:1707:HOH:O	2.17	0.58
1:A:999:C:H2'	1:A:1000:A:C8	2.39	0.58
1:A:1463:U:OP1	36:o:109:ARG:HD2	2.03	0.58
22:a:305:C:H2'	22:a:306:U:C6	2.39	0.58
22:a:720:U:H2'	22:a:721:A:C8	2.39	0.58
22:a:806:C:OP1	62:a:6328:HOH:O	2.17	0.58
22:a:2491:U:H5"	22:a:2570:G:H5"	1.86	0.58
22:a:1412:U:H2'	22:a:1413:A:H8	1.69	0.58
22:a:1484:U:H2'	22:a:1485:U:C6	2.39	0.58
22:a:2902:C:H2'	22:a:2903:U:O4'	2.04	0.58
34:m:51:LEU:CD2	62:m:211:HOH:O	2.52	0.58
2:B:97:LEU:HB2	2:B:100:MET:HG3	1.86	0.57
25:d:14:ILE:HA	36:o:12:GLN:HE22	1.69	0.57
32:k:69:ARG:O	62:k:201:HOH:O	2.17	0.57
1:A:1463:U:H2'	1:A:1464:U:C6	2.39	0.57
6:F:88:MET:HG2	6:F:90:MET:HE2	1.86	0.57
12:L:14:ARG:NH2	62:L:204:HOH:O	2.36	0.57
22:a:1761:C:OP2	62:a:6327:HOH:O	2.17	0.57
22:a:2505:G:N2	22:a:2506:U:O4	2.37	0.57
38:q:41:ILE:HD12	38:q:103:ALA:HA	1.86	0.57
54:Y:50:G:H1	54:Y:64:U:H3	1.51	0.57
8:H:96:MET:HE2	8:H:99:LEU:HB2	1.85	0.57
22:a:1486:U:H2'	22:a:1487:U:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2052:A:H4'	25:d:148:GLN:O	2.04	0.57
26:e:125:SER:O	26:e:137:LYS:NZ	2.32	0.57
38:q:1:MET:HE3	38:q:43:ASN:HD21	1.69	0.57
2:B:76:ALA:O	2:B:80:VAL:HG23	2.04	0.57
7:G:82:GLY:CA	53:X:13:A:C8	2.87	0.57
22:a:155:A:H2'	22:a:156:A:C8	2.40	0.57
22:a:349:U:H2'	22:a:350:G:H8	1.69	0.57
22:a:503:A:H5'	22:a:505:A:OP1	2.04	0.57
25:d:110:THR:HG23	25:d:202:ILE:HB	1.86	0.57
27:f:142:ASP:HB3	27:f:145:LYS:HB2	1.86	0.57
22:a:1486:U:H2'	22:a:1487:U:H6	1.68	0.57
22:a:2402:U:C1'	62:a:6572:HOH:O	2.45	0.57
28:g:140:VAL:O	28:g:144:VAL:HG23	2.04	0.57
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.37	0.57
1:A:1398:A:OP1	62:A:1709:HOH:O	2.17	0.57
22:a:219:A:N3	22:a:234:U:O2'	2.36	0.57
1:A:883:C:OP2	62:A:1708:HOH:O	2.17	0.57
12:L:55:VAL:O	12:L:62:GLU:HA	2.05	0.57
22:a:1028:A:N6	22:a:1125:G:H2'	2.20	0.57
59:a:6216:SPD:C2	62:a:8233:HOH:O	2.48	0.57
62:a:9067:HOH:O	48:0:38:LYS:HE3	2.03	0.57
31:j:109:SER:O	31:j:113:MET:HG2	2.04	0.57
41:t:26:LYS:HD3	41:t:37:GLU:HB3	1.86	0.57
1:A:171:A:H2'	1:A:172:A:C8	2.39	0.57
1:A:189:A:H2'	1:A:190:A:C8	2.40	0.57
22:a:851:C:H2'	22:a:852:U:H6	1.70	0.57
5:E:34:THR:HG22	5:E:52:LYS:HG2	1.87	0.57
22:a:593:U:H2'	22:a:594:U:C6	2.40	0.57
41:t:47:LYS:HD2	41:t:48:PRO:HD2	1.87	0.57
42:u:86:LEU:HD13	42:u:89:ILE:HD11	1.87	0.57
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.86	0.57
22:a:1179:G:H2'	22:a:1180:U:C6	2.40	0.57
22:a:1484:U:H2'	22:a:1485:U:H6	1.70	0.57
1:A:476:U:H2'	1:A:477:C:C6	2.40	0.56
4:D:172:GLU:O	4:D:180:GLY:HA2	2.05	0.56
33:l:50:ARG:HG2	33:l:50:ARG:HH21	1.69	0.56
33:l:77:PRO:HG2	33:l:80:VAL:HG21	1.87	0.56
34:m:51:LEU:HD23	62:m:211:HOH:O	2.03	0.56
22:a:2850:A:OP2	59:a:6210:SPD:H92	2.04	0.56
44:w:54:LYS:HD2	44:w:54:LYS:O	2.05	0.56
1:A:89:U:H2'	1:A:90:C:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:G:O6	4:D:2:ALA:N	2.38	0.56
1:A:1412:C:H2'	1:A:1413:A:C8	2.40	0.56
9:I:31:ASN:HD21	9:I:67:VAL:H	1.53	0.56
22:a:414:C:H2'	22:a:415:A:C8	2.40	0.56
22:a:695:G:O6	60:a:6223:SPM:H121	2.05	0.56
22:a:721:A:OP2	22:a:721:A:H8	1.87	0.56
22:a:1794:A:H2'	22:a:1795:C:C6	2.40	0.56
27:f:140:GLU:OE2	52:4:26:SER:OG	2.19	0.56
22:a:784:G:H5'	22:a:785:G:OP1	2.06	0.56
1:A:1273:C:H2'	1:A:1274:A:O4'	2.04	0.56
3:C:85:GLU:O	3:C:89:LYS:HD2	2.05	0.56
1:A:728:A:H2'	1:A:729:A:C8	2.41	0.56
2:B:115:LYS:O	2:B:119:THR:HG23	2.05	0.56
22:a:1733:G:H2'	22:a:1734:G:C8	2.41	0.56
1:A:17:U:H2'	1:A:18:C:C6	2.40	0.56
1:A:1218:C:H2'	1:A:1219:A:C8	2.39	0.56
34:m:28:LEU:HD23	34:m:48:VAL:HG21	1.88	0.56
1:A:1323:G:H2'	1:A:1324:A:C8	2.40	0.56
54:Y:62:C:H2'	54:Y:63:G:H8	1.70	0.56
1:A:746:A:H2'	1:A:747:A:C8	2.41	0.56
1:A:1000:A:H2'	1:A:1001:C:C6	2.41	0.56
1:A:1530:G:O6	21:U:46:LYS:NZ	2.36	0.56
22:a:871:U:H2'	22:a:872:U:C6	2.41	0.56
22:a:1177:G:H2'	22:a:1178:C:C6	2.41	0.56
22:a:846:U:H5'	22:a:847:U:OP1	2.05	0.56
35:n:56:LYS:NZ	62:n:203:HOH:O	2.38	0.56
54:Y:2:G:H2'	54:Y:3:G:C8	2.41	0.56
1:A:275:G:H5'	17:Q:16:LYS:HB3	1.88	0.55
5:E:127:ALA:HB1	62:E:208:HOH:O	2.06	0.55
12:L:15:LYS:NZ	62:L:202:HOH:O	2.33	0.55
22:a:264:C:O2	62:a:6329:HOH:O	2.18	0.55
33:l:51:ARG:HD2	54:Y:54:U:H4'	1.87	0.55
17:Q:47:HIS:HB3	17:Q:74:THR:HG22	1.88	0.55
22:a:2294:G:H5"	35:n:10:ARG:HD2	1.87	0.55
29:h:32:PRO:HA	44:w:39:TRP:CD1	2.42	0.55
1:A:1130:A:H2'	1:A:1131:G:H8	1.70	0.55
5:E:161:VAL:O	5:E:165:LEU:N	2.38	0.55
22:a:1499:C:H2'	22:a:1500:G:H8	1.70	0.55
22:a:2032:G:N7	62:a:6408:HOH:O	2.33	0.55
29:h:6:LEU:HD13	29:h:37:VAL:HG12	1.89	0.55
2:B:7:ARG:HH22	2:B:11:LYS:HE2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:h:34:GLY:O	29:h:36:ALA:N	2.39	0.55
48:0:11:LEU:HD23	48:0:51:GLU:HA	1.88	0.55
22:a:813:U:H2'	22:a:814:C:C6	2.42	0.55
22:a:2377:A:H5"	22:a:2377:A:H8	1.71	0.55
26:e:2:GLU:OE1	26:e:11:ALA:HB1	2.06	0.55
22:a:2895:G:H2'	22:a:2896:C:C6	2.41	0.55
30:i:125:TYR:HH	30:i:132:HIS:HE2	1.54	0.55
1:A:769:G:H4'	1:A:1513:A:H4'	1.89	0.55
22:a:1378:A:O2'	22:a:1380:G:N7	2.40	0.55
22:a:2291:U:H2'	22:a:2292:U:C6	2.42	0.55
62:a:7347:HOH:O	24:c:243:HIS:HD2	1.89	0.55
29:h:9:VAL:HA	62:h:202:HOH:O	2.05	0.55
44:w:43:GLU:CD	62:w:101:HOH:O	2.50	0.55
1:A:404:G:N7	4:D:2:ALA:HB3	2.22	0.55
1:A:459:A:H2'	1:A:460:A:H8	1.72	0.55
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.89	0.55
1:A:140:U:H2'	1:A:141:G:O4'	2.06	0.55
1:A:1120:C:H2'	1:A:1121:U:C6	2.42	0.55
2:B:133:GLU:O	2:B:137:ARG:HG3	2.07	0.55
22:a:936:A:H2'	22:a:937:C:C6	2.41	0.55
2:B:80:VAL:HG22	2:B:214:LEU:HD11	1.89	0.54
6:F:18:VAL:O	6:F:22:ILE:HG13	2.07	0.54
22:a:717:C:H3'	22:a:718:A:H8	1.72	0.54
22:a:1386:C:H2'	22:a:1387:A:C8	2.42	0.54
28:g:54:PRO:HB3	28:g:61:GLY:HA2	1.89	0.54
22:a:1485:U:H2'	22:a:1486:U:C6	2.42	0.54
22:a:896:A:H2'	54:Y:56:C:C2	2.41	0.54
22:a:2491:U:H4'	22:a:2492:U:OP1	2.07	0.54
31:j:105:ARG:HG3	31:j:108:ARG:HG3	1.88	0.54
38:q:57:GLY:HA2	38:q:102:SER:O	2.07	0.54
45:x:2:LYS:O	45:x:6:LEU:HB2	2.08	0.54
45:x:18:LEU:HB2	45:x:53:VAL:HG11	1.89	0.54
2:B:67:ILE:H	2:B:89:GLN:HE21	1.54	0.54
4:D:170:TRP:CD1	4:D:186:PRO:HD3	2.42	0.54
42:u:4:ILE:HG13	42:u:50:MET:HE1	1.89	0.54
54:Y:65:C:H2'	54:Y:66:A:H8	1.72	0.54
1:A:1027:C:H2'	1:A:1028:C:C6	2.42	0.54
1:A:1286:U:H2'	1:A:1287:A:H5'	1.90	0.54
5:E:45:ARG:HH11	5:E:73:ASN:ND2	2.05	0.54
13:M:89:LEU:O	13:M:93:ARG:HD2	2.08	0.54
16:P:45:GLU:O	16:P:46:LYS:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2204:G:H4'	24:c:150:LYS:HG3	1.89	0.54
3:C:179:ARG:HG3	3:C:206:GLU:HG3	1.89	0.54
44:w:39:TRP:NE1	44:w:41:GLU:HG2	2.23	0.54
1:A:85:U:H4'	1:A:86:G:N2	2.23	0.54
35:n:56:LYS:HD2	35:n:56:LYS:N	2.23	0.54
52:4:42:PRO:HB3	52:4:47:LYS:HB2	1.89	0.54
1:A:1171:A:H2'	1:A:1172:C:C6	2.42	0.54
1:A:543:U:OP1	4:D:14:ARG:HD2	2.07	0.54
5:E:83:HIS:CD2	8:H:96:MET:HE3	2.43	0.54
7:G:79:ARG:HA	7:G:84:THR:HA	1.90	0.54
22:a:1786:A:H1'	22:a:1938:A:N6	2.23	0.54
26:e:132:LYS:HB2	62:e:327:HOH:O	2.08	0.54
22:a:1799:G:O2'	24:c:180:GLU:OE2	2.22	0.54
22:a:2467:C:OP1	51:3:8:LYS:NZ	2.24	0.54
55:Z:56:C:C2	55:Z:57:A:C8	2.95	0.54
2:B:188:ASP:HB2	2:B:204:ASP:OD2	2.08	0.53
22:a:548:G:H2'	22:a:549:G:H1'	1.90	0.53
22:a:2196:C:H2'	22:a:2197:U:C6	2.43	0.53
45:x:42:LEU:O	45:x:46:VAL:HG23	2.08	0.53
1:A:559:A:OP2	62:A:1711:HOH:O	2.19	0.53
22:a:1655:A:N1	62:a:6414:HOH:O	2.34	0.53
22:a:1937:A:OP2	59:a:6211:SPD:H51	2.09	0.53
26:e:171:ASP:OD2	26:e:173:THR:OG1	2.26	0.53
30:i:114:LEU:HG	30:i:118:MET:HE3	1.90	0.53
44:w:41:GLU:O	44:w:44:LYS:HD2	2.09	0.53
1:A:50:A:O2'	1:A:360:G:N2	2.41	0.53
1:A:473:U:H2'	1:A:474:G:H8	1.73	0.53
1:A:1171:A:H2'	1:A:1172:C:H6	1.73	0.53
17:Q:5:ILE:HD13	17:Q:7:THR:HG23	1.90	0.53
22:a:1853:A:N1	22:a:2087:G:H1'	2.23	0.53
22:a:2020:A:H5'	47:z:9:THR:CG2	2.38	0.53
1:A:409:U:H5"	4:D:25:VAL:HG21	1.91	0.53
22:a:352:A:H2'	22:a:353:C:O4'	2.08	0.53
22:a:1939:5MU:OP1	22:a:2604:PSU:O2'	2.27	0.53
22:a:2377:A:OP1	62:a:6330:HOH:O	2.18	0.53
24:c:163:GLN:OE1	24:c:175:ARG:NH1	2.41	0.53
55:Z:9:G:O4'	55:Z:46:G:H1'	2.08	0.53
6:F:3:HIS:NE2	6:F:65:GLU:OE1	2.42	0.53
11:K:42:LEU:HD12	11:K:79:ILE:HD11	1.90	0.53
22:a:2420:C:OP1	62:a:6331:HOH:O	2.19	0.53
26:e:1:MET:HB3	26:e:14:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:G:H2'	1:A:715:A:C8	2.43	0.53
22:a:727:A:N1	62:a:6412:HOH:O	2.34	0.53
22:a:856:G:H2'	22:a:857:G:C8	2.44	0.53
22:a:969:G:H2'	22:a:970:U:C6	2.44	0.53
26:e:125:SER:H	26:e:137:LYS:NZ	2.07	0.53
9:I:118:LEU:HD22	9:I:124:ARG:HG2	1.90	0.53
11:K:72:ASP:O	11:K:75:LYS:HG2	2.09	0.53
11:K:111:THR:HG23	21:U:3:VAL:HB	1.91	0.53
22:a:290:U:H2'	22:a:291:G:O4'	2.09	0.53
22:a:1563:U:H2'	22:a:1564:C:C6	2.43	0.53
22:a:1715:G:O2'	22:a:1743:G:O6	2.21	0.53
62:a:7938:HOH:O	33:l:13:HIS:HE1	1.90	0.53
33:l:53:MET:HE1	33:l:103:TYR:CD2	2.43	0.53
1:A:8:A:N6	4:D:202:GLU:O	2.42	0.53
1:A:1120:C:H2'	1:A:1121:U:H6	1.74	0.53
22:a:2086:U:H2'	22:a:2087:G:C8	2.44	0.53
62:a:6668:HOH:O	26:e:98:LYS:HD3	2.09	0.53
27:f:61:SER:HB2	27:f:91:LEU:HD21	1.91	0.53
28:g:35:ARG:H	28:g:75:MET:HE1	1.74	0.53
1:A:73:C:O2'	1:A:74:A:O5'	2.27	0.53
1:A:470:C:H2'	1:A:471:U:H6	1.73	0.53
1:A:1225:A:H2'	1:A:1226:C:C5	2.43	0.53
4:D:168:PRO:HB3	4:D:170:TRP:CZ3	2.43	0.53
19:S:41:PHE:H	19:S:44:MET:HE3	1.73	0.53
22:a:366:C:H2'	22:a:367:G:O4'	2.09	0.53
22:a:1530:G:H2'	22:a:1531:C:C6	2.43	0.53
28:g:20:ASN:N	28:g:20:ASN:OD1	2.41	0.53
22:a:351:C:H2'	22:a:352:A:C8	2.44	0.52
22:a:1183:U:H2'	22:a:1184:U:C6	2.44	0.52
22:a:1482:G:N1	22:a:1508:A:H2	2.07	0.52
23:b:89:U:C1'	62:b:301:HOH:O	2.41	0.52
32:k:110:VAL:HG11	32:k:135:ILE:HD11	1.91	0.52
46:y:41:THR:HB	46:y:44:ILE:H	1.74	0.52
55:Z:11:A:H2'	55:Z:12:G:C8	2.44	0.52
8:H:89:LYS:CE	62:H:221:HOH:O	2.58	0.52
11:K:67:ALA:HB2	11:K:96:THR:HG23	1.91	0.52
22:a:1790:C:H2'	22:a:1791:A:C5	2.44	0.52
33:l:56:ALA:HB2	33:l:119:LEU:HD12	1.91	0.52
1:A:588:G:OP1	62:A:1710:HOH:O	2.18	0.52
1:A:999:C:H2'	1:A:1000:A:H8	1.75	0.52
22:a:547:A:H4'	22:a:548:G:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:694:U:O4	60:a:6223:SPM:H112	2.08	0.52
22:a:1287:A:H5'	34:m:103:ARG:HD2	1.90	0.52
22:a:1682:G:H2'	22:a:1683:U:C6	2.45	0.52
22:a:2522:U:O2'	22:a:2647:U:OP1	2.17	0.52
26:e:41:GLN:HG2	26:e:43:THR:HG23	1.91	0.52
31:j:40:LYS:HE3	31:j:57:VAL:HG12	1.91	0.52
38:q:71:LYS:HG2	38:q:73:LYS:HE2	1.92	0.52
41:t:98:SER:O	41:t:98:SER:OG	2.23	0.52
54:Y:49:G:O6	54:Y:66:A:N6	2.42	0.52
1:A:1513:A:H2'	1:A:1514:G:C8	2.44	0.52
62:A:2185:HOH:O	17:Q:68:SER:HB2	2.10	0.52
13:M:3:ARG:HH11	13:M:3:ARG:HG3	1.75	0.52
22:a:2478:A:H5'	51:3:32:LYS:HE2	1.91	0.52
23:b:66:A:H61	23:b:107:G:H2'	1.75	0.52
29:h:34:GLY:C	29:h:36:ALA:H	2.17	0.52
32:k:141:LYS:NZ	32:k:143:GLU:OE2	2.42	0.52
1:A:56:U:H2'	1:A:57:G:H8	1.75	0.52
22:a:224:U:O4	22:a:420:C:H5'	2.09	0.52
22:a:788:A:OP1	22:a:790:U:H5	1.93	0.52
22:a:1747:U:H2'	22:a:1748:C:C6	2.44	0.52
22:a:2430:A:N3	22:a:2430:A:H2'	2.24	0.52
23:b:39:A:H4'	62:b:341:HOH:O	2.08	0.52
24:c:200:HIS:CE1	24:c:203:ARG:HH11	2.27	0.52
27:f:116:GLY:HA3	27:f:178:ARG:HB3	1.91	0.52
28:g:26:ILE:HB	28:g:75:MET:HG2	1.91	0.52
1:A:455:G:H2'	1:A:456:A:C8	2.45	0.52
11:K:87:LYS:HB2	11:K:113:VAL:HG23	1.92	0.52
22:a:327:G:O6	59:a:6216:SPD:H81	2.10	0.52
22:a:386:G:O3'	59:a:6215:SPD:H91	2.09	0.52
22:a:2071:A:H2'	22:a:2072:C:C6	2.45	0.52
28:g:35:ARG:NE	28:g:71:LEU:HD13	2.24	0.52
47:z:33:THR:HB	47:z:51:GLY:HA2	1.91	0.52
55:Z:71:C:H2'	55:Z:72:A:H8	1.74	0.52
1:A:313:A:H2'	1:A:314:C:C6	2.44	0.52
1:A:1444:U:H2'	1:A:1445:U:C6	2.45	0.52
22:a:197:A:N6	22:a:2430:A:O2'	2.43	0.52
22:a:849:A:H2'	22:a:850:U:C6	2.45	0.52
22:a:2329:U:H2'	22:a:2330:G:C8	2.45	0.52
22:a:2469:A:N6	22:a:2481:G:O2'	2.43	0.52
59:a:6215:SPD:H102	44:w:22:LEU:HD21	1.73	0.52
32:k:78:ARG:HG2	32:k:113:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Z:28:C:H2'	55:Z:29:G:H8	1.74	0.52
7:G:85:TYR:OH	11:K:55:SER:OG	2.25	0.52
22:a:543:G:H5'	22:a:543:G:H8	1.75	0.52
22:a:728:G:O6	59:a:6217:SPD:H71	2.10	0.52
37:p:109:LEU:HD11	38:q:40:MET:HE1	1.92	0.52
1:A:51:A:N7	1:A:114:U:O2'	2.42	0.52
1:A:219:U:H2'	1:A:220:G:H8	1.74	0.52
62:A:2618:HOH:O	10:J:56:HIS:HD2	1.93	0.52
22:a:909:A:H2'	22:a:912:C:C5	2.45	0.52
22:a:1187:G:H5"	38:q:83:TYR:CE1	2.45	0.52
24:c:79:GLU:OE2	24:c:101:ARG:NE	2.39	0.52
39:r:29:VAL:HB	39:r:55:ILE:HD11	1.92	0.52
54:Y:3:G:H2'	54:Y:4:U:C6	2.44	0.52
1:A:246:A:N1	1:A:278:G:O2'	2.39	0.51
1:A:384:G:H2'	1:A:385:C:C6	2.44	0.51
1:A:1410:A:H2'	1:A:1411:C:C6	2.45	0.51
1:A:1478:U:H2'	1:A:1479:C:C6	2.46	0.51
2:B:106:THR:HA	2:B:109:GLN:NE2	2.24	0.51
22:a:811:U:H2'	32:k:21:ARG:HA	1.92	0.51
22:a:1182:G:H2'	22:a:1183:U:O4'	2.10	0.51
25:d:1:MET:HE3	25:d:100:LEU:HD23	1.92	0.51
1:A:470:C:H2'	1:A:471:U:C6	2.45	0.51
1:A:645:G:OP1	62:A:1712:HOH:O	2.19	0.51
1:A:736:C:H2'	1:A:737:C:C6	2.45	0.51
1:A:1032:G:C6	1:A:1033:G:H1'	2.45	0.51
4:D:105:MET:HE1	4:D:143:VAL:HB	1.92	0.51
9:I:24:GLY:HA3	9:I:62:ASP:CG	2.36	0.51
22:a:2529:G:H4'	28:g:175:LYS:HE3	1.92	0.51
22:a:2649:C:H2'	22:a:2650:U:C6	2.46	0.51
1:A:97:G:H2'	1:A:98:A:O4'	2.10	0.51
1:A:268:U:H2'	1:A:269:C:C6	2.46	0.51
1:A:461:A:H2'	1:A:462:G:H8	1.75	0.51
7:G:5:ARG:C	7:G:6:VAL:HG23	2.36	0.51
9:I:7:TYR:HH	9:I:9:THR:HG1	1.58	0.51
55:Z:72:A:H2'	55:Z:73:A:O4'	2.11	0.51
1:A:924:C:OP1	62:A:1713:HOH:O	2.19	0.51
33:l:106:ASP:OD1	33:l:107:GLY:N	2.40	0.51
22:a:325:G:O6	59:a:6216:SPD:C3	2.59	0.51
22:a:542:C:C2'	22:a:543:G:H5"	2.40	0.51
22:a:2247:A:N6	62:a:6578:HOH:O	2.43	0.51
26:e:106:LYS:HE2	26:e:201:ALA:OXT	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Y:19:G:H4'	54:Y:20:G:OP1	2.09	0.51
9:I:65:ILE:HG21	9:I:79:ILE:HG12	1.93	0.51
22:a:1528:A:H2'	22:a:1529:G:O4'	2.11	0.51
22:a:1802:A:H2'	22:a:1803:A:C8	2.46	0.51
62:a:9232:HOH:O	25:d:128:ARG:HD3	2.10	0.51
27:f:135:GLN:HG2	27:f:141:ILE:HG21	1.92	0.51
34:m:86:ARG:NE	34:m:117:ASP:OD2	2.39	0.51
41:t:53:ASN:ND2	41:t:55:PRO:HG2	2.26	0.51
22:a:2304:G:H22	22:a:2312:U:H3	1.59	0.51
33:l:50:ARG:HG2	33:l:50:ARG:NH2	2.24	0.51
47:z:46:ASP:O	47:z:53:LYS:NZ	2.41	0.51
1:A:450:G:N7	62:A:1787:HOH:O	2.34	0.51
12:L:36:ARG:HG2	12:L:38:TYR:CD1	2.46	0.51
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.91	0.51
22:a:581:C:H2'	22:a:582:A:C8	2.46	0.51
22:a:695:G:O6	60:a:6223:SPM:H122	2.11	0.51
22:a:1509:A:O2'	22:a:1510:G:H8	1.94	0.51
23:b:112:G:H2'	23:b:113:C:C6	2.46	0.51
55:Z:28:C:H2'	55:Z:29:G:C8	2.46	0.51
1:A:190:A:H8	1:A:190:A:O5'	1.93	0.51
6:F:37:HIS:HB3	6:F:97:THR:HG22	1.91	0.51
22:a:95:A:H4'	45:x:38:GLN:O	2.11	0.51
22:a:1414:C:H2'	22:a:1415:U:O4'	2.10	0.51
40:s:48:GLN:HE21	40:s:54:GLU:HG3	1.75	0.51
1:A:381:C:H2'	1:A:382:A:O4'	2.10	0.51
9:I:33:ARG:HG2	9:I:33:ARG:HH11	1.76	0.51
19:S:11:ILE:HD11	19:S:15:LEU:HD22	1.93	0.51
32:k:77:ILE:CD1	32:k:108:ALA:HB1	2.40	0.51
32:k:77:ILE:HG23	32:k:81:ASP:HB2	1.93	0.51
32:k:93:ASN:ND2	62:k:204:HOH:O	2.44	0.51
39:r:72:THR:HG22	39:r:73:LYS:HG3	1.93	0.51
1:A:71:A:H61	1:A:99:C:H1'	1.75	0.50
1:A:460:A:H2'	1:A:461:A:H8	1.76	0.50
1:A:555:U:H2'	1:A:556:C:C6	2.47	0.50
2:B:119:THR:O	2:B:123:ASP:CB	2.49	0.50
18:R:9:LYS:HA	18:R:46:GLY:HA3	1.93	0.50
22:a:150:U:H2'	22:a:151:C:C6	2.47	0.50
22:a:1904:G:O2'	22:a:1928:A:N1	2.39	0.50
22:a:2096:C:H2'	22:a:2097:A:H8	1.77	0.50
25:d:35:THR:HG22	25:d:73:VAL:HG21	1.93	0.50
38:q:33:VAL:HG23	38:q:61:ALA:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:U:H2'	1:A:217:C:H6	1.77	0.50
1:A:1443:C:H2'	1:A:1444:U:O4'	2.11	0.50
13:M:40:ALA:HB3	13:M:43:VAL:HG23	1.94	0.50
13:M:51:GLY:O	13:M:55:THR:HG23	2.10	0.50
22:a:114:U:O4	62:a:6332:HOH:O	2.19	0.50
22:a:2482:A:O3'	54:Y:63:G:H4'	2.12	0.50
45:x:14:LEU:HD13	62:x:101:HOH:O	2.11	0.50
1:A:28:A:O2'	1:A:296:U:OP1	2.24	0.50
1:A:1302:C:C5	13:M:17:ILE:HG13	2.46	0.50
1:A:1446:A:H8	1:A:1446:A:OP1	1.94	0.50
14:N:29:ALA:O	14:N:33:ASP:HB2	2.11	0.50
22:a:355:U:H2'	22:a:356:G:H8	1.77	0.50
22:a:493:G:H2'	22:a:494:G:O4'	2.10	0.50
22:a:1469:A:H2'	22:a:1470:A:H8	1.75	0.50
22:a:2478:A:OP2	51:3:2:LYS:NZ	2.30	0.50
22:a:2845:U:H5"	36:o:52:ASN:O	2.11	0.50
27:f:117:LEU:HD12	27:f:176:PRO:HD2	1.94	0.50
54:Y:20:G:H21	54:Y:48:C:H5	1.59	0.50
22:a:2585:U:H3	54:Y:76:A:HO3'	1.58	0.50
62:a:9606:HOH:O	44:w:36:HIS:HD2	1.94	0.50
32:k:93:ASN:CG	62:k:204:HOH:O	2.54	0.50
3:C:36:ASP:OD1	3:C:59:ARG:NH2	2.35	0.50
19:S:29:LYS:HG2	19:S:30:PRO:HD2	1.93	0.50
22:a:155:A:H2'	22:a:156:A:H8	1.75	0.50
22:a:299:A:N3	22:a:319:G:O2'	2.39	0.50
22:a:1509:A:HO2'	22:a:1510:G:H8	1.57	0.50
22:a:1723:G:C2	22:a:1724:G:H1'	2.47	0.50
28:g:54:PRO:HB3	28:g:61:GLY:CA	2.42	0.50
1:A:160:A:H2'	1:A:161:A:C8	2.47	0.50
22:a:898:C:H2'	22:a:899:A:O4'	2.12	0.50
28:g:158:LYS:CE	28:g:160:LYS:HD2	2.40	0.50
33:l:80:VAL:HG13	62:l:201:HOH:O	2.12	0.50
38:q:16:GLU:HG2	38:q:101:ILE:HG13	1.93	0.50
1:A:41:G:H2'	1:A:42:G:C8	2.47	0.50
22:a:892:A:H8	22:a:892:A:O5'	1.95	0.50
22:a:1506:U:H2'	22:a:1507:C:C6	2.46	0.50
55:Z:8:U:H5'	55:Z:49:G:H5'	1.94	0.50
1:A:404:G:O2'	1:A:498:A:N1	2.42	0.50
14:N:31:ILE:O	14:N:41:ARG:HD3	2.12	0.50
22:a:338:G:N2	59:a:6216:SPD:H32	2.26	0.50
22:a:642:U:O2'	22:a:644:A:N7	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:A:H2'	1:A:1131:G:C8	2.46	0.50
16:P:18:GLN:OE1	16:P:35:ARG:NE	2.44	0.50
1:A:553:A:H5"	12:L:21:VAL:HG21	1.93	0.49
1:A:1477:U:H2'	1:A:1478:U:C6	2.47	0.49
62:A:3467:HOH:O	8:H:76:GLN:HG2	2.10	0.49
4:D:54:GLN:HB3	4:D:203:LEU:HD13	1.94	0.49
9:I:47:VAL:HG13	9:I:80:ARG:HD3	1.94	0.49
22:a:1530:G:H2'	22:a:1531:C:H6	1.77	0.49
22:a:1880:U:H2'	22:a:1881:C:C6	2.47	0.49
22:a:1882:U:H2'	22:a:1883:U:C6	2.47	0.49
22:a:2649:C:H2'	22:a:2650:U:H6	1.77	0.49
34:m:8:ARG:HD2	34:m:43:GLU:HG2	1.93	0.49
43:v:37:ILE:HD11	43:v:82:ILE:HD11	1.94	0.49
44:w:3:ARG:O	44:w:12:PRO:HD3	2.12	0.49
1:A:789:U:O2'	1:A:791:G:N7	2.40	0.49
1:A:1441:A:H62	1:A:1461:G:H21	1.59	0.49
22:a:1441:G:H2'	22:a:1442:U:C6	2.47	0.49
22:a:1493:C:N4	62:a:6647:HOH:O	2.46	0.49
22:a:2395:C:H5"	59:a:6215:SPD:H21	1.94	0.49
28:g:35:ARG:N	28:g:75:MET:HE1	2.27	0.49
1:A:545:C:OP1	4:D:58:LYS:NZ	2.45	0.49
11:K:52:PHE:O	11:K:53:ARG:HD2	2.12	0.49
22:a:2310:C:O4'	62:a:6335:HOH:O	2.20	0.49
55:Z:67:C:C2'	55:Z:68:C:H5'	2.42	0.49
7:G:4:ARG:O	7:G:5:ARG:HB3	2.11	0.49
22:a:272:A:O2'	22:a:273:G:H5'	2.12	0.49
22:a:1599:U:H2'	22:a:1600:C:C6	2.48	0.49
22:a:1913:A:N1	54:Y:37:A:O2'	2.39	0.49
22:a:2406:A:H1'	59:a:6214:SPD:H51	1.95	0.49
23:b:1:U:H2'	23:b:2:G:H8	1.77	0.49
26:e:135:ALA:O	26:e:139:LYS:HG2	2.11	0.49
36:o:5:ILE:O	36:o:9:GLU:HG3	2.13	0.49
1:A:269:C:H2'	1:A:270:A:H8	1.77	0.49
1:A:1405:G:OP1	62:A:1715:HOH:O	2.20	0.49
22:a:594:U:H2'	22:a:595:C:C6	2.46	0.49
26:e:176:ASP:OD1	26:e:179:SER:OG	2.24	0.49
1:A:1397:C:OP2	5:E:29:ARG:NH2	2.46	0.49
22:a:347:A:H2'	22:a:348:A:C8	2.48	0.49
22:a:2687:U:H2'	22:a:2688:G:O4'	2.11	0.49
40:s:6:ARG:O	40:s:10:VAL:HG13	2.13	0.49
46:y:30:ARG:NH2	62:y:102:HOH:O	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:A:2218:HOH:O	12:L:43:LYS:HD2	2.12	0.49
6:F:17:GLN:OE1	6:F:17:GLN:N	2.45	0.49
15:O:47:LYS:HA	15:O:53:ARG:HH22	1.78	0.49
22:a:742:A:H2'	22:a:743:A:C8	2.48	0.49
22:a:2202:U:O2'	22:a:2204:G:OP1	2.24	0.49
27:f:44:ILE:HA	27:f:83:TYR:CE2	2.48	0.49
28:g:94:TYR:HA	28:g:106:SER:O	2.13	0.49
41:t:7:ARG:O	41:t:8:ASP:HB2	2.12	0.49
1:A:1465:A:H2'	1:A:1466:C:C6	2.47	0.49
19:S:56:GLN:NE2	62:S:105:HOH:O	2.44	0.49
22:a:1499:C:H2'	22:a:1500:G:C8	2.46	0.49
23:b:89:U:C6	62:b:301:HOH:O	2.59	0.49
28:g:84:THR:OG1	28:g:134:LYS:NZ	2.45	0.49
54:Y:68:C:H2'	54:Y:69:A:C8	2.48	0.49
1:A:5:U:OP1	1:A:5:U:H6	1.96	0.49
1:A:1428:A:H2'	1:A:1429:A:O4'	2.12	0.49
1:A:1491:G:H5"	12:L:43:LYS:HG3	1.95	0.49
4:D:107:PHE:CG	4:D:145:ILE:HD11	2.48	0.49
5:E:85:VAL:HG23	5:E:96:MET:HE3	1.94	0.49
22:a:829:A:N7	22:a:2248:C:H5'	2.28	0.49
22:a:2567:G:H2'	22:a:2568:U:C6	2.48	0.49
24:c:117:GLN:NE2	24:c:121:ASP:OD1	2.45	0.49
55:Z:71:C:H2'	55:Z:72:A:C8	2.48	0.49
1:A:79:G:H22	1:A:90:C:H42	1.59	0.49
1:A:540:G:H21	4:D:40:GLN:NE2	2.11	0.49
1:A:654:G:N7	62:A:1792:HOH:O	2.35	0.49
7:G:102:ARG:O	7:G:106:GLU:HG3	2.12	0.49
12:L:25:GLU:OE2	12:L:59:ASN:ND2	2.46	0.49
36:o:78:SER:OG	36:o:80:VAL:HG12	2.13	0.49
1:A:67:C:H2'	1:A:68:G:C8	2.48	0.48
1:A:1072:G:H2'	1:A:1073:U:C6	2.47	0.48
2:B:56:GLU:HG2	2:B:198:PHE:CZ	2.48	0.48
1:A:1315:U:H2'	1:A:1316:G:O4'	2.13	0.48
62:A:2787:HOH:O	4:D:2:ALA:HB1	2.13	0.48
22:a:1:G:H2'	22:a:2:G:C8	2.48	0.48
22:a:272:A:H2'	22:a:273:G:H8	1.78	0.48
22:a:1009:A:N3	22:a:1153:C:O2'	2.44	0.48
29:h:41:LYS:HD3	29:h:41:LYS:HA	1.61	0.48
20:T:61:GLN:OE1	20:T:61:GLN:HA	2.14	0.48
22:a:272:A:H2'	22:a:273:G:C8	2.49	0.48
22:a:1043:C:N3	22:a:1112:G:N1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1141:U:H4'	22:a:1142:A:O4'	2.13	0.48
22:a:1754:A:N1	22:a:2716:C:O2'	2.38	0.48
22:a:2025:C:H2'	22:a:2026:U:C6	2.48	0.48
62:a:7513:HOH:O	33:l:14:LYS:HE2	2.13	0.48
1:A:1148:U:H2'	1:A:1149:C:O4'	2.13	0.48
1:A:1435:G:H2'	1:A:1436:U:C6	2.48	0.48
5:E:142:ASP:O	5:E:146:ASN:ND2	2.47	0.48
10:J:20:GLN:O	10:J:24:GLU:HG2	2.14	0.48
10:J:65:TYR:HB3	14:N:96:LEU:HD11	1.94	0.48
22:a:363:G:H2'	22:a:364:C:C6	2.49	0.48
22:a:1149:G:H2'	22:a:1150:C:C6	2.48	0.48
22:a:1703:G:H2'	22:a:1704:C:C6	2.49	0.48
54:Y:70:C:O2	54:Y:70:C:H2'	2.12	0.48
22:a:1442:U:H2'	22:a:1443:U:C6	2.49	0.48
22:a:1902:C:H4'	24:c:242:LYS:O	2.14	0.48
22:a:2299:U:H2'	22:a:2300:C:C6	2.48	0.48
22:a:2328:A:H2'	22:a:2329:U:C6	2.48	0.48
22:a:2788:C:H2'	22:a:2789:C:C6	2.49	0.48
23:b:66:A:OP2	23:b:108:A:N6	2.45	0.48
38:q:36:ALA:HA	38:q:58:VAL:HG23	1.94	0.48
43:v:25:ARG:HD2	43:v:31:VAL:HG12	1.94	0.48
1:A:444:G:H2'	1:A:445:G:C8	2.49	0.48
1:A:1127:G:H5'	1:A:1280:A:O2'	2.14	0.48
1:A:1320:C:O2	19:S:36:ARG:NH2	2.46	0.48
6:F:18:VAL:HA	6:F:21:MET:HE2	1.94	0.48
20:T:39:ILE:HD11	20:T:83:ILE:HG13	1.95	0.48
22:a:169:G:H2'	22:a:170:U:H6	1.78	0.48
22:a:340:A:H2'	22:a:341:C:O4'	2.13	0.48
22:a:574:A:H5'	62:a:9438:HOH:O	2.13	0.48
38:q:27:ILE:O	38:q:66:HIS:HE1	1.95	0.48
1:A:739:C:OP2	6:F:2:ARG:NH2	2.45	0.48
1:A:920:U:H2'	1:A:921:U:C6	2.49	0.48
1:A:1516:2MG:N2	1:A:1519:MA6:OP2	2.43	0.48
22:a:608:A:H2'	22:a:609:A:C8	2.48	0.48
22:a:1874:C:H2'	22:a:1875:G:O4'	2.13	0.48
22:a:2462:C:H2'	22:a:2463:C:C6	2.48	0.48
6:F:43:GLY:HA2	6:F:58:HIS:CE1	2.49	0.48
22:a:2012:G:OP1	39:r:98:LYS:HE3	2.14	0.48
1:A:451:A:H61	1:A:481:G:H5'	1.77	0.48
1:A:1427:C:H2'	1:A:1428:A:C8	2.49	0.48
6:F:6:ILE:HG12	6:F:89:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:64:CYS:SG	17:Q:74:THR:HG23	2.54	0.48
1:A:613:C:H2'	1:A:614:C:C6	2.49	0.48
17:Q:5:ILE:HD11	17:Q:62:ARG:HD3	1.95	0.48
22:a:54:G:O6	62:a:6334:HOH:O	2.20	0.48
22:a:2064:C:H2'	22:a:2065:C:C6	2.49	0.48
1:A:234:C:H4'	17:Q:66:PRO:HG3	1.95	0.47
2:B:162:PHE:CE1	2:B:217:VAL:HG11	2.49	0.47
22:a:26:G:H1'	22:a:514:A:N6	2.28	0.47
22:a:153:U:H2'	22:a:154:U:H6	1.75	0.47
26:e:136:GLN:O	26:e:139:LYS:HG3	2.14	0.47
39:r:4:ILE:HG12	39:r:106:VAL:HG22	1.96	0.47
54:Y:66:A:C6	54:Y:67:U:C4	3.02	0.47
1:A:340:U:P	31:j:98:ARG:HH21	2.38	0.47
22:a:101:A:H2'	22:a:101:A:N3	2.29	0.47
22:a:349:U:H2'	22:a:350:G:C8	2.49	0.47
22:a:644:A:H2'	22:a:645:C:O4'	2.14	0.47
22:a:1432:G:H5"	59:a:6217:SPD:H92	1.96	0.47
37:p:85:LYS:HB3	37:p:116:ALA:HB1	1.97	0.47
54:Y:67:U:H2'	54:Y:68:C:C6	2.49	0.47
55:Z:2:G:H8	55:Z:2:G:OP2	1.97	0.47
1:A:707:U:OP1	62:A:1716:HOH:O	2.20	0.47
62:A:3277:HOH:O	21:U:46:LYS:HD2	2.13	0.47
4:D:100:ASN:ND2	4:D:111:ARG:HH21	2.12	0.47
22:a:476:G:H4'	22:a:502:A:N1	2.29	0.47
22:a:1446:C:H2'	22:a:1447:C:C6	2.48	0.47
35:n:4:LYS:O	35:n:8:ILE:HG12	2.14	0.47
1:A:678:U:H2'	1:A:679:C:C6	2.50	0.47
11:K:16:VAL:HG13	11:K:17:SER:H	1.79	0.47
22:a:766:U:O4	60:a:6223:SPM:H82	2.14	0.47
22:a:1867:G:H2'	22:a:1868:C:C6	2.50	0.47
22:a:1942:C:OP2	62:a:6338:HOH:O	2.20	0.47
22:a:2305:U:H5"	27:f:131:GLY:HA3	1.96	0.47
22:a:2671:G:H2'	22:a:2672:U:O4'	2.15	0.47
54:Y:13:C:H2'	54:Y:14:A:C8	2.49	0.47
1:A:1067:A:N1	1:A:1108:G:O2'	2.39	0.47
1:A:1095:U:H2'	1:A:1096:C:C6	2.50	0.47
1:A:1314:C:OP2	19:S:4:SER:OG	2.22	0.47
22:a:325:G:O6	59:a:6216:SPD:H31	2.14	0.47
22:a:2292:U:H2'	22:a:2293:G:C8	2.49	0.47
22:a:2783:U:H2'	22:a:2784:U:C6	2.50	0.47
22:a:2804:U:H2'	22:a:2805:C:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:n:53:THR:HG21	35:n:70:ALA:HB1	1.95	0.47
48:0:30:LYS:HD3	48:0:30:LYS:HA	1.57	0.47
22:a:839:U:H2'	22:a:840:C:C6	2.49	0.47
22:a:2820:A:O2'	22:a:2821:A:OP1	2.30	0.47
32:k:77:ILE:HD11	32:k:108:ALA:HB1	1.97	0.47
33:l:53:MET:HG3	33:l:120:ALA:HB2	1.96	0.47
1:A:41:G:H2'	1:A:42:G:H8	1.79	0.47
1:A:579:A:H2'	1:A:580:C:C6	2.50	0.47
1:A:985:C:H2'	1:A:986:U:C6	2.50	0.47
1:A:1062:U:H2'	1:A:1063:C:C6	2.49	0.47
22:a:78:U:H2'	22:a:79:C:C6	2.49	0.47
22:a:483:A:C8	41:t:45:HIS:HD2	2.33	0.47
22:a:634:C:H2'	22:a:635:C:C6	2.50	0.47
22:a:1901:A:H2'	22:a:1902:C:C6	2.49	0.47
22:a:2074:U:H2'	22:a:2075:U:C6	2.49	0.47
22:a:2859:G:H2'	22:a:2860:A:C8	2.50	0.47
23:b:49:C:H2'	23:b:50:A:C8	2.49	0.47
28:g:152:ARG:HB3	28:g:162:VAL:HG23	1.97	0.47
32:k:123:ARG:HG3	32:k:143:GLU:HB2	1.97	0.47
48:0:25:LYS:NZ	48:0:32:GLU:O	2.48	0.47
1:A:537:G:H2'	1:A:538:G:C8	2.49	0.47
11:K:97:ILE:HG22	21:U:12:PHE:HZ	1.79	0.47
22:a:64:A:H2'	22:a:65:U:H6	1.78	0.47
22:a:1548:A:H2'	22:a:1549:A:C8	2.50	0.47
22:a:2780:G:OP2	30:i:120:ARG:HD3	2.15	0.47
27:f:120:LYS:HB2	27:f:120:LYS:HE3	1.70	0.47
32:k:82:LEU:HD22	32:k:90:VAL:HG21	1.95	0.47
52:4:41:HIS:CD2	52:4:43:PHE:H	2.33	0.47
1:A:376:G:H5"	16:P:5:ARG:HB2	1.97	0.47
7:G:16:PRO:HD2	7:G:44:TYR:OH	2.15	0.47
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.96	0.47
11:K:113:VAL:HG12	18:R:73:ARG:HD3	1.96	0.47
12:L:43:LYS:HE2	12:L:89:D2T:H7	1.95	0.47
22:a:185:G:H4'	22:a:218:A:H4'	1.97	0.47
22:a:1007:C:OP1	30:i:37:ARG:NH2	2.48	0.47
22:a:1180:U:H2'	22:a:1181:U:O4'	2.15	0.47
22:a:1726:C:H2'	22:a:1727:C:C6	2.49	0.47
46:y:31:ARG:HG2	46:y:34:HIS:HB2	1.97	0.47
1:A:444:G:H2'	1:A:445:G:H8	1.80	0.47
1:A:476:U:H2'	1:A:477:C:H6	1.79	0.47
1:A:500:G:H2'	1:A:501:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:357:C:H2'	22:a:358:U:O4'	2.15	0.47
22:a:2312:U:H5'	27:f:85:ILE:HD11	1.95	0.47
22:a:2702:G:H2'	22:a:2703:C:H6	1.80	0.47
29:h:29:PHE:C	29:h:32:PRO:HD2	2.40	0.47
1:A:858:G:O6	62:A:1714:HOH:O	2.20	0.46
1:A:1043:G:HO2'	1:A:1044:A:H8	1.63	0.46
1:A:1314:C:H2'	1:A:1315:U:C6	2.50	0.46
2:B:93:ASN:H	2:B:93:ASN:HD22	1.63	0.46
7:G:116:MET:HA	7:G:119:ARG:HE	1.79	0.46
22:a:208:C:H2'	22:a:209:C:C6	2.49	0.46
22:a:768:G:O6	60:a:6223:SPM:H132	2.15	0.46
22:a:1882:U:H2'	22:a:1883:U:H6	1.80	0.46
62:a:9393:HOH:O	25:d:143:PRO:HG2	2.15	0.46
28:g:115:HIS:HE1	28:g:144:VAL:HG13	1.79	0.46
30:i:34:ARG:HG3	30:i:39:LYS:HB2	1.97	0.46
1:A:649:A:H2'	1:A:650:G:O4'	2.15	0.46
1:A:1001:C:C2	1:A:1002:G:C8	3.04	0.46
26:e:23:PHE:HB2	26:e:111:GLU:HG2	1.96	0.46
46:y:41:THR:O	46:y:45:ARG:HG2	2.15	0.46
1:A:35:G:H2'	1:A:36:C:C6	2.50	0.46
17:Q:53:CYS:SG	17:Q:75:LEU:HD11	2.54	0.46
22:a:1580:A:C8	22:a:1581:G:C8	3.03	0.46
22:a:1723:G:H2'	22:a:1724:G:O4'	2.15	0.46
24:c:5:LYS:HD2	24:c:5:LYS:HA	1.64	0.46
39:r:7:HIS:CD2	62:r:216:HOH:O	2.68	0.46
1:A:177:G:OP1	20:T:24:ARG:NH2	2.48	0.46
1:A:337:G:H2'	1:A:338:A:H8	1.78	0.46
1:A:619:U:H3	4:D:131:ASN:ND2	2.13	0.46
1:A:1082:A:N7	62:A:1805:HOH:O	2.36	0.46
1:A:1286:U:N3	1:A:1288:A:OP1	2.49	0.46
1:A:1427:C:H2'	1:A:1428:A:H8	1.81	0.46
8:H:64:LYS:HG3	8:H:71:VAL:HG21	1.97	0.46
22:a:857:G:H2'	22:a:858:G:O4'	2.15	0.46
23:b:1:U:H2'	23:b:2:G:C8	2.51	0.46
27:f:162:SER:OG	27:f:165:GLU:OE2	2.31	0.46
36:o:25:THR:HB	36:o:88:ARG:HB3	1.98	0.46
1:A:1474:U:H4'	22:a:1701:A:N3	2.30	0.46
19:S:12:ASP:OD2	19:S:35:SER:OG	2.23	0.46
19:S:28:LYS:HD2	19:S:29:LYS:N	2.31	0.46
22:a:2514:U:H2'	22:a:2515:C:C6	2.50	0.46
22:a:2590:A:H2'	22:a:2591:C:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2804:U:H2'	22:a:2805:C:C6	2.49	0.46
30:i:58:ASN:HD21	30:i:128:ASN:HD22	1.62	0.46
33:l:75:GLU:HB2	33:l:90:GLU:HG3	1.96	0.46
10:J:10:LEU:HD22	10:J:98:VAL:HG22	1.96	0.46
22:a:468:G:N7	49:1:39:ARG:NH2	2.55	0.46
22:a:505:A:OP2	59:a:6213:SPD:C2	2.62	0.46
22:a:684:G:OP1	49:1:16:HIS:ND1	2.47	0.46
22:a:936:A:H2'	22:a:937:C:H6	1.81	0.46
22:a:2591:C:H2'	22:a:2592:G:C8	2.51	0.46
23:b:48:U:H2'	23:b:49:C:H6	1.79	0.46
29:h:33:GLN:O	29:h:35:LYS:HG3	2.16	0.46
37:p:72:ASN:HB3	37:p:110:VAL:HG11	1.96	0.46
1:A:190:A:H2'	1:A:191:G:O4'	2.16	0.46
1:A:663:A:H5'	1:A:836:G:OP1	2.16	0.46
1:A:946:A:H2'	1:A:947:G:H8	1.74	0.46
12:L:43:LYS:HE2	12:L:43:LYS:HB3	1.72	0.46
22:a:332:A:H2'	59:a:6216:SPD:H92	1.98	0.46
22:a:609:A:H2'	22:a:610:C:O4'	2.16	0.46
22:a:1108:U:O5'	22:a:1108:U:H6	1.99	0.46
22:a:1168:G:O6	22:a:1181:U:O2	2.34	0.46
22:a:1370:C:H2'	22:a:1371:G:O4'	2.15	0.46
22:a:2242:G:OP2	62:a:6337:HOH:O	2.20	0.46
22:a:2578:G:OP2	59:a:6222:SPD:H21	2.16	0.46
62:a:7938:HOH:O	33:l:13:HIS:CE1	2.67	0.46
31:j:10:VAL:HG12	31:j:12:ASP:H	1.79	0.46
38:q:6:GLN:HE22	38:q:9:GLY:H	1.62	0.46
1:A:416:G:H2'	1:A:417:G:H5"	1.98	0.46
62:A:2884:HOH:O	19:S:52:HIS:HE1	1.97	0.46
22:a:169:G:H2'	22:a:170:U:C6	2.50	0.46
22:a:546:U:O2'	22:a:547:A:H5'	2.16	0.46
22:a:729:G:C6	24:c:207:LYS:HB2	2.51	0.46
22:a:1690:A:H2'	22:a:1691:C:O4'	2.16	0.46
22:a:1746:A:H2'	22:a:1747:U:C6	2.51	0.46
22:a:1889:A:H2'	22:a:1890:A:C8	2.51	0.46
43:v:53:CYS:SG	43:v:57:HIS:HA	2.55	0.46
1:A:515:G:N7	62:A:1797:HOH:O	2.35	0.46
1:A:692:U:H2'	1:A:694:A:OP2	2.16	0.46
1:A:1489:G:P	57:A:1601:PAR:HN61	2.38	0.46
2:B:20:THR:HG22	2:B:39:HIS:CE1	2.50	0.46
4:D:71:GLN:HE22	4:D:97:ARG:NH1	2.14	0.46
20:T:24:ARG:HD2	20:T:24:ARG:HA	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:o:27:GLU:OE1	36:o:87:LYS:NZ	2.41	0.46
44:w:8:THR:HG21	44:w:54:LYS:CE	2.42	0.46
45:x:19:LEU:HD23	45:x:19:LEU:HA	1.71	0.46
55:Z:54:U:H2'	55:Z:55:U:C6	2.51	0.46
1:A:224:U:H2'	1:A:225:C:C6	2.50	0.46
1:A:1032:G:H2'	1:A:1033:G:H4'	1.98	0.46
1:A:1088:G:H4'	21:U:70:LEU:HD13	1.98	0.46
2:B:102:THR:HA	2:B:179:LEU:HD11	1.98	0.46
22:a:635:C:O2'	22:a:639:U:OP1	2.28	0.46
22:a:721:A:H2'	22:a:722:A:C8	2.51	0.46
22:a:1646:C:H3'	62:a:9763:HOH:O	2.15	0.46
22:a:2389:G:H5"	22:a:2390:U:O4'	2.16	0.46
22:a:2901:C:C4	22:a:2902:C:N4	2.84	0.46
23:b:49:C:H2'	23:b:50:A:H8	1.79	0.46
28:g:26:ILE:HD12	28:g:75:MET:HB3	1.97	0.46
37:p:76:TYR:CZ	37:p:80:ILE:HG13	2.51	0.46
46:y:6:LYS:HB2	46:y:6:LYS:HE3	1.71	0.46
48:0:7:GLU:HG2	48:0:27:LYS:HG3	1.98	0.46
1:A:73:C:O2'	1:A:74:A:H8	1.99	0.45
1:A:188:C:H6	1:A:188:C:OP1	1.99	0.45
1:A:524:G:H2'	1:A:525:C:C6	2.51	0.45
1:A:600:A:H3'	62:A:1991:HOH:O	2.15	0.45
1:A:1309:G:N7	13:M:98:ARG:NH2	2.65	0.45
2:B:94:HIS:ND1	2:B:146:ASN:O	2.49	0.45
18:R:10:PHE:O	18:R:10:PHE:CG	2.68	0.45
22:a:883:G:C4	22:a:884:U:C5	3.04	0.45
22:a:1432:G:H2'	22:a:1433:A:C8	2.51	0.45
22:a:2820:A:N3	22:a:2820:A:H2'	2.31	0.45
26:e:118:LEU:HD11	26:e:188:MET:SD	2.57	0.45
42:u:72:VAL:HA	42:u:94:ALA:H	1.81	0.45
55:Z:69:C:H2'	55:Z:70:G:C8	2.51	0.45
1:A:181:A:N6	1:A:195:A:C8	2.84	0.45
1:A:481:G:O2'	1:A:483:C:N4	2.49	0.45
1:A:1026:G:O2'	1:A:1027:C:OP1	2.27	0.45
2:B:26:LYS:HD2	2:B:192:ASP:OD1	2.17	0.45
9:I:100:LYS:HE3	9:I:100:LYS:HB3	1.68	0.45
10:J:28:THR:HG23	10:J:87:LEU:HD23	1.98	0.45
15:O:45:GLU:O	15:O:45:GLU:HG2	2.15	0.45
22:a:1496:A:N3	22:a:1577:C:O2'	2.48	0.45
23:b:36:C:N4	23:b:49:C:O2	2.49	0.45
28:g:11:VAL:HB	28:g:48:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:28:LEU:HD12	45:x:46:VAL:HG21	1.98	0.45
1:A:1236:A:H2'	1:A:1237:C:C6	2.52	0.45
3:C:24:ALA:HB1	3:C:28:GLU:HB2	1.98	0.45
3:C:162:ILE:HD13	53:X:24:A:O3'	2.16	0.45
11:K:114:THR:HG21	21:U:32:VAL:HG21	1.99	0.45
22:a:338:G:C6	59:a:6216:SPD:H21	2.48	0.45
22:a:543:G:C6	22:a:551:G:C6	3.04	0.45
22:a:1269:A:H2'	22:a:1270:C:C6	2.52	0.45
22:a:1496:A:H2'	22:a:1498:C:C5	2.51	0.45
22:a:1680:U:H2'	22:a:1681:G:O4'	2.16	0.45
22:a:1916:A:H2'	22:a:1917:PSU:O4'	2.16	0.45
22:a:2557:G:H2'	22:a:2558:C:C6	2.51	0.45
34:m:22:ARG:HG3	34:m:70:THR:HA	1.98	0.45
36:o:2:SER:O	36:o:6:LYS:HG3	2.17	0.45
1:A:382:A:H2'	1:A:383:A:C8	2.52	0.45
1:A:695:A:H2'	1:A:696:A:C8	2.52	0.45
7:G:49:THR:O	7:G:53:ARG:HG3	2.16	0.45
10:J:67:ILE:HG13	14:N:96:LEU:HD13	1.97	0.45
11:K:79:ILE:HB	11:K:105:PHE:HE1	1.81	0.45
16:P:56:ARG:HA	16:P:56:ARG:HD2	1.72	0.45
22:a:12:U:O2	22:a:2626:C:H4'	2.16	0.45
22:a:27:G:OP1	59:a:6218:SPD:N1	2.49	0.45
22:a:1683:U:H2'	22:a:1684:G:C8	2.51	0.45
22:a:1796:U:H2'	22:a:1797:G:C8	2.51	0.45
22:a:2336:A:H4'	62:a:6321:HOH:O	2.16	0.45
22:a:2698:U:H2'	22:a:2699:C:C6	2.52	0.45
22:a:2749:A:H5"	28:g:2:SER:N	2.31	0.45
22:a:2895:G:H2'	22:a:2896:C:H6	1.78	0.45
3:C:15:VAL:HG11	3:C:179:ARG:O	2.17	0.45
13:M:68:ASP:O	13:M:72:GLU:HG3	2.16	0.45
15:O:17:ARG:HE	15:O:17:ARG:HB2	1.63	0.45
22:a:249:C:C5	59:a:6215:SPD:H22	2.51	0.45
22:a:657:U:H2'	22:a:658:U:C6	2.52	0.45
22:a:1614:A:C2	39:r:93:ALA:HB2	2.52	0.45
22:a:1871:A:H2'	22:a:1872:A:C8	2.52	0.45
22:a:2334:U:C4	35:n:16:ARG:HG3	2.51	0.45
22:a:2627:G:O2'	22:a:2781:A:N1	2.39	0.45
22:a:2902:C:O5'	22:a:2902:C:H6	1.99	0.45
34:m:55:ALA:HA	34:m:80:PHE:CE2	2.52	0.45
38:q:60:LYS:HB3	38:q:60:LYS:HE3	1.74	0.45
54:Y:68:C:H2'	54:Y:69:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Z:43:A:H2'	55:Z:44:A:H8	1.79	0.45
1:A:1028:C:H6	1:A:1028:C:O5'	1.99	0.45
2:B:90:PHE:CZ	2:B:154:MET:HA	2.52	0.45
4:D:147:GLU:OE1	4:D:147:GLU:N	2.50	0.45
8:H:10:MET:HG3	8:H:27:MET:SD	2.57	0.45
12:L:66:TYR:O	12:L:97:THR:HG23	2.17	0.45
22:a:822:G:OP2	62:a:6342:HOH:O	2.21	0.45
22:a:1199:U:H2'	22:a:1200:C:C6	2.52	0.45
22:a:1585:C:H2'	22:a:1586:A:C8	2.52	0.45
22:a:2799:A:O2'	22:a:2800:A:H5"	2.16	0.45
27:f:36:LEU:HD22	27:f:154:ILE:HG12	1.97	0.45
27:f:36:LEU:O	27:f:88:LYS:HA	2.17	0.45
31:j:14:SER:O	31:j:52:VAL:HG22	2.16	0.45
36:o:26:VAL:HG12	36:o:86:VAL:HG22	1.98	0.45
42:u:35:GLU:HG3	42:u:36:ALA:N	2.32	0.45
1:A:429:U:H3'	4:D:9:LEU:HD12	1.99	0.45
1:A:502:A:H2'	1:A:503:C:O4'	2.16	0.45
1:A:1140:C:H2'	1:A:1141:C:C6	2.51	0.45
22:a:191:A:H2'	22:a:192:C:C6	2.52	0.45
22:a:358:U:N3	22:a:359:G:N7	2.65	0.45
22:a:1338:G:O2'	22:a:1393:A:N1	2.44	0.45
22:a:1537:G:C5'	62:a:6416:HOH:O	2.64	0.45
22:a:1794:A:H2'	22:a:1795:C:H6	1.82	0.45
22:a:1946:U:H2'	22:a:1947:C:C6	2.52	0.45
22:a:2743:U:H2'	22:a:2744:G:O4'	2.17	0.45
55:Z:3:C:H2'	55:Z:4:G:H8	1.81	0.45
1:A:87:C:OP1	1:A:87:C:H4'	2.16	0.45
22:a:165:A:H2'	22:a:166:U:O4'	2.17	0.45
22:a:534:U:O2'	37:p:49:ASP:OD2	2.27	0.45
22:a:914:G:H5'	22:a:915:C:OP2	2.17	0.45
22:a:1266:G:O2'	22:a:2012:G:O6	2.26	0.45
22:a:1416:G:C4	22:a:1417:C:C5	3.04	0.45
22:a:1726:C:H2'	22:a:1727:C:H6	1.82	0.45
59:a:6215:SPD:C5	62:a:9858:HOH:O	2.30	0.45
62:a:6994:HOH:O	47:z:12:LYS:HE3	2.17	0.45
25:d:181:ASP:HB3	25:d:186:LEU:HB2	1.98	0.45
54:Y:18:G:O2'	54:Y:57:G:N2	2.44	0.45
1:A:501:C:H2'	1:A:502:A:C8	2.52	0.45
6:F:52:ASN:OD1	6:F:52:ASN:O	2.34	0.45
7:G:103:TRP:CD1	7:G:137:LYS:HD3	2.52	0.45
22:a:364:C:H2'	22:a:365:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1209:U:O2'	22:a:1237:A:N1	2.45	0.45
22:a:1827:U:OP2	24:c:221:ARG:HD2	2.16	0.45
38:q:26:ASP:O	38:q:27:ILE:HD13	2.17	0.45
41:t:54:GLN:H	41:t:54:GLN:CD	2.20	0.45
54:Y:6:A:C8	54:Y:6:A:OP2	2.70	0.45
1:A:1014:A:C2	1:A:1219:A:H1'	2.52	0.45
5:E:105:ILE:O	5:E:112:ARG:NH1	2.47	0.45
6:F:4:TYR:CE2	6:F:71:ILE:HG13	2.51	0.45
22:a:306:U:H2'	22:a:307:G:O4'	2.17	0.45
22:a:1721:G:O2'	22:a:1739:A:N6	2.44	0.45
27:f:52:ASN:HB3	27:f:150:ARG:HH22	1.81	0.45
40:s:9:LYS:HD3	40:s:9:LYS:HA	1.79	0.45
1:A:215:C:O2'	1:A:465:A:N7	2.48	0.44
1:A:371:A:H2'	1:A:372:C:O4'	2.17	0.44
1:A:1326:U:H2'	1:A:1327:C:C6	2.53	0.44
3:C:191:THR:HG21	3:C:196:ILE:HD12	1.98	0.44
7:G:5:ARG:O	7:G:5:ARG:HG3	2.17	0.44
8:H:66:PHE:CD2	8:H:67:GLN:HG2	2.52	0.44
18:R:72:ASP:OD1	18:R:72:ASP:N	2.47	0.44
22:a:405:U:O2'	22:a:406:G:H5'	2.18	0.44
22:a:2555:U:OP2	62:a:6341:HOH:O	2.21	0.44
28:g:98:VAL:HG23	28:g:125:CYS:SG	2.57	0.44
31:j:108:ARG:HH11	31:j:116:ILE:HG21	1.82	0.44
32:k:70:LYS:HE3	32:k:107:PHE:CE2	2.52	0.44
1:A:244:U:O4	1:A:906:A:H1'	2.17	0.44
1:A:678:U:H2'	1:A:679:C:H6	1.82	0.44
1:A:718:A:H5'	11:K:119:IAS:C	2.47	0.44
10:J:21:ALA:O	10:J:25:ILE:HG13	2.17	0.44
11:K:36:ASP:OD2	11:K:40:ASN:HB2	2.16	0.44
22:a:414:C:H2'	22:a:415:A:H8	1.80	0.44
22:a:861:A:H2'	22:a:862:G:O4'	2.17	0.44
22:a:1668:A:O2'	22:a:1674:G:N7	2.38	0.44
22:a:2196:C:O2'	22:a:2197:U:H5'	2.17	0.44
23:b:42:C:C6	27:f:66:LEU:HB2	2.52	0.44
32:k:137:ALA:C	32:k:139:GLY:N	2.74	0.44
43:v:50:ASN:HA	62:v:117:HOH:O	2.17	0.44
51:3:4:ARG:O	51:3:37:GLN:HA	2.18	0.44
1:A:411:A:P	4:D:26:ARG:HH12	2.40	0.44
11:K:88:GLY:O	11:K:93:ARG:NH1	2.46	0.44
22:a:285:G:O6	22:a:355:U:O2	2.34	0.44
22:a:570:G:H2'	22:a:2030:6MZ:N7	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1049:C:H2'	22:a:1050:A:C8	2.52	0.44
22:a:1153:C:H2'	22:a:1154:G:O4'	2.18	0.44
22:a:1482:G:N1	22:a:1508:A:C2	2.86	0.44
22:a:2063:C:O2	22:a:2450:A:N1	2.51	0.44
22:a:2291:U:OP1	22:a:2380:C:O2'	2.31	0.44
27:f:14:LYS:HD2	27:f:14:LYS:N	2.33	0.44
45:x:54:LYS:HA	45:x:57:LEU:HD12	1.98	0.44
17:Q:15:ASP:OD1	17:Q:54:GLY:HA2	2.18	0.44
22:a:586:A:N1	22:a:809:G:O2'	2.48	0.44
22:a:1536:C:H4'	22:a:1537:G:C4	2.53	0.44
22:a:1808:A:H3'	22:a:1809:A:C8	2.52	0.44
28:g:38:ASN:ND2	28:g:64:GLN:HG3	2.33	0.44
34:m:66:ALA:O	34:m:69:ARG:O	2.36	0.44
41:t:14:LEU:HD11	41:t:71:ALA:HB2	1.99	0.44
1:A:666:G:H5'	1:A:726:C:H1'	1.99	0.44
1:A:736:C:H2'	1:A:737:C:H6	1.83	0.44
1:A:903:G:OP1	62:A:1717:HOH:O	2.21	0.44
1:A:1179:A:H2'	1:A:1180:A:O4'	2.18	0.44
2:B:100:MET:HA	2:B:107:VAL:HG21	1.98	0.44
8:H:54:ASP:OD1	8:H:54:ASP:N	2.46	0.44
22:a:39:G:H2'	22:a:40:U:C6	2.52	0.44
22:a:909:A:H2'	22:a:912:C:H5	1.82	0.44
22:a:1930:G:N2	22:a:1968:G:H2'	2.33	0.44
22:a:2590:A:H2'	22:a:2591:C:C6	2.53	0.44
37:p:15:LYS:HE2	37:p:15:LYS:HB3	1.74	0.44
39:r:7:HIS:HD2	62:r:216:HOH:O	2.00	0.44
45:x:6:LEU:C	45:x:8:GLU:H	2.25	0.44
1:A:299:G:H2'	1:A:300:A:C8	2.52	0.44
1:A:537:G:H2'	1:A:538:G:H8	1.82	0.44
1:A:1169:A:H2'	1:A:1170:A:C8	2.53	0.44
1:A:1307:U:H2'	1:A:1308:U:C6	2.53	0.44
7:G:110:LYS:HE2	7:G:110:LYS:HB3	1.72	0.44
25:d:110:THR:CG2	25:d:202:ILE:HB	2.45	0.44
33:l:51:ARG:CD	54:Y:54:U:H4'	2.48	0.44
54:Y:9:A:C8	54:Y:46:G:N2	2.85	0.44
1:A:166:U:H2'	1:A:167:A:H8	1.83	0.44
1:A:580:C:H2'	1:A:581:G:O4'	2.18	0.44
1:A:1073:U:O2'	2:B:105:LYS:HE3	2.18	0.44
1:A:1220:G:O2'	19:S:52:HIS:HD2	1.99	0.44
4:D:9:LEU:HD21	4:D:22:LYS:HG2	2.00	0.44
4:D:34:ILE:HD13	4:D:34:ILE:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:GLY:HA2	5:E:71:MET:HE3	1.99	0.44
17:Q:28:PHE:CE2	17:Q:37:PHE:HB3	2.53	0.44
22:a:645:C:H2'	22:a:647:G:C8	2.53	0.44
22:a:890:C:H3'	22:a:891:G:O4'	2.18	0.44
22:a:1872:A:C5	22:a:1873:G:H1'	2.52	0.44
22:a:2752:C:H2'	22:a:2753:A:O4'	2.17	0.44
59:a:6222:SPD:H71	62:a:8593:HOH:O	2.16	0.44
45:x:14:LEU:HA	45:x:14:LEU:HD12	1.59	0.44
1:A:235:C:H2'	1:A:236:A:C8	2.52	0.44
2:B:71:GLY:O	2:B:93:ASN:HA	2.18	0.44
3:C:148:GLY:HA3	3:C:172:ARG:O	2.17	0.44
7:G:138:ARG:NH1	7:G:139:GLU:HG3	2.33	0.44
9:I:19:VAL:HG22	9:I:65:ILE:HG12	1.99	0.44
22:a:542:C:H2'	22:a:543:G:H5"	2.00	0.44
22:a:588:U:H2'	22:a:589:U:C6	2.52	0.44
22:a:887:U:O2'	22:a:889:C:OP2	2.30	0.44
25:d:7:LYS:HB2	25:d:7:LYS:HE3	1.78	0.44
31:j:116:ILE:HD13	31:j:116:ILE:HA	1.91	0.44
32:k:95:LEU:HB3	32:k:101:ILE:HG12	1.99	0.44
54:Y:11:C:H2'	54:Y:12:U:C6	2.53	0.44
55:Z:18:G:O6	55:Z:55:U:H1'	2.17	0.44
1:A:501:C:H2'	1:A:502:A:H8	1.83	0.44
1:A:983:A:H5'	1:A:984:C:OP2	2.18	0.44
4:D:124:MET:O	4:D:143:VAL:HA	2.18	0.44
22:a:1271:G:O6	59:a:6219:SPD:H42	2.18	0.44
22:a:2233:U:H2'	22:a:2234:G:C8	2.52	0.44
33:l:110:GLU:O	33:l:114:ARG:HG3	2.17	0.44
1:A:1250:A:H2'	1:A:1251:A:C8	2.52	0.43
6:F:98:GLU:HG2	6:F:99:ALA:H	1.83	0.43
7:G:76:LYS:HE3	7:G:89:VAL:HG21	1.99	0.43
22:a:1127:A:O4'	59:a:6212:SPD:H91	2.18	0.43
22:a:1637:A:H5'	22:a:1760:C:O2'	2.18	0.43
24:c:76:ALA:HB2	24:c:96:TYR:CD1	2.53	0.43
24:c:108:LYS:HB3	62:c:450:HOH:O	2.18	0.43
28:g:38:ASN:ND2	28:g:40:ALA:H	2.16	0.43
34:m:1:MET:HE3	34:m:3:HIS:CE1	2.53	0.43
37:p:49:ASP:HA	37:p:52:GLN:HB2	2.00	0.43
40:s:56:GLU:HB3	40:s:86:THR:HB	2.00	0.43
45:x:34:SER:HB2	45:x:36:GLN:HB2	2.00	0.43
1:A:62:U:OP1	1:A:385:C:O2'	2.35	0.43
1:A:182:A:C4	1:A:184:G:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:A:H4'	22:a:1837:C:OP1	2.18	0.43
1:A:1226:C:P	13:M:90:ARG:HH22	2.41	0.43
1:A:1438:G:OP1	20:T:33:LYS:NZ	2.50	0.43
5:E:76:LEU:HD21	5:E:120:VAL:HG22	2.00	0.43
16:P:74:LEU:HA	16:P:77:GLU:HG2	1.99	0.43
22:a:1309:G:H4'	49:1:7:PRO:HG2	2.01	0.43
38:q:85:LYS:HB2	38:q:85:LYS:HE2	1.81	0.43
55:Z:69:C:H2'	55:Z:70:G:H8	1.83	0.43
21:U:16:LEU:HG	21:U:20:LYS:HZ3	1.83	0.43
22:a:57:C:H2'	22:a:58:G:O4'	2.19	0.43
22:a:94:A:H2'	22:a:95:A:C8	2.53	0.43
22:a:103:A:H2'	22:a:104:A:O4'	2.19	0.43
22:a:180:G:OP1	62:a:6343:HOH:O	2.21	0.43
22:a:580:U:H2'	22:a:581:C:C6	2.53	0.43
22:a:696:G:O6	60:a:6223:SPM:C8	2.66	0.43
22:a:1377:G:N7	62:a:6445:HOH:O	2.36	0.43
22:a:1486:U:O2'	22:a:1487:U:H5'	2.18	0.43
22:a:2282:G:H4'	22:a:2389:G:O2'	2.18	0.43
28:g:48:ASN:O	28:g:49:THR:HG23	2.18	0.43
1:A:461:A:H2'	1:A:462:G:C8	2.53	0.43
1:A:919:A:OP1	62:A:1718:HOH:O	2.21	0.43
6:F:36:ILE:HD13	6:F:64:VAL:HG22	2.01	0.43
22:a:967:U:H2'	22:a:968:C:C6	2.53	0.43
22:a:1198:U:H2'	22:a:1199:U:C6	2.52	0.43
22:a:2038:G:H2'	22:a:2039:U:O4'	2.17	0.43
26:e:136:GLN:CD	26:e:139:LYS:HD2	2.43	0.43
54:Y:14:A:H2'	54:Y:15:G:O4'	2.17	0.43
54:Y:21:A:C5	54:Y:46:G:C6	3.06	0.43
1:A:1074:G:H5'	2:B:105:LYS:HE3	2.00	0.43
1:A:1465:A:H2'	1:A:1466:C:H6	1.82	0.43
62:C:314:HOH:O	14:N:65:ARG:HD3	2.18	0.43
10:J:5:ARG:HD3	10:J:7:ARG:HG2	1.99	0.43
12:L:33:VAL:HG22	12:L:79:VAL:HG22	2.00	0.43
13:M:49:SER:O	13:M:53:ILE:HG12	2.18	0.43
22:a:911:A:P	59:a:6220:SPD:H51	2.58	0.43
22:a:1047:G:O3'	22:a:1048:A:H8	2.01	0.43
22:a:1736:U:H2'	22:a:1737:G:O4'	2.19	0.43
22:a:1932:A:H2'	22:a:1933:G:O4'	2.19	0.43
22:a:1971:U:C4	62:a:8102:HOH:O	2.70	0.43
22:a:2537:U:H2'	22:a:2538:C:H6	1.81	0.43
26:e:121:VAL:O	26:e:189:THR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:y:24:LEU:HD11	46:y:54:MET:HE2	2.00	0.43
52:4:3:LYS:O	52:4:5:ILE:HG23	2.19	0.43
54:Y:29:U:H2'	54:Y:30:C:H6	1.84	0.43
1:A:232:G:H1'	1:A:262:A:N1	2.34	0.43
1:A:358:U:H2'	1:A:359:G:C8	2.53	0.43
1:A:1352:C:H2'	1:A:1353:G:C8	2.54	0.43
12:L:79:VAL:O	12:L:103:ASP:HB2	2.19	0.43
16:P:40:ASN:HB3	16:P:43:ALA:HB2	2.00	0.43
22:a:138:U:O2'	22:a:139:U:H5"	2.18	0.43
22:a:1181:U:H2'	22:a:1182:G:H8	1.77	0.43
22:a:1913:A:C6	54:Y:38:A:H5'	2.54	0.43
28:g:95:ARG:HG2	28:g:128:GLN:HG2	2.00	0.43
33:l:1:MET:HE3	62:l:220:HOH:O	2.17	0.43
40:s:71:GLY:O	40:s:72:GLN:HG2	2.19	0.43
55:Z:18:G:N2	55:Z:57:A:H2'	2.33	0.43
1:A:767:A:H2'	1:A:768:A:O4'	2.19	0.43
1:A:945:G:C2	1:A:946:A:C8	3.06	0.43
1:A:1033:G:C8	1:A:1034:G:C8	3.07	0.43
4:D:13:ARG:NH2	4:D:38:PRO:HA	2.33	0.43
22:a:696:G:O6	60:a:6223:SPM:H81	2.19	0.43
22:a:1412:U:C2	22:a:1413:A:C8	3.07	0.43
22:a:2345:G:N3	22:a:2381:A:H2'	2.33	0.43
22:a:2462:C:H2'	22:a:2463:C:H6	1.83	0.43
22:a:2585:U:N3	54:Y:76:A:O3'	2.42	0.43
1:A:73:C:C2	1:A:74:A:C8	3.06	0.43
1:A:84:U:H4'	1:A:85:U:OP2	2.18	0.43
1:A:607:A:H2'	1:A:608:A:C8	2.53	0.43
1:A:1397:C:P	5:E:29:ARG:HH22	2.41	0.43
4:D:197:GLU:HG2	4:D:198:HIS:N	2.33	0.43
22:a:282:A:H2'	22:a:283:G:H8	1.84	0.43
22:a:412:A:N7	22:a:2411:A:H2	2.16	0.43
22:a:2096:C:H2'	22:a:2097:A:C8	2.54	0.43
22:a:2292:U:H2'	22:a:2293:G:H8	1.84	0.43
22:a:2799:A:O2'	22:a:2801:G:OP2	2.27	0.43
1:A:1118:U:H2'	1:A:1119:C:H6	1.83	0.43
1:A:1225:A:H2'	1:A:1226:C:C6	2.54	0.43
15:O:17:ARG:NH1	15:O:26:GLU:OE1	2.52	0.43
18:R:18:VAL:HG13	18:R:20:GLU:O	2.19	0.43
22:a:1589:U:H2'	22:a:1590:A:C8	2.53	0.43
22:a:1593:A:H2'	22:a:1594:U:C6	2.53	0.43
22:a:2648:G:H2'	22:a:2649:C:C6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:115:A:H2'	23:b:116:G:C8	2.54	0.43
28:g:44:LYS:HG3	28:g:51:THR:OG1	2.18	0.43
28:g:105:LEU:HB3	28:g:107:LEU:HG	2.01	0.43
31:j:58:LEU:HA	31:j:89:ASN:ND2	2.33	0.43
36:o:2:SER:HB2	36:o:3:ASN:H	1.57	0.43
37:p:58:ARG:HA	37:p:61:TRP:CE3	2.54	0.43
1:A:73:C:HO2'	1:A:74:A:H8	1.67	0.43
1:A:264:C:H2'	1:A:265:G:O4'	2.18	0.43
5:E:45:ARG:HH11	5:E:73:ASN:HD22	1.67	0.43
7:G:93:PRO:HD3	7:G:96:ARG:NH2	2.34	0.43
8:H:50:LYS:HB2	8:H:50:LYS:HE3	1.61	0.43
22:a:105:C:H2'	22:a:106:C:C6	2.53	0.43
22:a:386:G:O3'	59:a:6215:SPD:C9	2.67	0.43
22:a:454:A:H4'	22:a:455:C:OP2	2.18	0.43
22:a:1117:C:H2'	22:a:1118:C:C6	2.53	0.43
25:d:55:LYS:HD3	25:d:60:VAL:HG22	1.99	0.43
54:Y:2:G:H2'	54:Y:3:G:O4'	2.19	0.43
1:A:119:A:H5"	1:A:120:A:O4'	2.19	0.42
1:A:390:U:H2'	1:A:391:G:H8	1.78	0.42
1:A:489:C:H2'	1:A:490:C:C6	2.54	0.42
1:A:505:G:H2'	1:A:506:G:H8	1.84	0.42
1:A:745:G:H2'	1:A:746:A:C8	2.54	0.42
1:A:1088:G:H2'	1:A:1089:G:O4'	2.19	0.42
2:B:128:LYS:H	2:B:128:LYS:CD	2.32	0.42
8:H:55:THR:C	8:H:57:PRO:HD3	2.44	0.42
17:Q:60:GLU:HB2	17:Q:77:ARG:HG2	2.01	0.42
18:R:32:TYR:HB3	18:R:55:LEU:HD21	2.01	0.42
22:a:639:U:H2'	22:a:640:C:H6	1.82	0.42
22:a:922:C:O2'	43:v:29:GLU:OE2	2.36	0.42
22:a:947:A:H2'	22:a:948:C:C6	2.54	0.42
22:a:1047:G:O2'	22:a:1110:G:N1	2.25	0.42
22:a:1881:C:H2'	22:a:1882:U:O4'	2.19	0.42
22:a:2070:A:H2'	22:a:2071:A:O4'	2.19	0.42
23:b:42:C:O2'	27:f:63:GLN:HG2	2.18	0.42
33:l:53:MET:SD	33:l:117:PHE:HE1	2.42	0.42
38:q:51:VAL:HG23	38:q:51:VAL:O	2.19	0.42
1:A:33:A:H2'	1:A:34:C:C6	2.53	0.42
1:A:77:A:H2'	1:A:78:A:C8	2.54	0.42
1:A:473:U:H2'	1:A:474:G:C8	2.53	0.42
21:U:10:GLU:CD	21:U:18:ARG:HH21	2.27	0.42
22:a:248:G:O5'	22:a:249:C:H5"	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:277:G:H5'	22:a:278:A:OP1	2.19	0.42
22:a:387:U:OP1	59:a:6215:SPD:H92	2.18	0.42
22:a:483:A:H5"	41:t:47:LYS:HD3	2.01	0.42
22:a:717:C:H3'	22:a:718:A:C8	2.54	0.42
22:a:1733:G:H2'	22:a:1734:G:H8	1.85	0.42
22:a:1796:U:H2'	22:a:1797:G:H8	1.82	0.42
22:a:2723:C:H2'	22:a:2724:U:O4'	2.19	0.42
28:g:154:PRO:HA	28:g:160:LYS:O	2.19	0.42
33:l:17:ASN:O	33:l:38:ARG:HD3	2.19	0.42
1:A:410:G:P	4:D:26:ARG:HH11	2.42	0.42
1:A:493:A:H2'	1:A:494:G:N9	2.34	0.42
1:A:672:U:H2'	1:A:673:A:C8	2.54	0.42
3:C:85:GLU:OE1	3:C:89:LYS:HE3	2.19	0.42
13:M:19:LEU:HB2	13:M:30:SER:OG	2.19	0.42
13:M:68:ASP:OD1	13:M:71:ARG:NH1	2.53	0.42
22:a:1019:U:OP1	22:a:1035:U:O2'	2.27	0.42
22:a:2583:G:N3	54:Y:76:A:C2	2.87	0.42
25:d:149:ASN:OD1	25:d:150:MEQ:N	2.51	0.42
27:f:80:ARG:CZ	55:Z:56:C:C5	3.01	0.42
31:j:41:ILE:HD11	31:j:58:LEU:HG	2.01	0.42
14:N:10:GLU:HG3	14:N:63:ARG:HD2	2.02	0.42
22:a:297:G:H2'	22:a:298:G:O4'	2.20	0.42
22:a:1805:A:N3	24:c:50:THR:HB	2.34	0.42
22:a:2680:U:H5'	25:d:194:PRO:HA	2.01	0.42
22:a:2900:A:C6	22:a:2901:C:C4	3.07	0.42
59:a:6217:SPD:H22	62:a:7142:HOH:O	2.18	0.42
24:c:119:GLY:HA2	24:c:189:ARG:HH12	1.84	0.42
1:A:629:A:H2'	1:A:630:A:O4'	2.19	0.42
1:A:1002:G:H2'	1:A:1003:G:O4'	2.20	0.42
6:F:38:ARG:HB3	6:F:63:ASN:HB2	2.01	0.42
22:a:365:U:H2'	22:a:366:C:C6	2.54	0.42
22:a:818:G:H4'	22:a:838:C:O3'	2.19	0.42
22:a:1049:C:C2	22:a:1050:A:C8	3.07	0.42
22:a:1385:A:H1'	22:a:1386:C:C6	2.54	0.42
22:a:1607:C:H4'	22:a:1608:A:O5'	2.20	0.42
22:a:2241:A:H2'	22:a:2242:G:C8	2.54	0.42
22:a:2646:C:H2'	22:a:2647:U:O4'	2.19	0.42
26:e:136:GLN:HA	26:e:139:LYS:CG	2.50	0.42
26:e:152:GLU:O	26:e:153:LEU:C	2.63	0.42
26:e:170:ARG:NH2	26:e:176:ASP:OD1	2.45	0.42
28:g:75:MET:O	28:g:79:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:G:H2'	1:A:58:C:C6	2.54	0.42
1:A:635:A:H2'	1:A:636:U:C6	2.54	0.42
1:A:1202:U:OP1	62:A:1720:HOH:O	2.22	0.42
6:F:22:ILE:O	6:F:26:THR:HG23	2.19	0.42
10:J:7:ARG:HD3	10:J:73:LEU:HD11	2.01	0.42
18:R:13:PHE:O	18:R:18:VAL:HB	2.19	0.42
22:a:2421:G:N7	50:2:31:HIS:HD2	2.18	0.42
62:a:9687:HOH:O	33:l:7:THR:HG22	2.19	0.42
35:n:53:THR:HB	35:n:65:THR:HB	2.01	0.42
48:0:17:THR:HG21	48:0:43:VAL:HG13	2.02	0.42
1:A:5:U:H4'	1:A:6:G:O5'	2.20	0.42
1:A:66:A:N3	62:A:1811:HOH:O	2.37	0.42
1:A:675:A:O2'	11:K:116:ILE:O	2.35	0.42
1:A:868:C:H2'	1:A:869:G:O4'	2.20	0.42
1:A:1043:G:O2'	1:A:1044:A:H8	2.02	0.42
5:E:89:HIS:O	5:E:90:THR:C	2.63	0.42
5:E:164:ILE:O	5:E:165:LEU:HD23	2.20	0.42
17:Q:11:ARG:NH1	17:Q:56:GLY:HA2	2.35	0.42
22:a:848:C:H2'	22:a:849:A:C8	2.54	0.42
1:A:1003:G:N2	1:A:1004:A:O2'	2.52	0.42
3:C:140:ASN:O	3:C:144:LEU:HD23	2.20	0.42
4:D:43:ALA:O	4:D:45:LYS:HE2	2.19	0.42
4:D:100:ASN:HD22	4:D:111:ARG:HE	1.67	0.42
22:a:118:A:N3	22:a:178:G:H1'	2.35	0.42
22:a:249:C:O2	50:2:12:LYS:NZ	2.51	0.42
22:a:1015:U:H2'	22:a:1016:G:C8	2.55	0.42
22:a:1778:U:H2'	22:a:1784:A:N6	2.34	0.42
22:a:2412:A:H2'	22:a:2413:G:O4'	2.20	0.42
62:a:7362:HOH:O	47:z:42:HIS:CE1	2.71	0.42
23:b:40:U:H4'	62:b:374:HOH:O	2.19	0.42
26:e:127:GLU:CD	26:e:127:GLU:H	2.27	0.42
27:f:119:ALA:O	27:f:167:ARG:NH1	2.38	0.42
28:g:69:ARG:O	28:g:73:ASN:HB2	2.19	0.42
40:s:26:LYS:O	40:s:26:LYS:HG2	2.20	0.42
41:t:53:ASN:ND2	41:t:55:PRO:O	2.52	0.42
1:A:1333:A:H2'	1:A:1334:G:O4'	2.20	0.42
1:A:1412:C:H2'	1:A:1413:A:H8	1.85	0.42
1:A:1464:U:P	36:o:109:ARG:HH22	2.43	0.42
2:B:36:ASN:O	2:B:38:VAL:HG23	2.20	0.42
3:C:77:ILE:HG22	3:C:81:GLY:HA2	2.01	0.42
4:D:85:ASN:O	4:D:88:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:33:ARG:HG2	9:I:33:ARG:NH1	2.34	0.42
21:U:2:PRO:HG2	21:U:23:CYS:HA	2.01	0.42
22:a:1668:A:OP2	62:a:6346:HOH:O	2.22	0.42
22:a:1709:U:H2'	22:a:1710:G:C8	2.55	0.42
22:a:2030:6MZ:C2	22:a:2499:C:H5"	2.49	0.42
24:c:24:LEU:HD13	24:c:83:TYR:HB2	2.01	0.42
24:c:115:GLN:HE21	24:c:115:GLN:HB3	1.63	0.42
40:s:30:ILE:HG13	40:s:85:VAL:HB	2.01	0.42
54:Y:5:G:H2'	54:Y:6:A:C8	2.54	0.42
1:A:109:A:C6	1:A:326:G:C6	3.08	0.42
1:A:309:A:O2'	1:A:607:A:N1	2.45	0.42
1:A:1000:A:H2'	1:A:1001:C:H6	1.84	0.42
5:E:156:LYS:HD3	8:H:71:VAL:HG13	2.02	0.42
7:G:56:LYS:HB3	7:G:57:SER:H	1.74	0.42
12:L:110:ARG:HD2	12:L:110:ARG:HA	1.88	0.42
22:a:80:G:H5'	22:a:346:A:H1'	2.02	0.42
22:a:247:G:H4'	22:a:386:G:C5	2.55	0.42
22:a:747:5MU:O2	22:a:2014:A:H1'	2.19	0.42
22:a:1365:A:OP1	44:w:3:ARG:HD2	2.20	0.42
22:a:1412:U:H2'	22:a:1413:A:C8	2.51	0.42
22:a:2216:G:H2'	22:a:2217:G:C8	2.55	0.42
22:a:2786:U:O2'	22:a:2787:C:H5'	2.19	0.42
26:e:125:SER:H	26:e:137:LYS:HZ3	1.68	0.42
30:i:31:GLU:OE2	30:i:34:ARG:NH1	2.53	0.42
31:j:1:MET:SD	31:j:67:LYS:HD3	2.60	0.42
38:q:2:TYR:CE2	38:q:42:ALA:HB3	2.55	0.42
51:3:16:ILE:CD1	51:3:25:VAL:HG22	2.50	0.42
55:Z:14:A:H5'	55:Z:15:G:OP2	2.20	0.42
1:A:113:G:H2'	1:A:114:U:C6	2.55	0.41
1:A:475:C:H2'	1:A:476:U:O4'	2.20	0.41
1:A:519:C:H2'	1:A:520:A:O4'	2.19	0.41
17:Q:9:GLN:HA	17:Q:59:VAL:O	2.20	0.41
22:a:1259:G:O3'	59:a:6218:SPD:H21	2.20	0.41
26:e:134:LEU:HD23	26:e:164:LEU:HD12	2.01	0.41
33:l:1:MET:HE2	33:l:1:MET:HB3	1.57	0.41
38:q:27:ILE:HG13	38:q:33:VAL:CG1	2.50	0.41
44:w:40:VAL:HG13	44:w:43:GLU:HB2	2.01	0.41
44:w:68:LEU:HD22	44:w:78:TYR:CE1	2.56	0.41
47:z:52:ARG:CZ	47:z:54:VAL:HG12	2.49	0.41
1:A:218:U:H2'	1:A:219:U:O4'	2.19	0.41
1:A:1005:A:C6	1:A:1006:G:H1'	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:G:C5	1:A:1140:C:H1'	2.54	0.41
8:H:11:LEU:HD22	8:H:75:ILE:HD11	2.01	0.41
22:a:2721:A:H1'	22:a:2873:A:O2'	2.20	0.41
24:c:72:ASP:HB2	24:c:119:GLY:HA3	2.01	0.41
28:g:93:GLY:O	28:g:95:ARG:HD3	2.19	0.41
54:Y:59:U:O2'	54:Y:60:C:H5'	2.19	0.41
54:Y:69:A:H3'	54:Y:70:C:H6	1.84	0.41
1:A:107:G:P	59:A:1696:SPD:H101	2.43	0.41
1:A:399:G:H2'	1:A:400:C:C6	2.55	0.41
1:A:513:C:H2'	1:A:514:C:C6	2.54	0.41
3:C:132:ARG:O	3:C:136:ARG:HG3	2.21	0.41
5:E:150:PRO:HG3	8:H:99:LEU:HD21	2.03	0.41
6:F:20:GLY:O	6:F:23:GLU:HG3	2.21	0.41
8:H:3:MET:HE1	62:H:212:HOH:O	2.21	0.41
8:H:88:ARG:NH2	8:H:91:GLU:OE2	2.54	0.41
13:M:83:LEU:HD23	13:M:83:LEU:HA	1.84	0.41
22:a:144:A:H2'	22:a:145:C:C6	2.55	0.41
22:a:434:U:H1'	22:a:435:C:H5	1.86	0.41
22:a:1672:A:C2	22:a:2582:G:H5'	2.56	0.41
22:a:2299:U:H2'	22:a:2300:C:H6	1.85	0.41
27:f:22:TYR:OH	27:f:165:GLU:HG2	2.20	0.41
28:g:89:LEU:HD22	28:g:162:VAL:HG22	2.02	0.41
31:j:39:ILE:HG13	31:j:41:ILE:HG23	2.02	0.41
34:m:18:GLN:HE21	34:m:22:ARG:NH1	2.18	0.41
41:t:85:PHE:CE1	41:t:94:ARG:HG2	2.55	0.41
41:t:96:PHE:CZ	41:t:103:ILE:HG12	2.55	0.41
50:2:62:LEU:HB3	50:2:65:ALA:HB2	2.03	0.41
1:A:539:A:H2'	1:A:540:G:C8	2.55	0.41
1:A:779:C:H2'	1:A:780:A:O4'	2.20	0.41
59:A:1696:SPD:HN11	59:A:1696:SPD:H52	1.84	0.41
15:O:88:ARG:NH2	22:a:714:U:OP2	2.54	0.41
21:U:8:GLU:C	21:U:10:GLU:H	2.27	0.41
22:a:337:C:OP2	41:t:4:LYS:NZ	2.50	0.41
22:a:937:C:P	50:2:52:LYS:HE3	2.59	0.41
22:a:1316:U:H2'	22:a:1317:G:H8	1.85	0.41
22:a:1588:G:H2'	22:a:1589:U:H6	1.86	0.41
22:a:2295:C:OP2	35:n:10:ARG:HD3	2.20	0.41
22:a:2552:OMU:HM23	22:a:2554:U:C6	2.55	0.41
22:a:2822:G:O2'	22:a:2824:C:OP2	2.34	0.41
23:b:112:G:H2'	23:b:113:C:H6	1.85	0.41
24:c:37:ASN:O	24:c:37:ASN:CG	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:71:LYS:HG3	24:c:102:ARG:NH2	2.35	0.41
24:c:133:ARG:HB3	24:c:186:ALA:HB1	2.02	0.41
30:i:125:TYR:OH	30:i:132:HIS:NE2	2.45	0.41
31:j:105:ARG:HB2	31:j:123:LEU:O	2.20	0.41
38:q:27:ILE:O	38:q:66:HIS:CE1	2.73	0.41
54:Y:25:C:H2'	54:Y:26:A:H8	1.85	0.41
1:A:165:G:H2'	1:A:166:U:C6	2.55	0.41
4:D:70:ARG:CZ	62:D:305:HOH:O	2.67	0.41
7:G:7:ILE:HD13	7:G:7:ILE:N	2.34	0.41
7:G:151:PHE:C	7:G:153:HIS:H	2.28	0.41
22:a:244:A:H2'	22:a:245:G:O4'	2.20	0.41
22:a:327:G:H2'	22:a:328:U:O4'	2.19	0.41
54:Y:13:C:O2'	54:Y:14:A:OP1	2.28	0.41
55:Z:25:C:H2'	55:Z:26:G:O4'	2.21	0.41
2:B:129:LEU:HD22	2:B:137:ARG:HE	1.86	0.41
4:D:51:TYR:OH	62:D:302:HOH:O	2.20	0.41
8:H:101:ILE:HG12	8:H:129:VAL:HB	2.02	0.41
22:a:84:A:H4'	22:a:85:G:O5'	2.21	0.41
22:a:361:G:O2'	22:a:362:A:H8	2.04	0.41
22:a:362:A:H2'	22:a:363:G:H5'	2.02	0.41
22:a:601:C:O2'	22:a:605:G:OP1	2.28	0.41
22:a:910:A:H2'	22:a:911:A:C8	2.55	0.41
22:a:1405:U:H2'	22:a:1406:U:H6	1.83	0.41
22:a:1528:A:N6	22:a:1543:G:O2'	2.53	0.41
22:a:2019:A:H4'	37:p:34:VAL:HG21	2.02	0.41
22:a:2680:U:O2'	22:a:2681:C:H5'	2.21	0.41
22:a:2802:G:H2'	22:a:2803:G:C8	2.55	0.41
1:A:546:A:P	4:D:69:GLU:HB3	2.61	0.41
1:A:628:G:H2'	1:A:629:A:C8	2.56	0.41
1:A:860:A:H2'	1:A:861:G:O4'	2.20	0.41
1:A:881:G:P	12:L:9:ARG:HH22	2.43	0.41
1:A:1216:A:H5"	14:N:5:SER:HB3	2.03	0.41
4:D:184:ARG:NH2	4:D:186:PRO:HA	2.33	0.41
22:a:176:A:O2'	22:a:177:G:H5'	2.21	0.41
22:a:282:A:H2'	22:a:283:G:C8	2.56	0.41
22:a:401:A:N1	62:a:6460:HOH:O	2.37	0.41
22:a:576:U:H2'	22:a:577:G:C8	2.55	0.41
22:a:1538:G:H2'	22:a:1539:U:C6	2.55	0.41
22:a:1589:U:H2'	22:a:1590:A:H8	1.86	0.41
22:a:2783:U:H2'	22:a:2784:U:H6	1.84	0.41
62:a:7362:HOH:O	47:z:42:HIS:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:142:ASP:O	27:f:146:VAL:HG23	2.20	0.41
30:i:95:ARG:HG2	30:i:96:ARG:HD3	2.02	0.41
30:i:110:PRO:O	30:i:115:GLY:HA3	2.21	0.41
1:A:272:C:H2'	1:A:273:U:C6	2.55	0.41
1:A:404:G:H4'	1:A:439:U:O2	2.21	0.41
1:A:575:G:O2'	1:A:821:G:H5'	2.21	0.41
1:A:718:A:C2	18:R:38:LYS:HG2	2.56	0.41
1:A:1071:C:H2'	1:A:1072:G:H8	1.84	0.41
22:a:144:A:H2'	22:a:145:C:H6	1.86	0.41
22:a:896:A:C2'	54:Y:56:C:O2	2.61	0.41
22:a:1225:G:OP1	38:q:71:LYS:NZ	2.48	0.41
22:a:1259:G:O2'	59:a:6218:SPD:H32	2.20	0.41
22:a:1357:C:H2'	22:a:1358:G:O4'	2.21	0.41
22:a:1428:C:C5	22:a:1569:A:H5"	2.56	0.41
22:a:1440:U:H2'	22:a:1441:G:C8	2.56	0.41
22:a:2020:A:H62	47:z:6:ASN:ND2	2.19	0.41
22:a:2543:G:H2'	22:a:2544:G:C8	2.56	0.41
22:a:2702:G:H2'	22:a:2703:C:C6	2.55	0.41
22:a:2756:U:H1'	22:a:2757:A:H5"	2.02	0.41
22:a:2849:U:H4'	22:a:2868:A:C2	2.55	0.41
28:g:42:GLU:HB2	28:g:53:GLY:O	2.20	0.41
32:k:39:LYS:HZ2	32:k:39:LYS:HG3	1.72	0.41
54:Y:21:A:C5	54:Y:46:G:C5	3.09	0.41
55:Z:3:C:H2'	55:Z:4:G:C8	2.56	0.41
1:A:34:C:H2'	1:A:35:G:H8	1.85	0.41
1:A:128:G:O2'	1:A:129:A:H5'	2.21	0.41
1:A:155:A:H2'	1:A:156:C:C6	2.56	0.41
1:A:373:A:O2'	1:A:451:A:N7	2.54	0.41
1:A:464:U:H2'	1:A:465:A:H5"	2.02	0.41
1:A:1077:G:N2	1:A:1080:A:OP2	2.45	0.41
1:A:1220:G:O3'	19:S:36:ARG:HD3	2.21	0.41
1:A:1496:C:H2'	1:A:1497:G:O4'	2.21	0.41
4:D:48:LEU:HD12	4:D:48:LEU:HA	1.92	0.41
4:D:107:PHE:CD2	4:D:145:ILE:HD11	2.56	0.41
4:D:142:VAL:HA	4:D:180:GLY:O	2.20	0.41
5:E:156:LYS:HD3	8:H:71:VAL:HA	2.03	0.41
6:F:96:VAL:O	6:F:96:VAL:HG12	2.20	0.41
10:J:85:ASP:O	10:J:89:ARG:HG2	2.21	0.41
14:N:5:SER:O	14:N:9:ARG:HG3	2.21	0.41
18:R:9:LYS:HA	18:R:9:LYS:HD3	1.92	0.41
20:T:57:ILE:O	20:T:61:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:151:C:H2'	22:a:152:A:H8	1.85	0.41
22:a:325:G:O6	59:a:6216:SPD:H32	2.20	0.41
22:a:537:G:H5"	30:i:5:THR:HG21	2.03	0.41
22:a:581:C:H2'	22:a:582:A:H8	1.84	0.41
22:a:720:U:H6	22:a:720:U:O5'	2.04	0.41
22:a:894:U:H2'	22:a:895:U:C6	2.56	0.41
22:a:933:A:H5'	22:a:934:U:OP2	2.20	0.41
22:a:1490:A:H2'	24:c:98:ASP:HB3	2.03	0.41
22:a:1531:C:C2'	22:a:1532:A:H5'	2.50	0.41
22:a:2333:A:H3'	43:v:75:LYS:NZ	2.35	0.41
60:a:6223:SPM:N10	62:a:6301:HOH:O	1.89	0.41
26:e:184:ASP:HA	32:k:2:ARG:HH12	1.86	0.41
28:g:42:GLU:O	28:g:52:PHE:HA	2.20	0.41
41:t:13:VAL:HA	41:t:70:VAL:HG12	2.03	0.41
41:t:54:GLN:HG2	41:t:55:PRO:HD3	2.03	0.41
44:w:6:GLN:NE2	44:w:50:ARG:H	2.16	0.41
54:Y:24:G:H3'	54:Y:25:C:H6	1.85	0.41
1:A:592:G:H2'	1:A:593:U:C6	2.56	0.41
1:A:1436:U:H2'	1:A:1437:A:C8	2.56	0.41
1:A:1478:U:H2'	1:A:1479:C:H6	1.84	0.41
1:A:1530:G:H2'	1:A:1531:A:C8	2.56	0.41
3:C:6:HIS:CG	14:N:89:MET:HB3	2.56	0.41
22:a:460:A:H2'	22:a:461:C:O4'	2.21	0.41
22:a:703:U:H2'	22:a:704:G:O4'	2.21	0.41
22:a:883:G:H2'	22:a:884:U:H6	1.86	0.41
22:a:1420:A:O2'	22:a:1421:G:H5'	2.21	0.41
22:a:1676:A:H2'	22:a:1677:A:O4'	2.21	0.41
22:a:2407:A:H2'	22:a:2408:U:C6	2.56	0.41
22:a:2443:C:OP1	26:e:63:LYS:HD3	2.21	0.41
59:a:6215:SPD:H102	44:w:22:LEU:HD22	1.80	0.41
25:d:1:MET:HE2	25:d:205:PRO:CG	2.51	0.41
42:u:44:HIS:O	42:u:48:MET:HB2	2.21	0.41
43:v:37:ILE:HG21	43:v:80:ILE:HG21	2.03	0.41
1:A:16:A:N1	1:A:919:A:H2	2.20	0.40
1:A:252:U:C2	1:A:253:A:N7	2.89	0.40
1:A:259:G:OP1	20:T:36:TYR:OH	2.32	0.40
1:A:750:C:O2	15:O:23:GLY:HA3	2.20	0.40
1:A:892:A:H2'	1:A:893:C:C6	2.56	0.40
1:A:927:G:O2'	1:A:1503:A:N7	2.43	0.40
1:A:1022:A:H2'	1:A:1023:U:O4'	2.21	0.40
1:A:1424:U:H2'	1:A:1425:U:C6	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:MET:HE3	2:B:158:PRO:HD3	2.03	0.40
62:C:302:HOH:O	14:N:97:LYS:HB2	2.22	0.40
5:E:34:THR:HB	5:E:50:TYR:CE1	2.55	0.40
21:U:7:ARG:O	21:U:10:GLU:HB3	2.21	0.40
21:U:39:GLU:HG3	21:U:43:THR:HB	2.03	0.40
22:a:181:A:H2'	22:a:182:A:C8	2.56	0.40
22:a:273:G:H2'	22:a:274:C:C5	2.54	0.40
22:a:472:A:OP2	62:a:6344:HOH:O	2.22	0.40
22:a:667:U:H2'	22:a:668:A:O4'	2.21	0.40
22:a:1385:A:C4	22:a:1386:C:C5	3.09	0.40
22:a:1582:C:H2'	22:a:1583:A:O4'	2.20	0.40
22:a:1586:A:C5	22:a:1587:G:C8	3.09	0.40
22:a:2066:C:O2'	22:a:2067:G:H5'	2.20	0.40
22:a:2246:G:H2'	22:a:2247:A:C8	2.55	0.40
22:a:2648:G:H2'	22:a:2649:C:H6	1.86	0.40
23:b:106:G:H2'	23:b:107:G:O4'	2.21	0.40
25:d:121:THR:HB	25:d:127:PHE:CD2	2.56	0.40
28:g:90:VAL:HG23	28:g:160:LYS:HA	2.03	0.40
32:k:123:ARG:HE	32:k:143:GLU:HG3	1.85	0.40
1:A:110:C:H2'	1:A:111:G:O4'	2.21	0.40
1:A:745:G:O2'	1:A:746:A:H5'	2.20	0.40
7:G:76:LYS:HG3	7:G:89:VAL:HG21	2.03	0.40
12:L:66:TYR:HB2	12:L:87:VAL:HG21	2.03	0.40
15:O:80:GLN:O	15:O:84:ARG:HG3	2.20	0.40
22:a:72:U:H4'	62:a:9384:HOH:O	2.22	0.40
22:a:140:C:H5'	22:a:141:G:C4	2.56	0.40
22:a:228:C:H4'	22:a:229:C:H5"	2.02	0.40
22:a:278:A:C6	22:a:362:A:C5	3.09	0.40
22:a:948:C:H1'	22:a:984:A:C8	2.56	0.40
22:a:1115:G:C4	22:a:1116:G:C8	3.08	0.40
22:a:1199:U:H1'	37:p:4:VAL:HG22	2.03	0.40
22:a:1316:U:H2'	22:a:1317:G:C8	2.56	0.40
23:b:29:A:H2'	23:b:30:C:O4'	2.21	0.40
54:Y:18:G:O2'	54:Y:57:G:N1	2.50	0.40
54:Y:29:U:H2'	54:Y:30:C:C6	2.56	0.40
1:A:253:A:H2'	1:A:254:G:C8	2.56	0.40
1:A:410:G:H2'	1:A:429:U:C5	2.56	0.40
1:A:426:U:OP1	4:D:33:LYS:HD3	2.22	0.40
22:a:20:C:H2'	22:a:21:A:C8	2.57	0.40
22:a:264:C:N3	62:a:6329:HOH:O	2.51	0.40
22:a:543:G:H8	22:a:543:G:C5'	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2395:C:OP1	62:a:6345:HOH:O	2.22	0.40
25:d:46:ARG:NH1	25:d:86:GLU:HA	2.37	0.40
33:l:53:MET:HE1	33:l:103:TYR:CE2	2.56	0.40
35:n:88:LYS:O	35:n:116:GLN:HG3	2.21	0.40
42:u:20:LEU:HD21	42:u:41:GLU:CD	2.46	0.40
54:Y:50:G:H2'	54:Y:51:C:C6	2.56	0.40
1:A:216:U:H4'	1:A:464:U:H4'	2.02	0.40
1:A:1468:A:H2'	1:A:1469:C:O4'	2.21	0.40
6:F:20:GLY:O	6:F:21:MET:C	2.64	0.40
7:G:149:LYS:HE2	7:G:149:LYS:HB2	1.74	0.40
22:a:415:A:H2'	22:a:416:U:C6	2.56	0.40
22:a:2271:G:OP1	43:v:18:ALA:HB1	2.20	0.40
62:a:9374:HOH:O	24:c:242:LYS:CE	2.55	0.40
24:c:163:GLN:CD	24:c:175:ARG:HH11	2.29	0.40
28:g:9:VAL:HG11	28:g:50:LEU:HB2	2.03	0.40
29:h:37:VAL:HG22	29:h:38:PRO:O	2.21	0.40
1:A:197:A:C6	1:A:221:C:H4'	2.56	0.40
1:A:302:G:O2'	1:A:556:C:H5"	2.21	0.40
1:A:857:C:H2'	1:A:858:G:O4'	2.21	0.40
1:A:977:A:O2'	1:A:979:C:OP2	2.35	0.40
1:A:1005:A:H3'	1:A:1006:G:H8	1.86	0.40
5:E:23:LYS:HE2	5:E:23:LYS:HB2	1.82	0.40
12:L:110:ARG:HB3	12:L:119:VAL:HG21	2.04	0.40
13:M:96:PRO:HG2	13:M:102:THR:CG2	2.51	0.40
22:a:1797:G:C6	22:a:1798:U:C4	3.10	0.40
22:a:2461:A:H2'	22:a:2462:C:C6	2.56	0.40
27:f:10:ASP:O	27:f:14:LYS:HD3	2.21	0.40
36:o:114:LEU:HD23	36:o:114:LEU:HA	1.58	0.40
48:0:26:ASN:O	48:0:30:LYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
3	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
4	D	203/206 (98%)	194 (96%)	9 (4%)	0	100	100
5	E	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
6	F	101/135 (75%)	94 (93%)	7 (7%)	0	100	100
7	G	151/179 (84%)	137 (91%)	12 (8%)	2 (1%)	9	3
8	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	I	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
10	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	5
11	K	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
12	L	120/124 (97%)	115 (96%)	4 (3%)	1 (1%)	16	7
13	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
14	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
15	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
18	R	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
19	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
20	T	84/87 (97%)	84 (100%)	0	0	100	100
21	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
24	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
25	d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
26	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
27	f	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
28	g	174/177 (98%)	151 (87%)	21 (12%)	2 (1%)	11	4
29	h	39/149 (26%)	32 (82%)	7 (18%)	0	100	100
30	i	140/142 (99%)	140 (100%)	0	0	100	100
31	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
32	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	18	9
33	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
34	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
35	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
37	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
38	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
39	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
40	s	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
41	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
42	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
43	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
44	w	75/78 (96%)	75 (100%)	0	0	100	100
45	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
48	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
All	All	5481/5913 (93%)	5262 (96%)	212 (4%)	7 (0%)	49	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	6	VAL
28	g	47	ASP
10	J	57	VAL
7	G	5	ARG
12	L	102	LEU
32	k	138	ALA
28	g	92	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	186/199 (94%)	171 (92%)	15 (8%)	11 3
3	C	170/190 (90%)	161 (95%)	9 (5%)	20 9
4	D	172/173 (99%)	151 (88%)	21 (12%)	5 1
5	E	119/126 (94%)	110 (92%)	9 (8%)	12 4
6	F	90/116 (78%)	82 (91%)	8 (9%)	9 2
7	G	126/147 (86%)	114 (90%)	12 (10%)	8 2
8	H	104/105 (99%)	103 (99%)	1 (1%)	68 65
9	I	105/107 (98%)	102 (97%)	3 (3%)	37 28
10	J	86/90 (96%)	80 (93%)	6 (7%)	14 5
11	K	89/98 (91%)	81 (91%)	8 (9%)	9 2
12	L	102/103 (99%)	96 (94%)	6 (6%)	18 8
13	M	93/96 (97%)	83 (89%)	10 (11%)	6 1
14	N	83/84 (99%)	82 (99%)	1 (1%)	63 58
15	O	76/77 (99%)	72 (95%)	4 (5%)	20 9
16	P	65/65 (100%)	61 (94%)	4 (6%)	16 7
17	Q	73/78 (94%)	68 (93%)	5 (7%)	14 5
18	R	57/65 (88%)	52 (91%)	5 (9%)	9 2
19	S	72/79 (91%)	67 (93%)	5 (7%)	14 5
20	T	65/66 (98%)	59 (91%)	6 (9%)	8 2
21	U	60/61 (98%)	53 (88%)	7 (12%)	5 1
24	c	216/218 (99%)	209 (97%)	7 (3%)	34 24
25	d	163/163 (100%)	161 (99%)	2 (1%)	63 58
26	e	165/165 (100%)	154 (93%)	11 (7%)	15 5
27	f	148/150 (99%)	139 (94%)	9 (6%)	17 7
28	g	137/138 (99%)	116 (85%)	21 (15%)	3 0
29	h	32/114 (28%)	28 (88%)	4 (12%)	4 1
30	i	116/116 (100%)	113 (97%)	3 (3%)	40 32
31	j	104/104 (100%)	98 (94%)	6 (6%)	18 8
32	k	103/103 (100%)	98 (95%)	5 (5%)	22 10
33	l	107/107 (100%)	103 (96%)	4 (4%)	30 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	m	98/103 (95%)	96 (98%)	2 (2%)	48 42
35	n	86/87 (99%)	80 (93%)	6 (7%)	14 5
36	o	99/100 (99%)	98 (99%)	1 (1%)	68 65
37	p	89/90 (99%)	86 (97%)	3 (3%)	32 22
38	q	84/84 (100%)	77 (92%)	7 (8%)	10 3
39	r	93/93 (100%)	92 (99%)	1 (1%)	65 61
40	s	80/84 (95%)	76 (95%)	4 (5%)	22 10
41	t	83/85 (98%)	76 (92%)	7 (8%)	10 3
42	u	78/78 (100%)	71 (91%)	7 (9%)	9 2
43	v	58/63 (92%)	55 (95%)	3 (5%)	21 9
44	w	67/68 (98%)	64 (96%)	3 (4%)	24 13
45	x	54/55 (98%)	46 (85%)	8 (15%)	3 1
46	y	48/49 (98%)	44 (92%)	4 (8%)	10 3
47	z	47/48 (98%)	45 (96%)	2 (4%)	26 14
48	0	46/49 (94%)	41 (89%)	5 (11%)	6 1
49	1	38/38 (100%)	38 (100%)	0	100 100
50	2	51/52 (98%)	49 (96%)	2 (4%)	28 17
51	3	34/34 (100%)	33 (97%)	1 (3%)	37 28
52	4	55/62 (89%)	50 (91%)	5 (9%)	9 2
All	All	4572/4825 (95%)	4284 (94%)	288 (6%)	18 6

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	ASP
2	B	20	THR
2	B	58	ASN
2	B	62	SER
2	B	63	ARG
2	B	67	ILE
2	B	70	VAL
2	B	93	ASN
2	B	107	VAL
2	B	117	LEU
2	B	133	GLU

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Mol	Chain	Res	Type
2	B	161	LEU
2	B	188	ASP
2	B	205	ASP
2	B	211	THR
3	C	75	ILE
3	C	85	GLU
3	C	107	ARG
3	C	108	LYS
3	C	111	LEU
3	C	147	LYS
3	C	170	GLU
3	C	178	LEU
3	C	207	ILE
4	D	25	VAL
4	D	26	ARG
4	D	34	ILE
4	D	48	LEU
4	D	50	ASP
4	D	85	ASN
4	D	138	SER
4	D	142	VAL
4	D	143	VAL
4	D	144	SER
4	D	146	ARG
4	D	166	GLU
4	D	167	LYS
4	D	177	LYS
4	D	181	THR
4	D	184	ARG
4	D	188	ARG
4	D	192	SER
4	D	202	GLU
4	D	205	SER
4	D	206	LYS
5	E	14	LYS
5	E	22	SER
5	E	55	GLU
5	E	64	MET
5	E	72	ILE
5	E	73	ASN
5	E	145	GLU
5	E	159	LYS

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Mol	Chain	Res	Type
5	E	164	ILE
6	F	2	ARG
6	F	14	GLN
6	F	15	SER
6	F	53	LYS
6	F	62	MET
6	F	82	ASP
6	F	102	MET
6	F	103	VAL
7	G	7	ILE
7	G	9	GLN
7	G	22	LEU
7	G	50	LEU
7	G	72	THR
7	G	77	SER
7	G	89	VAL
7	G	90	GLU
7	G	113	ASP
7	G	129	GLU
7	G	144	MET
7	G	149	LYS
8	H	56	LYS
9	I	43	THR
9	I	59	GLU
9	I	85	ARG
10	J	7	ARG
10	J	17	LEU
10	J	27	GLU
10	J	28	THR
10	J	46	LYS
10	J	92	LEU
11	K	14	LYS
11	K	35	THR
11	K	36	ASP
11	K	72	ASP
11	K	75	LYS
11	K	86	VAL
11	K	87	LYS
11	K	129	VAL
12	L	4	VAL
12	L	14	ARG
12	L	43	LYS

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Mol	Chain	Res	Type
12	L	54	ARG
12	L	55	VAL
12	L	62	GLU
13	M	3	ARG
13	M	4	ILE
13	M	7	ILE
13	M	16	VAL
13	M	27	LYS
13	M	49	SER
13	M	53	ILE
13	M	75	MET
13	M	82	ASP
13	M	114	LYS
14	N	34	VAL
15	O	3	LEU
15	O	18	ASP
15	O	47	LYS
15	O	75	VAL
16	P	3	THR
16	P	42	ILE
16	P	47	GLU
16	P	48	GLU
17	Q	5	ILE
17	Q	16	LYS
17	Q	41	THR
17	Q	42	THR
17	Q	50	ASN
18	R	14	THR
18	R	21	ILE
18	R	35	GLU
18	R	36	SER
18	R	50	LYS
19	S	5	LEU
19	S	24	GLU
19	S	28	LYS
19	S	29	LYS
19	S	43	ASN
20	T	6	SER
20	T	13	GLN
20	T	44	LYS
20	T	54	MET
20	T	84	ASN

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Mol	Chain	Res	Type
20	T	85	LYS
21	U	3	VAL
21	U	4	ILE
21	U	8	GLU
21	U	44	GLU
21	U	54	LYS
21	U	59	LYS
21	U	60	LEU
24	c	4	VAL
24	c	28	LYS
24	c	37	ASN
24	c	111	LYS
24	c	140	THR
24	c	242	LYS
24	c	272	SER
25	d	12	THR
25	d	92	VAL
26	e	4	VAL
26	e	9	GLN
26	e	14	VAL
26	e	65	THR
26	e	107	SER
26	e	114	ARG
26	e	123	LYS
26	e	146	VAL
26	e	150	THR
26	e	153	LEU
26	e	175	ILE
27	f	32	GLU
27	f	47	LYS
27	f	50	LEU
27	f	85	ILE
27	f	112	ARG
27	f	120	LYS
27	f	136	ILE
27	f	150	ARG
27	f	165	GLU
28	g	9	VAL
28	g	20	ASN
28	g	27	LYS
28	g	34	THR
28	g	36	THR

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Mol	Chain	Res	Type
28	g	43	VAL
28	g	44	LYS
28	g	49	THR
28	g	75	MET
28	g	76	VAL
28	g	77	ILE
28	g	79	VAL
28	g	90	VAL
28	g	101	ASN
28	g	103	ILE
28	g	122	THR
28	g	127	THR
28	g	129	THR
28	g	171	THR
28	g	173	GLU
28	g	175	LYS
29	h	6	LEU
29	h	9	VAL
29	h	17	ASP
29	h	21	VAL
30	i	1	MET
30	i	9	GLU
30	i	11	VAL
31	j	51	LYS
31	j	58	LEU
31	j	88	ASN
31	j	95	ILE
31	j	109	SER
31	j	123	LEU
32	k	115	GLU
32	k	117	THR
32	k	118	THR
32	k	120	VAL
32	k	129	LYS
33	l	7	THR
33	l	51	ARG
33	l	78	LEU
33	l	135	VAL
34	m	6	SER
34	m	48	VAL
35	n	2	ASP
35	n	16	ARG

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Mol	Chain	Res	Type
35	n	45	SER
35	n	85	LYS
35	n	87	ILE
35	n	89	ASP
36	o	2	SER
37	p	85	LYS
37	p	87	SER
37	p	112	LYS
38	q	6	GLN
38	q	33	VAL
38	q	41	ILE
38	q	47	VAL
38	q	55	ASP
38	q	71	LYS
38	q	72	VAL
39	r	66	ILE
40	s	36	LYS
40	s	74	ILE
40	s	86	THR
40	s	93	LEU
41	t	8	ASP
41	t	15	THR
41	t	24	LYS
41	t	39	ILE
41	t	60	GLU
41	t	74	ASN
41	t	98	SER
42	u	3	THR
42	u	11	GLU
42	u	58	SER
42	u	60	VAL
42	u	62	THR
42	u	63	ILE
42	u	77	VAL
43	v	10	THR
43	v	30	SER
43	v	44	LYS
44	w	54	LYS
44	w	56	MET
44	w	71	LEU
45	x	2	LYS
45	x	4	LYS

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Mol	Chain	Res	Type
45	x	5	GLU
45	x	8	GLU
45	x	13	GLU
45	x	14	LEU
45	x	24	GLU
45	x	58	ASN
46	y	3	LYS
46	y	4	THR
46	y	41	THR
46	y	59	GLU
47	z	26	THR
47	z	54	VAL
48	0	5	ILE
48	0	32	GLU
48	0	35	GLU
48	0	37	LYS
48	0	54	ILE
50	2	15	LYS
50	2	31	HIS
51	3	36	ARG
52	4	8	LYS
52	4	13	THR
52	4	17	SER
52	4	24	ILE
52	4	66	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	39	HIS
2	B	58	ASN
2	B	89	GLN
2	B	103	ASN
2	B	109	GLN
3	C	3	GLN
3	C	100	GLN
3	C	123	GLN
3	C	140	ASN
4	D	40	GLN
4	D	71	GLN
4	D	100	ASN
4	D	131	ASN

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Mol	Chain	Res	Type
4	D	140	ASN
5	E	12	GLN
5	E	73	ASN
5	E	82	GLN
5	E	146	ASN
5	E	148	ASN
6	F	37	HIS
6	F	46	GLN
6	F	55	HIS
7	G	68	ASN
7	G	86	GLN
9	I	31	ASN
9	I	32	GLN
9	I	110	GLN
10	J	15	HIS
10	J	56	HIS
11	K	24	HIS
11	K	38	GLN
11	K	40	ASN
12	L	112	GLN
13	M	8	ASN
14	N	35	ASN
15	O	35	GLN
15	O	40	GLN
15	O	50	HIS
16	P	9	HIS
19	S	52	HIS
19	S	56	GLN
19	S	57	HIS
19	S	83	HIS
20	T	48	GLN
20	T	68	HIS
20	T	84	ASN
21	U	56	HIS
24	c	60	GLN
24	c	90	ASN
24	c	115	GLN
24	c	117	GLN
24	c	197	ASN
24	c	243	HIS
26	e	94	GLN
26	e	136	GLN

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Mol	Chain	Res	Type
27	f	37	ASN
28	g	38	ASN
28	g	48	ASN
28	g	101	ASN
28	g	104	ASN
28	g	115	HIS
29	h	20	ASN
30	i	47	HIS
30	i	58	ASN
30	i	86	GLN
30	i	128	ASN
31	j	9	ASN
32	k	35	HIS
32	k	93	ASN
33	l	13	HIS
34	m	18	GLN
34	m	31	HIS
35	n	100	HIS
36	o	10	GLN
36	o	12	GLN
36	o	41	GLN
37	p	37	GLN
37	p	52	GLN
38	q	6	GLN
38	q	43	ASN
39	r	7	HIS
39	r	9	HIS
39	r	31	GLN
39	r	40	ASN
40	s	48	GLN
40	s	72	GLN
41	t	40	ASN
41	t	53	ASN
41	t	74	ASN
42	u	5	ASN
42	u	49	ASN
43	v	57	HIS
44	w	6	GLN
44	w	20	HIS
44	w	36	HIS
45	x	15	ASN
45	x	31	GLN

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Mol	Chain	Res	Type
46	y	20	HIS
46	y	49	ASN
47	z	6	ASN
47	z	42	HIS
50	2	31	HIS
50	2	43	HIS
52	4	20	ASN
52	4	30	HIS
52	4	41	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1516/1542 (98%)	219 (14%)	6 (0%)
22	a	2749/2904 (94%)	350 (12%)	0
23	b	118/120 (98%)	13 (11%)	0
53	X	11/28 (39%)	3 (27%)	0
54	Y	72/76 (94%)	32 (44%)	3 (4%)
55	Z	75/76 (98%)	31 (41%)	1 (1%)
56	5	1/2 (50%)	1 (100%)	0
All	All	4542/4748 (95%)	649 (14%)	10 (0%)

All (649) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	74	A
1	A	75	G
1	A	80	A
1	A	83	C
1	A	84	U
1	A	85	U

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Mol	Chain	Res	Type
1	A	86	G
1	A	87	C
1	A	88	U
1	A	89	U
1	A	94	G
1	A	95	C
1	A	96	U
1	A	121	U
1	A	122	G
1	A	131	A
1	A	141	G
1	A	144	G
1	A	146	G
1	A	149	A
1	A	166	U
1	A	177	G
1	A	181	A
1	A	182	A
1	A	183	C
1	A	189	A
1	A	197	A
1	A	202	G
1	A	203	G
1	A	204	G
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	271	C
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	345	C
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C

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Mol	Chain	Res	Type
1	A	373	A
1	A	384	G
1	A	398	U
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	417	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	436	C
1	A	446	G
1	A	453	G
1	A	456	A
1	A	457	G
1	A	458	U
1	A	459	A
1	A	463	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	474	G
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	490	C
1	A	495	A
1	A	511	C
1	A	518	C
1	A	531	U
1	A	547	A
1	A	559	A
1	A	572	A
1	A	573	A
1	A	575	G

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Mol	Chain	Res	Type
1	A	576	C
1	A	577	G
1	A	579	A
1	A	596	A
1	A	615	G
1	A	633	G
1	A	648	A
1	A	650	G
1	A	653	U
1	A	665	A
1	A	702	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	746	A
1	A	747	A
1	A	748	G
1	A	755	G
1	A	774	G
1	A	777	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	832	G
1	A	840	C
1	A	890	G
1	A	914	A
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	984	C
1	A	993	G
1	A	997	U
1	A	998	C
1	A	1004	A

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Mol	Chain	Res	Type
1	A	1006	G
1	A	1008	U
1	A	1009	U
1	A	1027	C
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1037	C
1	A	1043	G
1	A	1044	A
1	A	1045	C
1	A	1046	A
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1137	C
1	A	1139	G
1	A	1143	G
1	A	1144	G
1	A	1159	U
1	A	1169	A
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1256	A
1	A	1258	G
1	A	1275	A
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1302	C
1	A	1317	C

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Mol	Chain	Res	Type
1	A	1320	C
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1419	G
1	A	1427	C
1	A	1432	G
1	A	1440	U
1	A	1441	A
1	A	1442	G
1	A	1444	U
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1479	C
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1503	A
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
22	a	10	A
22	a	15	G
22	a	34	U
22	a	42	A
22	a	45	G
22	a	58	G
22	a	71	A

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Mol	Chain	Res	Type
22	a	74	A
22	a	75	G
22	a	84	A
22	a	101	A
22	a	102	U
22	a	110	G
22	a	118	A
22	a	119	A
22	a	120	U
22	a	139	U
22	a	140	C
22	a	163	C
22	a	165	A
22	a	181	A
22	a	196	A
22	a	215	G
22	a	216	A
22	a	221	A
22	a	222	A
22	a	231	A
22	a	248	G
22	a	264	C
22	a	265	A
22	a	272	A
22	a	274	C
22	a	278	A
22	a	279	A
22	a	280	U
22	a	282	A
22	a	285	G
22	a	286	U
22	a	289	G
22	a	292	U
22	a	294	A
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	357	C
22	a	361	G
22	a	362	A
22	a	386	G

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Mol	Chain	Res	Type
22	a	404	A
22	a	405	U
22	a	406	G
22	a	411	G
22	a	412	A
22	a	451	U
22	a	481	G
22	a	491	G
22	a	504	A
22	a	505	A
22	a	508	A
22	a	509	C
22	a	530	G
22	a	531	C
22	a	532	A
22	a	533	G
22	a	543	G
22	a	544	C
22	a	545	U
22	a	546	U
22	a	548	G
22	a	549	G
22	a	563	A
22	a	573	U
22	a	575	A
22	a	603	A
22	a	614	A
22	a	615	U
22	a	627	A
22	a	637	A
22	a	645	C
22	a	646	U
22	a	647	G
22	a	653	U
22	a	654	A
22	a	685	A
22	a	686	U
22	a	714	U
22	a	717	C
22	a	721	A
22	a	730	A
22	a	747	5MU

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Mol	Chain	Res	Type
22	a	764	A
22	a	765	C
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	792	A
22	a	805	G
22	a	812	C
22	a	827	U
22	a	828	U
22	a	846	U
22	a	847	U
22	a	856	G
22	a	859	G
22	a	869	G
22	a	879	G
22	a	882	G
22	a	883	G
22	a	884	U
22	a	885	C
22	a	888	C
22	a	890	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	897	C
22	a	898	C
22	a	899	A
22	a	905	A
22	a	910	A
22	a	914	G
22	a	915	C
22	a	934	U
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	984	A
22	a	985	C
22	a	996	A

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Mol	Chain	Res	Type
22	a	1012	U
22	a	1013	C
22	a	1017	G
22	a	1033	U
22	a	1041	G
22	a	1045	C
22	a	1046	A
22	a	1047	G
22	a	1048	A
22	a	1051	G
22	a	1108	U
22	a	1111	A
22	a	1112	G
22	a	1115	G
22	a	1116	G
22	a	1120	G
22	a	1122	G
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1171	G
22	a	1227	G
22	a	1253	A
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1273	U
22	a	1294	U
22	a	1300	G
22	a	1301	A
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1409	U
22	a	1411	U
22	a	1416	G
22	a	1417	C
22	a	1420	A
22	a	1421	G
22	a	1427	A

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Mol	Chain	Res	Type
22	a	1428	C
22	a	1452	G
22	a	1453	A
22	a	1468	U
22	a	1476	U
22	a	1482	G
22	a	1486	U
22	a	1487	U
22	a	1493	C
22	a	1497	U
22	a	1504	A
22	a	1506	U
22	a	1508	A
22	a	1509	A
22	a	1510	G
22	a	1515	A
22	a	1529	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1559	U
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1586	A
22	a	1590	A
22	a	1593	A
22	a	1608	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1715	G
22	a	1722	A
22	a	1729	U
22	a	1730	C
22	a	1731	G
22	a	1732	C

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Mol	Chain	Res	Type
22	a	1733	G
22	a	1736	U
22	a	1738	G
22	a	1750	G
22	a	1764	C
22	a	1773	A
22	a	1782	U
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1847	A
22	a	1858	A
22	a	1859	U
22	a	1866	A
22	a	1867	G
22	a	1868	C
22	a	1870	C
22	a	1871	A
22	a	1873	G
22	a	1906	G
22	a	1907	G
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2023	C
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G

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Mol	Chain	Res	Type
22	a	2062	A
22	a	2069	G7M
22	a	2194	U
22	a	2198	A
22	a	2203	U
22	a	2204	G
22	a	2208	C
22	a	2211	A
22	a	2223	G
22	a	2225	A
22	a	2238	G
22	a	2268	A
22	a	2279	G
22	a	2283	C
22	a	2287	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2335	A
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2377	A
22	a	2383	G
22	a	2385	C
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2424	C
22	a	2425	A
22	a	2429	G
22	a	2430	A
22	a	2431	U
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2470	G
22	a	2476	A
22	a	2480	C
22	a	2491	U

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Mol	Chain	Res	Type
22	a	2502	G
22	a	2505	G
22	a	2518	A
22	a	2529	G
22	a	2535	G
22	a	2547	A
22	a	2554	U
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2585	U
22	a	2586	U
22	a	2602	A
22	a	2603	G
22	a	2609	U
22	a	2613	U
22	a	2629	U
22	a	2630	G
22	a	2670	A
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2716	C
22	a	2726	A
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2751	G
22	a	2752	C
22	a	2757	A
22	a	2765	A
22	a	2778	A
22	a	2790	U
22	a	2792	A
22	a	2795	C
22	a	2798	U
22	a	2799	A
22	a	2802	G
22	a	2820	A
22	a	2821	A
22	a	2835	A
22	a	2861	U

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Mol	Chain	Res	Type
22	a	2873	A
22	a	2883	A
22	a	2884	U
22	a	2891	U
22	a	2899	A
22	a	2901	C
22	a	2902	C
23	b	9	G
23	b	13	G
23	b	34	A
23	b	35	C
23	b	36	C
23	b	45	A
23	b	56	G
23	b	57	A
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	109	A
53	X	14	A
53	X	15	A
53	X	24	A
54	Y	2	G
54	Y	3	G
54	Y	5	G
54	Y	6	A
54	Y	8	U
54	Y	9	A
54	Y	11	C
54	Y	13	C
54	Y	14	A
54	Y	15	G
54	Y	19	G
54	Y	20	G
54	Y	21	A
54	Y	23	A
54	Y	24	G
54	Y	25	C
54	Y	26	A
54	Y	45	G
54	Y	46	G

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Mol	Chain	Res	Type
54	Y	47	U
54	Y	48	C
54	Y	49	G
54	Y	50	G
54	Y	57	G
54	Y	59	U
54	Y	64	U
54	Y	66	A
54	Y	67	U
54	Y	70	C
54	Y	71	C
54	Y	73	A
54	Y	75	C
55	Z	6	G
55	Z	8	U
55	Z	9	G
55	Z	14	A
55	Z	16	C
55	Z	17	C
55	Z	17(A)	U
55	Z	18	G
55	Z	19	G
55	Z	20	U
55	Z	21	A
55	Z	22	G
55	Z	31	G
55	Z	46	G
55	Z	47	U
55	Z	49	G
55	Z	50	U
55	Z	51	C
55	Z	52	G
55	Z	53	G
55	Z	54	U
55	Z	56	C
55	Z	58	A
55	Z	59	A
55	Z	62	C
55	Z	65	C
55	Z	66	C
55	Z	68	C
55	Z	69	C

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Mol	Chain	Res	Type
55	Z	71	C
55	Z	76	A
56	5	76	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	250	A
1	A	467	U
1	A	575	G
1	A	1026	G
1	A	1035	A
54	Y	13	C
54	Y	45	G
54	Y	60	C
55	Z	58	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	PSU	a	1917	22	18,21,22	1.46	3 (16%)	21,30,33	2.07	5 (23%)
12	D2T	L	89	12	8,9,10	2.47	3 (37%)	6,11,13	1.50	1 (16%)
22	H2U	a	2449	22	18,21,22	1.19	2 (11%)	19,30,33	1.06	2 (10%)
22	OMG	a	2251	55,22	23,26,27	1.23	3 (13%)	32,38,41	2.12	6 (18%)
1	2MG	A	1207	1	23,26,27	1.24	4 (17%)	33,38,41	2.23	7 (21%)
1	MA6	A	1518	1	23,26,27	1.47	4 (17%)	33,38,41	2.11	10 (30%)
22	2MA	a	2503	58,22	22,25,26	1.45	5 (22%)	32,37,40	2.34	10 (31%)
1	G7M	A	527	1	23,26,27	1.62	4 (17%)	34,39,42	1.85	6 (17%)
1	2MG	A	1516	1	23,26,27	1.23	4 (17%)	33,38,41	2.21	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	5MU	a	1939	22	19,22,23	1.49	5 (26%)	27,32,35	2.34	6 (22%)
1	5MC	A	967	1	19,22,23	1.67	3 (15%)	26,32,35	1.10	3 (11%)
1	2MG	A	966	1	23,26,27	1.23	3 (13%)	33,38,41	2.31	10 (30%)
1	MA6	A	1519	1	23,26,27	1.58	5 (21%)	33,38,41	2.09	11 (33%)
1	5MC	A	1407	1	19,22,23	1.72	3 (15%)	26,32,35	1.17	2 (7%)
22	2MG	a	1835	22	23,26,27	1.27	4 (17%)	33,38,41	2.27	8 (24%)
33	MS6	l	82	33	5,7,8	0.23	0	2,7,9	0.25	0
1	UR3	A	1498	1	19,22,23	0.87	1 (5%)	26,32,35	1.67	4 (15%)
22	1MG	a	745	22	23,26,27	1.16	4 (17%)	33,39,42	1.80	9 (27%)
22	2MG	a	2445	22	23,26,27	1.24	3 (13%)	33,38,41	2.08	7 (21%)
22	PSU	a	2604	22	18,21,22	1.51	1 (5%)	21,30,33	1.47	3 (14%)
11	IAS	K	119	11	6,7,8	1.34	1 (16%)	3,8,10	0.65	0
22	PSU	a	955	22	18,21,22	1.40	3 (16%)	21,30,33	2.10	4 (19%)
22	OMU	a	2552	22	19,22,23	1.23	2 (10%)	25,31,34	1.84	5 (20%)
22	3TD	a	1915	22	19,22,23	1.63	5 (26%)	23,32,35	2.27	5 (21%)
22	PSU	a	2605	22	18,21,22	1.32	2 (11%)	21,30,33	2.27	6 (28%)
22	PSU	a	2504	22	18,21,22	1.48	3 (16%)	21,30,33	1.89	5 (23%)
22	PSU	a	746	58,22	18,21,22	1.37	3 (16%)	21,30,33	2.11	5 (23%)
22	OMC	a	2498	58,22	19,22,23	0.79	1 (5%)	25,31,34	0.86	0
1	PSU	A	516	1	18,21,22	1.37	2 (11%)	21,30,33	2.00	4 (19%)
22	5MC	a	1962	22	19,22,23	1.75	3 (15%)	26,32,35	1.19	3 (11%)
22	G7M	a	2069	22	23,26,27	1.48	4 (17%)	34,39,42	1.81	5 (14%)
22	6MZ	a	1618	22	22,25,26	1.37	4 (18%)	29,36,39	2.24	10 (34%)
33	4D4	l	81	33	9,11,12	1.97	2 (22%)	7,13,15	1.38	0
22	6MZ	a	2030	22	22,25,26	1.50	5 (22%)	29,36,39	2.25	12 (41%)
1	4OC	A	1402	1	20,23,24	0.67	0	25,32,35	1.00	1 (4%)
22	PSU	a	2457	22	18,21,22	1.45	2 (11%)	21,30,33	2.08	3 (14%)
22	5MU	a	747	22	19,22,23	1.46	6 (31%)	27,32,35	2.12	6 (22%)
25	MEQ	d	150	25	8,9,10	0.47	0	5,10,12	0.26	0
22	PSU	a	1911	22	18,21,22	1.36	3 (16%)	21,30,33	1.92	4 (19%)
22	PSU	a	2580	22	18,21,22	1.42	3 (16%)	21,30,33	2.02	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
22	PSU	a	1917	22	-	1/7/25/26	0/2/2/2
12	D2T	L	89	12	-	5/7/12/14	-
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
22	OMG	a	2251	55,22	-	0/9/27/28	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
22	2MA	a	2503	58,22	-	1/7/25/26	0/3/3/3
1	G7M	A	527	1	-	1/7/25/26	0/3/3/3
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	1/9/27/28	0/3/3/3
1	MA6	A	1519	1	-	1/11/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
33	MS6	l	82	33	-	1/4/6/8	-
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
22	2MG	a	2445	22	-	1/9/27/28	0/3/3/3
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
11	IAS	K	119	11	-	0/7/7/8	-
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2504	22	-	2/7/25/26	0/2/2/2
22	PSU	a	746	58,22	-	3/7/25/26	0/2/2/2
22	OMC	a	2498	58,22	-	0/9/27/28	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
22	G7M	a	2069	22	-	0/7/25/26	0/3/3/3
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
33	4D4	l	81	33	-	1/11/12/14	-
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
1	4OC	A	1402	1	-	1/9/29/30	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	5MU	a	747	22	-	1/7/25/26	0/2/2/2
25	MEQ	d	150	25	-	2/8/9/11	-
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1962	5MC	C5-C4	6.58	1.49	1.44
1	A	1407	5MC	C5-C4	6.30	1.48	1.44
1	A	967	5MC	C5-C4	6.23	1.48	1.44
1	A	527	G7M	C5-N7	-5.48	1.32	1.39
22	a	2604	PSU	C2-N1	5.28	1.43	1.36
1	A	1519	MA6	C5-C4	4.90	1.47	1.39
12	L	89	D2T	CB-CA	4.66	1.56	1.54
22	a	2069	G7M	C5-N7	-4.60	1.33	1.39
1	A	1518	MA6	C5-C4	4.16	1.46	1.39
22	a	2503	2MA	C5-C4	4.11	1.46	1.39
33	l	81	4D4	CZ-NE	4.10	1.41	1.33
12	L	89	D2T	CB-CG	4.08	1.59	1.52
22	a	2030	6MZ	C5-C4	4.03	1.46	1.39
22	a	1618	6MZ	C5-C4	4.00	1.46	1.39
22	a	2457	PSU	C6-C5	3.93	1.39	1.35
22	a	2504	PSU	C6-C5	3.91	1.39	1.35
22	a	1911	PSU	C6-C5	3.79	1.39	1.35
1	A	516	PSU	C6-C5	3.78	1.39	1.35
22	a	1915	3TD	C4-N3	-3.64	1.32	1.40
22	a	746	PSU	C6-C5	3.45	1.39	1.35
22	a	1915	3TD	C10-N3	3.41	1.53	1.47
22	a	1915	3TD	C6-C5	3.30	1.38	1.35
22	a	2580	PSU	C6-C5	3.30	1.38	1.35
22	a	1917	PSU	C6-C5	3.26	1.38	1.35
22	a	1917	PSU	C4-N3	-3.23	1.32	1.38
33	l	81	4D4	CZ-NH2	3.20	1.43	1.32
22	a	2605	PSU	C4-N3	-3.19	1.32	1.38
22	a	2251	OMG	C5-C4	3.17	1.47	1.38
22	a	2605	PSU	C6-C5	3.15	1.38	1.35
22	a	1835	2MG	C5-C4	3.10	1.47	1.38
22	a	955	PSU	C4-N3	-3.04	1.33	1.38
1	A	966	2MG	C5-C4	3.02	1.47	1.38
1	A	1207	2MG	C5-C4	2.99	1.46	1.38
22	a	955	PSU	C6-C5	2.93	1.38	1.35
22	a	2504	PSU	C4-N3	-2.92	1.33	1.38
22	a	2449	H2U	C2-N3	-2.90	1.32	1.38
22	a	747	5MU	C6-C5	2.90	1.39	1.34
22	a	2030	6MZ	C5-N7	-2.89	1.33	1.39
1	A	527	G7M	C5-C4	2.88	1.45	1.38
22	a	2445	2MG	C5-C4	2.88	1.46	1.38
22	a	2457	PSU	C4-N3	-2.87	1.33	1.38
1	A	1407	5MC	C6-C5	2.86	1.39	1.34
22	a	1939	5MU	C6-N1	-2.85	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	745	1MG	C5-C4	2.84	1.46	1.38
22	a	2030	6MZ	C4-N9	-2.83	1.31	1.37
1	A	1518	MA6	C5-C6	2.82	1.48	1.41
22	a	1939	5MU	C6-C5	2.82	1.39	1.34
22	a	1911	PSU	C4-N3	-2.81	1.33	1.38
22	a	2580	PSU	C4-N3	-2.80	1.33	1.38
22	a	2552	OMU	C4-N3	-2.80	1.33	1.38
22	a	2449	H2U	C4-N3	-2.79	1.32	1.37
22	a	1618	6MZ	C5-C6	2.76	1.48	1.41
22	a	1939	5MU	C2-N3	-2.76	1.33	1.38
22	a	1835	2MG	C6-N1	-2.76	1.33	1.38
1	A	1519	MA6	C5-C6	2.74	1.48	1.41
1	A	1516	2MG	C5-C4	2.74	1.46	1.38
22	a	747	5MU	C4-N3	-2.74	1.33	1.38
22	a	1939	5MU	C4-N3	-2.73	1.33	1.38
22	a	1917	PSU	C2-N3	-2.72	1.33	1.37
22	a	2069	G7M	C5-C4	2.71	1.45	1.38
22	a	747	5MU	C4-C5	2.68	1.49	1.44
1	A	1518	MA6	C4-N9	-2.67	1.32	1.37
1	A	1519	MA6	C4-N9	-2.66	1.32	1.37
22	a	2503	2MA	C5-C6	2.63	1.48	1.41
11	K	119	IAS	CB-CG	2.63	1.56	1.50
22	a	1962	5MC	C6-N1	-2.63	1.33	1.38
22	a	2445	2MG	C6-N1	-2.62	1.33	1.38
1	A	1516	2MG	C6-N1	-2.61	1.34	1.38
22	a	2251	OMG	C6-N1	-2.60	1.34	1.38
1	A	516	PSU	C4-N3	-2.58	1.34	1.38
22	a	2552	OMU	C2-N3	-2.56	1.33	1.38
22	a	745	1MG	C2-N1	2.54	1.41	1.37
22	a	1939	5MU	C4-C5	2.51	1.48	1.44
1	A	1518	MA6	C5-N7	-2.46	1.34	1.39
1	A	967	5MC	C6-C5	2.45	1.38	1.34
12	L	89	D2T	CB-SB	2.45	1.84	1.82
22	a	745	1MG	C4-N9	-2.44	1.31	1.38
22	a	1618	6MZ	C5-N7	-2.44	1.34	1.39
22	a	2580	PSU	C2-N3	-2.43	1.33	1.37
22	a	746	PSU	C4-N3	-2.42	1.34	1.38
22	a	2445	2MG	C4-N9	-2.42	1.31	1.38
1	A	1519	MA6	C5-N7	-2.41	1.34	1.39
1	A	527	G7M	C6-N1	-2.40	1.34	1.38
22	a	2030	6MZ	C5-C6	2.40	1.47	1.41
22	a	2069	G7M	C6-N1	-2.37	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2251	OMG	C5-N7	-2.37	1.34	1.39
22	a	747	5MU	C2-N3	-2.37	1.33	1.38
22	a	2030	6MZ	C8-N7	2.36	1.36	1.31
1	A	966	2MG	C6-N1	-2.35	1.34	1.38
22	a	2069	G7M	C4-N9	-2.35	1.32	1.38
1	A	967	5MC	C6-N1	-2.34	1.34	1.38
22	a	1915	3TD	C2-N3	-2.34	1.33	1.38
22	a	2503	2MA	C8-N7	2.33	1.36	1.31
22	a	1835	2MG	C2-N3	2.32	1.36	1.32
22	a	747	5MU	C6-N1	-2.30	1.34	1.38
22	a	2504	PSU	C2-N3	-2.30	1.33	1.37
1	A	966	2MG	C5-N7	-2.29	1.34	1.39
22	a	746	PSU	C2-N3	-2.27	1.33	1.37
22	a	2503	2MA	C5-N7	-2.27	1.34	1.39
1	A	1207	2MG	C6-N1	-2.26	1.34	1.38
22	a	2503	2MA	C4-N9	-2.24	1.33	1.37
22	a	1962	5MC	C6-C5	2.23	1.38	1.34
1	A	1516	2MG	C5-N7	-2.21	1.34	1.39
1	A	1519	MA6	C8-N7	2.21	1.35	1.31
22	a	955	PSU	C2-N3	-2.19	1.33	1.37
1	A	1407	5MC	C6-N1	-2.18	1.34	1.38
22	a	1835	2MG	C5-N7	-2.15	1.34	1.39
22	a	747	5MU	C2-N1	2.15	1.41	1.38
1	A	527	G7M	C4-N9	-2.13	1.32	1.38
1	A	1516	2MG	C4-N9	-2.13	1.32	1.38
1	A	1207	2MG	C2-N3	2.12	1.36	1.32
22	a	1915	3TD	C2-N1	-2.10	1.34	1.37
22	a	745	1MG	C5-N7	-2.08	1.34	1.39
1	A	1207	2MG	C5-N7	-2.06	1.34	1.39
22	a	2498	OMC	C6-C5	2.03	1.39	1.35
1	A	1498	UR3	C6-C5	2.03	1.39	1.35
22	a	1911	PSU	C2-N3	-2.01	1.34	1.37
22	a	1618	6MZ	C4-N9	-2.01	1.33	1.37

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	1915	3TD	N1-C2-N3	8.41	122.24	116.13
1	A	966	2MG	C2-N3-C4	7.51	121.40	112.00
22	a	2503	2MA	C5-C4-N3	-7.47	119.31	127.18
22	a	1835	2MG	C2-N3-C4	7.37	121.21	112.00
1	A	1207	2MG	C2-N3-C4	7.34	121.18	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1516	2MG	C2-N3-C4	7.03	120.79	112.00
22	a	955	PSU	N1-C2-N3	6.84	122.38	115.17
22	a	2605	PSU	N1-C2-N3	6.75	122.29	115.17
22	a	746	PSU	N1-C2-N3	6.72	122.26	115.17
22	a	2445	2MG	C2-N3-C4	6.71	120.39	112.00
22	a	1917	PSU	N1-C2-N3	6.65	122.19	115.17
22	a	1835	2MG	C5-C4-N3	-6.57	117.93	128.39
22	a	2251	OMG	C5-C4-N3	-6.57	117.94	128.39
1	A	1498	UR3	C4-N3-C2	-6.53	119.33	124.58
22	a	2457	PSU	N1-C2-N3	6.41	121.94	115.17
22	a	2503	2MA	N3-C4-N9	6.23	134.90	126.99
1	A	516	PSU	N1-C2-N3	6.17	121.68	115.17
22	a	2504	PSU	N1-C2-N3	6.16	121.66	115.17
1	A	966	2MG	C5-C4-N3	-6.12	118.65	128.39
22	a	2580	PSU	N1-C2-N3	6.01	121.51	115.17
1	A	1207	2MG	C5-C4-N3	-5.87	119.05	128.39
22	a	1911	PSU	N1-C2-N3	5.82	121.31	115.17
22	a	1939	5MU	C4-N3-C2	-5.62	119.98	127.34
22	a	2251	OMG	C2-N3-C4	5.55	121.87	112.30
22	a	1618	6MZ	C5-C4-N3	-5.53	119.11	126.72
22	a	747	5MU	N3-C2-N1	5.51	122.07	114.89
1	A	1516	2MG	C5-C4-N3	-5.45	119.71	128.39
22	a	1835	2MG	N9-C4-N3	5.34	136.63	125.95
22	a	2445	2MG	C5-C4-N3	-5.30	119.95	128.39
22	a	2069	G7M	C5-C4-N3	-5.13	118.46	128.15
22	a	2069	G7M	C2-N3-C4	5.12	121.12	112.30
1	A	527	G7M	C5-C4-N3	-5.11	118.50	128.15
1	A	527	G7M	N9-C4-N3	5.08	136.11	125.95
22	a	1939	5MU	N3-C2-N1	5.08	121.50	114.89
22	a	2605	PSU	C4-N3-C2	-5.08	119.38	126.37
22	a	1939	5MU	C5-C6-N1	-5.08	117.80	123.31
22	a	747	5MU	C4-N3-C2	-5.06	120.71	127.34
22	a	2069	G7M	N9-C4-N3	4.90	135.74	125.95
22	a	2552	OMU	C4-N3-C2	-4.83	120.62	126.61
1	A	1518	MA6	C5-C4-N3	-4.83	120.07	126.72
1	A	527	G7M	C2-N3-C4	4.77	120.52	112.30
1	A	1519	MA6	C2-N1-C6	4.77	123.47	111.83
22	a	746	PSU	C4-N3-C2	-4.67	119.94	126.37
22	a	1618	6MZ	N3-C4-N9	4.66	135.09	127.17
22	a	1939	5MU	C5-C4-N3	4.65	119.37	115.32
1	A	966	2MG	N9-C4-N3	4.61	135.18	125.95
22	a	745	1MG	C2-N3-C4	4.57	122.25	111.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	2251	OMG	N9-C4-N3	4.55	135.06	125.95
1	A	1518	MA6	C2-N1-C6	4.50	122.83	111.83
22	a	1915	3TD	C4-N3-C2	-4.39	119.97	124.61
22	a	2552	OMU	N3-C2-N1	4.35	120.56	114.89
22	a	745	1MG	C5-C4-N3	-4.29	121.56	128.39
22	a	2030	6MZ	C5-C4-N3	-4.28	120.82	126.72
1	A	1519	MA6	C5-C4-N3	-4.25	120.87	126.72
22	a	2030	6MZ	C9-N6-C6	-4.23	118.93	122.85
1	A	1207	2MG	N9-C4-N3	4.20	134.35	125.95
22	a	1917	PSU	C4-N3-C2	-4.17	120.63	126.37
22	a	955	PSU	C4-N3-C2	-4.12	120.70	126.37
1	A	1518	MA6	C4-C5-N7	-4.08	105.92	110.58
22	a	1939	5MU	O4-C4-C5	-4.08	120.25	124.92
22	a	2457	PSU	C4-N3-C2	-4.07	120.77	126.37
22	a	2445	2MG	N9-C4-N3	4.03	134.01	125.95
22	a	2030	6MZ	C4-N9-C8	4.01	109.95	105.74
22	a	2580	PSU	C4-N3-C2	-3.98	120.88	126.37
1	A	1519	MA6	C4-C5-N7	-3.93	106.09	110.58
1	A	1518	MA6	N1-C2-N3	-3.91	122.66	128.58
1	A	1516	2MG	N9-C4-N3	3.90	133.75	125.95
22	a	1618	6MZ	C9-N6-C6	-3.88	119.25	122.85
22	a	747	5MU	C5-C4-N3	3.86	118.68	115.32
22	a	1911	PSU	C4-N3-C2	-3.86	121.05	126.37
22	a	2552	OMU	C5-C4-N3	3.86	120.20	114.80
22	a	1939	5MU	O2-C2-N1	-3.80	117.85	122.80
1	A	516	PSU	C4-N3-C2	-3.78	121.16	126.37
22	a	1618	6MZ	C2-N3-C4	3.74	120.96	111.83
22	a	2503	2MA	C4-N9-C8	3.73	109.65	105.74
1	A	1518	MA6	C2-N3-C4	3.70	120.87	111.83
1	A	1407	5MC	C5-C6-N1	-3.68	119.31	123.31
22	a	2251	OMG	C6-C5-N7	3.67	136.98	130.29
22	a	2030	6MZ	C6-C5-N7	3.67	136.43	132.43
1	A	1516	2MG	C6-C5-N7	3.66	136.95	130.29
22	a	747	5MU	O4-C4-C5	-3.65	120.75	124.92
22	a	2445	2MG	C6-C5-N7	3.62	136.87	130.29
22	a	2504	PSU	C4-N3-C2	-3.61	121.40	126.37
22	a	2030	6MZ	N3-C4-N9	3.57	133.23	127.17
22	a	2604	PSU	C6-C5-C4	3.56	120.57	118.17
1	A	1207	2MG	C6-C5-N7	3.55	136.76	130.29
22	a	747	5MU	C5-C6-N1	-3.55	119.45	123.31
1	A	1519	MA6	N1-C2-N3	-3.55	123.21	128.58
1	A	1518	MA6	N3-C4-N9	3.55	133.20	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	G7M	C2'-C1'-N9	-3.53	103.43	113.25
22	a	2580	PSU	O2-C2-N1	-3.45	119.23	122.79
22	a	1618	6MZ	N1-C2-N3	-3.44	123.37	128.58
22	a	747	5MU	O2-C2-N1	-3.44	118.32	122.80
1	A	1519	MA6	C4-N9-C8	3.41	109.32	105.74
22	a	745	1MG	C6-C5-N7	3.40	136.91	129.36
22	a	2030	6MZ	C4-C5-N7	-3.38	106.72	110.58
1	A	1519	MA6	N3-C4-N9	3.34	132.84	127.17
1	A	966	2MG	C6-C5-N7	3.33	136.34	130.29
22	a	2457	PSU	O2-C2-N1	-3.31	119.38	122.79
22	a	1618	6MZ	C6-C5-N7	3.30	136.02	132.43
1	A	516	PSU	O2-C2-N1	-3.30	119.39	122.79
22	a	745	1MG	N9-C4-N3	3.27	132.50	125.95
22	a	2030	6MZ	N1-C2-N3	-3.27	123.63	128.58
22	a	2604	PSU	O2-C2-N1	3.25	126.14	122.79
1	A	1519	MA6	C2-N3-C4	3.22	119.70	111.83
22	a	1962	5MC	C5-C6-N1	-3.21	119.82	123.31
22	a	2605	PSU	O2-C2-N1	-3.20	119.49	122.79
22	a	1618	6MZ	C4-N9-C8	3.17	109.06	105.74
22	a	2030	6MZ	N9-C8-N7	-3.15	109.47	113.94
22	a	2552	OMU	O2-C2-N1	-3.14	118.71	122.80
22	a	1618	6MZ	C4-C5-N7	-3.12	107.01	110.58
22	a	2251	OMG	C4-C5-N7	-3.12	105.73	110.67
22	a	2503	2MA	C4-C5-N7	-3.12	107.02	110.58
1	A	1498	UR3	C5-C4-N3	3.10	119.13	115.04
1	A	966	2MG	N1-C2-N2	3.06	119.69	116.56
22	a	745	1MG	C6-C5-C4	-3.03	116.54	119.97
22	a	2604	PSU	C6-N1-C2	-3.02	119.89	122.69
22	a	2069	G7M	O6-C6-C5	-3.01	121.29	128.01
1	A	1518	MA6	C4-N9-C8	3.00	108.89	105.74
22	a	2030	6MZ	C2-N3-C4	2.99	119.13	111.83
1	A	967	5MC	C5-C6-N1	-2.99	120.07	123.31
22	a	1962	5MC	C5-C4-N3	-2.98	118.70	121.75
22	a	955	PSU	O2-C2-N1	-2.98	119.72	122.79
1	A	1516	2MG	N1-C2-N2	2.94	119.56	116.56
22	a	1835	2MG	C6-C5-N7	2.92	135.60	130.29
22	a	1915	3TD	C5-C6-N1	-2.90	118.12	122.14
1	A	1518	MA6	C5-N7-C8	2.89	108.00	103.45
22	a	2503	2MA	C2-N1-C6	2.89	122.54	118.10
1	A	1519	MA6	C6-C5-N7	2.88	138.03	133.43
1	A	1518	MA6	C6-C5-N7	2.85	137.99	133.43
22	a	2030	6MZ	C5-N7-C8	2.84	107.92	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1407	5MC	C5-C4-N3	-2.82	118.87	121.75
1	A	1519	MA6	C5-N7-C8	2.81	107.87	103.45
22	a	2503	2MA	N9-C8-N7	-2.80	109.97	113.94
22	a	2503	2MA	C6-C5-N7	2.75	137.39	132.09
1	A	1207	2MG	C4-C5-N7	-2.71	106.37	110.67
1	A	527	G7M	O6-C6-C5	-2.69	122.01	128.01
22	a	2552	OMU	O4-C4-C5	-2.68	120.55	125.16
22	a	1618	6MZ	C5-N7-C8	2.63	107.59	103.45
22	a	2503	2MA	C5-N7-C8	2.62	107.57	103.45
22	a	745	1MG	C4-C5-N7	-2.60	106.55	110.67
22	a	746	PSU	O2-C2-N1	-2.58	120.13	122.79
22	a	2605	PSU	C5-C6-N1	-2.56	118.58	122.14
22	a	2449	H2U	N3-C2-N1	2.56	119.22	116.65
22	a	2030	6MZ	C4-N9-C1'	-2.52	120.75	126.63
1	A	1207	2MG	N1-C2-N2	2.52	119.13	116.56
1	A	1402	4OC	C6-C5-C4	2.51	120.03	117.00
22	a	1917	PSU	O2-C2-N3	-2.51	117.40	121.86
1	A	1519	MA6	N9-C8-N7	-2.49	110.40	113.94
22	a	2445	2MG	N1-C2-N2	2.49	119.11	116.56
22	a	745	1MG	N2-C2-N1	2.48	120.78	118.79
22	a	1911	PSU	O2-C2-N1	-2.48	120.23	122.79
22	a	2069	G7M	C5-C6-N1	2.48	116.96	111.84
1	A	967	5MC	C5-C4-N3	-2.46	119.23	121.75
1	A	1516	2MG	O6-C6-C5	-2.46	120.04	126.53
1	A	1498	UR3	C6-N1-C2	-2.46	119.79	121.80
1	A	1518	MA6	N9-C8-N7	-2.45	110.46	113.94
22	a	1835	2MG	C4-C5-N7	-2.44	106.80	110.67
22	a	1917	PSU	C5-C6-N1	-2.44	118.75	122.14
22	a	1962	5MC	CM5-C5-C6	-2.44	119.55	122.85
12	L	89	D2T	OD1-CG-CB	-2.43	117.36	122.44
22	a	1618	6MZ	N9-C8-N7	-2.40	110.54	113.94
22	a	746	PSU	O2-C2-N3	-2.39	117.61	121.86
22	a	2503	2MA	N3-C2-N1	-2.39	121.55	125.77
1	A	966	2MG	O6-C6-C5	-2.38	120.25	126.53
1	A	966	2MG	C4-C5-N7	-2.38	106.90	110.67
1	A	1519	MA6	C4-N9-C1'	-2.38	121.07	126.63
22	a	2030	6MZ	C2-N1-C6	2.37	123.10	115.24
22	a	2580	PSU	O4'-C1'-C2'	2.37	108.43	105.15
1	A	1516	2MG	C4-C5-N7	-2.36	106.93	110.67
22	a	2445	2MG	C4-C5-N7	-2.31	107.00	110.67
22	a	1917	PSU	O2-C2-N1	-2.31	120.41	122.79
1	A	527	G7M	C5-C6-N1	2.30	116.60	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	1835	2MG	O6-C6-C5	-2.30	120.46	126.53
22	a	2251	OMG	C8-N7-C5	2.27	108.31	104.26
22	a	2504	PSU	O2-C2-N3	-2.26	117.84	121.86
22	a	746	PSU	C5-C6-N1	-2.25	119.02	122.14
1	A	966	2MG	N2-C2-N3	-2.25	117.65	120.51
1	A	1207	2MG	O6-C6-C5	-2.24	120.63	126.53
22	a	955	PSU	O2-C2-N3	-2.23	117.89	121.86
22	a	2504	PSU	O2-C2-N1	-2.23	120.49	122.79
22	a	2504	PSU	C5-C6-N1	-2.22	119.06	122.14
22	a	1915	3TD	O4'-C1'-C2'	2.18	108.17	105.15
22	a	745	1MG	C8-N9-C4	2.17	110.10	106.03
22	a	1911	PSU	C5-C6-N1	-2.16	119.15	122.14
1	A	1516	2MG	C5-C6-N1	2.15	118.71	113.25
22	a	1915	3TD	O2-C2-N3	-2.14	118.80	121.82
22	a	1835	2MG	C2-N1-C6	-2.12	121.99	124.55
22	a	2503	2MA	N6-C6-N1	2.10	119.87	117.03
1	A	967	5MC	CM5-C5-C6	-2.10	120.00	122.85
1	A	1498	UR3	C3U-N3-C4	2.09	120.77	117.87
1	A	966	2MG	C2-N1-C6	-2.08	122.04	124.55
1	A	516	PSU	O4'-C1'-C2'	2.07	108.02	105.15
1	A	966	2MG	C5-C6-N1	2.06	118.50	113.25
22	a	2605	PSU	O2-C2-N3	-2.05	118.22	121.86
22	a	2449	H2U	C5-C6-N1	-2.04	105.33	111.52
22	a	745	1MG	N9-C8-N7	-2.04	109.61	113.40
22	a	2605	PSU	O4-C4-C5	-2.04	118.94	124.01
1	A	1516	2MG	N2-C2-N3	-2.04	117.92	120.51
22	a	1835	2MG	C5-C6-N1	2.01	118.38	113.25
22	a	2445	2MG	O6-C6-C5	-2.00	121.24	126.53

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	CG-CB-SB-CB1
12	L	89	D2T	CA-CB-CG-OD1
12	L	89	D2T	CA-CB-CG-OD2
22	a	746	PSU	O4'-C1'-C5-C6
25	d	150	MEQ	NE2-CD-CG-CB
25	d	150	MEQ	OE1-CD-CG-CB
22	a	2030	6MZ	O4'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
22	a	2504	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	O4'-C4'-C5'-O5'
22	a	2445	2MG	C3'-C4'-C5'-O5'
22	a	746	PSU	O4'-C1'-C5-C4
22	a	747	5MU	C3'-C4'-C5'-O5'
22	a	2504	PSU	C3'-C4'-C5'-O5'
1	A	527	G7M	C4'-C5'-O5'-P
22	a	2503	2MA	C4'-C5'-O5'-P
22	a	1917	PSU	O4'-C4'-C5'-O5'
12	L	89	D2T	CA-CB-SB-CB1
12	L	89	D2T	SB-CB-CG-OD2
1	A	966	2MG	C3'-C4'-C5'-O5'
33	l	82	MS6	CB-CG-SD-CE
22	a	746	PSU	C2'-C1'-C5-C6
33	l	81	4D4	O-C-CA-CB
1	A	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	1917	PSU	1	0
12	L	89	D2T	1	0
1	A	1518	MA6	1	0
1	A	1516	2MG	1	0
22	a	1939	5MU	1	0
1	A	1519	MA6	2	0
22	a	2604	PSU	1	0
11	K	119	IAS	1	0
22	a	2552	OMU	1	0
22	a	2069	G7M	1	0
22	a	2030	6MZ	3	0
22	a	747	5MU	1	0
25	d	150	MEQ	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 329 ligands modelled in this entry, 311 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	SPD	a	6209	-	9,9,9	0.21	0	8,8,8	0.27	0
59	SPD	a	6218	-	9,9,9	0.18	0	8,8,8	0.19	0
59	SPD	a	6222	-	9,9,9	0.18	0	8,8,8	0.16	0
59	SPD	a	6220	-	9,9,9	0.22	0	8,8,8	0.26	0
59	SPD	A	1695	-	9,9,9	0.17	0	8,8,8	0.34	0
59	SPD	a	6215	-	9,9,9	0.19	0	8,8,8	0.19	0
59	SPD	a	6221	-	9,9,9	0.21	0	8,8,8	0.17	0
57	PAR	A	1601	-	44,45,45	0.50	0	63,67,67	0.88	1 (1%)
59	SPD	a	6212	-	9,9,9	0.18	0	8,8,8	0.17	0
59	SPD	a	6213	-	9,9,9	0.19	0	8,8,8	0.20	0
59	SPD	a	6216	-	9,9,9	0.17	0	8,8,8	0.21	0
59	SPD	A	1696	-	9,9,9	0.17	0	8,8,8	0.25	0
59	SPD	a	6217	-	9,9,9	0.17	0	8,8,8	0.17	0
59	SPD	a	6219	-	9,9,9	0.18	0	8,8,8	0.18	0
59	SPD	a	6214	-	9,9,9	0.19	0	8,8,8	0.19	0
59	SPD	a	6210	-	9,9,9	0.20	0	8,8,8	0.18	0
60	SPM	a	6223	-	13,13,13	0.17	0	12,12,12	0.18	0
59	SPD	a	6211	-	9,9,9	0.19	0	8,8,8	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SPD	a	6209	-	-	0/7/7/7	-
59	SPD	a	6218	-	-	3/7/7/7	-
59	SPD	a	6222	-	-	2/7/7/7	-
59	SPD	a	6220	-	-	1/7/7/7	-
59	SPD	A	1695	-	-	2/7/7/7	-
59	SPD	a	6215	-	-	4/7/7/7	-
59	SPD	a	6221	-	-	2/7/7/7	-
57	PAR	A	1601	-	-	4/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SPD	a	6212	-	-	5/7/7/7	-
59	SPD	a	6213	-	-	3/7/7/7	-
59	SPD	a	6216	-	-	3/7/7/7	-
59	SPD	A	1696	-	-	4/7/7/7	-
59	SPD	a	6217	-	-	4/7/7/7	-
59	SPD	a	6219	-	-	7/7/7/7	-
59	SPD	a	6214	-	-	5/7/7/7	-
59	SPD	a	6210	-	-	4/7/7/7	-
60	SPM	a	6223	-	-	9/11/11/11	-
59	SPD	a	6211	-	-	3/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	A	1601	PAR	C13-O52-C52	-2.44	112.20	117.98

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	1601	PAR	C44-C54-C64-N64
57	A	1601	PAR	O54-C54-C64-N64
59	a	6212	SPD	C3-C4-C5-N6
59	a	6211	SPD	N6-C7-C8-C9
59	a	6219	SPD	C3-C4-C5-N6
59	a	6211	SPD	C3-C4-C5-N6
59	A	1695	SPD	C3-C4-C5-N6
59	a	6216	SPD	N6-C7-C8-C9
59	a	6210	SPD	C3-C4-C5-N6
59	a	6219	SPD	N6-C7-C8-C9
59	a	6219	SPD	C8-C7-N6-C5
60	a	6223	SPM	C3-C4-N5-C6
59	a	6222	SPD	C4-C5-N6-C7
60	a	6223	SPM	C8-C9-N10-C11
60	a	6223	SPM	C7-C8-C9-N10
59	a	6214	SPD	N6-C7-C8-C9
59	a	6213	SPD	N6-C7-C8-C9
59	a	6215	SPD	C3-C4-C5-N6

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Mol	Chain	Res	Type	Atoms
59	A	1696	SPD	N6-C7-C8-C9
59	a	6210	SPD	C8-C7-N6-C5
59	a	6213	SPD	C3-C4-C5-N6
60	a	6223	SPM	C2-C3-C4-N5
59	a	6219	SPD	C2-C3-C4-C5
59	a	6216	SPD	C2-C3-C4-C5
59	a	6212	SPD	C2-C3-C4-C5
59	A	1695	SPD	C4-C5-N6-C7
59	a	6210	SPD	C7-C8-C9-N10
59	a	6212	SPD	C4-C5-N6-C7
59	a	6215	SPD	C7-C8-C9-N10
59	a	6216	SPD	C4-C5-N6-C7
59	a	6215	SPD	N6-C7-C8-C9
59	a	6213	SPD	C8-C7-N6-C5
59	a	6222	SPD	C8-C7-N6-C5
59	a	6217	SPD	C3-C4-C5-N6
59	a	6212	SPD	N6-C7-C8-C9
59	a	6218	SPD	N1-C2-C3-C4
59	a	6214	SPD	C3-C4-C5-N6
59	A	1696	SPD	C2-C3-C4-C5
57	A	1601	PAR	C52-C42-O11-C11
59	a	6217	SPD	C7-C8-C9-N10
59	a	6219	SPD	C7-C8-C9-N10
59	a	6221	SPD	C7-C8-C9-N10
60	a	6223	SPM	N1-C2-C3-C4
60	a	6223	SPM	C12-C11-N10-C9
60	a	6223	SPM	C11-C12-C13-N14
59	a	6215	SPD	N1-C2-C3-C4
59	a	6217	SPD	N6-C7-C8-C9
59	a	6211	SPD	C4-C5-N6-C7
57	A	1601	PAR	C23-C33-O33-C14
60	a	6223	SPM	C6-C7-C8-C9
59	a	6214	SPD	C4-C5-N6-C7
59	A	1696	SPD	C3-C4-C5-N6
59	a	6220	SPD	C3-C4-C5-N6
59	a	6218	SPD	C2-C3-C4-C5
59	a	6210	SPD	C2-C3-C4-C5
59	a	6214	SPD	C8-C7-N6-C5
59	a	6214	SPD	C2-C3-C4-C5
59	a	6212	SPD	N1-C2-C3-C4
59	a	6219	SPD	C4-C5-N6-C7
59	a	6217	SPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
60	a	6223	SPM	C7-C6-N5-C4
59	A	1696	SPD	C7-C8-C9-N10
59	a	6218	SPD	C7-C8-C9-N10
59	a	6219	SPD	N1-C2-C3-C4
59	a	6221	SPD	N1-C2-C3-C4

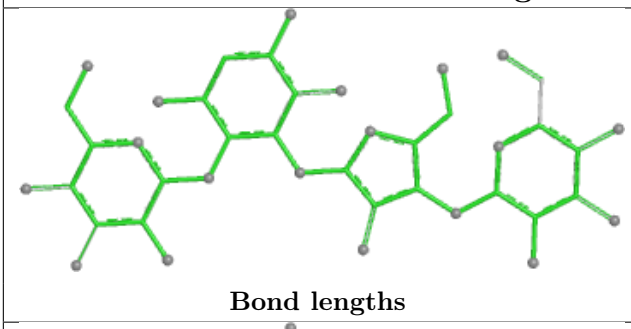
There are no ring outliers.

16 monomers are involved in 68 short contacts:

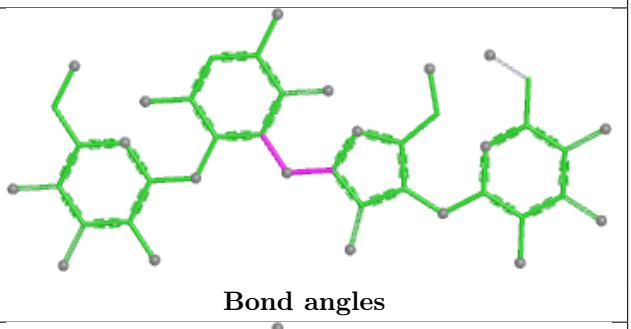
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	a	6218	SPD	3	0
59	a	6222	SPD	2	0
59	a	6220	SPD	2	0
59	a	6215	SPD	10	0
59	a	6221	SPD	1	0
57	A	1601	PAR	1	0
59	a	6212	SPD	3	0
59	a	6213	SPD	4	0
59	a	6216	SPD	14	0
59	A	1696	SPD	2	0
59	a	6217	SPD	4	0
59	a	6219	SPD	3	0
59	a	6214	SPD	1	0
59	a	6210	SPD	7	0
60	a	6223	SPM	10	0
59	a	6211	SPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

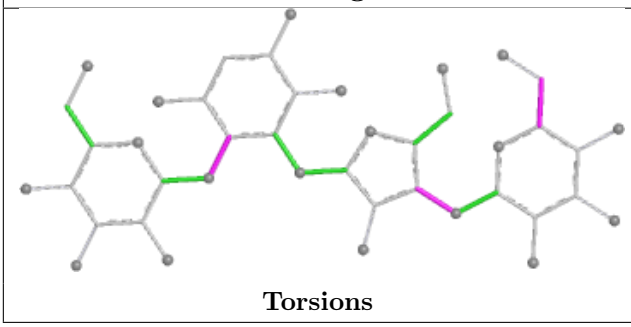
Ligand PAR A 1601



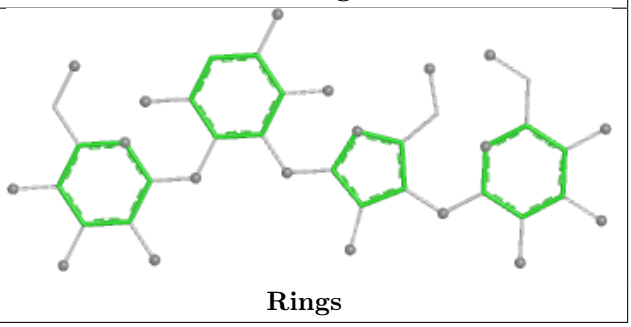
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

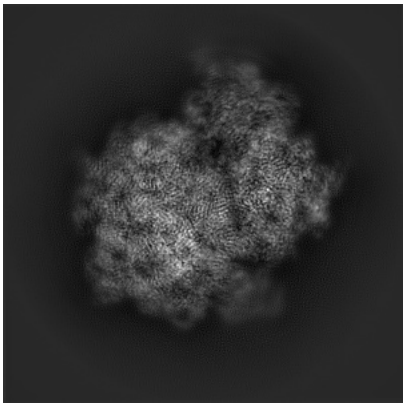
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22586. These allow visual inspection of the internal detail of the map and identification of artifacts.

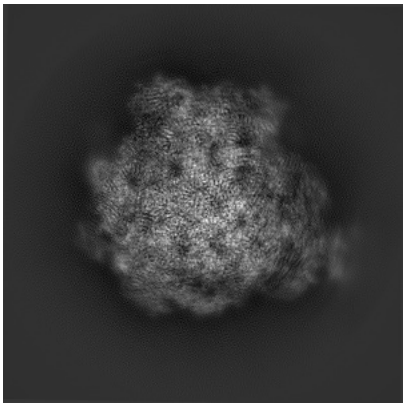
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

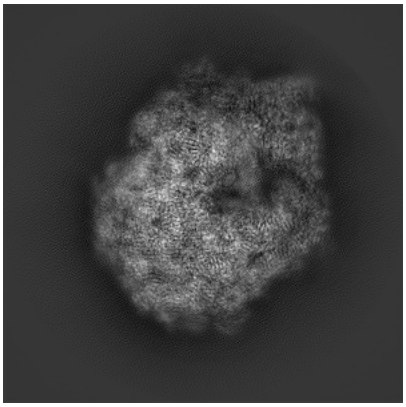
6.1.1 Primary map



X



Y

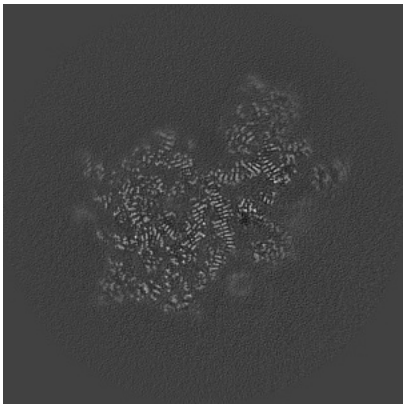


Z

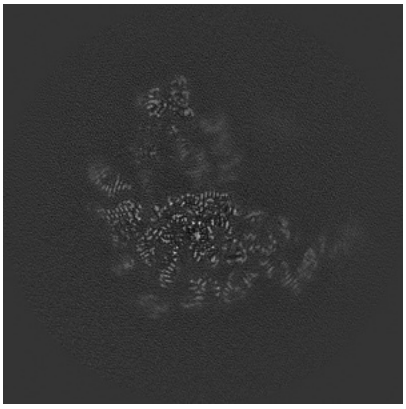
The images above show the map projected in three orthogonal directions.

6.2 Central slices

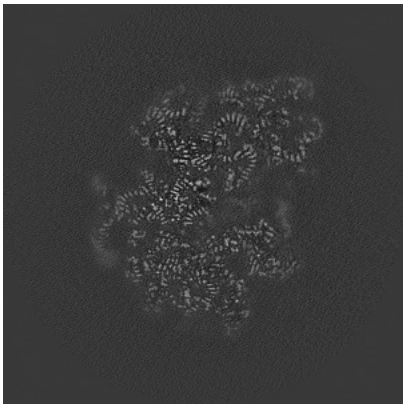
6.2.1 Primary map



X Index: 248



Y Index: 248

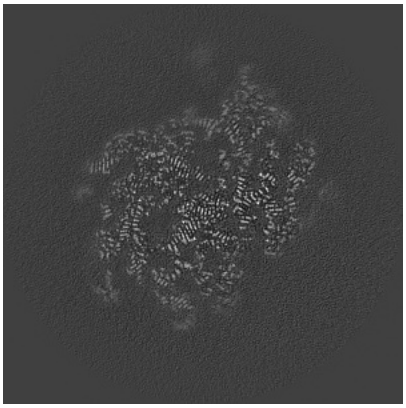


Z Index: 248

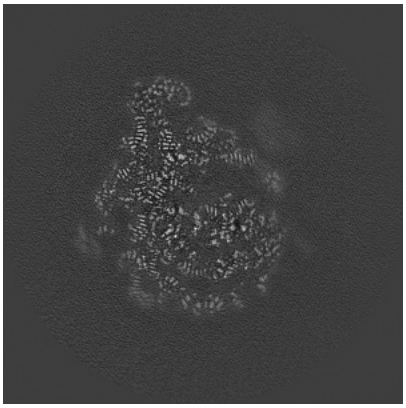
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

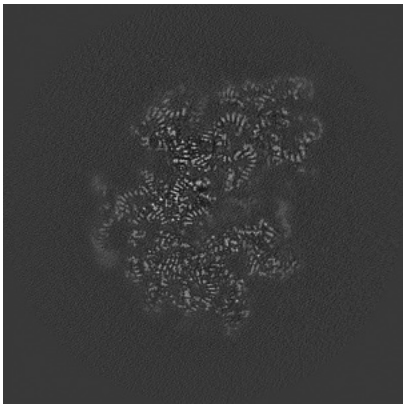
6.3.1 Primary map



X Index: 216



Y Index: 218

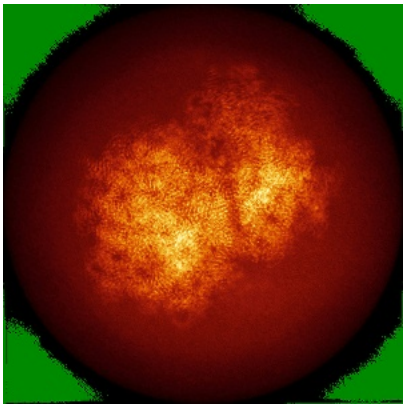


Z Index: 248

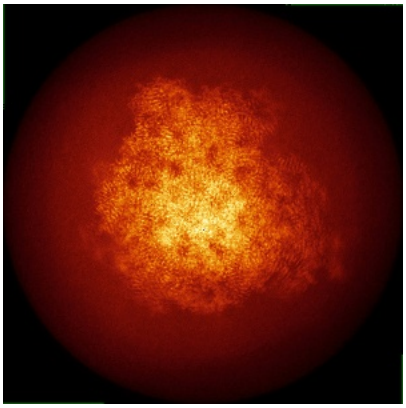
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

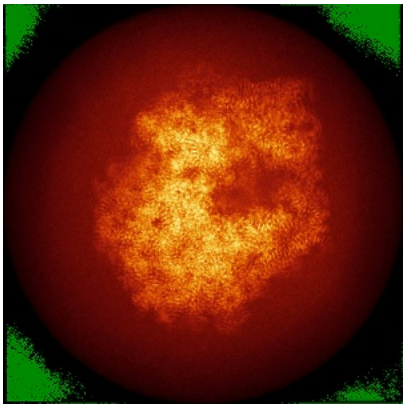
6.4.1 Primary map



X



Y

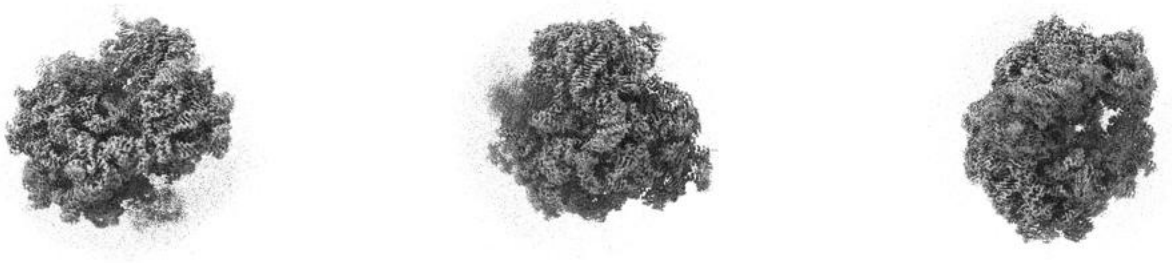


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

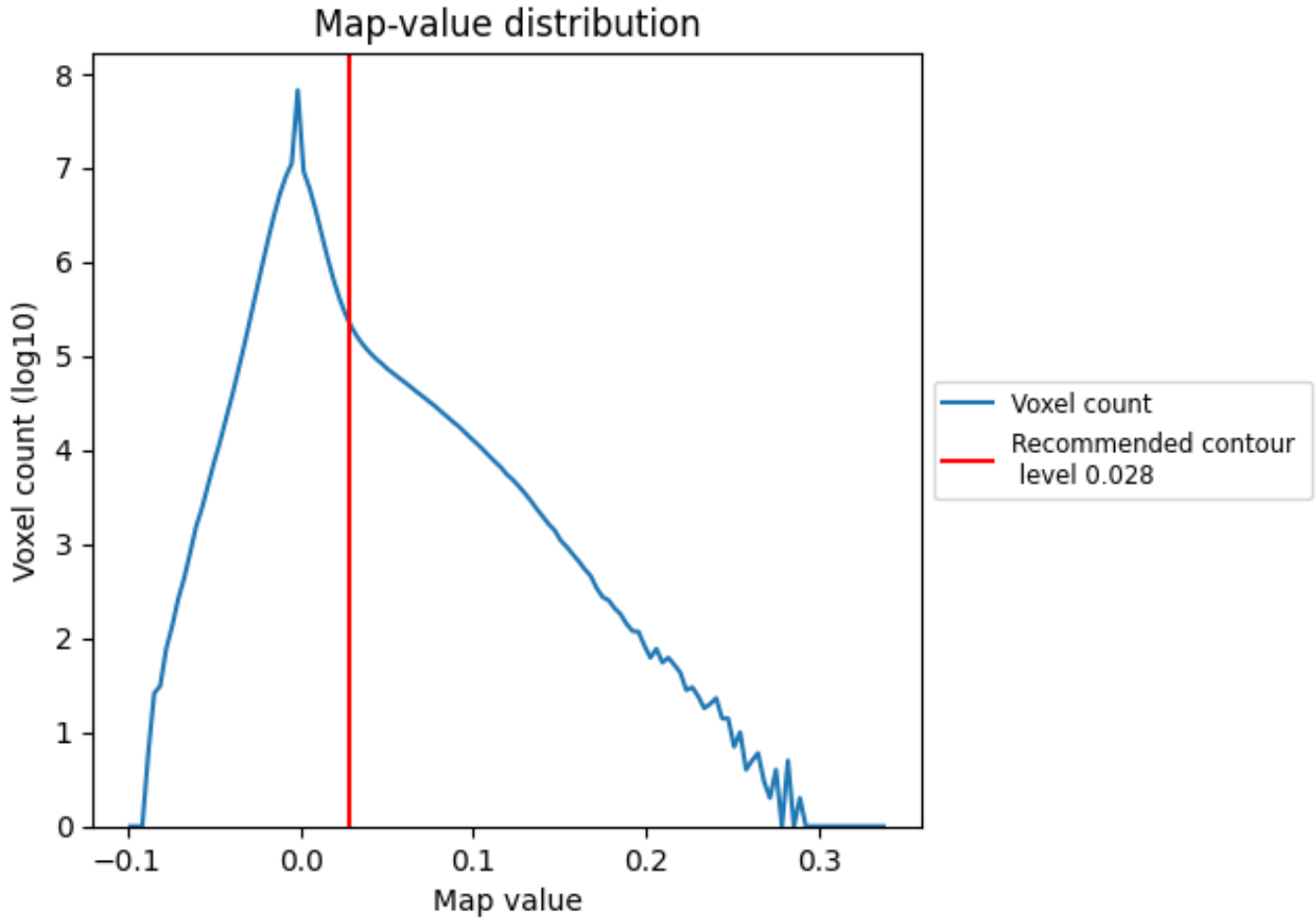
6.6 Mask visualisation (i)

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

7 Map analysis

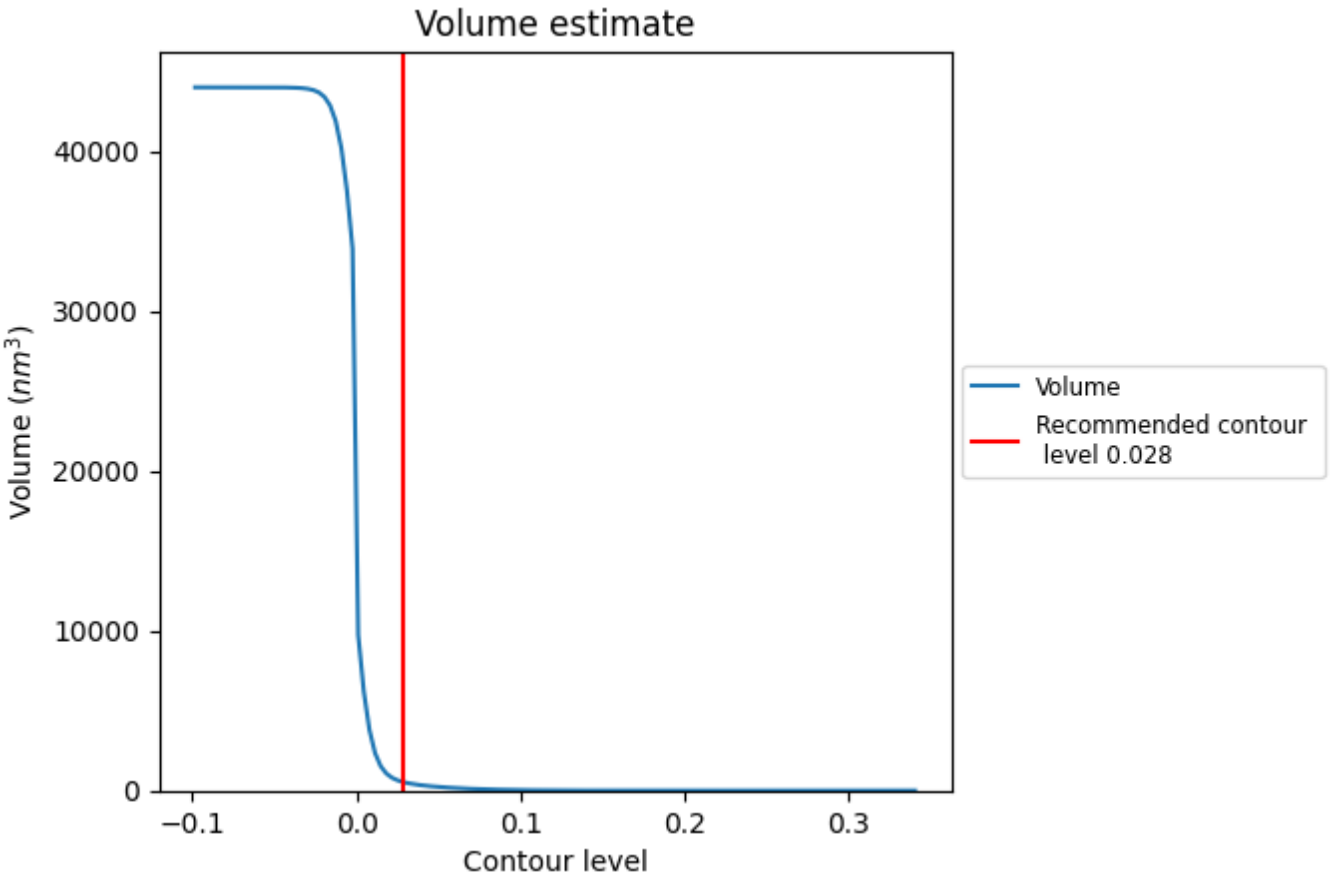
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

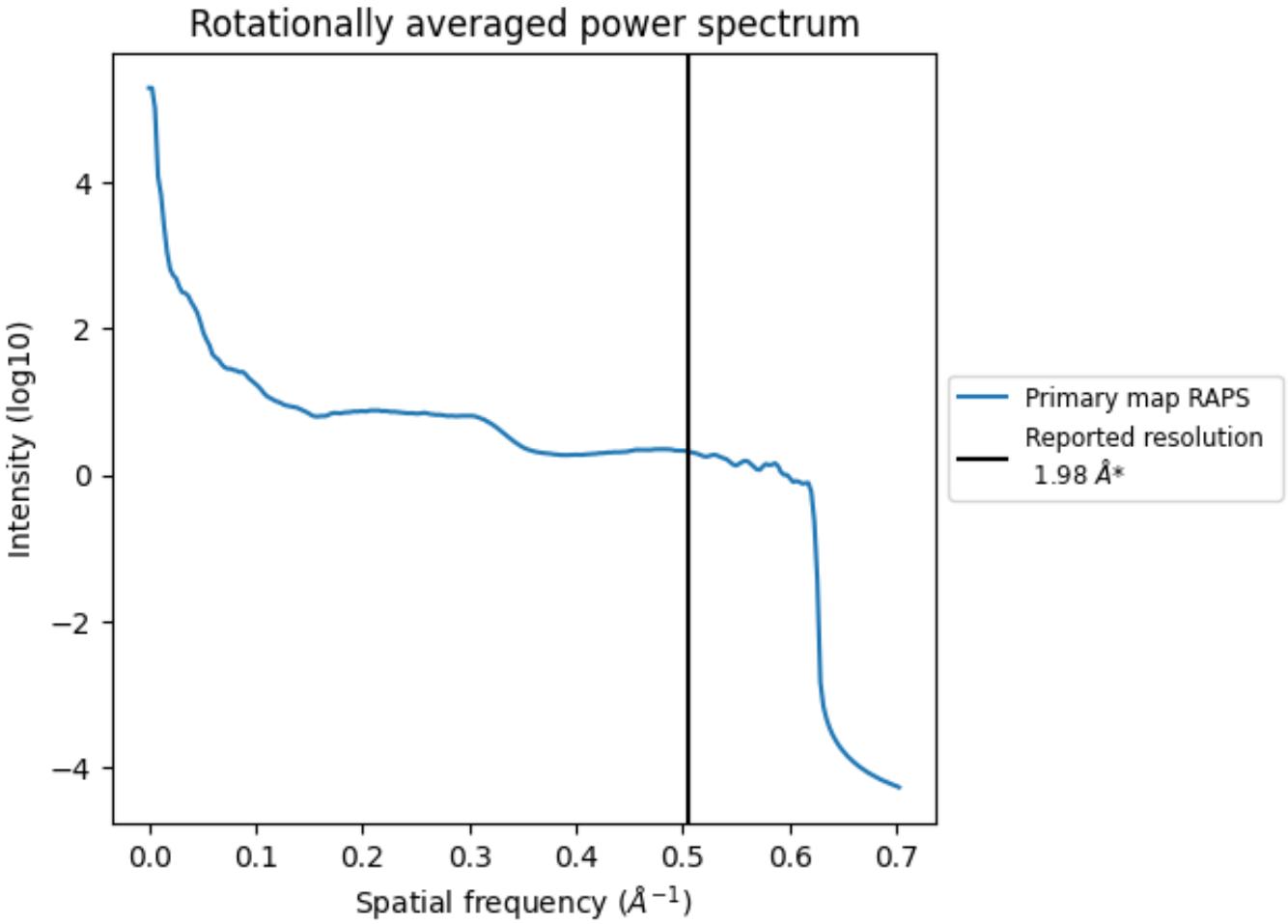
7.2 Volume estimate



The volume at the recommended contour level is 549 nm^3; this corresponds to an approximate mass of 496 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 (i)



*Reported resolution corresponds to spatial frequency of 0.505 Å^{-1}

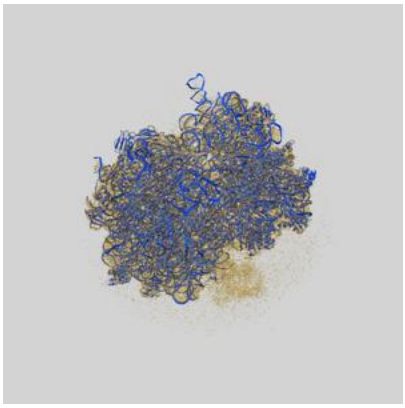
8 Fourier-Shell correlation

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

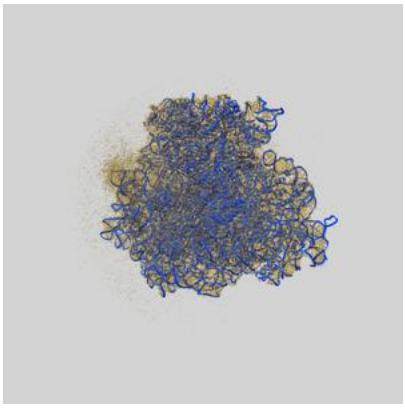
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22586 and PDB model 7K00. Per-residue inclusion information can be found in section 3 on page 20.

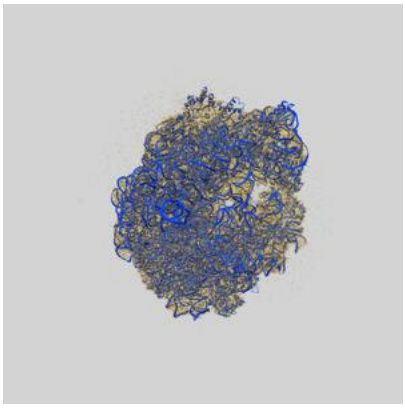
9.1 Map-model overlay



X



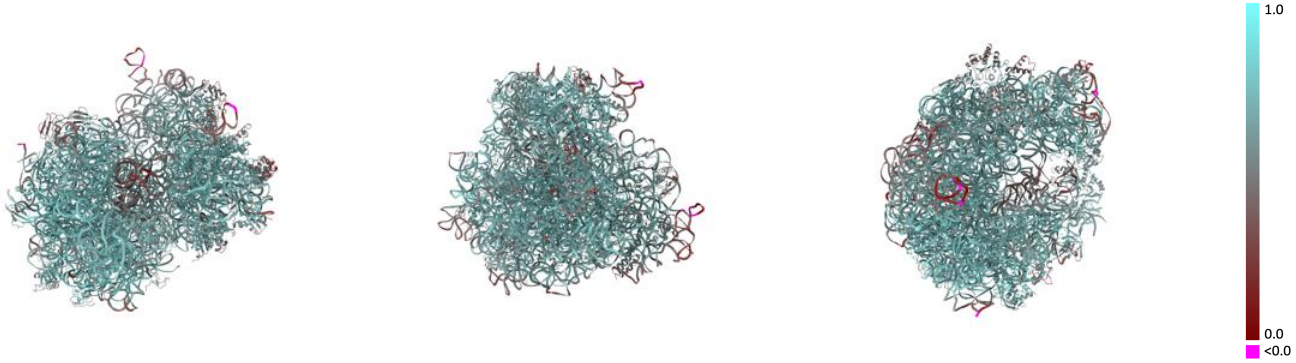
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 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.

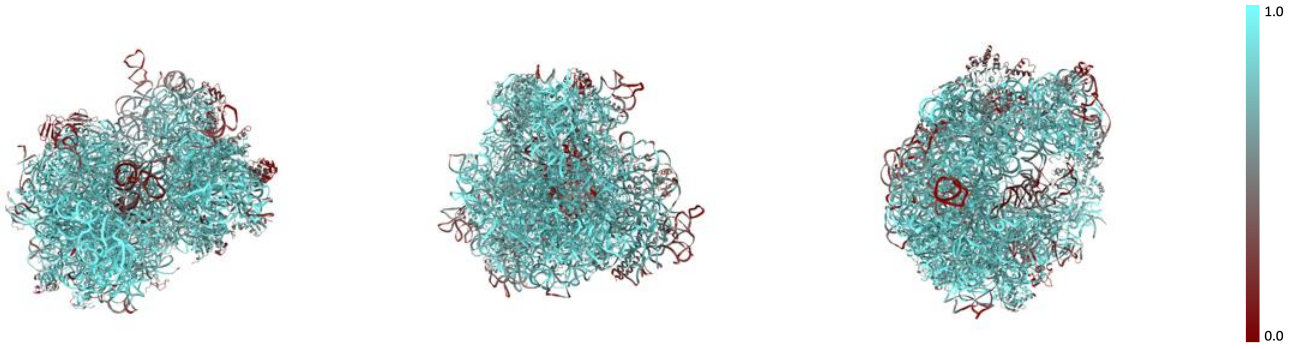
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

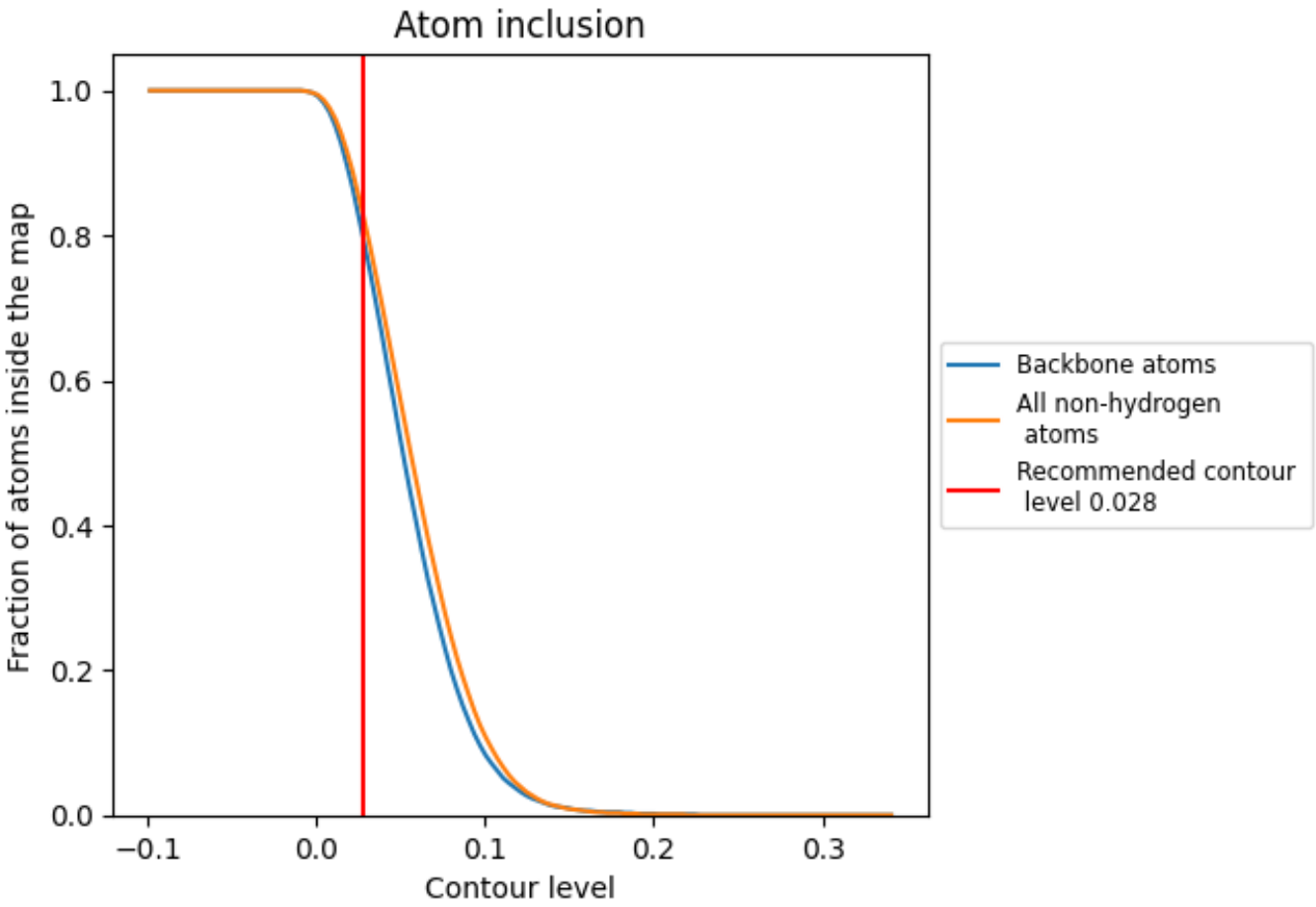
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 83% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8270	0.6770
0	0.8290	0.7010
1	0.9550	0.7930
2	0.9610	0.7840
3	0.7880	0.7110
4	0.6020	0.5410
5	0.7620	0.6520
A	0.8420	0.6520
B	0.4410	0.5030
C	0.7620	0.6510
D	0.4470	0.5260
E	0.8270	0.6710
F	0.6760	0.5710
G	0.6010	0.5560
H	0.8580	0.6910
I	0.7380	0.6370
J	0.5280	0.5540
K	0.7990	0.6430
L	0.7870	0.6700
M	0.7380	0.6290
N	0.8090	0.6810
O	0.8120	0.6390
P	0.6070	0.5960
Q	0.6180	0.5790
R	0.7840	0.6430
S	0.7510	0.6460
T	0.4900	0.5400
U	0.5040	0.5150
X	0.7390	0.6520
Y	0.3480	0.4370
Z	0.5390	0.5090
a	0.9070	0.7200
b	0.9240	0.6830
c	0.9210	0.7550
d	0.8530	0.7460



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Chain	Atom inclusion	Q-score
e	0.7350	0.6750
f	0.7560	0.6070
g	0.2810	0.4700
h	0.4430	0.5260
i	0.8750	0.7410
j	0.8130	0.7220
k	0.8570	0.7240
l	0.8670	0.7410
m	0.9260	0.7730
n	0.8620	0.6810
o	0.7930	0.7110
p	0.8980	0.7730
q	0.7490	0.6820
r	0.8330	0.7400
s	0.7040	0.6700
t	0.5950	0.5900
u	0.7140	0.6440
v	0.9110	0.7500
w	0.8500	0.7170
x	0.4990	0.5590
y	0.8400	0.7190
z	0.8350	0.7340