



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 09:03 AM EDT

PDB ID : 7KGB / pdb_00007kgb
EMDB ID : EMD-22865
Title : CryoEM structure of A2296-methylated Mycobacterium tuberculosis ribosome bound with SEQ-9
Authors : Cui, Z.; Zhang, J.
Deposited on : 2020-10-16
Resolution : 2.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

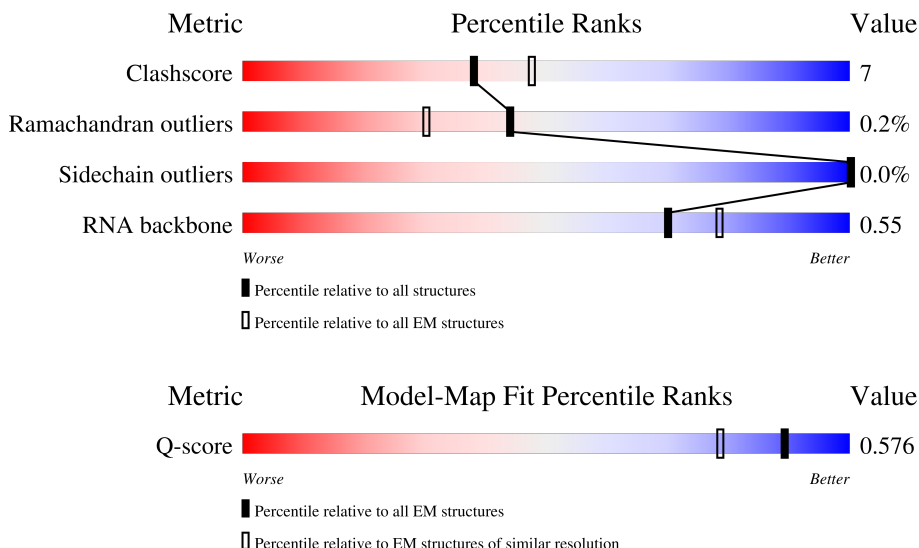
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.



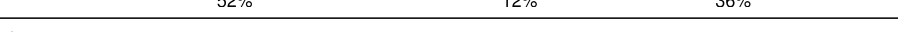
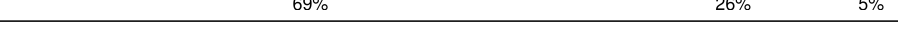
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	57	
2	1	55	
3	2	47	

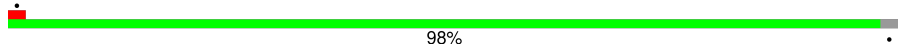
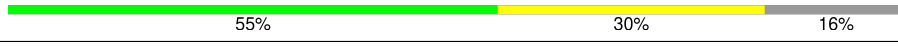
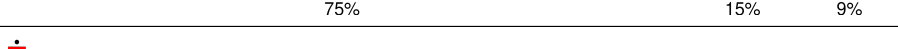
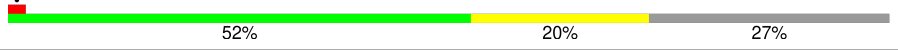
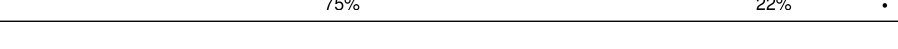
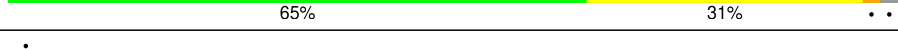
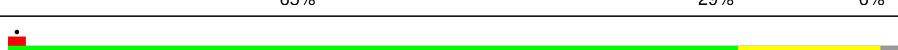
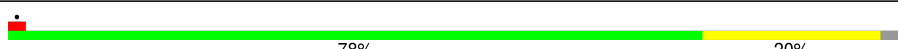
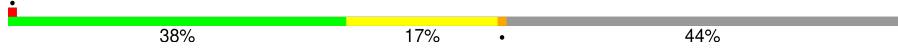
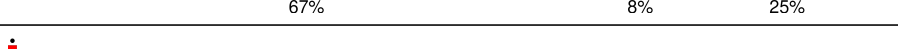
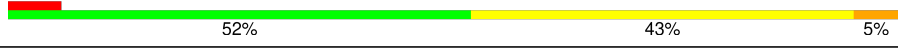
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Mol	Chain	Length	Quality of chain
4	3	64	
5	4	37	
6	6	80	
7	A	3138	
8	B	115	
9	C	280	
10	D	217	
11	E	223	
12	F	187	
13	G	179	
14	H	152	
15	J	195	
16	K	122	
17	L	146	
18	M	138	
19	N	180	
20	O	122	
21	P	113	
22	Q	129	
23	R	104	
24	S	197	
25	T	100	
26	U	105	
27	V	215	
28	W	86	

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Mol	Chain	Length	Quality of chain
29	X	64	
30	Y	77	
31	Z	65	
32	a	1537	
33	c	274	
34	d	201	
35	e	220	
36	f	96	
37	g	156	
38	h	132	
39	i	151	
40	j	101	
41	k	139	
42	l	124	
43	m	124	
44	n	61	
45	o	89	
46	p	162	
47	q	135	
48	r	84	
49	s	93	
50	t	86	
51	v	24	
52	y	77	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 145319 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 protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	54	Total	C	N	O	0	0
			429	266	94	69		

- Molecule 2 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			400	245	84	67	4		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	42	Total	C	N	O	S	0	0
			358	212	94	51	1		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	62	Total	C	N	O	0	0
			494	298	112	84		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			299	182	66	47	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	VAL	MET	conflict	UNP P9WH89

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	57	Total	C	N	O	S	0	0
			446	277	82	82	5		

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	3118	Total	C	N	O	P	0	0
			66962	29851	12340	21653	3118		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	115	Total	C	N	O	P	0	0
			2458	1097	456	790	115		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	272	Total	C	N	O	S	0	0
			2088	1277	437	369	5		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	213	Total	C	N	O	S	0	0
			1590	985	307	292	6		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	207	Total	C	N	O	S	0	0
			1552	958	303	289	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	178	Total	C	N	O	S	0	0
			1408	885	267	251	5		

- Molecule 13 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	174	Total	C	N	O	S	0	0
			1330	836	249	244	1		

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	47	Total	C	N	O	S	0	0
			350	220	64	65	1		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	146	Total	C	N	O	S	0	0
			1143	724	217	199	3		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	121	Total	C	N	O	S	0	0
			934	585	179	168	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	VAL	MET	conflict	UNP A0A045HTP7

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	143	Total	C	N	O	S	0	0
			1068	662	216	188	2		

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	134	Total	C	N	O	S	0	0
			1072	679	215	177	1		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	116	Total	C	N	O	S	0	0
			908	574	175	158	1		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	116	Total	C	N	O		0	0
			886	541	188	157			

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	112	Total	C	N	O	S	0	0
			907	573	174	159	1		

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	122	Total	C	N	O		0	0
			980	608	205	167			

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	100	Total	C	N	O		0	0
			757	482	138	137			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	insertion	UNP P9WHC3

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	113	Total	C	N	O		0	0
			860	533	178	149			

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	T	98	Total	C	N	O	0	0
			759	480	141	138		

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	90	Total	C	N	O	S	0
			699	430	138	129	2	0

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	V	95	Total	C	N	O		0
			735	456	152	127		0

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	W	71	Total	C	N	O	0	0
			526	325	108	93		

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	X	63	Total	C	N	O	S	0
			476	289	101	81	5	0

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Y	65	Total	C	N	O	S	0
			541	331	106	103	1	0

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Z	59	Total	C	N	O	0	0
			476	293	101	82		

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1519	Total	C	N	O	P	0	0
			32621	14536	5961	10605	1519		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	207	Total	C	N	O	S	0	0
			1654	1030	322	298	4		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	200	Total	C	N	O	S	0	0
			1650	1036	316	296	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	160	Total	C	N	O	S	0	0
			1149	726	214	206	3		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	95	Total	C	N	O	S	0	0
			757	480	133	141	3		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	152	Total	C	N	O	S	0	0
			1193	742	234	215	2		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			999	627	187	184	1		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	i	127	Total	C	N	O	0	0
			993	628	195	170		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	99	Total	C	N	O	S	0	0
			789	496	146	144	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	k	117	Total	C	N	O	0	0
			873	540	175	158		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			959	594	197	166	2		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	116	Total	C	N	O	S	0	0
			945	578	196	168	3		

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			468	294	96	73	5		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	o	87	Total	C	N	O	0	0
			718	449	144	125		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	p	91	Total	C	N	O	0	0
			728	462	140	126		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	94	Total	C	N	O	S	0	0
			763	477	151	132	3		

- Molecule 48 is a protein called 30S ribosomal protein S18 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	63	Total	C	N	O	S	0	0
			497	309	96	89	3		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	83	Total	C	N	O	S	0	0
			672	432	125	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	t	82	Total	C	N	O	0	0
			631	381	137	113		

- Molecule 51 is a protein called 50S ribosomal protein L37.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	v	22	Total	C	N	O	0	0
			186	111	47	28		

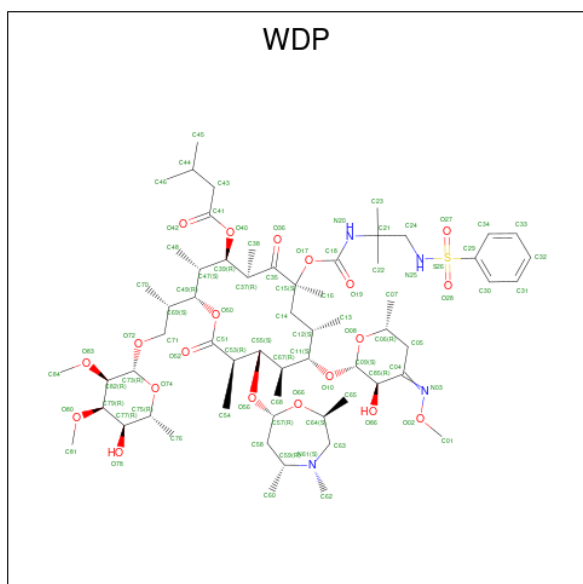
- Molecule 52 is a RNA chain called tRNA-initiator Met(CAU).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	77	Total	C	N	O	P	0	0
			1644	732	297	538	77		

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	1	1	Total	Zn	0
			1	1	
53	4	1	Total	Zn	0
			1	1	
53	6	1	Total	Zn	0
			1	1	
53	X	1	Total	Zn	0
			1	1	
53	n	1	Total	Zn	0
			1	1	
53	r	1	Total	Zn	0
			1	1	

- Molecule 54 is Sequanamycin 9 (CCD ID: WDP) (formula: $C_{61}H_{102}N_4O_{20}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
54	A	1	Total	C	N	O	S	0
			86	61	4	20	1	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	A	306	Total	Mg	0
			306	306	
55	B	7	Total	Mg	0
			7	7	

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Mol	Chain	Residues	Atoms		AltConf
55	C	3	Total 3	Mg 3	0
55	D	1	Total 1	Mg 1	0
55	L	1	Total 1	Mg 1	0
55	M	1	Total 1	Mg 1	0
55	a	126	Total 126	Mg 126	0
55	t	1	Total 1	Mg 1	0
55	y	1	Total 1	Mg 1	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.

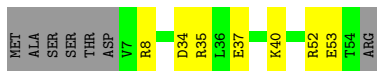
- Molecule 1: 50S ribosomal protein L32

Chain 0: 



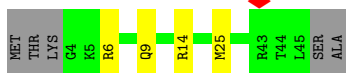
- Molecule 2: 50S ribosomal protein L33 2

Chain 1: 



- Molecule 3: 50S ribosomal protein L34

Chain 2: 



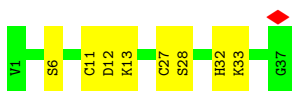
- Molecule 4: 50S ribosomal protein L35

Chain 3: 

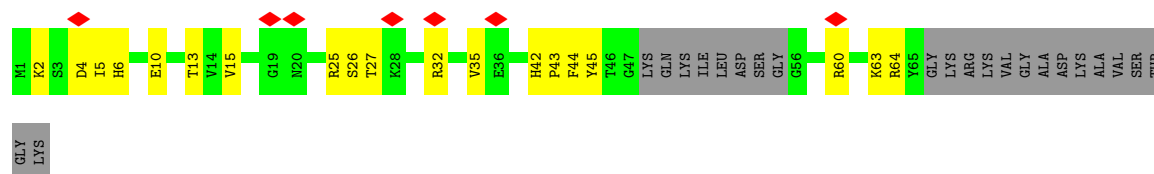


- Molecule 5: 50S ribosomal protein L36

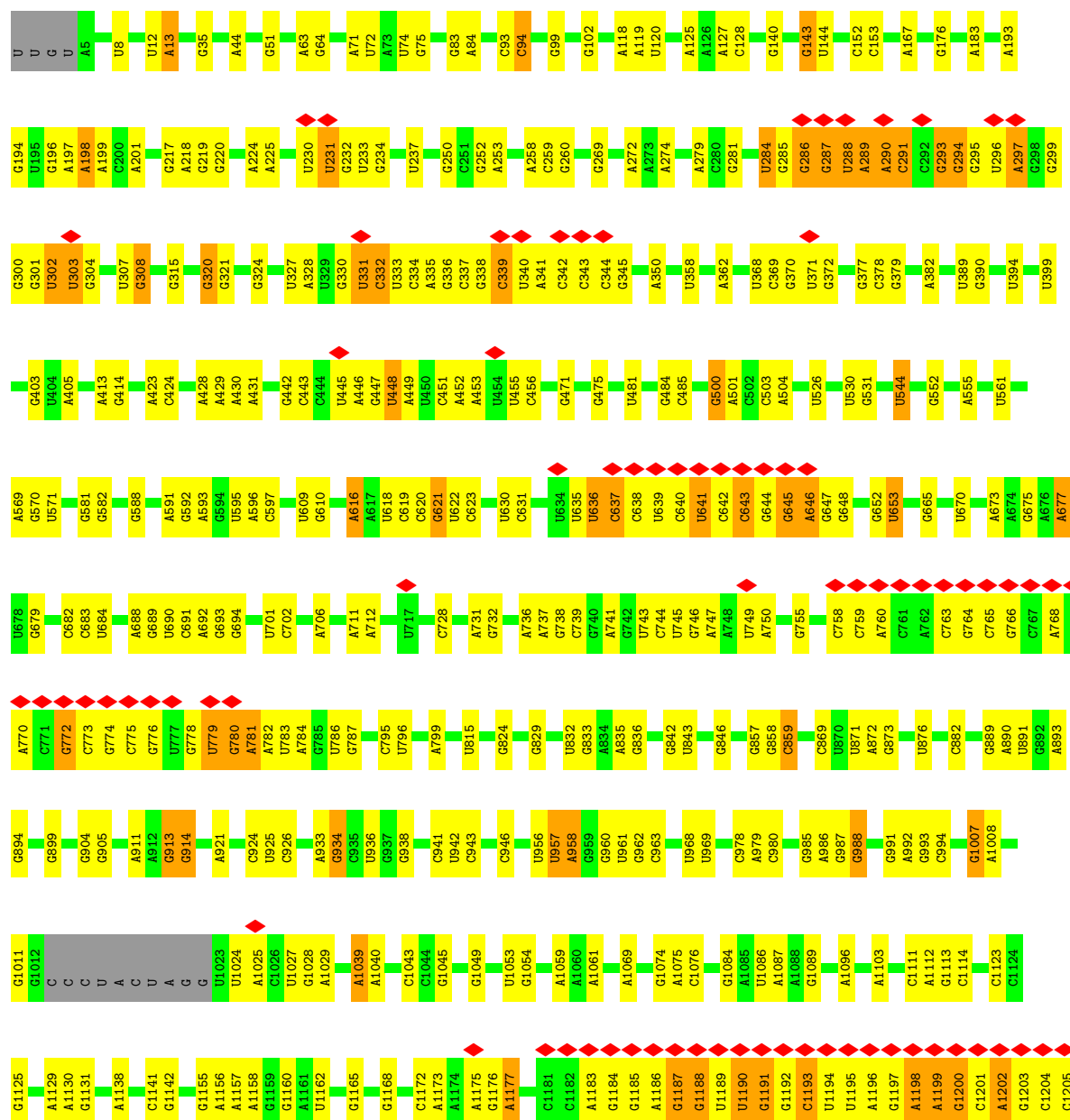
Chain 4: 

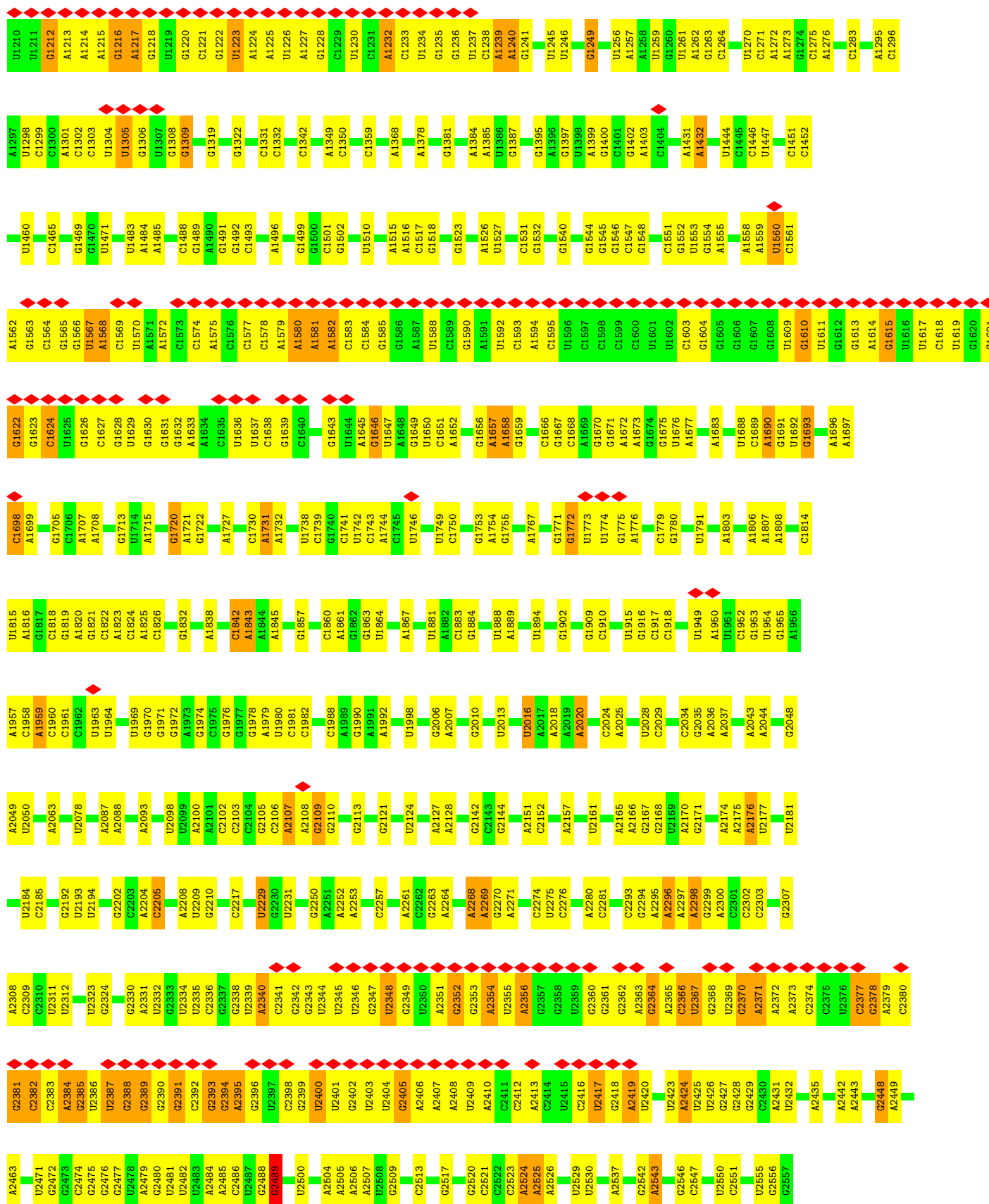


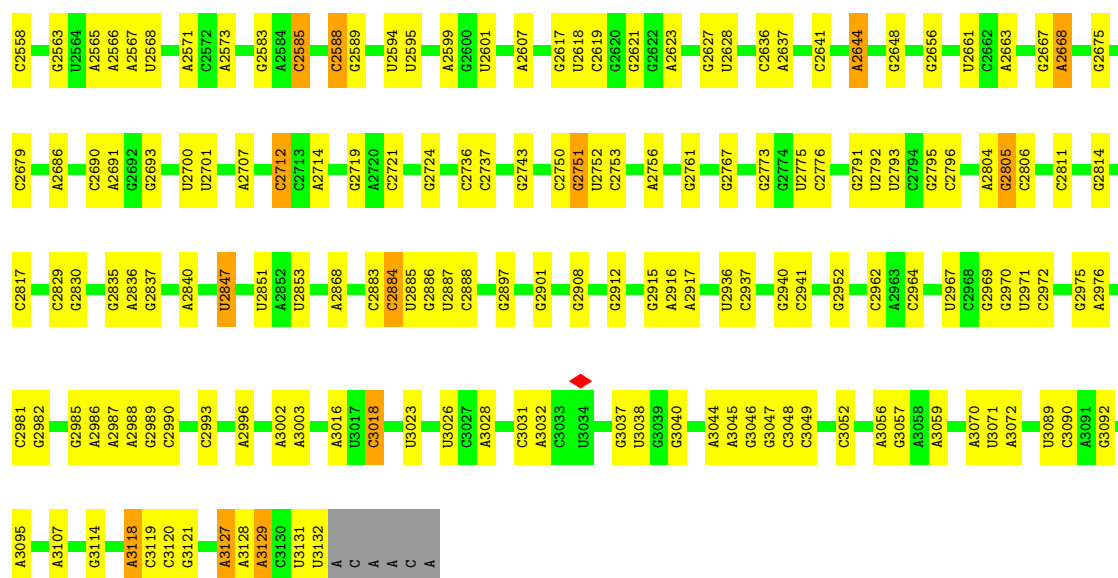
- Molecule 6: 50S ribosomal protein L31



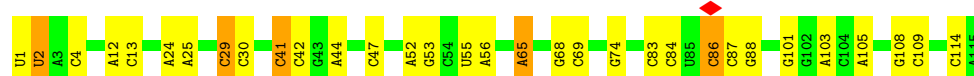
• Molecule 7: 23S rRNA



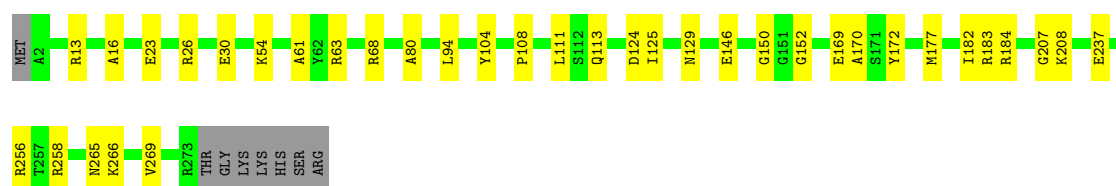
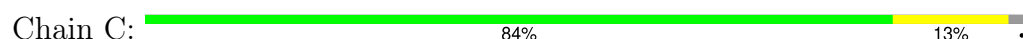




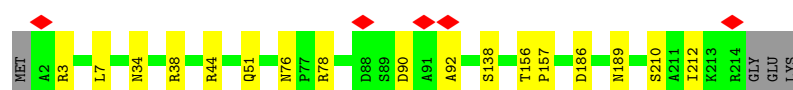
• Molecule 8: 5S rRNA



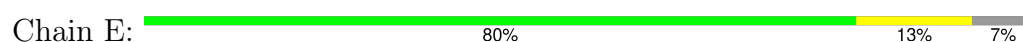
• Molecule 9: 50S ribosomal protein L2



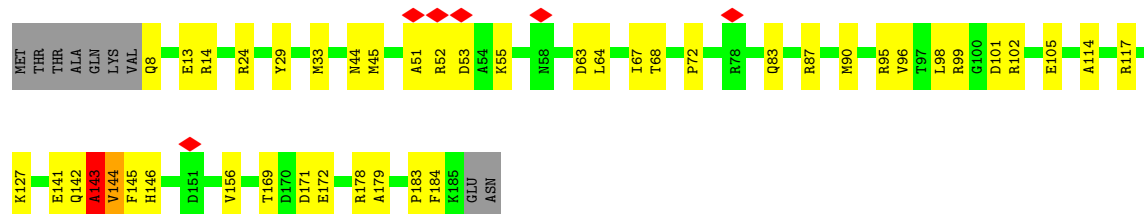
• Molecule 10: 50S ribosomal protein L3



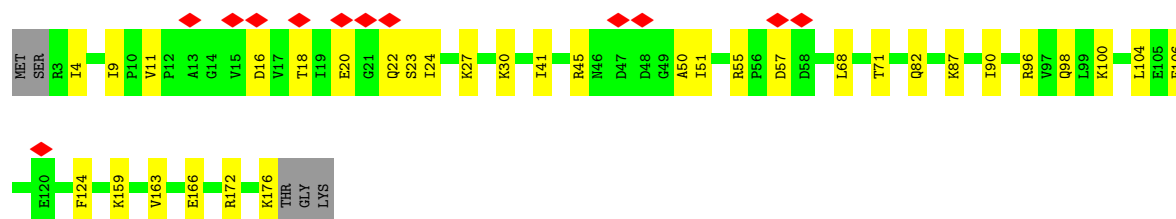
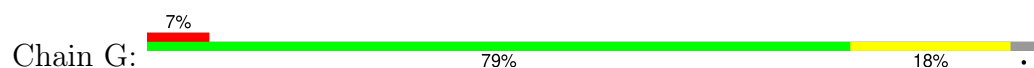
• Molecule 11: 50S ribosomal protein L4



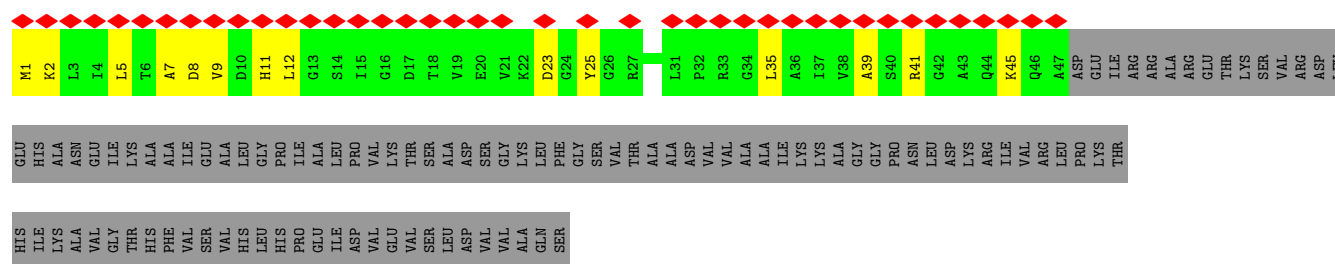
- Molecule 12: 50S ribosomal protein L5



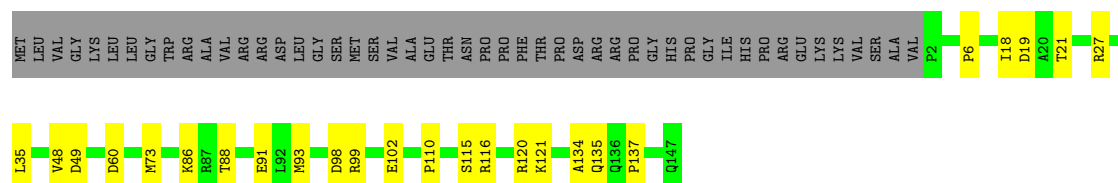
- Molecule 13: 50S ribosomal protein L6



- Molecule 14: 50S ribosomal protein L9

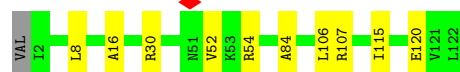


- Molecule 15: 50S ribosomal protein L13



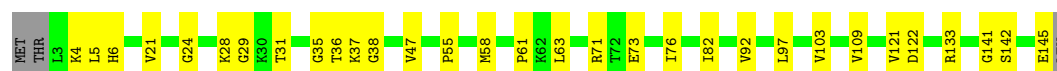
- Molecule 16: 50S ribosomal protein L14

Chain K:  91% 8%



- Molecule 17: 50S ribosomal protein L15

Chain L:  77% 21%



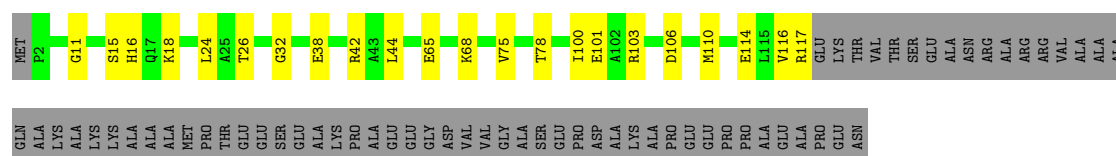
- Molecule 18: 50S ribosomal protein L16

Chain M:  78% 19%



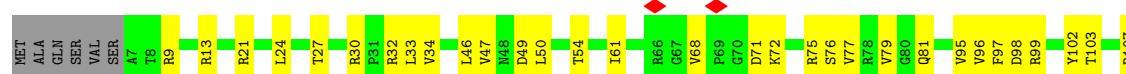
- Molecule 19: 50S ribosomal protein L17

Chain N:  52% 12% 36%



- Molecule 20: 50S ribosomal protein L18

Chain O:  69% 26% 5%



- Molecule 21: 50S ribosomal protein L19

Chain P:  91% 8%

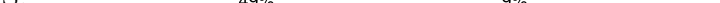


- Molecule 22: 50S ribosomal protein L20

MET
A2
K12
K19
R22
R28
L31
Q38
D49
R63
E66
Y76
I80
V88
E89
V90
D91
R92
K93
N94
E119
D120
A123
PRO
SER
GLY
GIU
ALA
ALA

- Chain R: 87% 8% . .

Category	Count
MET	1
MET ALA	1
T4	1
I7	1
E29	1
S30	1
E31	1
E34	1
S37	1
L38	1
L42	1
D45	1
T50	1
T51	1
D52	1
Y85	1
I103	1
ALA	1

- Chain S: 

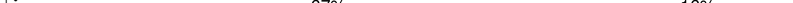
MET	THR	ALA	ALA	THR	LYS	ALA	THR	E9	K16	R25	K26	R35	D44	I45	P56	V60	V84	K93	R98	A99	Q100	G101	R102	A103	F104	R105	E118	S119	R120	P121	ALA	LVS	ASP	GLN	ARG	ARG	SER	ALA	LVS	SER	SER	ARG	ALA	ALA	ARG	THR	GLU	ALA	SER
-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

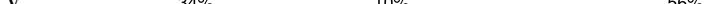
ALA	ALA	SER	VAL	GLY	ALA	ALA	ALA	ALA	ALA	LYS	LYS	ALA	ALA	PRO	PRO	SER	GLY	VAL	LYS	LYS	THR	PRO	ALA	LYS	LYS	ALA	ALA	ALA	ALA	LYS	LYS	THR	SER	GLY	GLY	SER
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- Chain T:  8% 81% 17%

Number of amino acids

MET ALA T3 I11 P14 E18 K19 S20 L23 L24 V28 F50 V57 P68 T69 R70 T71 G72 V84 R91 D94 L95 F96 G97 A98 A99 A100

- Chain U:  6% 67% 16% 14%

- Chain V: 

[illegible]

GLU	GLY	GLN	ALA	GLY	PRO	ASP	THR	LEU	VAL	THR	GLN	GLU	THR	ASN	SER	ILE	GLU	ILE	GLU	GLY	GLN	LEU	THR	VAL	SER	ILE	GLU	GLY	ALA	GLU	PRO	THR	THR	GLN	LEU	THR	THR	GLY	ALA	GLY	GLN	ILE	ALA	LEU	PRO	GLY	VAL	SER	LEU	ILE	SER	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

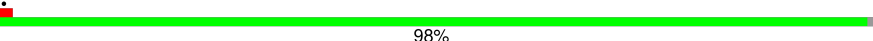
ASP	LEU	LEU	VAL	VAL	ASN	VAL	VAL	LYS	ALA	PRO	THR	ALA	GLU	GLU	LEU	GLY	GLY	GLU	VAL	ALA	GLY	ALA	GLU	GLU	ALA	GLU	GLU	GLU	ALA	ALA	VAL	GLU	ALA	GLY	GLY	GLU	SER	GLI
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- Molecule 28: 50S ribosomal protein L27

Chain W: 



- Molecule 29: 50S ribosomal protein L28

Chain X: 



- Molecule 30: 50S ribosomal protein L29

Chain Y: 



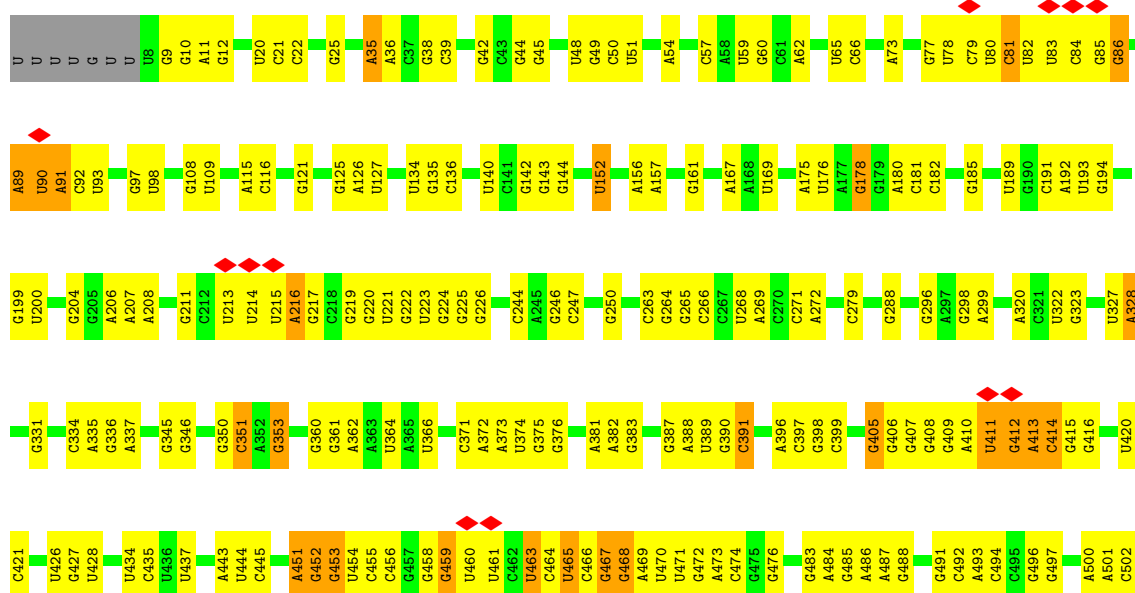
- Molecule 31: 50S ribosomal protein L30

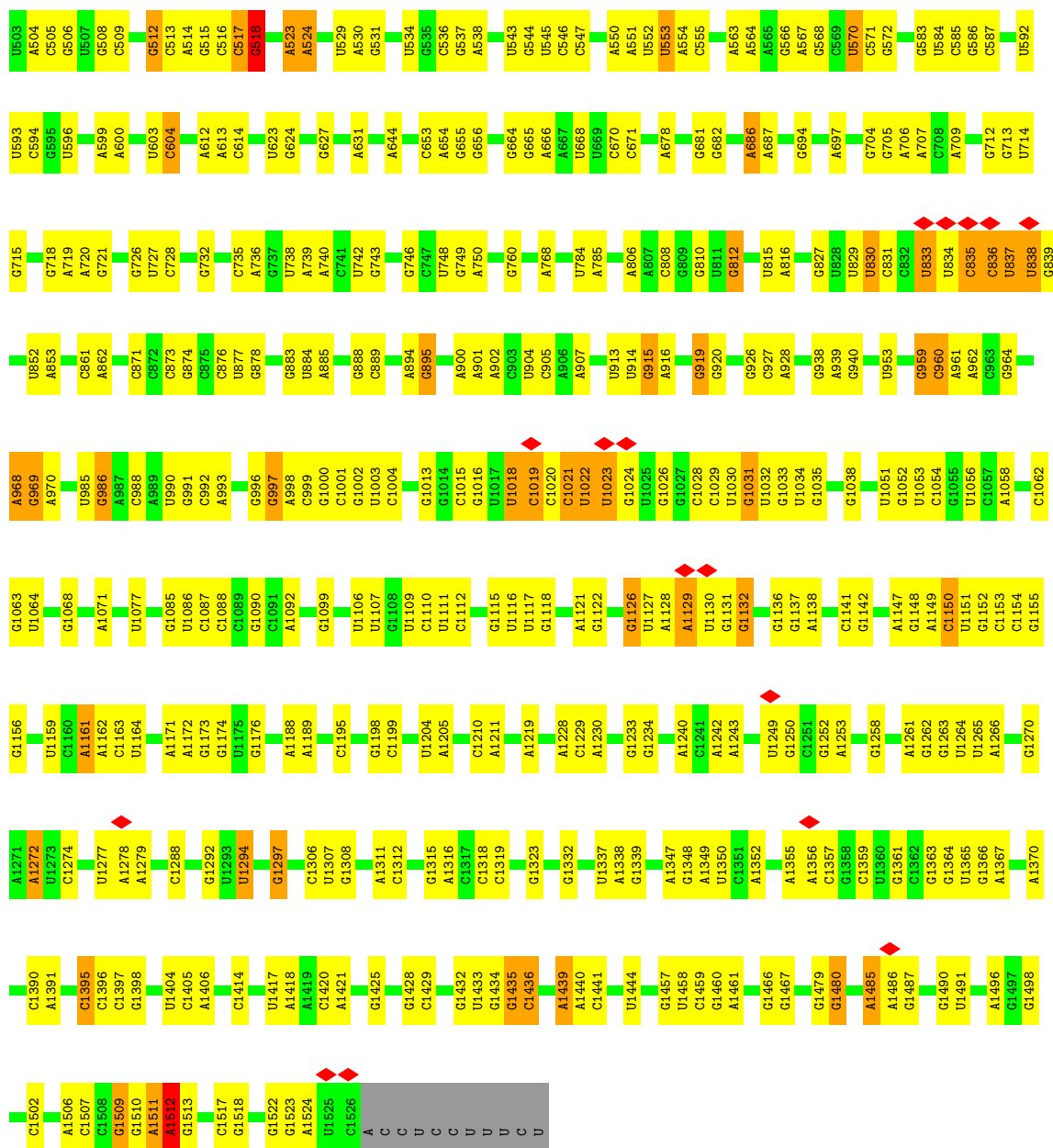
Chain Z: 



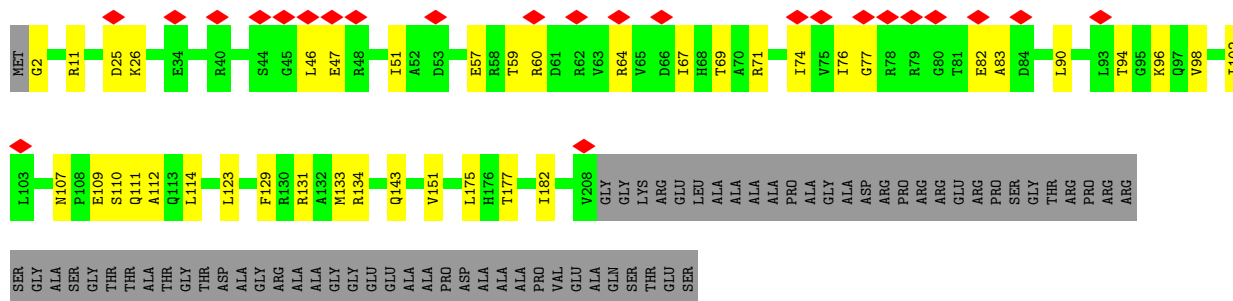
- Molecule 32: 16S rRNA

Chain a: 

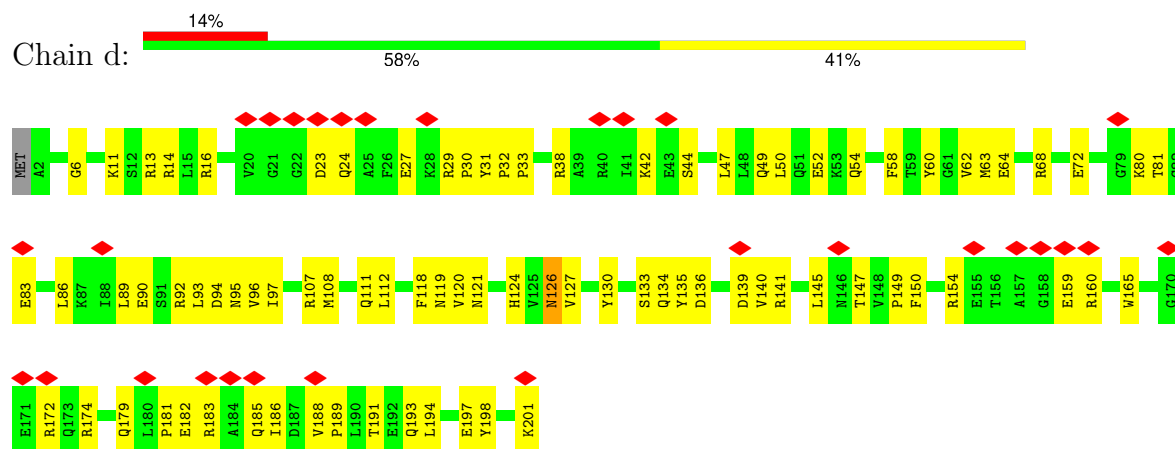




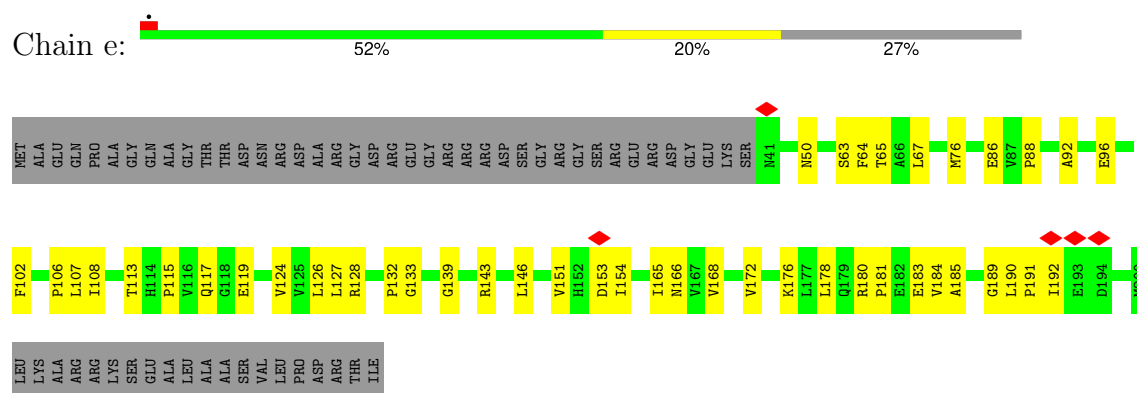
• Molecule 33: 30S ribosomal protein S3



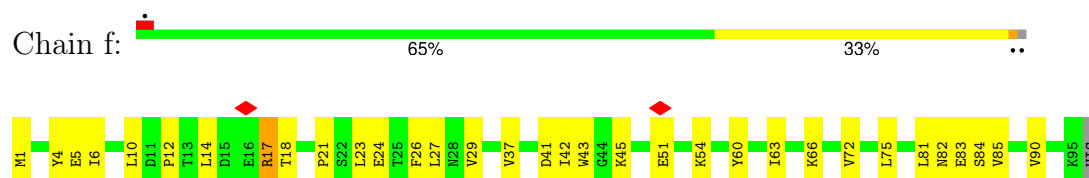
- Molecule 34: 30S ribosomal protein S4



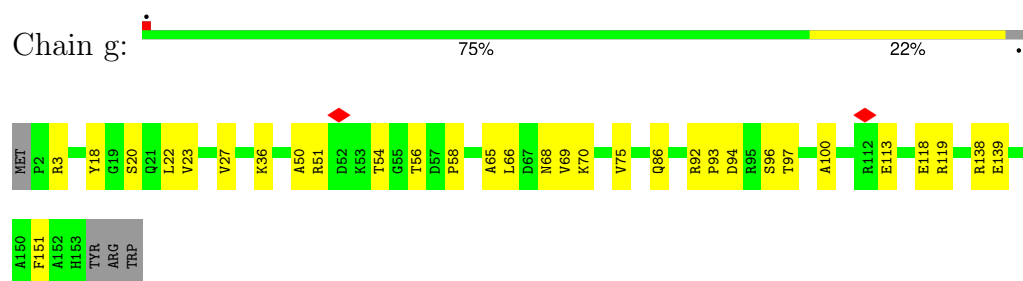
- Molecule 35: 30S ribosomal protein S5



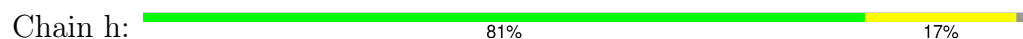
- Molecule 36: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S7

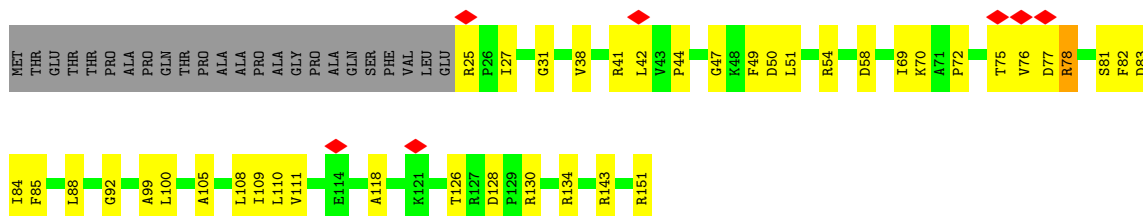


- Molecule 38: 30S ribosomal protein S8

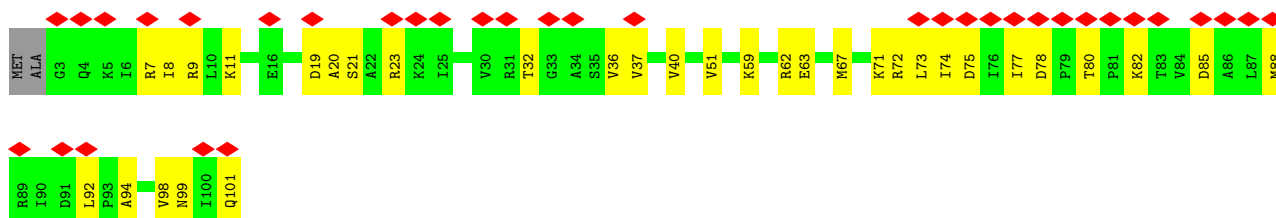




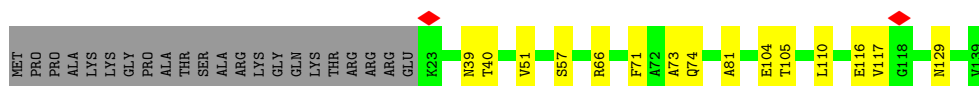
- Molecule 39: 30S ribosomal protein S9



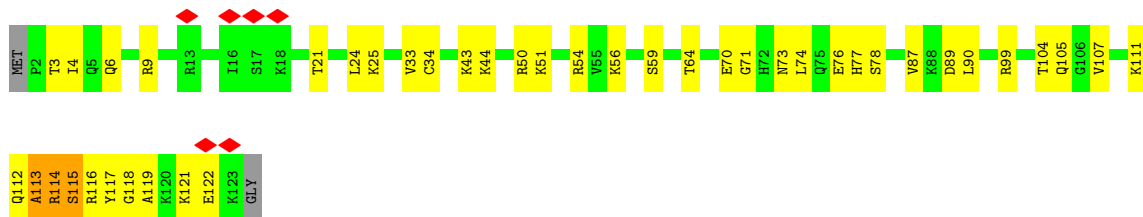
- Molecule 40: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S11



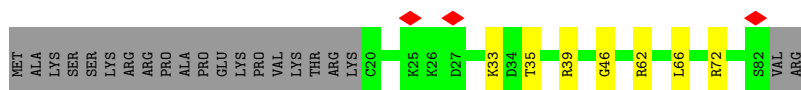
- Molecule 42: 30S ribosomal protein S12



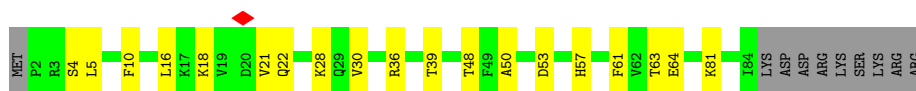
- Molecule 43: 30S ribosomal protein S13



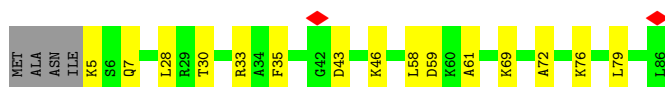
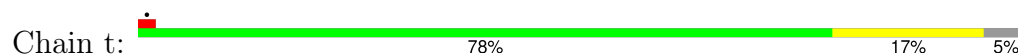




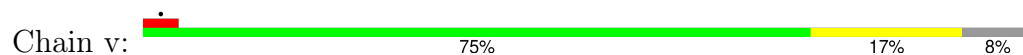
- Molecule 49: 30S ribosomal protein S19



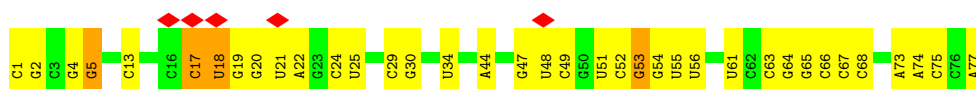
- Molecule 50: 30S ribosomal protein S20



- Molecule 51: 50S ribosomal protein L37



- Molecule 52: tRNA-initiator Met(CAU)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1065544	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, MA6, 4OC, 6MZ, OMG, ZN, G7M, UR3, 2MG, OMC, WDP, 5MC

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	0	0.34	0/435	0.36	0/581
2	1	0.29	0/407	0.37	0/543
3	2	0.36	0/361	0.43	0/473
4	3	0.32	0/499	0.37	0/664
5	4	0.28	0/303	0.37	0/402
6	6	0.21	0/455	0.51	0/611
7	A	0.36	0/74825	0.32	0/116743
8	B	0.28	0/2749	0.27	0/4284
9	C	0.34	0/2129	0.37	0/2861
10	D	0.33	0/1613	0.41	0/2174
11	E	0.30	0/1575	0.40	0/2129
12	F	0.28	0/1429	0.50	0/1921
13	G	0.20	0/1351	0.34	0/1824
14	H	0.14	0/353	0.41	0/474
15	J	0.32	0/1170	0.39	0/1584
16	K	0.32	0/944	0.40	0/1268
17	L	0.31	0/1081	0.41	0/1443
18	M	0.32	0/1098	0.46	0/1481
19	N	0.33	0/925	0.36	0/1242
20	O	0.28	0/895	0.45	0/1202
21	P	0.32	0/922	0.40	0/1236
22	Q	0.35	0/992	0.41	0/1329
23	R	0.31	0/766	0.39	0/1030
24	S	0.32	0/874	0.32	0/1186
25	T	0.30	0/770	0.38	0/1038
26	U	0.28	0/705	0.68	2/941 (0.2%)
27	V	0.24	0/747	0.39	0/1010
28	W	0.34	0/531	0.43	0/707
29	X	0.33	0/484	0.37	0/648
30	Y	0.29	0/544	0.47	0/727
31	Z	0.31	0/480	0.38	0/645
32	a	0.30	0/36305	0.29	0/56645

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.23	0/1678	0.39	0/2254
34	d	0.22	0/1683	0.48	0/2269
35	e	0.27	0/1165	0.49	0/1578
36	f	0.28	0/767	0.42	0/1036
37	g	0.23	0/1210	0.36	0/1631
38	h	0.28	0/1014	0.40	0/1369
39	i	0.24	0/1011	0.50	0/1356
40	j	0.24	0/803	0.47	0/1086
41	k	0.25	0/891	0.39	0/1204
42	l	0.29	0/970	0.51	0/1295
43	m	0.23	0/953	0.44	0/1274
44	n	0.27	0/477	0.38	0/634
45	o	0.27	0/727	0.51	0/973
46	p	0.26	0/742	0.53	0/1000
47	q	0.27	0/774	0.50	1/1032 (0.1%)
48	r	0.28	0/502	0.44	0/674
49	s	0.23	0/690	0.47	0/928
50	t	0.23	0/633	0.34	0/838
51	v	0.28	0/188	0.32	0/243
52	y	0.25	0/1836	0.27	0/2859
All	All	0.33	0/157431	0.34	3/236579 (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	F	0	1
23	R	0	1
26	U	0	1
36	f	0	1
39	i	0	1
42	l	0	2
46	p	0	1
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U	89	GLU	CA-C-N	7.53	135.25	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U	89	GLU	C-N-CA	7.53	135.25	121.70
47	q	54	PRO	CA-N-CD	-6.39	103.06	112.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	F	143	ALA	Peptide
23	R	50	THR	Peptide
26	U	90	GLU	Peptide
36	f	17	ARG	Sidechain
39	i	78	ARG	Peptide
42	l	113	ALA	Peptide
42	l	115	SER	Peptide
46	p	45	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	429	0	465	8	0
2	1	400	0	409	7	0
3	2	358	0	390	3	0
4	3	494	0	533	7	0
5	4	299	0	323	6	0
6	6	446	0	430	16	0
7	A	66962	0	33732	685	0
8	B	2458	0	1253	18	0
9	C	2088	0	2123	24	0
10	D	1590	0	1633	11	0
11	E	1552	0	1593	16	0
12	F	1408	0	1449	34	0
13	G	1330	0	1390	23	0
14	H	350	0	367	12	0
15	J	1143	0	1173	18	0
16	K	934	0	993	7	0
17	L	1068	0	1129	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	M	1072	0	1115	18	0
19	N	908	0	956	14	0
20	O	886	0	924	22	0
21	P	907	0	947	8	0
22	Q	980	0	1028	13	0
23	R	757	0	817	7	0
24	S	860	0	903	11	0
25	T	759	0	809	17	0
26	U	699	0	737	20	0
27	V	735	0	767	13	0
28	W	526	0	548	9	0
29	X	476	0	492	0	0
30	Y	541	0	551	17	0
31	Z	476	0	509	6	0
32	a	32621	0	16429	390	0
33	c	1654	0	1694	30	0
34	d	1650	0	1671	74	0
35	e	1149	0	1207	29	0
36	f	757	0	796	21	0
37	g	1193	0	1256	25	0
38	h	999	0	1034	15	0
39	i	993	0	1052	31	0
40	j	789	0	821	27	0
41	k	873	0	887	10	0
42	l	959	0	1045	37	0
43	m	945	0	992	23	0
44	n	468	0	492	8	0
45	o	718	0	760	11	0
46	p	728	0	764	30	0
47	q	763	0	823	22	0
48	r	497	0	514	5	0
49	s	672	0	690	13	0
50	t	631	0	681	12	0
51	v	186	0	202	4	0
52	y	1644	0	836	20	0
53	1	1	0	0	0	0
53	4	1	0	0	0	0
53	6	1	0	0	0	0
53	X	1	0	0	0	0
53	n	1	0	0	0	0
53	r	1	0	0	0	0
54	A	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	A	306	0	0	0	0
55	B	7	0	0	0	0
55	C	3	0	0	0	0
55	D	1	0	0	0	0
55	L	1	0	0	0	0
55	M	1	0	0	0	0
55	a	126	0	0	0	0
55	t	1	0	0	0	0
55	y	1	0	0	0	0
All	All	145319	0	95134	1743	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 (1743) 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)
7:A:1959:A:H2	7:A:1970:G:N1	1.28	1.30
7:A:1959:A:C2	7:A:1970:G:N1	2.02	1.18
7:A:2335:U:H3	7:A:2428:G:H1	1.03	0.99
52:y:1:C:H42	52:y:73:A:H61	1.12	0.94
7:A:2309:C:H5	7:A:2675:G:H1	1.16	0.92
7:A:2542:G:H22	7:A:2550:U:H3	1.20	0.89
32:a:1002:G:N2	32:a:1013:G:N7	2.19	0.89
52:y:51:U:H3	52:y:65:G:H1	0.94	0.89
32:a:467:G:H2'	32:a:468:G:H8	1.38	0.88
39:i:77:ASP:HB2	39:i:78:ARG:HB3	1.52	0.88
7:A:289:A:HO2'	7:A:304:G:HO2'	1.21	0.88
32:a:1019:C:H42	32:a:1026:G:H1	1.24	0.86
7:A:1517:C:H5	7:A:1532:G:H1	1.23	0.85
7:A:1592:U:H3	7:A:1613:G:H1	1.19	0.85
7:A:732:G:H1	7:A:739:C:H5	1.20	0.85
7:A:1235:G:C6	7:A:1236:G:O6	2.30	0.84
34:d:29:ARG:HH12	34:d:32:PRO:HD2	1.40	0.84
7:A:1465:C:OP1	25:T:68:ARG:NH2	2.11	0.84
7:A:1658:A:H61	7:A:1815:U:H3	1.22	0.83
7:A:1959:A:N1	7:A:1970:G:O6	2.11	0.83
10:D:3:ARG:NH1	10:D:210:SER:O	2.11	0.83
32:a:926:G:N7	37:g:3:ARG:NH1	2.27	0.83
11:E:24:ILE:HD11	11:E:204:VAL:HG23	1.60	0.82
40:j:11:LYS:HG2	40:j:71:LYS:HG2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:113:ALA:O	42:l:115:SER:N	2.11	0.82
35:e:86:GLU:HG3	35:e:88:PRO:HD2	1.60	0.81
7:A:873:G:H1	7:A:882:C:H5	1.25	0.81
7:A:1772:G:H21	7:A:1775:G:H1	1.28	0.80
7:A:638:C:N3	7:A:640:C:N4	2.29	0.80
32:a:413:A:H3'	32:a:414:C:H6	1.47	0.79
42:l:76:GLU:HG3	42:l:77:HIS:H	1.46	0.79
7:A:637:C:O2	7:A:646:A:N6	2.16	0.79
7:A:2174:A:H2	7:A:2181:U:H3	1.30	0.79
7:A:1628:G:N3	36:f:17:ARG:NH1	2.30	0.78
32:a:709:A:H5'	41:k:129:ASN:HB2	1.65	0.78
7:A:1558:A:H5''	7:A:1645:A:H61	1.47	0.78
32:a:517:C:O2'	32:a:518:G7M:O4'	2.02	0.77
40:j:85:ASP:HA	40:j:88:MET:HE2	1.64	0.77
7:A:2006:G:H1	7:A:2217:C:H5	1.31	0.77
11:E:123:ASP:O	11:E:127:ASN:ND2	2.17	0.77
34:d:68:ARG:NH1	34:d:72:GLU:OE2	2.17	0.77
7:A:1953:G:N2	7:A:1976:G:H22	1.83	0.77
12:F:117:ARG:HD3	12:F:144:VAL:HA	1.68	0.76
7:A:645:G:N2	7:A:646:A:N7	2.32	0.76
27:V:15:THR:OG1	27:V:16:GLU:OE1	2.03	0.76
7:A:3018:C:OP2	15:J:120:ARG:NH1	2.19	0.76
6:6:64:ARG:HG2	49:s:5:LEU:HD11	1.69	0.75
40:j:9:ARG:HB2	40:j:99:ASN:HB2	1.68	0.75
7:A:1959:A:H2	7:A:1970:G:C2	2.02	0.75
32:a:1020:C:N4	32:a:1023:U:OP1	2.20	0.75
7:A:1953:G:H22	7:A:1976:G:H1	1.34	0.74
7:A:946:C:H5	7:A:1322:G:H1	1.35	0.74
7:A:2338:G:N1	7:A:2425:U:N3	2.34	0.74
7:A:1842:C:N4	7:A:1857:G:OP2	2.21	0.74
7:A:1955:G:N2	7:A:1974:G:H1	1.86	0.74
7:A:1203:G:H5'	7:A:2712:C:H4'	1.70	0.74
7:A:1959:A:N1	7:A:1970:G:C6	2.56	0.74
32:a:968:A:H4'	32:a:969:G:H5''	1.69	0.74
36:f:6:ILE:HG12	36:f:90:VAL:HG22	1.69	0.74
38:h:5:ASP:OD1	38:h:79:ARG:NH1	2.20	0.73
7:A:1955:G:H22	7:A:1974:G:H1	1.33	0.73
6:6:25:ARG:NH1	12:F:105:GLU:OE2	2.22	0.73
32:a:514:A:OP1	42:l:116:ARG:NH2	2.20	0.73
8:B:42:C:O2	12:F:99:ARG:NH1	2.22	0.73
12:F:87:ARG:H	12:F:90:MET:HE2	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:638:C:N4	7:A:641:U:O4	2.21	0.73
7:A:1212:G:N2	7:A:1215:A:C8	2.57	0.73
32:a:211:G:O2'	32:a:216:A:N6	2.22	0.73
12:F:14:ARG:NH2	12:F:179:ALA:O	2.22	0.72
33:c:59:THR:HG22	40:j:94:ALA:HB2	1.71	0.72
34:d:86:LEU:HB3	34:d:183:ARG:HB3	1.71	0.72
35:e:180:ARG:HB2	35:e:183:GLU:OE1	1.89	0.72
13:G:87:LYS:HB2	13:G:166:GLU:HG3	1.71	0.72
18:M:32:TYR:OH	18:M:111:GLU:OE2	2.01	0.72
7:A:1212:G:N1	7:A:1215:A:OP2	2.23	0.72
40:j:32:THR:O	40:j:82:LYS:NZ	2.22	0.72
7:A:1566:G:H1	7:A:1637:U:H3	0.81	0.72
7:A:1953:G:H22	7:A:1976:G:H22	1.35	0.72
18:M:77:LYS:NZ	18:M:86:GLY:O	2.22	0.72
34:d:120:VAL:HG23	34:d:121:ASN:H	1.54	0.72
7:A:1656:G:O2'	7:A:1816:A:N6	2.22	0.72
32:a:472:G:O2'	32:a:474:C:N4	2.22	0.72
34:d:147:THR:HG22	34:d:149:PRO:HD2	1.70	0.71
32:a:1077:U:H3	32:a:1090:G:H22	1.38	0.71
7:A:616:A:OP2	15:J:116:ARG:NH1	2.24	0.71
7:A:1569:C:N4	7:A:1633:A:OP2	2.24	0.71
11:E:143:SER:OG	11:E:146:SER:OG	2.07	0.71
13:G:9:ILE:HB	13:G:51:ILE:HB	1.72	0.71
43:m:12:ASP:OD1	43:m:44:ARG:NE	2.22	0.71
37:g:75:VAL:HG22	37:g:86:GLN:HB3	1.72	0.71
43:m:3:ARG:HG2	43:m:7:VAL:HA	1.71	0.71
7:A:1988:C:H5	21:P:93:ARG:HH22	1.39	0.71
39:i:50:ASP:HB3	39:i:85:PHE:HB3	1.73	0.71
46:p:45:GLU:HG3	46:p:46:PRO:HD3	1.72	0.71
32:a:1002:G:N1	32:a:1013:G:O6	2.19	0.71
7:A:1952:C:H2'	7:A:1953:G:C8	2.26	0.70
33:c:51:ILE:HD12	33:c:67:ILE:HD11	1.72	0.70
11:E:155:THR:HG22	11:E:157:ARG:H	1.56	0.70
39:i:151:ARG:NH2	52:y:34:U:OP2	2.23	0.70
12:F:68:THR:HG21	12:F:96:VAL:HG11	1.73	0.70
32:a:413:A:H5'	32:a:414:C:H5	1.56	0.70
32:a:664:G:H2'	32:a:665:G:C8	2.26	0.70
15:J:60:ASP:HA	15:J:93:MET:HE1	1.73	0.70
32:a:514:A:N6	42:l:89:ASP:OD2	2.20	0.70
7:A:1683:A:OP1	7:A:1698:C:N4	2.25	0.69
3:2:14:ARG:NH2	7:A:899:G:OP2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:635:U:O2	7:A:648:G:N2	2.21	0.69
47:q:58:ARG:HB2	47:q:115:MET:HE2	1.72	0.69
7:A:1771:G:H1	7:A:1776:A:H61	1.41	0.69
46:p:41:HIS:HB2	46:p:48:LEU:HB3	1.73	0.69
46:p:45:GLU:HG3	46:p:46:PRO:CD	2.22	0.69
7:A:2351:A:N1	7:A:2356:A:N6	2.41	0.69
7:A:2338:G:N2	7:A:2425:U:O2	2.26	0.69
12:F:68:THR:HB	12:F:98:LEU:HD21	1.73	0.69
32:a:1068:G:N2	32:a:1071:A:OP2	2.24	0.69
34:d:90:GLU:HA	34:d:95:ASN:HD22	1.56	0.69
7:A:2566:A:H2'	7:A:2567:A:C8	2.28	0.69
16:K:120:GLU:OE1	21:P:64:SER:OG	2.09	0.69
38:h:11:LEU:HD22	38:h:77:LEU:HD22	1.75	0.69
7:A:2363:A:O2'	7:A:2410:A:N6	2.26	0.69
40:j:80:THR:HG21	40:j:82:LYS:HE3	1.75	0.68
33:c:69:THR:HG22	33:c:102:ILE:HD11	1.75	0.68
34:d:80:LYS:HG3	35:e:133:GLY:HA2	1.73	0.68
49:s:18:LYS:O	49:s:22:GLN:NE2	2.27	0.68
32:a:77:G:H1	32:a:91:A:H2	1.39	0.68
7:A:8:U:H3	7:A:3129:A:H62	1.38	0.68
7:A:1577:C:H42	7:A:1627:C:H42	1.41	0.68
19:N:116:VAL:HG12	19:N:117:ARG:HD3	1.75	0.68
2:l:8:ARG:NH1	7:A:2523:C:OP2	2.27	0.68
26:U:89:GLU:HA	26:U:91:THR:N	2.09	0.68
32:a:206:A:H8	32:a:221:U:HO2'	1.40	0.68
7:A:1553:U:H2'	7:A:1554:G:C8	2.29	0.68
16:K:107:ARG:HH12	21:P:33:GLU:HB3	1.59	0.68
32:a:1001:C:H2'	32:a:1002:G:C8	2.29	0.68
7:A:635:U:H3	7:A:648:G:H1	0.74	0.68
24:S:118:GLU:OE2	24:S:120:ARG:NH1	2.27	0.68
7:A:2707:A:N6	7:A:2719:G:O2'	2.27	0.68
17:L:122:ASP:OD2	17:L:142:SER:OG	2.12	0.68
32:a:451:A:N7	46:p:47:SER:OG	2.26	0.68
32:a:1425:G:O2'	32:a:1461:A:N6	2.27	0.68
41:k:74:GLN:HB3	41:k:105:THR:HG22	1.76	0.67
7:A:64:G:H1'	25:T:69:THR:HG21	1.77	0.67
7:A:1570:U:H3	7:A:1632:G:H2'	1.58	0.67
47:q:46:LYS:HG3	47:q:47:HIS:H	1.58	0.67
7:A:1743:C:H2'	7:A:1744:A:H8	1.60	0.67
39:i:44:PRO:HA	39:i:82:PHE:HB2	1.75	0.67
7:A:2380:C:H1'	7:A:2385:G:H22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:86:ARG:HH21	26:U:95:VAL:HG21	1.59	0.67
31:Z:7:THR:OG1	31:Z:34:SER:OG	2.11	0.67
34:d:29:ARG:NH1	34:d:30:PRO:O	2.27	0.67
7:A:1629:U:H2'	7:A:1630:G:C8	2.30	0.67
26:U:88:ASP:OD1	26:U:89:GLU:N	2.27	0.67
32:a:59:U:H2'	32:a:60:G:H8	1.61	0.66
7:A:2426:U:H2'	7:A:2427:G:H8	1.59	0.66
37:g:54:THR:HG23	37:g:56:THR:H	1.60	0.66
30:Y:14:THR:O	30:Y:64:ARG:NH1	2.29	0.66
34:d:80:LYS:HG2	34:d:81:THR:H	1.59	0.66
38:h:15:ARG:NH1	38:h:77:LEU:O	2.28	0.66
21:P:38:ARG:NH2	32:a:345:G:OP1	2.28	0.66
7:A:2897:G:O2'	13:G:176:LYS:NZ	2.29	0.66
32:a:1428:G:H2'	32:a:1429:C:C6	2.31	0.66
43:m:108:ARG:HH21	43:m:111:LYS:HE3	1.61	0.66
7:A:1172:C:H2'	7:A:1173:A:C8	2.31	0.66
7:A:1953:G:H22	7:A:1976:G:N2	1.93	0.66
32:a:207:A:H8	32:a:220:G:H21	1.41	0.66
32:a:1352:A:OP2	44:n:35:ARG:NH2	2.29	0.65
20:O:99:ARG:NH1	20:O:102:TYR:O	2.29	0.65
7:A:289:A:N6	7:A:300:G:N1	2.43	0.65
7:A:544:U:HO2'	7:A:561:U:H3	1.43	0.65
7:A:2418:G:OP2	7:A:2419:A:N6	2.29	0.65
30:Y:11:ARG:NH1	30:Y:63:GLU:OE1	2.29	0.65
7:A:2106:C:N4	7:A:2109:G:N3	2.44	0.65
33:c:25:ASP:OD2	33:c:26:LYS:N	2.30	0.65
7:A:1235:G:O6	7:A:1236:G:O6	2.15	0.65
17:L:36:THR:HG22	17:L:38:GLY:H	1.62	0.65
7:A:1206:A:OP1	7:A:1207:C:N4	2.28	0.65
32:a:408:G:H5''	34:d:24:GLN:HE21	1.62	0.65
1:O:45:LYS:HD2	7:A:3118:A:OP1	1.97	0.64
7:A:2571:A:OP1	28:W:75:ARG:NH2	2.30	0.64
32:a:655:G:H22	32:a:732:G:H1	1.46	0.64
7:A:635:U:O4	7:A:648:G:O6	2.15	0.64
40:j:37:VAL:N	40:j:75:ASP:OD1	2.30	0.64
7:A:1172:C:H2'	7:A:1173:A:H8	1.61	0.64
40:j:7:ARG:HH21	40:j:74:ILE:HB	1.62	0.64
7:A:297:A:N1	7:A:341:A:N6	2.46	0.64
4:3:43:ARG:NH2	7:A:2601:U:OP2	2.30	0.64
7:A:1011:G:O6	7:A:1024:U:C2	2.50	0.64
32:a:223:U:OP1	50:t:69:LYS:NZ	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:471:G:H22	7:A:481:U:H3	1.44	0.64
7:A:1176:G:H21	7:A:1240:A:H62	1.46	0.64
24:S:35:ARG:NH1	24:S:84:VAL:O	2.30	0.64
7:A:763:C:N4	7:A:764:G:O6	2.31	0.64
32:a:515:G:H2'	32:a:516:C:C6	2.33	0.64
32:a:919:G:H2'	32:a:1498:G:C8	2.33	0.64
7:A:1198:A:O2'	7:A:1204:C:N4	2.31	0.63
7:A:2543:A:N6	12:F:45:MET:O	2.30	0.63
7:A:296:U:O4	7:A:297:A:N6	2.30	0.63
46:p:92:ARG:NH1	46:p:92:ARG:O	2.30	0.63
7:A:768:A:N6	7:A:772:G:O6	2.31	0.63
7:A:1657:A:H4'	7:A:1658:A:H5''	1.79	0.63
37:g:113:GLU:HB3	37:g:118:GLU:OE2	1.99	0.63
2:l:37:GLU:OE2	2:l:52:ARG:NH1	2.31	0.63
7:A:640:C:N3	7:A:643:C:N4	2.46	0.63
20:O:72:LYS:HB3	20:O:107:ARG:HD3	1.79	0.63
32:a:361:G:N2	32:a:364:U:OP2	2.30	0.63
7:A:636:U:H5	7:A:647:G:H1	1.44	0.63
7:A:1193:C:H42	7:A:1198:A:H3'	1.63	0.63
7:A:1628:G:H2'	7:A:1629:U:C6	2.33	0.63
47:q:111:ARG:NE	47:q:133:GLU:OE2	2.32	0.63
7:A:1011:G:C6	7:A:1024:U:O2	2.52	0.63
7:A:2381:G:OP1	7:A:2382:C:N4	2.30	0.63
9:C:258:ARG:NH1	9:C:265:ASN:OD1	2.32	0.63
6:6:42:HIS:ND1	6:6:43:PRO:O	2.30	0.63
39:i:69:ILE:HG12	39:i:100:LEU:HD23	1.81	0.63
7:A:1578:C:H2'	7:A:1579:A:H8	1.63	0.63
12:F:143:ALA:O	12:F:145:PHE:N	2.32	0.63
31:Z:23:LEU:HG	31:Z:50:VAL:HG21	1.81	0.63
7:A:193:A:H2'	7:A:194:G:C8	2.34	0.62
7:A:307:U:O2'	14:H:41:ARG:NH1	2.32	0.62
28:W:56:ASP:OD1	28:W:58:THR:OG1	2.17	0.62
32:a:1370:A:OP1	37:g:92:ARG:NH2	2.31	0.62
7:A:2036:A:H2'	7:A:2037:A:C8	2.35	0.62
32:a:413:A:H3'	32:a:414:C:C6	2.33	0.62
32:a:1420:C:H2'	32:a:1421:A:C8	2.34	0.62
7:A:285:G:N1	7:A:303:U:N3	2.47	0.62
34:d:119:ASN:HD21	34:d:141:ARG:HE	1.46	0.62
42:l:74:LEU:HD11	42:l:104:THR:HG22	1.81	0.62
43:m:75:GLN:OE1	43:m:79:ARG:NH1	2.32	0.62
7:A:324:G:H22	7:A:452:A:H2	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1566:G:O6	7:A:1637:U:O4	2.17	0.62
7:A:2364:G:N2	7:A:2399:G:O4'	2.33	0.62
28:W:31:VAL:HB	28:W:35:GLU:HG3	1.81	0.62
32:a:665:G:H2'	32:a:666:A:H8	1.64	0.62
35:e:127:LEU:HB3	35:e:154:ILE:HD11	1.80	0.62
7:A:299:G:H2'	7:A:300:G:H8	1.62	0.62
7:A:3071:U:H2'	7:A:3072:A:C8	2.34	0.62
13:G:45:ARG:HH21	13:G:51:ILE:HA	1.64	0.62
13:G:98:GLN:OE1	13:G:100:LYS:NZ	2.30	0.62
7:A:1842:C:H4'	7:A:1843:A:H5''	1.82	0.62
34:d:62:VAL:HG21	34:d:89:LEU:HD11	1.82	0.62
20:O:81:GLN:HA	20:O:118:ASN:HD22	1.65	0.62
7:A:83:G:H1	7:A:102:G:HO2'	1.47	0.62
32:a:1348:G:H2'	32:a:1349:A:C8	2.34	0.62
7:A:942:U:H2'	7:A:943:C:C6	2.35	0.62
10:D:7:LEU:HB2	10:D:34:ASN:HD21	1.64	0.62
7:A:622:U:H2'	7:A:623:C:C6	2.35	0.61
34:d:86:LEU:HD22	34:d:183:ARG:HD3	1.81	0.61
40:j:59:LYS:HE2	40:j:62:ARG:NH2	2.15	0.61
34:d:60:TYR:OH	34:d:183:ARG:NE	2.33	0.61
7:A:1952:C:H2'	7:A:1953:G:H8	1.64	0.61
32:a:997:G:H2'	32:a:998:A:C8	2.35	0.61
7:A:1190:U:H3	7:A:1226:U:H4'	1.65	0.61
7:A:2370:G:H21	7:A:2394:G:H3'	1.65	0.61
15:J:73:MET:HE3	15:J:86:LYS:HD3	1.82	0.61
32:a:627:G:O3'	47:q:57:ARG:NH1	2.33	0.61
32:a:1272:A:OP2	40:j:71:LYS:NZ	2.33	0.61
32:a:1315:G:H2'	32:a:1316:A:C8	2.35	0.61
7:A:1707:A:H2'	7:A:1708:A:C8	2.35	0.61
7:A:289:A:N6	7:A:300:G:C6	2.68	0.61
7:A:1011:G:O6	7:A:1024:U:O2	2.18	0.61
7:A:1544:G:H2'	7:A:1545:G:C8	2.36	0.61
7:A:1581:A:OP1	7:A:1622:G:N1	2.34	0.61
15:J:6:PRO:HG2	15:J:48:VAL:HG21	1.81	0.61
7:A:746:G:N2	7:A:749:U:OP2	2.28	0.61
36:f:51:GLU:OE2	36:f:54:LYS:N	2.29	0.61
7:A:2377:C:OP1	7:A:2389:G:N2	2.34	0.61
32:a:59:U:H2'	32:a:60:G:C8	2.36	0.61
32:a:466:C:H2'	32:a:467:G:C8	2.35	0.61
32:a:1029:C:H2'	32:a:1030:U:C6	2.36	0.61
32:a:1121:A:H2'	32:a:1122:G:H8	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:139:ASP:OD1	34:d:174:ARG:NE	2.34	0.61
32:a:143:G:H2'	32:a:144:G:C8	2.35	0.60
34:d:183:ARG:HA	34:d:186:ILE:HB	1.83	0.60
47:q:132:LEU:HD12	47:q:133:GLU:HG2	1.83	0.60
52:y:51:U:O4	52:y:65:G:O6	2.19	0.60
15:J:73:MET:SD	15:J:88:THR:HG22	2.41	0.60
32:a:1308:G:N1	32:a:1311:A:OP2	2.33	0.60
7:A:1359:C:OP1	22:Q:12:LYS:NZ	2.34	0.60
33:c:110:SER:HB3	33:c:143:GLN:HG3	1.83	0.60
7:A:2405:G:O2'	7:A:2406:A:N7	2.34	0.60
18:M:78:PRO:HG2	18:M:81:THR:HG21	1.83	0.60
32:a:512:G:OP2	42:l:51:LYS:NZ	2.34	0.60
7:A:1007:G:N1	7:A:1028:G:O2'	2.34	0.60
7:A:2409:U:H4'	7:A:2410:A:H5'	1.82	0.60
28:W:53:ARG:O	28:W:59:LEU:N	2.34	0.60
33:c:76:ILE:HA	33:c:83:ALA:HB2	1.81	0.60
7:A:2481:U:H2'	7:A:2482:U:C6	2.37	0.60
32:a:1030:U:H2'	32:a:1031:G:C8	2.36	0.60
7:A:284:U:O2	7:A:304:G:O6	2.19	0.60
7:A:338:G:OP2	7:A:338:G:N2	2.25	0.60
7:A:766:G:O6	7:A:774:G:N1	2.35	0.60
32:a:500:A:H4'	34:d:47:LEU:HD13	1.82	0.60
7:A:1658:A:H3'	7:A:1659:G:H8	1.67	0.60
12:F:63:ASP:O	12:F:67:ILE:HD12	2.02	0.60
32:a:492:C:H2'	32:a:493:A:H8	1.66	0.60
7:A:1223:U:O4'	7:A:1227:A:N6	2.35	0.60
7:A:1554:G:H2'	7:A:1555:A:H8	1.67	0.60
7:A:3023:U:OP1	10:D:44:ARG:NH1	2.34	0.60
32:a:554:A:H62	32:a:877:U:H3	1.48	0.60
33:c:94:THR:HG23	33:c:96:LYS:H	1.67	0.60
7:A:293:G:H2'	7:A:294:G:C8	2.37	0.59
32:a:121:G:OP1	32:a:596:U:O2'	2.15	0.59
7:A:2448:G:H21	7:A:2449:A:H5''	1.66	0.59
36:f:12:PRO:O	36:f:45:LYS:NZ	2.35	0.59
45:o:5:ALA:O	45:o:9:LYS:HG2	2.02	0.59
7:A:2529:U:H2'	7:A:2530:U:C6	2.37	0.59
32:a:375:G:H5''	46:p:6:LYS:HB2	1.84	0.59
34:d:127:VAL:HG23	34:d:130:TYR:HB2	1.84	0.59
37:g:22:LEU:HD21	37:g:66:LEU:HD12	1.84	0.59
7:A:287:G:H8	7:A:302:U:H2'	1.67	0.59
26:U:29:ASP:OD1	26:U:30:ARG:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1156:G:H1	32:a:1164:U:H3	1.51	0.59
32:a:1420:C:H2'	32:a:1421:A:H8	1.68	0.59
33:c:57:GLU:HB3	33:c:64:ARG:HB3	1.84	0.59
7:A:647:G:H2'	7:A:648:G:H8	1.66	0.59
32:a:268:U:H2'	32:a:269:A:C8	2.37	0.59
9:C:169:GLU:HG2	9:C:170:ALA:H	1.68	0.59
32:a:415:G:H2'	32:a:416:G:H8	1.66	0.59
32:a:704:G:H2'	32:a:705:G:C8	2.37	0.59
34:d:49:GLN:HB3	34:d:198:TYR:HB2	1.85	0.59
42:l:33:VAL:HG12	42:l:56:LYS:HB3	1.84	0.59
7:A:1235:G:C6	7:A:1236:G:C6	2.90	0.59
24:S:56:PRO:O	24:S:60:VAL:HG23	2.03	0.59
32:a:491:G:H2'	32:a:492:C:C6	2.37	0.59
32:a:991:G:H1	32:a:1034:U:H3	1.51	0.59
45:o:18:HIS:O	45:o:20:THR:N	2.36	0.59
42:l:3:THR:HG22	42:l:6:GLN:H	1.67	0.59
6:6:4:ASP:H	6:6:5:ILE:HD12	1.67	0.58
6:6:60:ARG:HD2	6:6:63:LYS:HD3	1.84	0.58
7:A:1953:G:N2	7:A:1976:G:H1	2.01	0.58
2:1:35:ARG:NH1	2:1:52:ARG:HE	2.00	0.58
7:A:1953:G:H1	7:A:1976:G:H1	1.50	0.58
7:A:1198:A:N6	7:A:1202:A:OP1	2.37	0.58
13:G:11:VAL:HG23	13:G:50:ALA:HA	1.84	0.58
35:e:132:PRO:HA	35:e:153:ASP:OD2	2.02	0.58
7:A:334:C:H2'	7:A:335:A:H8	1.67	0.58
9:C:108:PRO:HD2	9:C:111:LEU:HD22	1.85	0.58
32:a:20:U:H2'	32:a:21:C:C6	2.38	0.58
32:a:408:G:H5'	34:d:23:ASP:HB3	1.84	0.58
32:a:492:C:H2'	32:a:493:A:C8	2.38	0.58
7:A:307:U:O2	14:H:45:LYS:NZ	2.36	0.58
7:A:1628:G:H2'	7:A:1629:U:H6	1.69	0.58
7:A:2348:U:O2	7:A:2351:A:N6	2.37	0.58
13:G:22:GLN:NE2	13:G:41:ILE:O	2.37	0.58
37:g:113:GLU:HB2	37:g:119:ARG:HG2	1.85	0.58
32:a:451:A:N7	46:p:46:PRO:HB2	2.19	0.58
7:A:334:C:H2'	7:A:335:A:C8	2.39	0.58
32:a:414:C:H2'	32:a:415:G:O4'	2.02	0.58
32:a:873:C:OP2	42:l:3:THR:HG21	2.03	0.58
32:a:1506:A:H2'	32:a:1507:C:C6	2.39	0.58
52:y:1:C:H2'	52:y:2:G:H8	1.67	0.58
7:A:2936:U:H2'	7:A:2937:C:C6	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:135:GLN:O	15:J:137:PRO:HD3	2.04	0.58
7:A:1574:C:H2'	7:A:1575:A:H8	1.69	0.58
7:A:2087:A:H2'	7:A:2088:A:C8	2.38	0.58
7:A:2426:U:H2'	7:A:2427:G:C8	2.38	0.58
32:a:529:U:H5''	42:l:111:LYS:HB2	1.85	0.58
32:a:1509:2MG:N2	32:a:1512:MA6:OP2	2.31	0.58
12:F:141:GLU:HG2	12:F:143:ALA:H	1.69	0.58
32:a:411:U:H3'	32:a:412:G:H4'	1.85	0.58
36:f:27:LEU:HD13	36:f:37:VAL:HG11	1.85	0.58
7:A:1567:U:O2'	7:A:1568:A:N7	2.36	0.57
7:A:2389:G:H2'	7:A:2390:G:C8	2.39	0.57
17:L:36:THR:HG22	17:L:37:LYS:H	1.69	0.57
6:6:44:PHE:HE2	12:F:183:PRO:HB2	1.69	0.57
7:A:1263:G:OP1	51:v:3:LYS:NZ	2.29	0.57
32:a:191:C:N4	47:q:56:GLY:O	2.37	0.57
32:a:464:C:H2'	32:a:465:U:C6	2.39	0.57
46:p:52:ASN:OD1	46:p:55:ARG:N	2.26	0.57
7:A:1431:A:H4'	7:A:1432:A:H5''	1.84	0.57
7:A:1465:C:H5''	25:T:68:ARG:HH21	1.69	0.57
7:A:1484:A:H2'	7:A:1485:A:C8	2.39	0.57
7:A:2151:A:N6	32:a:1487:G:OP2	2.36	0.57
10:D:38:ARG:HB3	10:D:51:GLN:HB2	1.85	0.57
32:a:719:A:H2'	32:a:720:A:C8	2.40	0.57
32:a:1117:U:O4	40:j:9:ARG:NH1	2.37	0.57
32:a:1347:A:H2'	32:a:1348:G:H8	1.69	0.57
32:a:11:A:C6	34:d:201:LYS:HB2	2.40	0.57
32:a:108:G:H1'	32:a:353:G:H5'	1.87	0.57
32:a:705:G:H2'	32:a:706:A:C8	2.39	0.57
7:A:1176:G:O2'	7:A:1239:A:N1	2.32	0.57
7:A:1200:G:N7	7:A:1218:G:H2'	2.18	0.57
7:A:1884:G:O2'	19:N:106:ASP:OD1	2.21	0.57
10:D:3:ARG:NH1	10:D:212:ILE:HG23	2.20	0.57
26:U:89:GLU:HA	26:U:91:THR:H	1.68	0.57
32:a:513:C:H41	42:l:50:ARG:NH2	2.02	0.57
7:A:1185:G:H4'	7:A:1215:A:H1'	1.87	0.57
7:A:1206:A:H5''	7:A:1207:C:H5	1.68	0.57
7:A:1577:C:H42	7:A:1627:C:N4	2.03	0.57
11:E:175:VAL:HG23	11:E:183:ILE:HD11	1.87	0.57
19:N:26:THR:HG23	19:N:75:VAL:HG21	1.87	0.57
32:a:1001:C:H2'	32:a:1002:G:H8	1.70	0.57
7:A:1623:G:H5''	7:A:1624:C:H5'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2098:U:OP1	7:A:2648:G:O2'	2.23	0.57
32:a:298:G:H2'	32:a:299:A:C8	2.40	0.57
7:A:1959:A:C2	7:A:1970:G:C6	2.90	0.57
8:B:1:U:H2'	8:B:2:U:C6	2.40	0.57
32:a:665:G:H2'	32:a:666:A:C8	2.40	0.57
32:a:22:C:OP1	35:e:166:ASN:ND2	2.35	0.56
32:a:390:G:H5''	46:p:9:ARG:HH11	1.70	0.56
7:A:484:G:H2'	7:A:485:C:C6	2.40	0.56
7:A:1471:U:OP1	25:T:19:LYS:NZ	2.36	0.56
32:a:406:G:H2'	32:a:407:G:C8	2.40	0.56
32:a:412:G:O2'	32:a:427:G:N2	2.31	0.56
7:A:871:U:H2'	7:A:872:A:C8	2.41	0.56
7:A:2106:C:H2'	7:A:2107:A:O3'	2.04	0.56
8:B:74:G:H5''	27:V:17:THR:HG21	1.86	0.56
9:C:61:ALA:O	9:C:63:ARG:NH1	2.38	0.56
32:a:406:G:H2'	32:a:407:G:H8	1.70	0.56
32:a:426:U:OP2	32:a:427:G:O2'	2.21	0.56
32:a:1031:G:H2'	32:a:1032:U:C6	2.41	0.56
52:y:17:C:OP1	52:y:61:U:O2'	2.21	0.56
7:A:1523:G:O6	25:T:18:GLU:HG3	2.06	0.56
7:A:1622:G:H2'	7:A:1623:G:O4'	2.05	0.56
7:A:1672:A:H2'	7:A:1673:A:C8	2.41	0.56
7:A:3028:A:H62	7:A:3127:A:H2	1.51	0.56
32:a:296:G:N2	32:a:299:A:OP2	2.32	0.56
7:A:988:G:O2'	7:A:1045:G:O6	2.23	0.56
7:A:1958:C:H5	7:A:1971:G:H21	1.51	0.56
32:a:939:A:H2'	32:a:940:G:C8	2.40	0.56
7:A:2354:A:O2'	7:A:2407:A:N6	2.39	0.56
7:A:2583:G:N3	7:A:2619:C:H2'	2.21	0.56
20:O:61:ILE:O	20:O:61:ILE:HG13	2.05	0.56
32:a:178:G:O2'	32:a:180:A:N1	2.39	0.56
32:a:513:C:H41	42:l:50:ARG:HH22	1.53	0.56
7:A:1129:A:H2'	7:A:1130:A:C8	2.41	0.56
7:A:1200:G:O6	7:A:1218:G:O2'	2.20	0.56
32:a:206:A:H8	32:a:221:U:O2'	1.88	0.56
42:l:43:LYS:HG2	42:l:44:LYS:H	1.70	0.56
46:p:10:LEU:HD21	46:p:19:ARG:HG3	1.87	0.56
7:A:630:U:H2'	7:A:631:C:C6	2.41	0.56
7:A:670:U:H1'	7:A:2268:6MZ:H9C1	1.86	0.56
7:A:992:A:H2'	7:A:993:G:C8	2.41	0.56
7:A:2996:A:C4	13:G:68:LEU:HD21	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:80:THR:HG22	40:j:82:LYS:HG3	1.88	0.56
7:A:1567:U:H2'	7:A:1569:C:H41	1.70	0.56
7:A:1578:C:H2'	7:A:1579:A:C8	2.39	0.56
7:A:1980:U:H2'	7:A:1981:C:C6	2.40	0.56
7:A:2332:U:OP1	14:H:11:HIS:ND1	2.40	0.56
16:K:54:ARG:NH1	32:a:1414:C:OP1	2.39	0.56
32:a:1337:U:OP1	39:i:143:ARG:NH1	2.39	0.56
6:6:15:VAL:HG11	6:6:32:ARG:HH21	1.71	0.55
7:A:1637:U:H2'	7:A:1638:C:C6	2.41	0.55
7:A:2151:A:N6	32:a:1485:A:O2'	2.39	0.55
26:U:89:GLU:N	26:U:90:GLU:HB2	2.21	0.55
7:A:342:C:H2'	7:A:343:C:C6	2.42	0.55
7:A:1008:A:C2	7:A:1028:G:N2	2.74	0.55
20:O:77:VAL:O	20:O:81:GLN:HG3	2.06	0.55
25:T:50:PHE:O	25:T:91:ARG:NH2	2.39	0.55
7:A:428:A:H1'	7:A:429:A:C2	2.41	0.55
47:q:110:ASP:O	47:q:112:VAL:HG13	2.07	0.55
7:A:569:A:OP2	26:U:43:LYS:NZ	2.33	0.55
32:a:1367:A:OP1	37:g:36:LYS:NZ	2.31	0.55
35:e:146:LEU:HD13	35:e:154:ILE:HG21	1.89	0.55
7:A:368:U:H2'	7:A:369:C:C6	2.41	0.55
7:A:1771:G:H22	7:A:1776:A:N6	2.04	0.55
7:A:1592:U:O4	7:A:1613:G:O6	2.25	0.55
7:A:778:G:O2'	7:A:779:U:H5'	2.07	0.55
32:a:221:U:H2'	32:a:222:G:H8	1.72	0.55
32:a:920:G:O2'	32:a:1496:A:N7	2.37	0.55
32:a:1210:C:H2'	32:a:1211:A:C8	2.41	0.55
39:i:126:THR:HG22	39:i:128:ASP:H	1.71	0.55
43:m:23:PHE:HB3	43:m:67:GLU:HG3	1.88	0.55
46:p:39:ARG:HD2	46:p:41:HIS:HE1	1.71	0.55
7:A:1194:U:H1'	7:A:1203:G:H1	1.71	0.55
7:A:1577:C:C2	36:f:17:ARG:NH2	2.75	0.55
32:a:727:U:H2'	32:a:728:C:C6	2.42	0.55
32:a:1242:A:H2'	32:a:1243:A:C8	2.41	0.55
7:A:1558:A:H5''	7:A:1645:A:N6	2.21	0.55
7:A:1824:C:H2'	7:A:1825:A:H8	1.72	0.55
34:d:165:TRP:CE2	34:d:181:PRO:HB3	2.41	0.55
1:0:16:ARG:NH2	7:A:1395:G:OP1	2.35	0.55
7:A:942:U:H2'	7:A:943:C:H6	1.72	0.55
7:A:978:C:H2'	7:A:979:A:H8	1.71	0.55
7:A:1157:A:H2'	7:A:1158:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2761:G:HO2'	7:A:3002:A:HO2'	1.55	0.55
16:K:16:ALA:HB2	16:K:52:VAL:HG21	1.89	0.55
32:a:135:G:O2'	47:q:44:GLY:O	2.24	0.55
32:a:1021:C:O2'	32:a:1023:U:OP1	2.18	0.55
32:a:1405:C:H2'	32:a:1406:A:C8	2.41	0.55
7:A:2013:U:H5	7:A:2018:A:N7	2.05	0.54
9:C:124:ASP:O	9:C:129:ASN:ND2	2.30	0.54
12:F:142:GLN:HE22	12:F:156:VAL:HA	1.72	0.54
32:a:500:A:N3	32:a:534:U:O2'	2.39	0.54
32:a:1053:U:H2'	32:a:1054:C:C6	2.42	0.54
38:h:7:ILE:HB	38:h:79:ARG:NH1	2.22	0.54
39:i:81:SER:OG	39:i:82:PHE:N	2.26	0.54
2:1:40:LYS:NZ	7:A:2585:C:OP1	2.36	0.54
7:A:1185:G:O2'	7:A:1215:A:O2'	2.20	0.54
9:C:177:MET:HE2	9:C:183:ARG:HB2	1.90	0.54
20:O:68:VAL:HG22	20:O:75:ARG:HD3	1.89	0.54
32:a:1127:U:H2'	32:a:1128:A:C8	2.42	0.54
7:A:1617:U:H2'	7:A:1618:C:C6	2.42	0.54
31:Z:46:LEU:O	31:Z:50:VAL:HG12	2.07	0.54
32:a:134:U:H2'	32:a:135:G:H8	1.73	0.54
32:a:336:G:H2'	32:a:337:A:C8	2.42	0.54
37:g:69:VAL:HG23	37:g:100:ALA:HB1	1.88	0.54
7:A:691:C:H2'	7:A:692:A:H8	1.72	0.54
32:a:458:G:C6	32:a:459:G:H1'	2.43	0.54
39:i:27:ILE:HG23	39:i:110:LEU:HD22	1.90	0.54
7:A:333:U:H2'	7:A:334:C:C6	2.42	0.54
7:A:2912:G:H4'	16:K:30:ARG:HD2	1.90	0.54
32:a:73:A:N1	32:a:89:A:N6	2.55	0.54
33:c:123:LEU:HD11	33:c:129:PHE:HB3	1.90	0.54
43:m:2:ALA:HB3	43:m:9:LEU:HD13	1.90	0.54
50:t:43:ASP:OD2	50:t:46:LYS:NZ	2.26	0.54
7:A:1011:G:H1	7:A:1024:U:H1'	1.72	0.54
7:A:1235:G:N1	7:A:1236:G:C6	2.76	0.54
7:A:2513:C:O2'	18:M:84:GLY:O	2.26	0.54
34:d:27:GLU:OE1	34:d:27:GLU:N	2.40	0.54
36:f:14:LEU:HD11	36:f:84:SER:HB3	1.89	0.54
7:A:1202:A:H2'	7:A:1203:G:C8	2.43	0.54
26:U:88:ASP:CG	26:U:89:GLU:H	2.13	0.54
34:d:159:GLU:HG2	34:d:160:ARG:N	2.23	0.54
43:m:27:ARG:O	43:m:31:ASN:ND2	2.29	0.54
7:A:1731:A:H2'	7:A:1732:A:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:24:GLY:O	17:L:29:GLY:HA2	2.08	0.54
32:a:85:G:N2	32:a:86:G:N7	2.56	0.54
33:c:77:GLY:HA3	33:c:82:GLU:HB3	1.89	0.54
7:A:2338:G:O6	7:A:2425:U:O4	2.25	0.54
7:A:3057:G:O2'	7:A:3059:A:OP2	2.16	0.54
32:a:1121:A:O3'	39:i:41:ARG:NH2	2.33	0.54
42:l:54:ARG:NH1	42:l:64:THR:OG1	2.38	0.54
7:A:368:U:H2'	7:A:369:C:H6	1.72	0.53
7:A:832:U:H2'	7:A:833:G:O4'	2.08	0.53
7:A:1298:U:H2'	7:A:1299:C:C6	2.43	0.53
7:A:2378:G:O2'	7:A:2379:A:O4'	2.17	0.53
32:a:452:G:O2'	32:a:453:G:H8	1.91	0.53
32:a:1038:G:H5''	44:n:4:LYS:HD3	1.89	0.53
32:a:1154:C:H2'	32:a:1155:G:H8	1.72	0.53
32:a:1347:A:H2'	32:a:1348:G:C8	2.43	0.53
39:i:50:ASP:HB3	39:i:85:PHE:CB	2.38	0.53
46:p:17:GLN:HG3	46:p:41:HIS:CD2	2.42	0.53
7:A:688:A:N1	7:A:938:G:O2'	2.40	0.53
7:A:1621:G:H2'	7:A:1622:G:C8	2.43	0.53
32:a:990:U:H3	32:a:1035:G:H1	1.56	0.53
34:d:145:LEU:HD23	34:d:154:ARG:HH22	1.72	0.53
7:A:645:G:H22	7:A:646:A:H62	1.55	0.53
7:A:1186:A:N6	7:A:1216:G:OP2	2.42	0.53
7:A:382:A:OP2	26:U:82:ARG:NH2	2.42	0.53
7:A:1651:C:H2'	7:A:1652:A:C8	2.43	0.53
7:A:2250:G:N7	24:S:26:LYS:NZ	2.54	0.53
7:A:2263:G:H2'	7:A:2264:A:C8	2.43	0.53
37:g:151:PHE:HZ	41:k:66:ARG:HE	1.57	0.53
7:A:281:G:H1	7:A:307:U:H3	1.56	0.53
7:A:1574:C:H2'	7:A:1575:A:C8	2.43	0.53
7:A:2404:U:H3'	7:A:2405:G:H2'	1.90	0.53
7:A:2275:U:H2'	7:A:2276:C:C6	2.43	0.53
11:E:186:PRO:HG3	11:E:206:ALA:HB1	1.90	0.53
34:d:16:ARG:HH12	34:d:33:PRO:HG3	1.74	0.53
45:o:78:TYR:O	45:o:82:ILE:HG12	2.09	0.53
7:A:765:C:H2'	7:A:766:G:N7	2.24	0.53
7:A:2775:U:H2'	7:A:2776:C:C6	2.44	0.53
12:F:53:ASP:O	12:F:55:LYS:HG2	2.09	0.53
32:a:706:A:H2'	32:a:707:A:C8	2.43	0.53
32:a:830:U:C4	32:a:831:C:C4	2.97	0.53
32:a:1030:U:H2'	32:a:1031:G:H8	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1007:G:O2'	7:A:1029:A:N6	2.41	0.53
7:A:1195:U:H4'	7:A:1197:G:N7	2.24	0.53
8:B:12:A:N1	8:B:68:G:O2'	2.40	0.53
18:M:51:ARG:HD3	18:M:66:ILE:HD11	1.91	0.53
20:O:30:ARG:NH1	20:O:95:VAL:O	2.41	0.53
26:U:98:SER:OG	26:U:99:LYS:O	2.27	0.53
49:s:21:VAL:HG13	49:s:22:GLN:OE1	2.09	0.53
7:A:332:C:H2'	7:A:333:U:H6	1.74	0.53
7:A:552:G:N2	7:A:555:A:OP2	2.32	0.53
7:A:1516:A:O2'	7:A:1527:U:O2	2.27	0.53
7:A:2302:C:H2'	7:A:2303:C:C6	2.44	0.53
32:a:552:U:O2'	32:a:553:U:OP2	2.26	0.53
32:a:1466:G:H2'	32:a:1467:G:C8	2.44	0.53
7:A:1554:G:H2'	7:A:1555:A:C8	2.44	0.52
7:A:1560:U:O4	7:A:1643:G:O2'	2.26	0.52
7:A:2489:OMG:OP2	18:M:82:ARG:NH1	2.42	0.52
7:A:2565:A:H2'	7:A:2566:A:C8	2.44	0.52
22:Q:53:ARG:HA	22:Q:56:GLU:HB2	1.91	0.52
32:a:871:C:H5'	38:h:83:PRO:HG2	1.91	0.52
7:A:1123:C:OP1	22:Q:53:ARG:NH2	2.42	0.52
7:A:2127:A:H2'	7:A:2128:A:C8	2.43	0.52
34:d:92:ARG:O	34:d:96:VAL:HG23	2.09	0.52
7:A:1197:G:N3	7:A:1224:A:O2'	2.36	0.52
7:A:1969:U:H2'	7:A:1970:G:C8	2.44	0.52
7:A:2987:A:OP2	7:A:2988:A:O2'	2.21	0.52
32:a:381:A:H2'	32:a:382:A:C8	2.44	0.52
32:a:530:A:H2'	32:a:531:G:C8	2.43	0.52
34:d:29:ARG:NH1	34:d:32:PRO:HD2	2.18	0.52
39:i:76:VAL:HG11	39:i:118:ALA:HB1	1.91	0.52
45:o:10:GLU:HG3	45:o:13:ARG:HH22	1.74	0.52
7:A:691:C:H2'	7:A:692:A:C8	2.44	0.52
7:A:2100:A:N6	7:A:2113:G:O2'	2.42	0.52
32:a:1128:A:N3	32:a:1129:A:O2'	2.42	0.52
32:a:1141:C:H2'	32:a:1142:G:C8	2.44	0.52
2:l:35:ARG:HB3	2:l:53:GLU:HB2	1.90	0.52
7:A:2814:G:O2'	7:A:2817:C:OP2	2.24	0.52
18:M:111:GLU:OE1	18:M:115:ARG:NH2	2.40	0.52
25:T:11:ILE:O	30:Y:33:ARG:NH2	2.42	0.52
32:a:833:U:O4'	32:a:835:C:N4	2.33	0.52
32:a:997:G:C6	32:a:1018:U:H5'	2.44	0.52
32:a:1019:C:N4	32:a:1026:G:H1	2.00	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:21:SER:OG	40:j:92:LEU:HD23	2.09	0.52
7:A:1185:G:O2'	7:A:1232:A:N6	2.42	0.52
7:A:1221:C:H3'	7:A:1222:G:H8	1.74	0.52
7:A:1713:G:O2'	7:A:1753:G:O6	2.26	0.52
9:C:172:TYR:HB3	9:C:184:ARG:HG2	1.90	0.52
32:a:483:G:H2'	32:a:484:A:C8	2.44	0.52
8:B:53:G:H21	12:F:33:MET:HE1	1.74	0.52
25:T:70:ARG:HH11	25:T:72:GLY:H	1.58	0.52
32:a:175:A:H2'	32:a:176:U:C6	2.45	0.52
47:q:61:ARG:HE	47:q:78:LEU:HD23	1.75	0.52
7:A:2529:U:OP1	7:A:2618:U:O2'	2.28	0.52
13:G:30:LYS:HZ2	13:G:82:GLN:HA	1.75	0.52
32:a:90:U:O2'	32:a:91:A:H8	1.93	0.52
32:a:508:G:N2	32:a:524:A:OP2	2.27	0.52
35:e:139:GLY:O	35:e:143:ARG:HB3	2.10	0.52
32:a:408:G:OP2	34:d:24:GLN:NE2	2.42	0.52
36:f:10:LEU:HD23	36:f:85:VAL:HA	1.91	0.52
43:m:58:ASP:HA	43:m:61:GLU:OE2	2.10	0.52
45:o:18:HIS:C	45:o:20:THR:H	2.18	0.52
7:A:230:U:H4'	7:A:231:U:H5''	1.92	0.51
7:A:1690:A:H5''	7:A:1691:G:H5''	1.92	0.51
7:A:2829:C:H2'	7:A:2830:G:C8	2.46	0.51
34:d:140:VAL:HG21	34:d:150:PHE:CZ	2.45	0.51
41:k:81:ALA:HB2	41:k:110:LEU:HD23	1.91	0.51
6:6:60:ARG:HA	6:6:63:LYS:HG2	1.91	0.51
7:A:289:A:H2'	7:A:290:A:O4'	2.10	0.51
7:A:1444:U:H5	7:A:1838:A:N1	2.08	0.51
7:A:2202:G:O2'	7:A:2205:C:OP1	2.27	0.51
7:A:2391:G:H3'	7:A:2392:C:H6	1.76	0.51
17:L:82:ILE:HD11	17:L:97:LEU:HD21	1.92	0.51
25:T:23:LEU:HB3	25:T:28:VAL:HB	1.92	0.51
32:a:444:U:H2'	32:a:445:C:C6	2.44	0.51
32:a:592:U:H2'	32:a:593:U:C6	2.45	0.51
41:k:116:GLU:OE2	41:k:117:VAL:N	2.42	0.51
7:A:1236:G:H2'	7:A:1237:U:C6	2.46	0.51
7:A:3071:U:H2'	7:A:3072:A:H8	1.75	0.51
32:a:327:U:H3'	32:a:328:A:H5''	1.91	0.51
32:a:451:A:H4'	32:a:452:G:OP2	2.09	0.51
17:L:4:LYS:HB3	17:L:6:HIS:CE1	2.46	0.51
26:U:89:GLU:HB3	26:U:93:LYS:N	2.26	0.51
30:Y:22:LEU:HD21	30:Y:58:TYR:HE1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:226:G:P	47:q:50:ARG:HH21	2.34	0.51
32:a:413:A:H5'	32:a:414:C:C5	2.43	0.51
32:a:718:G:N2	32:a:721:G:OP2	2.41	0.51
32:a:1130:U:O2'	32:a:1132:G:OP1	2.27	0.51
36:f:5:GLU:OE2	48:r:33:LYS:NZ	2.35	0.51
7:A:332:C:H2'	7:A:333:U:C6	2.45	0.51
7:A:1675:G:O2'	7:A:1755:G:O2'	2.23	0.51
7:A:2386:U:O2'	7:A:2387:U:O4'	2.27	0.51
33:c:111:GLN:HG2	33:c:114:LEU:HD12	1.92	0.51
52:y:29:C:H2'	52:y:30:G:H8	1.75	0.51
7:A:2975:G:H2'	7:A:2976:A:C8	2.46	0.51
32:a:398:G:H2'	32:a:399:C:C6	2.45	0.51
42:l:73:ASN:ND2	42:l:105:GLN:OE1	2.44	0.51
7:A:285:G:N1	7:A:303:U:C2	2.79	0.51
7:A:1564:C:H2'	7:A:1565:G:C8	2.46	0.51
7:A:2311:U:H2'	7:A:2312:U:C6	2.46	0.51
7:A:3052:C:OP1	19:N:42:ARG:NH2	2.36	0.51
32:a:1031:G:H2'	32:a:1032:U:H6	1.74	0.51
7:A:2204:A:N3	7:A:2830:G:O2'	2.38	0.51
7:A:2627:G:H5''	7:A:2628:U:O4'	2.10	0.51
36:f:4:TYR:CD2	36:f:72:VAL:HG21	2.44	0.51
7:A:455:U:H2'	7:A:456:C:H6	1.76	0.51
7:A:1594:A:H2'	7:A:1595:C:C6	2.46	0.51
16:K:106:LEU:HB2	16:K:115:ILE:HD11	1.92	0.51
25:T:18:GLU:HG2	25:T:19:LYS:N	2.26	0.51
32:a:523:A:N6	32:a:1198:G:O2'	2.42	0.51
32:a:969:G:H5'	32:a:1350:U:O2'	2.10	0.51
7:A:289:A:H1'	7:A:304:G:H1'	1.92	0.51
7:A:339:C:H2'	7:A:340:U:C6	2.46	0.51
7:A:1215:A:H4'	7:A:1232:A:H61	1.74	0.51
7:A:2372:A:H3'	7:A:2373:A:H8	1.75	0.51
12:F:178:ARG:HH21	12:F:184:PHE:HB2	1.75	0.51
19:N:75:VAL:HA	19:N:78:THR:HG22	1.92	0.51
32:a:991:G:N2	32:a:1034:U:O2	2.40	0.51
7:A:636:U:HO2'	7:A:637:C:H6	1.59	0.50
7:A:1672:A:H2'	7:A:1673:A:H8	1.76	0.50
7:A:2269:A:N3	7:A:2693:G:O2'	2.41	0.50
8:B:29:C:OP1	20:O:9:ARG:NH1	2.42	0.50
32:a:492:C:OP1	42:l:114:ARG:NH2	2.44	0.50
32:a:1163:C:H2'	32:a:1164:U:H6	1.75	0.50
33:c:90:LEU:O	33:c:94:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:21:TYR:CE1	38:h:70:ARG:HG3	2.45	0.50
7:A:289:A:H2	7:A:303:U:H4'	1.76	0.50
21:P:105:LYS:HG2	32:a:1425:G:OP1	2.11	0.50
32:a:585:C:H2'	32:a:586:G:O4'	2.11	0.50
32:a:1457:G:H2'	32:a:1458:U:H6	1.76	0.50
35:e:172:VAL:O	35:e:176:LYS:HG2	2.11	0.50
39:i:25:ARG:N	39:i:25:ARG:HD2	2.26	0.50
40:j:8:ILE:HB	40:j:73:LEU:O	2.10	0.50
7:A:340:U:H2'	7:A:341:A:C8	2.46	0.50
7:A:636:U:O2'	7:A:637:C:H6	1.95	0.50
7:A:858:G:C5	9:C:208:LYS:HB2	2.47	0.50
10:D:7:LEU:H	10:D:34:ASN:HD21	1.60	0.50
25:T:14:PRO:HD3	30:Y:34:PHE:CD1	2.46	0.50
7:A:1917:C:H2'	7:A:1918:C:C6	2.46	0.50
7:A:2886:G:H2'	7:A:2887:U:C6	2.47	0.50
22:Q:91:ASP:OD1	22:Q:94:ASN:ND2	2.29	0.50
35:e:108:ILE:HB	35:e:113:THR:HG22	1.94	0.50
7:A:1184:G:HO2'	7:A:1213:A:H61	1.60	0.50
32:a:614:C:O2	46:p:12:LYS:NZ	2.31	0.50
34:d:27:GLU:H	34:d:27:GLU:CD	2.19	0.50
7:A:2102:C:H2'	7:A:2103:C:C6	2.47	0.50
7:A:2389:G:H2'	7:A:2390:G:H8	1.75	0.50
32:a:38:G:H2'	32:a:39:C:C6	2.46	0.50
39:i:38:VAL:HG22	39:i:88:LEU:HD13	1.94	0.50
41:k:39:ASN:OD1	41:k:57:SER:HB3	2.11	0.50
7:A:258:A:H2'	7:A:259:C:H6	1.77	0.50
7:A:1212:G:O2'	7:A:1215:A:N6	2.44	0.50
7:A:1954:U:H2'	7:A:1955:G:C8	2.47	0.50
19:N:15:SER:HA	19:N:18:LYS:HE2	1.93	0.50
7:A:307:U:H1'	14:H:45:LYS:NZ	2.27	0.50
7:A:1190:U:H2'	7:A:1199:A:N3	2.27	0.50
32:a:82:U:H2'	32:a:83:U:C6	2.47	0.50
32:a:1339:G:C8	39:i:130:ARG:HB3	2.47	0.50
35:e:181:PRO:HA	35:e:184:VAL:HG22	1.94	0.50
7:A:84:A:N1	7:A:99:G:O2'	2.43	0.50
7:A:682:C:H2'	7:A:683:C:C6	2.47	0.50
7:A:711:A:H2'	7:A:712:A:C8	2.47	0.50
7:A:1237:U:H2'	7:A:1238:C:C2	2.47	0.50
12:F:169:THR:OG1	12:F:171:ASP:OD1	2.22	0.50
15:J:73:MET:HE3	15:J:86:LYS:CD	2.41	0.50
30:Y:24:GLU:O	30:Y:28:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:852:U:H2'	32:a:853:A:H8	1.76	0.50
37:g:51:ARG:HD3	37:g:58:PRO:HD3	1.93	0.50
7:A:484:G:H2'	7:A:485:C:H6	1.77	0.49
7:A:728:C:O2'	7:A:786:U:OP1	2.30	0.49
7:A:1629:U:H2'	7:A:1630:G:H8	1.77	0.49
7:A:2093:A:H2	7:A:2121:G:H21	1.59	0.49
7:A:2537:A:H61	7:A:2555:U:H3	1.60	0.49
10:D:76:ASN:O	10:D:78:ARG:NH1	2.45	0.49
32:a:468:G:H2'	32:a:469:A:N3	2.27	0.49
32:a:516:C:O2'	32:a:517:C:H5'	2.11	0.49
11:E:36:ASN:HB3	11:E:39:LEU:HB3	1.93	0.49
32:a:1297:G:N2	32:a:1323:G:H1'	2.26	0.49
34:d:13:ARG:NH2	34:d:32:PRO:O	2.41	0.49
35:e:108:ILE:O	35:e:108:ILE:HG12	2.12	0.49
7:A:430:A:H2'	7:A:431:A:C8	2.48	0.49
7:A:442:G:H2'	7:A:443:C:C6	2.47	0.49
15:J:98:ASP:N	15:J:98:ASP:OD1	2.42	0.49
22:Q:28:ARG:HD3	22:Q:38:GLN:HG2	1.94	0.49
30:Y:6:SER:HB3	30:Y:9:GLU:HG2	1.93	0.49
34:d:134:GLN:HG2	34:d:179:GLN:HA	1.94	0.49
39:i:108:LEU:HA	39:i:111:VAL:HG12	1.94	0.49
43:m:14:ARG:NH1	43:m:16:GLU:OE1	2.42	0.49
7:A:2883:C:H4'	7:A:2970:G:O2'	2.12	0.49
12:F:24:ARG:NH1	12:F:29:TYR:O	2.46	0.49
32:a:1265:U:H2'	32:a:1266:A:O4'	2.11	0.49
42:l:3:THR:O	42:l:6:GLN:N	2.46	0.49
7:A:1187:G:H2'	7:A:1188:G:O4'	2.13	0.49
7:A:1234:U:H2'	7:A:1235:G:H8	1.78	0.49
7:A:2751:G:H2'	7:A:2752:U:C6	2.48	0.49
8:B:30:C:O2'	8:B:52:A:N1	2.38	0.49
32:a:48:U:H2'	32:a:49:G:C8	2.46	0.49
32:a:653:C:O2'	32:a:827:G:OP1	2.29	0.49
32:a:1359:C:O2'	40:j:62:ARG:NH1	2.43	0.49
7:A:571:U:H4'	26:U:44:HIS:ND1	2.28	0.49
7:A:736:A:H2'	7:A:737:A:C8	2.48	0.49
15:J:49:ASP:OD1	15:J:121:LYS:NZ	2.45	0.49
20:O:71:ASP:OD1	20:O:71:ASP:N	2.46	0.49
32:a:152:U:H3	32:a:161:G:H1	1.59	0.49
32:a:727:U:H2'	32:a:728:C:H6	1.77	0.49
32:a:1439:A:O2'	32:a:1440:A:H5'	2.13	0.49
33:c:46:LEU:HB3	33:c:51:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m:69:ASP:OD2	43:m:70:LEU:N	2.45	0.49
7:A:778:G:OP2	7:A:778:G:H8	1.95	0.49
7:A:1959:A:H2	7:A:1970:G:H1	0.55	0.49
7:A:2392:C:H2'	7:A:2393:G:C8	2.47	0.49
32:a:1498:G:N3	32:a:1498:G:H2'	2.28	0.49
42:l:87:VAL:HG21	42:l:90:LEU:HB2	1.95	0.49
52:y:29:C:H2'	52:y:30:G:C8	2.48	0.49
7:A:1825:A:H2'	7:A:1826:C:C6	2.48	0.49
7:A:1957:A:N6	7:A:1972:G:H1'	2.28	0.49
7:A:2365:A:H1'	7:A:2410:A:O2'	2.13	0.49
7:A:2795:G:H2'	7:A:2796:C:C6	2.47	0.49
17:L:31:THR:HB	17:L:35:GLY:H	1.77	0.49
32:a:415:G:H2'	32:a:416:G:C8	2.46	0.49
32:a:1432:G:H5''	50:t:33:ARG:HH12	1.77	0.49
34:d:90:GLU:HA	34:d:95:ASN:ND2	2.25	0.49
51:v:8:LYS:O	51:v:11:ARG:HG2	2.13	0.49
7:A:503:C:H2'	7:A:504:A:C8	2.47	0.49
7:A:3132:U:O2	15:J:134:ALA:HB1	2.12	0.49
27:V:14:ARG:HG2	27:V:46:GLU:CD	2.38	0.49
27:V:36:TYR:O	27:V:96:LEU:HA	2.12	0.49
32:a:938:G:C2	32:a:939:A:C8	3.00	0.49
44:n:15:ARG:HE	44:n:16:PHE:H	1.60	0.49
46:p:41:HIS:ND1	46:p:48:LEU:HD22	2.27	0.49
49:s:50:ALA:HB1	49:s:57:HIS:HB3	1.95	0.49
7:A:93:C:H2'	7:A:94:C:O4'	2.13	0.49
7:A:331:U:H5	7:A:445:U:H5''	1.78	0.49
7:A:333:U:H2'	7:A:334:C:H6	1.77	0.49
13:G:30:LYS:NZ	13:G:82:GLN:HA	2.27	0.49
24:S:100:GLN:OE1	24:S:102:ARG:NH2	2.46	0.49
32:a:79:C:H2'	32:a:80:U:O4'	2.13	0.49
32:a:969:G:OP2	32:a:1350:U:O2'	2.31	0.49
34:d:183:ARG:NH1	34:d:188:VAL:HA	2.28	0.49
3:2:6:ARG:O	3:2:9:GLN:NE2	2.41	0.48
7:A:1446:C:H2'	7:A:1447:U:C6	2.48	0.48
7:A:2479:A:H2'	7:A:2480:G:C8	2.48	0.48
7:A:2488:G:N2	18:M:84:GLY:HA3	2.28	0.48
12:F:72:PRO:HB3	12:F:96:VAL:HB	1.94	0.48
13:G:20:GLU:O	13:G:23:SER:OG	2.26	0.48
15:J:19:ASP:OD1	15:J:21:THR:OG1	2.24	0.48
32:a:11:A:N6	34:d:197:GLU:O	2.46	0.48
32:a:81:C:H2'	32:a:82:U:O4'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1122:G:P	39:i:41:ARG:HH22	2.36	0.48
34:d:165:TRP:CD2	34:d:181:PRO:HB3	2.48	0.48
37:g:23:VAL:O	37:g:27:VAL:HG13	2.13	0.48
43:m:87:TYR:CZ	43:m:91:ARG:HD2	2.48	0.48
7:A:1771:G:H22	7:A:1776:A:H61	1.61	0.48
7:A:2700:U:H2'	7:A:2701:U:C6	2.48	0.48
17:L:36:THR:HG22	17:L:37:LYS:N	2.27	0.48
32:a:1003:U:H2'	32:a:1004:C:C6	2.48	0.48
38:h:85:LEU:HD12	42:l:4:ILE:HG21	1.94	0.48
5:4:11:CYS:SG	5:4:32:HIS:CE1	3.06	0.48
7:A:1822:C:H2'	7:A:1823:A:C8	2.49	0.48
32:a:224:G:O2'	47:q:47:HIS:HB2	2.13	0.48
7:A:1349:A:H2'	7:A:1350:C:C6	2.48	0.48
7:A:1590:G:N1	7:A:1592:U:O4	2.47	0.48
7:A:1688:U:H2'	7:A:1689:C:C6	2.49	0.48
7:A:2524:A:H4'	7:A:2525:A:O4'	2.12	0.48
20:O:76:SER:HA	20:O:79:VAL:HG12	1.95	0.48
40:j:36:VAL:HG12	40:j:77:ILE:HG22	1.93	0.48
4:3:16:ARG:HH11	4:3:16:ARG:HG3	1.78	0.48
7:A:842:G:OP2	45:o:88:ARG:NH2	2.36	0.48
7:A:961:U:H2'	7:A:962:G:C8	2.49	0.48
7:A:1039:A:H2'	7:A:1040:A:C8	2.48	0.48
7:A:1176:G:N2	7:A:1240:A:H62	2.10	0.48
7:A:1659:G:O2'	7:A:1731:A:N6	2.46	0.48
25:T:70:ARG:NH1	25:T:72:GLY:H	2.11	0.48
32:a:1111:U:H2'	32:a:1112:C:C6	2.48	0.48
39:i:49:PHE:CD1	39:i:84:ILE:HD11	2.48	0.48
7:A:290:A:H1'	7:A:291:C:C5	2.48	0.48
7:A:378:C:H2'	7:A:379:G:H8	1.79	0.48
7:A:1275:C:H2'	7:A:1276:A:H8	1.78	0.48
7:A:1623:G:O2'	7:A:1624:C:H5	1.97	0.48
7:A:2339:U:H3	7:A:2424:A:N6	2.11	0.48
9:C:94:LEU:HB2	9:C:104:TYR:HE1	1.78	0.48
10:D:90:ASP:C	10:D:92:ALA:H	2.20	0.48
20:O:21:ARG:NE	20:O:32:ARG:NH1	2.62	0.48
20:O:34:VAL:HA	20:O:98:ASP:HB3	1.95	0.48
23:R:31:GLU:OE2	23:R:31:GLU:N	2.45	0.48
32:a:1306:C:H2'	32:a:1307:U:C6	2.48	0.48
37:g:68:ASN:O	37:g:138:ARG:NH1	2.38	0.48
39:i:72:PRO:O	39:i:75:THR:HG22	2.13	0.48
40:j:32:THR:HG22	40:j:82:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:114:ARG:HH22	42:l:121:LYS:HZ3	1.61	0.48
7:A:1558:A:P	7:A:1646:G:H22	2.36	0.48
12:F:51:ALA:HB3	12:F:52:ARG:HH11	1.77	0.48
32:a:382:A:C5	32:a:383:G:H1'	2.48	0.48
32:a:1062:C:H2'	32:a:1063:G:H8	1.78	0.48
37:g:75:VAL:HG21	37:g:144:MET:HG2	1.95	0.48
7:A:1322:G:OP1	17:L:31:THR:OG1	2.30	0.48
7:A:2323:U:H2'	7:A:2324:G:C8	2.49	0.48
9:C:68:ARG:NH1	9:C:150:GLY:O	2.47	0.48
20:O:32:ARG:HH21	20:O:47:VAL:HG21	1.78	0.48
30:Y:5:VAL:O	30:Y:56:ARG:NH1	2.46	0.48
32:a:939:A:H2'	32:a:940:G:H8	1.77	0.48
32:a:1028:C:H2'	32:a:1029:C:C6	2.49	0.48
1:O:8:LYS:HE3	1:O:12:ASN:HB3	1.96	0.48
7:A:1302:C:N4	7:A:1305:U:O2'	2.47	0.48
7:A:1559:A:N6	7:A:1645:A:OP1	2.46	0.48
7:A:1617:U:H2'	7:A:1618:C:H6	1.79	0.48
33:c:133:MET:HE3	33:c:151:VAL:HG12	1.95	0.48
34:d:133:SER:N	34:d:136:ASP:OD2	2.46	0.48
43:m:29:ARG:NH1	43:m:32:GLU:OE2	2.47	0.48
47:q:60:THR:HG22	47:q:115:MET:HG3	1.96	0.48
7:A:985:G:H2'	7:A:986:A:C8	2.48	0.48
7:A:1245:U:H2'	7:A:1246:U:C6	2.49	0.48
7:A:1676:U:H2'	7:A:1677:A:H8	1.79	0.48
7:A:2985:G:O6	7:A:2993:C:H5''	2.14	0.48
13:G:16:ASP:OD1	13:G:27:LYS:N	2.47	0.48
19:N:32:GLY:O	19:N:114:GLU:HB2	2.13	0.48
32:a:336:G:H2'	32:a:337:A:H8	1.77	0.48
32:a:834:U:O2'	32:a:836:C:H5''	2.14	0.48
32:a:991:G:H2'	32:a:992:C:C6	2.48	0.48
32:a:1115:G:O2'	32:a:1137:G:O6	2.31	0.48
7:A:220:G:H22	7:A:237:U:H4'	1.79	0.47
7:A:259:C:H2'	7:A:260:G:O4'	2.14	0.47
7:A:1184:G:N2	7:A:1214:A:O2'	2.47	0.47
7:A:1637:U:H2'	7:A:1638:C:H6	1.79	0.47
7:A:2971:U:H2'	7:A:2972:C:C6	2.49	0.47
8:B:53:G:H21	12:F:33:MET:CE	2.27	0.47
18:M:36:ALA:HB2	18:M:103:LEU:HD21	1.96	0.47
32:a:748:U:H2'	32:a:749:G:O4'	2.14	0.47
32:a:1028:C:H2'	32:a:1029:C:H6	1.78	0.47
32:a:1106:U:H2'	32:a:1107:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:o:70:ILE:HA	45:o:73:ILE:HG22	1.94	0.47
7:A:701:U:H2'	7:A:702:C:C6	2.49	0.47
7:A:1492:G:H2'	7:A:1493:C:C6	2.48	0.47
7:A:1593:C:H2'	7:A:1594:A:N7	2.29	0.47
17:L:103:VAL:HG21	17:L:109:VAL:HG22	1.96	0.47
32:a:434:U:H2'	32:a:435:C:C6	2.49	0.47
35:e:76:MET:HE2	35:e:102:PHE:HB3	1.96	0.47
49:s:61:PHE:HD2	49:s:63:THR:HG22	1.79	0.47
1:O:45:LYS:O	1:O:49:LEU:HG	2.14	0.47
7:A:285:G:H3'	7:A:286:G:H5''	1.95	0.47
7:A:1707:A:H2'	7:A:1708:A:H8	1.75	0.47
7:A:2566:A:H2'	7:A:2567:A:H8	1.77	0.47
14:H:9:VAL:HG21	14:H:12:LEU:HB2	1.96	0.47
22:Q:88:VAL:HG12	22:Q:90:VAL:HG12	1.95	0.47
30:Y:14:THR:OG1	30:Y:15:ASP:N	2.47	0.47
32:a:1013:G:OP2	32:a:1013:G:N2	2.42	0.47
32:a:1161:A:H2'	32:a:1162:A:C8	2.48	0.47
36:f:43:TRP:HB2	36:f:60:TYR:HB2	1.96	0.47
42:l:121:LYS:O	42:l:122:GLU:HG2	2.15	0.47
7:A:389:U:H2'	7:A:390:G:O4'	2.15	0.47
7:A:925:U:H2'	7:A:926:C:C6	2.50	0.47
7:A:1630:G:H2'	7:A:1631:G:H8	1.79	0.47
7:A:2307:G:H2'	7:A:2308:A:C8	2.49	0.47
7:A:2509:G:OP1	28:W:18:ALA:HB1	2.15	0.47
18:M:16:ARG:NH2	18:M:18:ARG:HD3	2.30	0.47
20:O:46:LEU:O	20:O:54:THR:HA	2.13	0.47
26:U:98:SER:HB3	26:U:102:GLY:HA2	1.96	0.47
27:V:31:ILE:HG12	27:V:49:GLY:HA2	1.96	0.47
28:W:39:ARG:HD3	28:W:58:THR:HG23	1.96	0.47
32:a:268:U:H2'	32:a:269:A:H8	1.77	0.47
32:a:390:G:H5''	46:p:9:ARG:NH1	2.29	0.47
39:i:69:ILE:H	39:i:69:ILE:HD12	1.79	0.47
7:A:616:A:C2	7:A:2280:A:H2'	2.49	0.47
7:A:1298:U:H2'	7:A:1299:C:H6	1.79	0.47
7:A:1603:C:O2	7:A:1604:G:N1	2.48	0.47
11:E:157:ARG:NH1	11:E:199:ASP:OD2	2.47	0.47
12:F:83:GLN:OE1	12:F:83:GLN:N	2.47	0.47
32:a:334:C:H2'	32:a:335:A:H8	1.79	0.47
32:a:517:C:H2'	32:a:517:C:OP2	2.14	0.47
32:a:1121:A:H61	32:a:1136:G:H1'	1.79	0.47
37:g:70:LYS:NZ	37:g:96:SER:OG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:5:ASP:HB2	38:h:83:PRO:HG3	1.96	0.47
7:A:199:A:H62	7:A:2668:A:H2'	1.79	0.47
7:A:2431:A:H2'	7:A:2432:U:H6	1.80	0.47
14:H:7:ALA:HB3	14:H:35:LEU:HG	1.96	0.47
32:a:389:U:H2'	32:a:390:G:C8	2.49	0.47
32:a:837:U:H1'	32:a:839:G:C8	2.48	0.47
34:d:16:ARG:HH12	34:d:33:PRO:CG	2.27	0.47
43:m:57:ARG:O	43:m:60:ILE:HG12	2.15	0.47
52:y:24:C:H2'	52:y:25:U:C6	2.49	0.47
7:A:872:A:O2'	7:A:1894:U:OP1	2.27	0.47
7:A:1191:G:H1'	7:A:1217:A:H62	1.78	0.47
7:A:1516:A:H1'	7:A:1517:C:O2	2.15	0.47
7:A:1614:A:H2'	7:A:1615:G:H4'	1.97	0.47
7:A:2617:G:H2'	7:A:2618:U:C6	2.50	0.47
7:A:3089:U:H2'	7:A:3090:C:C6	2.50	0.47
11:E:14:LYS:HD2	11:E:154:LEU:HD21	1.97	0.47
30:Y:17:GLU:O	30:Y:21:ARG:HG2	2.15	0.47
32:a:134:U:H2'	32:a:135:G:C8	2.48	0.47
32:a:1348:G:H2'	32:a:1349:A:H8	1.78	0.47
34:d:183:ARG:HH12	34:d:188:VAL:HA	1.80	0.47
35:e:115:PRO:HB3	35:e:128:ARG:HG2	1.97	0.47
37:g:94:ASP:OD2	37:g:94:ASP:N	2.47	0.47
38:h:43:GLU:HG3	38:h:103:VAL:HG21	1.97	0.47
49:s:63:THR:OG1	49:s:64:GLU:N	2.48	0.47
7:A:646:A:H2'	7:A:647:G:O4'	2.14	0.47
7:A:1245:U:H2'	7:A:1246:U:H6	1.79	0.47
7:A:1303:C:H5	7:A:1305:U:H1'	1.79	0.47
7:A:3044:A:H2'	7:A:3045:A:C8	2.49	0.47
14:H:2:LYS:HB3	14:H:39:ALA:HB3	1.97	0.47
15:J:110:PRO:O	15:J:115:SER:OG	2.30	0.47
32:a:852:U:H2'	32:a:853:A:C8	2.50	0.47
36:f:23:LEU:HA	36:f:26:PHE:HD2	1.79	0.47
50:t:43:ASP:OD2	50:t:46:LYS:HG2	2.14	0.47
7:A:1177:A:H1'	7:A:1241:G:H21	1.78	0.47
7:A:2500:U:OP2	28:W:16:SER:OG	2.27	0.47
7:A:2887:U:H2'	7:A:2888:C:H6	1.80	0.47
8:B:13:C:OP2	8:B:69:C:O2'	2.33	0.47
18:M:47:ILE:HD12	18:M:70:PRO:HG3	1.96	0.47
32:a:697:A:H2	41:k:51:VAL:HG21	1.80	0.47
32:a:999:C:H2'	32:a:1000:G:H8	1.79	0.47
43:m:40:ASP:OD1	43:m:40:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:13:LYS:HG3	5:4:27:CYS:SG	2.55	0.47
7:A:2378:G:N2	7:A:2388:G:O4'	2.44	0.47
7:A:2792:U:H2'	7:A:2793:U:C6	2.50	0.47
7:A:2971:U:H2'	7:A:2972:C:H6	1.79	0.47
7:A:2989:G:H4'	13:G:4:ILE:HG13	1.97	0.47
13:G:16:ASP:O	13:G:18:THR:HG23	2.14	0.47
32:a:405:G:H21	34:d:111:GLN:HE22	1.63	0.47
32:a:469:A:H2'	32:a:470:U:O4'	2.15	0.47
32:a:1115:G:N2	32:a:1116:U:O4	2.45	0.47
38:h:76:GLY:HA3	38:h:132:TRP:CZ2	2.50	0.47
45:o:10:GLU:HG3	45:o:13:ARG:NH2	2.30	0.47
7:A:637:C:H2'	7:A:638:C:C6	2.50	0.46
7:A:961:U:H2'	7:A:962:G:H8	1.79	0.46
7:A:2374:C:N4	7:A:2392:C:O2'	2.48	0.46
12:F:8:GLN:HG3	12:F:13:GLU:OE2	2.16	0.46
18:M:43:THR:HG22	18:M:45:ARG:H	1.79	0.46
22:Q:119:GLU:HG2	22:Q:120:ASP:N	2.30	0.46
30:Y:12:GLU:N	30:Y:12:GLU:OE2	2.48	0.46
32:a:35:A:H2'	32:a:36:A:C8	2.50	0.46
32:a:485:G:O2'	32:a:487:A:H1'	2.15	0.46
32:a:996:G:O2'	32:a:1022:U:N3	2.48	0.46
32:a:1195:C:OP1	44:n:2:ALA:N	2.48	0.46
42:l:114:ARG:NH1	42:l:121:LYS:HG3	2.30	0.46
7:A:143:G:H5'	7:A:144:U:OP2	2.14	0.46
7:A:1222:G:H21	7:A:1228:G:H1	1.61	0.46
7:A:2555:U:H2'	7:A:2556:G:O4'	2.15	0.46
32:a:546:C:H2'	32:a:547:C:C6	2.50	0.46
32:a:1258:G:N2	32:a:1261:A:OP2	2.27	0.46
40:j:7:ARG:HB2	40:j:101:GLN:HB2	1.97	0.46
40:j:63:GLU:OE1	44:n:58:LYS:NZ	2.43	0.46
6:6:26:SER:OG	6:6:27:THR:N	2.40	0.46
7:A:1618:C:H2'	7:A:1619:U:O4'	2.15	0.46
7:A:1721:A:H2'	7:A:1722:G:H8	1.80	0.46
7:A:2102:C:H2'	7:A:2103:C:H6	1.79	0.46
7:A:2431:A:H2'	7:A:2432:U:C6	2.50	0.46
9:C:80:ALA:O	9:C:113:GLN:NE2	2.46	0.46
30:Y:13:LEU:HB3	30:Y:17:GLU:HB2	1.97	0.46
32:a:226:G:OP2	47:q:50:ARG:NH2	2.48	0.46
32:a:837:U:O2'	32:a:838:U:O4'	2.32	0.46
32:a:901:A:H2'	32:a:902:A:C8	2.50	0.46
35:e:189:GLY:C	35:e:190:LEU:HD23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:p:77:THR:HG23	46:p:79:ASP:H	1.80	0.46
7:A:289:A:H5''	7:A:302:U:H3	1.79	0.46
7:A:644:G:C2	7:A:645:G:H1'	2.49	0.46
7:A:682:C:H4'	22:Q:31:LEU:HD13	1.98	0.46
7:A:1111:C:O2	51:v:21:ARG:NH2	2.48	0.46
7:A:1646:G:N2	7:A:1647:U:O4	2.39	0.46
18:M:17:GLN:NE2	18:M:39:HIS:HB3	2.30	0.46
27:V:69:ILE:N	27:V:72:LYS:O	2.48	0.46
32:a:90:U:O2'	32:a:91:A:O5'	2.33	0.46
32:a:529:U:OP2	42:l:112:GLN:HB2	2.15	0.46
32:a:530:A:H2'	32:a:531:G:H8	1.80	0.46
32:a:760:G:H4'	32:a:1506:A:H4'	1.97	0.46
32:a:833:U:H4'	32:a:834:U:H5'	1.98	0.46
1:0:6:ARG:HE	7:A:2257:C:H41	1.63	0.46
7:A:452:A:N6	7:A:453:A:N1	2.64	0.46
7:A:1570:U:N3	7:A:1633:A:OP2	2.48	0.46
32:a:655:G:OP1	48:r:62:ARG:NE	2.47	0.46
32:a:815:U:H2'	32:a:816:A:C8	2.50	0.46
32:a:1417:U:H2'	32:a:1418:A:C8	2.50	0.46
36:f:26:PHE:O	36:f:29:VAL:HG12	2.15	0.46
45:o:47:LYS:O	45:o:53:ARG:NH2	2.49	0.46
7:A:645:G:N2	7:A:646:A:H62	2.13	0.46
7:A:690:U:H2'	7:A:691:C:C6	2.51	0.46
7:A:1283:C:OP1	22:Q:92:ARG:NH2	2.43	0.46
7:A:2016:U:H1'	7:A:2847:U:H5''	1.98	0.46
7:A:2363:A:H5'	7:A:2364:G:H5'	1.96	0.46
7:A:2419:A:H2'	7:A:2420:U:C6	2.50	0.46
11:E:129:ARG:HD2	11:E:199:ASP:OD1	2.16	0.46
24:S:44:ASP:OD1	24:S:45:ILE:N	2.48	0.46
32:a:89:A:N6	32:a:92:C:H41	2.14	0.46
32:a:199:G:H2'	32:a:200:U:C6	2.51	0.46
32:a:1051:U:H2'	32:a:1052:G:H8	1.81	0.46
35:e:190:LEU:O	35:e:192:ILE:N	2.42	0.46
7:A:2372:A:N1	7:A:2393:G:O2'	2.49	0.46
12:F:127:LYS:HA	12:F:127:LYS:HD3	1.71	0.46
32:a:1051:U:C5	33:c:2:GLY:HA3	2.51	0.46
37:g:66:LEU:HD23	37:g:66:LEU:HA	1.80	0.46
47:q:54:PRO:HD2	47:q:54:PRO:O	2.16	0.46
52:y:53:G:C4	52:y:54:G:C8	3.04	0.46
7:A:198:A:H62	7:A:960:G:H21	1.63	0.46
7:A:640:C:H3'	7:A:641:U:C5'	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1007:G:N1	7:A:1028:G:N3	2.64	0.46
7:A:2335:U:O2	7:A:2428:G:N2	2.38	0.46
7:A:2529:U:H2'	7:A:2530:U:H6	1.80	0.46
7:A:2567:A:H2'	7:A:2568:U:C6	2.51	0.46
7:A:2636:C:H2'	7:A:2637:A:C8	2.51	0.46
12:F:171:ASP:OD1	12:F:172:GLU:N	2.49	0.46
24:S:98:ARG:HG3	24:S:104:PHE:CD2	2.51	0.46
32:a:65:U:H2'	32:a:66:C:C6	2.51	0.46
32:a:888:G:H2'	32:a:889:C:C6	2.51	0.46
32:a:1111:U:H2'	32:a:1112:C:H6	1.81	0.46
32:a:1253:A:H61	32:a:1266:A:H1'	1.81	0.46
34:d:13:ARG:O	34:d:16:ARG:NH1	2.49	0.46
35:e:67:LEU:HD21	35:e:168:VAL:HG21	1.98	0.46
36:f:82:ASN:OD1	36:f:83:GLU:N	2.48	0.46
7:A:1488:C:H2'	7:A:1489:G:O4'	2.16	0.46
7:A:2356:A:C2	7:A:2404:U:H1'	2.51	0.46
7:A:3026:U:O2'	7:A:3044:A:N3	2.43	0.46
25:T:57:VAL:HG22	25:T:84:VAL:HG22	1.98	0.46
31:Z:45:GLY:O	31:Z:49:VAL:HG23	2.15	0.46
32:a:1013:G:H21	32:a:1013:G:P	2.38	0.46
32:a:1152:G:C2	32:a:1153:C:C6	3.04	0.46
40:j:78:ASP:OD2	40:j:80:THR:OG1	2.25	0.46
47:q:110:ASP:OD1	47:q:134:LYS:HG2	2.16	0.46
7:A:1650:U:H2'	7:A:1651:C:C6	2.51	0.46
7:A:1767:A:N6	7:A:1780:G:O2'	2.49	0.46
20:O:30:ARG:HD3	20:O:96:VAL:HG13	1.98	0.46
20:O:49:ASP:O	20:O:50:LEU:HD23	2.15	0.46
32:a:443:A:H2'	32:a:444:U:C6	2.51	0.46
32:a:874:G:P	42:l:9:ARG:HH22	2.39	0.46
42:l:76:GLU:O	42:l:77:HIS:C	2.59	0.46
7:A:287:G:C8	7:A:302:U:H2'	2.48	0.45
7:A:978:C:H2'	7:A:979:A:C8	2.51	0.45
7:A:1141:C:N3	15:J:27:ARG:NH1	2.64	0.45
7:A:3031:C:H2'	7:A:3032:A:C8	2.51	0.45
9:C:182:ILE:HB	9:C:269:VAL:HB	1.97	0.45
17:L:55:PRO:HD2	17:L:58:MET:HB2	1.98	0.45
30:Y:44:ASN:OD1	30:Y:45:ARG:NH1	2.49	0.45
43:m:67:GLU:H	43:m:67:GLU:CD	2.23	0.45
52:y:4:G:O2'	52:y:5:G:H8	1.99	0.45
7:A:1824:C:H2'	7:A:1825:A:C8	2.51	0.45
24:S:93:LYS:HD3	24:S:105:ARG:HH11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:135:G:H1	32:a:223:U:H5	1.64	0.45
32:a:735:C:H2'	32:a:736:A:H8	1.82	0.45
32:a:1288:C:H4'	32:a:1294:U:O4	2.15	0.45
42:l:21:THR:OG1	42:l:24:LEU:HB2	2.16	0.45
45:o:12:LEU:HD13	45:o:22:THR:HG22	1.98	0.45
7:A:196:G:H2'	7:A:197:A:O4'	2.16	0.45
7:A:679:G:O2'	7:A:1385:A:OP1	2.34	0.45
7:A:993:G:H2'	7:A:994:C:H6	1.82	0.45
7:A:1232:A:N3	7:A:1232:A:H2'	2.30	0.45
7:A:1270:U:O2	7:A:1272:A:N6	2.49	0.45
7:A:1910:C:O2	10:D:138:SER:OG	2.30	0.45
7:A:2829:C:H2'	7:A:2830:G:H8	1.81	0.45
28:W:72:LYS:O	28:W:73:ARG:HG2	2.17	0.45
32:a:405:G:H21	34:d:111:GLN:NE2	2.14	0.45
4:3:25:GLN:HG3	17:L:63:LEU:HD23	1.97	0.45
7:A:455:U:H2'	7:A:456:C:C6	2.52	0.45
7:A:991:G:H2'	7:A:992:A:O4'	2.16	0.45
7:A:2048:G:OP2	7:A:2049:A:O2'	2.23	0.45
13:G:87:LYS:CB	13:G:166:GLU:HG3	2.44	0.45
32:a:463:U:H2'	32:a:464:C:C6	2.51	0.45
32:a:463:U:H2'	32:a:464:C:H6	1.80	0.45
32:a:1479:G:H2'	32:a:1480:G:O4'	2.16	0.45
37:g:54:THR:HG23	37:g:56:THR:N	2.30	0.45
43:m:58:ASP:OD1	43:m:59:TYR:N	2.50	0.45
50:t:28:LEU:HD23	50:t:58:LEU:HD23	1.97	0.45
7:A:140:G:H21	7:A:1540:G:H1'	1.81	0.45
7:A:343:C:H2'	7:A:344:C:C6	2.52	0.45
7:A:1215:A:H4'	7:A:1232:A:N1	2.32	0.45
8:B:108:G:H2'	8:B:109:C:C6	2.51	0.45
20:O:33:LEU:HD23	20:O:97:PHE:HD1	1.82	0.45
52:y:17:C:H5'	52:y:18:U:C5	2.51	0.45
7:A:1451:C:C5	7:A:1460:U:H5''	2.52	0.45
7:A:1558:A:O5'	7:A:1646:G:N2	2.45	0.45
14:H:1:MET:HE3	14:H:23:ASP:HA	1.99	0.45
14:H:5:LEU:HD23	14:H:5:LEU:H	1.82	0.45
17:L:71:ARG:NE	17:L:73:GLU:OE2	2.42	0.45
32:a:77:G:H2'	32:a:78:U:O4'	2.16	0.45
32:a:199:G:H2'	32:a:200:U:H6	1.80	0.45
32:a:491:G:H2'	32:a:492:C:H6	1.81	0.45
2:1:34:ASP:N	2:1:34:ASP:OD1	2.48	0.45
6:6:15:VAL:HG21	6:6:32:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1156:A:N1	7:A:1256:U:H5	2.15	0.45
7:A:3092:G:N2	7:A:3095:A:OP2	2.31	0.45
20:O:27:THR:HG23	20:O:30:ARG:H	1.82	0.45
46:p:30:ASP:OD1	46:p:30:ASP:N	2.47	0.45
46:p:72:LYS:HA	46:p:72:LYS:HD3	1.75	0.45
7:A:336:G:H2'	7:A:337:C:C6	2.51	0.45
15:J:88:THR:OG1	15:J:91:GLU:HG3	2.17	0.45
32:a:351:C:H4'	32:a:353:G:OP1	2.16	0.45
32:a:686:A:H2'	32:a:687:A:C8	2.51	0.45
32:a:1150:C:C4	32:a:1152:G:C8	3.05	0.45
32:a:1428:G:H2'	32:a:1429:C:H6	1.81	0.45
32:a:1433:U:H2'	32:a:1434:G:O4'	2.17	0.45
46:p:60:LEU:HD11	46:p:74:LEU:HD13	1.99	0.45
49:s:30:VAL:HA	49:s:48:THR:HG23	1.99	0.45
3:2:25:MET:HE3	3:2:25:MET:HB3	1.92	0.45
27:V:51:ASP:O	27:V:55:VAL:HG23	2.16	0.45
32:a:376:G:OP1	46:p:4:LYS:NZ	2.43	0.45
34:d:108:MET:O	34:d:112:LEU:HD23	2.17	0.45
36:f:41:ASP:OD1	36:f:42:ILE:N	2.50	0.45
37:g:149:ARG:HD2	41:k:71:PHE:CE1	2.51	0.45
48:r:46:GLY:O	48:r:72:ARG:NH2	2.42	0.45
52:y:55:U:H2'	52:y:56:U:O4'	2.16	0.45
4:3:19:THR:OG1	7:A:755:G:OP1	2.31	0.45
7:A:451:C:H2'	7:A:452:A:H8	1.82	0.45
7:A:588:G:N1	7:A:591:A:OP2	2.48	0.45
7:A:1295:A:H2'	7:A:1296:C:C6	2.52	0.45
7:A:1667:G:H2'	7:A:1668:C:C6	2.51	0.45
7:A:1969:U:H2'	7:A:1970:G:H8	1.82	0.45
7:A:2940:G:H2'	7:A:2941:C:H6	1.83	0.45
13:G:96:ARG:HE	13:G:98:GLN:NE2	2.15	0.45
32:a:986:G:H2'	32:a:988:C:H41	1.82	0.45
7:A:1053:U:H2'	7:A:1054:G:C8	2.52	0.44
7:A:1075:A:H2'	7:A:1076:C:C6	2.53	0.44
7:A:1197:G:H4'	7:A:1225:A:H4'	1.99	0.44
7:A:3131:U:H2'	7:A:3132:U:C6	2.52	0.44
32:a:505:C:H2'	32:a:506:G:H8	1.82	0.44
34:d:31:TYR:O	34:d:33:PRO:HD3	2.18	0.44
37:g:146:GLU:OE1	37:g:149:ARG:NH2	2.50	0.44
7:A:335:A:H2'	7:A:336:G:H8	1.82	0.44
7:A:503:C:H2'	7:A:504:A:H8	1.82	0.44
7:A:2170:A:H2'	7:A:2171:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2423:U:H3'	7:A:2424:A:H5''	2.00	0.44
7:A:2442:A:H2'	7:A:2443:A:H8	1.83	0.44
13:G:104:LEU:HD12	13:G:124:PHE:HB3	1.99	0.44
32:a:493:A:H2'	32:a:494:C:C6	2.52	0.44
34:d:52:GLU:HG2	34:d:194:LEU:HB2	1.99	0.44
34:d:191:THR:HG22	34:d:193:GLN:H	1.82	0.44
39:i:69:ILE:O	39:i:70:LYS:HG2	2.18	0.44
50:t:28:LEU:HD11	50:t:61:ALA:HB2	1.99	0.44
7:A:609:U:H2'	7:A:610:G:C8	2.53	0.44
7:A:993:G:H2'	7:A:994:C:C6	2.52	0.44
7:A:1623:G:H4'	7:A:1624:C:C6	2.52	0.44
7:A:1692:U:O2'	7:A:1693:G:N7	2.50	0.44
7:A:2106:C:N3	7:A:2109:G:H1'	2.32	0.44
7:A:2363:A:N7	7:A:2400:U:H1'	2.32	0.44
7:A:2750:C:H2'	7:A:2751:G:O4'	2.18	0.44
27:V:14:ARG:HG2	27:V:46:GLU:OE2	2.17	0.44
32:a:77:G:N1	32:a:91:A:H2	2.11	0.44
32:a:221:U:H2'	32:a:222:G:C8	2.52	0.44
32:a:1149:A:C2	32:a:1173:G:C4	3.05	0.44
33:c:57:GLU:OE2	40:j:94:ALA:HB3	2.18	0.44
36:f:6:ILE:HD13	36:f:75:LEU:HD22	1.99	0.44
49:s:22:GLN:HB3	49:s:28:LYS:HB2	2.00	0.44
1:0:41:ARG:HD2	7:A:3121:G:N3	2.33	0.44
6:6:13:THR:HB	6:6:32:ARG:HG2	1.99	0.44
7:A:1157:A:N3	7:A:2724:G:O2'	2.46	0.44
7:A:1517:C:H2'	7:A:1518:G:C8	2.52	0.44
18:M:83:MET:HE2	18:M:83:MET:HA	2.00	0.44
23:R:50:THR:O	23:R:52:ASP:N	2.51	0.44
23:R:51:THR:O	23:R:51:THR:OG1	2.29	0.44
32:a:38:G:H2'	32:a:39:C:H6	1.83	0.44
32:a:513:C:H5	42:l:50:ARG:HH12	1.66	0.44
32:a:1240:A:H4'	39:i:54:ARG:HH12	1.81	0.44
32:a:1264:U:H2'	32:a:1265:U:C6	2.51	0.44
34:d:183:ARG:C	34:d:186:ILE:H	2.25	0.44
38:h:117:GLN:O	38:h:121:GLN:HG3	2.18	0.44
7:A:252:G:H2'	7:A:253:A:C8	2.52	0.44
7:A:448:U:C2	7:A:449:A:C8	3.06	0.44
7:A:829:G:O2'	7:A:1867:A:N3	2.42	0.44
7:A:1577:C:H2'	7:A:1578:C:C6	2.52	0.44
7:A:1742:U:H2'	7:A:1743:C:C6	2.51	0.44
7:A:2489:OMG:HM23	7:A:2489:OMG:HI1'	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:169:GLU:OE2	9:C:184:ARG:HD2	2.17	0.44
10:D:186:ASP:OD1	10:D:189:ASN:ND2	2.47	0.44
21:P:33:GLU:OE1	21:P:38:ARG:HD3	2.17	0.44
32:a:443:A:H2'	32:a:444:U:H6	1.83	0.44
32:a:876:C:O2'	32:a:877:U:H5'	2.18	0.44
34:d:120:VAL:HG23	34:d:121:ASN:N	2.29	0.44
39:i:42:LEU:HD12	39:i:84:ILE:HG22	2.00	0.44
42:l:25:LYS:HD2	42:l:59:SER:HB2	2.00	0.44
43:m:23:PHE:N	43:m:67:GLU:OE2	2.46	0.44
47:q:50:ARG:HG3	47:q:51:THR:N	2.32	0.44
5:4:6:SER:HB2	7:A:1160:G:H4'	1.99	0.44
7:A:1649:G:H2'	7:A:1650:U:H6	1.83	0.44
7:A:2192:G:O2'	7:A:2194:U:O4	2.32	0.44
13:G:55:ARG:NH1	13:G:57:ASP:HA	2.32	0.44
19:N:100:ILE:HG22	19:N:101:GLU:N	2.32	0.44
32:a:360:G:H2'	32:a:361:G:O4'	2.17	0.44
32:a:996:G:N3	32:a:1022:U:N3	2.66	0.44
32:a:999:C:H2'	32:a:1000:G:C8	2.52	0.44
32:a:1277:U:H5'	32:a:1278:A:N7	2.33	0.44
52:y:24:C:H2'	52:y:25:U:H6	1.81	0.44
7:A:12:U:O2'	7:A:13:A:O5'	2.29	0.44
7:A:152:C:H2'	7:A:153:C:C6	2.53	0.44
7:A:423:A:H2'	7:A:424:C:O4'	2.17	0.44
7:A:2334:U:H2'	7:A:2335:U:C6	2.53	0.44
13:G:18:THR:O	13:G:24:ILE:HA	2.17	0.44
13:G:90:ILE:HG12	13:G:163:VAL:HG22	2.00	0.44
17:L:82:ILE:HD12	17:L:92:VAL:HG11	2.00	0.44
31:Z:6:ILE:HG22	31:Z:28:LEU:HD11	1.99	0.44
32:a:1404:U:H2'	32:a:1405:C:C6	2.52	0.44
36:f:6:ILE:HB	36:f:63:ILE:HB	1.99	0.44
46:p:55:ARG:HD2	46:p:55:ARG:HA	1.62	0.44
7:A:1331:C:H2'	7:A:1332:C:C6	2.53	0.44
7:A:1397:G:O5'	24:S:25:ARG:NH2	2.51	0.44
32:a:136:C:H4'	47:q:45:PRO:O	2.17	0.44
32:a:504:A:H2'	32:a:505:C:C6	2.53	0.44
33:c:67:ILE:O	33:c:102:ILE:HD12	2.17	0.44
34:d:6:GLY:H	34:d:107:ARG:HH22	1.66	0.44
34:d:80:LYS:HD3	34:d:83:GLU:CD	2.42	0.44
41:k:40:THR:HG21	41:k:73:ALA:HA	1.99	0.44
50:t:7:GLN:HG2	50:t:7:GLN:O	2.17	0.44
7:A:1775:G:H2'	7:A:1776:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2028:U:H2'	7:A:2029:C:C6	2.52	0.44
7:A:2837:G:N7	9:C:237:GLU:HG2	2.33	0.44
27:V:30:LYS:HB3	27:V:46:GLU:HB3	2.00	0.44
32:a:181:C:H2'	32:a:182:C:C6	2.53	0.44
32:a:406:G:O2'	34:d:108:MET:HB3	2.18	0.44
32:a:496:G:H2'	32:a:497:G:C8	2.53	0.44
32:a:1163:C:H2'	32:a:1164:U:C6	2.53	0.44
32:a:1459:C:H2'	32:a:1460:G:O4'	2.18	0.44
33:c:112:ALA:C	33:c:114:LEU:H	2.26	0.44
34:d:159:GLU:HG2	34:d:160:ARG:H	1.83	0.44
34:d:182:GLU:HB3	34:d:185:GLN:HG3	1.99	0.44
43:m:99:ARG:HB2	43:m:101:GLN:HE22	1.82	0.44
50:t:35:PHE:CD2	50:t:79:LEU:HD22	2.53	0.44
7:A:294:G:H2'	7:A:295:G:O4'	2.18	0.43
7:A:1141:C:O2	15:J:27:ARG:NH1	2.51	0.43
7:A:1670:G:H2'	7:A:1671:G:O4'	2.18	0.43
23:R:7:ILE:HD12	23:R:42:LEU:HD23	2.00	0.43
27:V:33:ALA:HB3	27:V:47:LEU:HD13	2.00	0.43
32:a:372:A:C2	32:a:373:A:C8	3.06	0.43
32:a:599:A:H2'	32:a:600:A:O4'	2.18	0.43
32:a:1063:G:H2'	32:a:1064:U:C6	2.53	0.43
34:d:126:ASN:HD22	34:d:126:ASN:N	2.16	0.43
6:6:2:LYS:HG2	6:6:6:HIS:CD2	2.53	0.43
7:A:924:C:H2'	7:A:925:U:C6	2.53	0.43
12:F:45:MET:HE3	12:F:64:LEU:HG	2.00	0.43
32:a:388:A:H3'	32:a:389:U:H6	1.83	0.43
32:a:603:U:H2'	32:a:604:C:C6	2.53	0.43
6:6:35:VAL:HG12	12:F:146:HIS:NE2	2.33	0.43
7:A:1715:A:N6	7:A:1753:G:O2'	2.46	0.43
8:B:83:C:H2'	8:B:84:C:O4'	2.19	0.43
27:V:66:THR:HA	27:V:75:LEU:HA	2.00	0.43
32:a:1240:A:H4'	39:i:54:ARG:HH22	1.83	0.43
32:a:1361:G:OP1	39:i:134:ARG:NH2	2.52	0.43
33:c:107:ASN:C	33:c:109:GLU:H	2.27	0.43
37:g:139:GLU:HG3	37:g:143:LYS:HE3	1.99	0.43
40:j:19:ASP:OD2	40:j:20:ALA:N	2.51	0.43
7:A:258:A:H2'	7:A:259:C:C6	2.53	0.43
7:A:1193:C:N4	7:A:1199:A:OP1	2.50	0.43
7:A:1958:C:H3'	7:A:1959:A:H8	1.82	0.43
7:A:2295:A:H2'	7:A:2296:6MZ:O4'	2.19	0.43
7:A:2752:U:H2'	7:A:2753:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:593:U:H2'	32:a:594:C:C6	2.53	0.43
33:c:47:GLU:H	33:c:47:GLU:CD	2.26	0.43
34:d:68:ARG:O	34:d:72:GLU:OE1	2.35	0.43
35:e:165:ILE:HD12	35:e:165:ILE:H	1.83	0.43
4:3:30:ARG:HH21	17:L:61:PRO:HB2	1.83	0.43
7:A:350:A:N6	7:A:445:U:H3	2.17	0.43
7:A:1177:A:N1	7:A:1241:G:O2'	2.45	0.43
7:A:1183:A:H2'	7:A:1184:G:O4'	2.18	0.43
7:A:1741:C:H2'	7:A:1742:U:C6	2.54	0.43
7:A:2354:A:C2	7:A:2407:A:H5''	2.53	0.43
7:A:2835:G:H2'	7:A:2836:A:C8	2.53	0.43
7:A:2916:A:H2'	7:A:2917:A:C8	2.53	0.43
8:B:47:C:H5'	20:O:103:THR:CG2	2.47	0.43
9:C:94:LEU:HD13	9:C:104:TYR:CE1	2.53	0.43
32:a:551:A:H4'	32:a:552:U:H5''	2.01	0.43
32:a:1116:U:C2	32:a:1118:G:C8	3.07	0.43
37:g:50:ALA:O	37:g:54:THR:HG22	2.19	0.43
39:i:54:ARG:HB3	39:i:58:ASP:HB2	1.99	0.43
42:l:34:CYS:HB3	42:l:78:SER:O	2.18	0.43
7:A:378:C:H2'	7:A:379:G:C8	2.54	0.43
7:A:1227:A:H3'	7:A:1228:G:C8	2.53	0.43
7:A:1263:G:N7	51:v:3:LYS:HE3	2.34	0.43
7:A:2078:U:H5''	9:C:256:ARG:HG2	1.99	0.43
7:A:2184:U:H2'	7:A:2185:C:C6	2.54	0.43
7:A:2936:U:H2'	7:A:2937:C:H6	1.84	0.43
7:A:2985:G:O3'	13:G:71:THR:HG21	2.19	0.43
11:E:124:ARG:HD3	11:E:124:ARG:HA	1.79	0.43
12:F:114:ALA:HB1	12:F:144:VAL:HG23	2.01	0.43
20:O:32:ARG:O	20:O:46:LEU:HA	2.19	0.43
32:a:57:C:H2'	32:a:351:C:H41	1.84	0.43
32:a:550:A:H4'	32:a:551:A:H3'	2.01	0.43
33:c:60:ARG:NH2	40:j:98:VAL:H	2.17	0.43
39:i:50:ASP:C	39:i:51:LEU:HD12	2.44	0.43
46:p:9:ARG:HE	46:p:16:PRO:HB3	1.84	0.43
46:p:24:ASP:OD2	46:p:25:ALA:N	2.52	0.43
48:r:66:LEU:HD23	48:r:66:LEU:HA	1.86	0.43
7:A:641:U:H1'	7:A:643:C:H5''	2.01	0.43
7:A:1184:G:HO2'	7:A:1213:A:N6	2.16	0.43
7:A:1331:C:H2'	7:A:1332:C:H6	1.82	0.43
7:A:1501:C:H2'	7:A:1502:G:O4'	2.18	0.43
7:A:1860:C:H2'	7:A:1861:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2093:A:H2	7:A:2121:G:N2	2.16	0.43
7:A:2371:A:H8	7:A:2395:A:H5'	1.84	0.43
11:E:60:THR:O	11:E:64:VAL:HG23	2.18	0.43
19:N:11:GLY:O	19:N:16:HIS:ND1	2.48	0.43
24:S:93:LYS:HD3	24:S:105:ARG:NH1	2.33	0.43
32:a:681:G:H2'	32:a:682:G:C8	2.54	0.43
34:d:11:LYS:HE2	34:d:58:PHE:CE2	2.53	0.43
7:A:1303:C:C2	7:A:1309:G:C2	3.07	0.43
7:A:1638:C:H2'	7:A:1639:G:C8	2.53	0.43
7:A:1738:U:H2'	7:A:1739:C:C6	2.53	0.43
7:A:1863:G:H2'	7:A:1864:U:C6	2.54	0.43
7:A:2020:A:H1'	7:A:2176:A:N6	2.34	0.43
25:T:94:ASP:OD1	25:T:94:ASP:N	2.43	0.43
32:a:453:G:H2'	32:a:454:U:H6	1.84	0.43
32:a:1147:A:H2'	32:a:1148:G:O4'	2.18	0.43
32:a:1228:A:H2'	32:a:1229:C:C6	2.53	0.43
7:A:428:A:H1'	7:A:429:A:H2	1.80	0.43
7:A:677:A:OP2	7:A:2737:C:O2'	2.36	0.43
7:A:1446:C:H2'	7:A:1447:U:H6	1.84	0.43
7:A:1582:A:H5''	7:A:1583:C:C5	2.54	0.43
7:A:2721:C:N3	18:M:124:LYS:NZ	2.67	0.43
7:A:2969:G:H2'	7:A:2970:G:C8	2.53	0.43
9:C:266:LYS:HE2	9:C:266:LYS:HB3	1.82	0.43
10:D:156:THR:HA	10:D:157:PRO:HA	1.90	0.43
19:N:103:ARG:HD3	19:N:110:MET:SD	2.58	0.43
32:a:334:C:H2'	32:a:335:A:C8	2.54	0.43
32:a:373:A:H2'	32:a:374:U:C6	2.54	0.43
32:a:516:C:C2'	32:a:517:C:H5'	2.49	0.43
36:f:21:PRO:HA	36:f:24:GLU:HG2	2.01	0.43
7:A:786:U:H2'	7:A:787:G:C8	2.54	0.43
7:A:1227:A:H3'	7:A:1228:G:H8	1.83	0.43
32:a:224:G:H2'	32:a:225:G:O4'	2.19	0.43
32:a:913:U:H2'	32:a:914:U:C6	2.54	0.43
32:a:1018:U:H4'	32:a:1019:C:C6	2.53	0.43
52:y:65:G:H2'	52:y:66:C:H6	1.84	0.43
4:3:57:ARG:NH1	17:L:47:VAL:O	2.52	0.42
7:A:936:U:O2'	7:A:2298:A:N1	2.46	0.42
7:A:968:U:H2'	7:A:969:U:C6	2.54	0.42
7:A:979:A:H2'	7:A:980:C:C6	2.54	0.42
7:A:1738:U:H2'	7:A:1739:C:H6	1.83	0.42
7:A:2471:U:H2'	7:A:2472:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:3031:C:H2'	7:A:3032:A:H8	1.83	0.42
9:C:26:ARG:HH22	9:C:30:GLU:HB2	1.84	0.42
17:L:121:VAL:O	17:L:141:GLY:HA3	2.19	0.42
17:L:133:ARG:NH2	17:L:145:GLU:OE2	2.52	0.42
30:Y:10:LEU:HD23	30:Y:10:LEU:HA	1.90	0.42
32:a:391:C:P	46:p:9:ARG:HH12	2.41	0.42
32:a:612:A:H2'	32:a:613:A:C8	2.54	0.42
32:a:884:U:H2'	32:a:885:A:H8	1.83	0.42
32:a:888:G:H2'	32:a:889:C:H6	1.84	0.42
32:a:1262:G:C2	32:a:1263:G:C8	3.07	0.42
33:c:71:ARG:HB3	33:c:74:ILE:HD13	2.01	0.42
43:m:108:ARG:NH2	43:m:111:LYS:HE3	2.31	0.42
45:o:37:ALA:O	45:o:41:GLU:OE1	2.36	0.42
46:p:59:TRP:HA	46:p:62:VAL:HG12	2.00	0.42
47:q:95:LYS:HB3	47:q:95:LYS:HE2	1.78	0.42
50:t:72:ALA:O	50:t:76:LYS:HG3	2.18	0.42
7:A:83:G:O6	26:U:93:LYS:HE3	2.18	0.42
7:A:747:A:N1	7:A:2607:A:O2'	2.48	0.42
7:A:774:G:H2'	7:A:775:C:C6	2.53	0.42
7:A:1546:G:H2'	7:A:1547:C:H6	1.83	0.42
7:A:1720:G:H2'	7:A:1721:A:C8	2.54	0.42
7:A:2588:C:H2'	7:A:2589:G:O4'	2.19	0.42
18:M:15:PRO:HG2	18:M:41:TYR:CE1	2.53	0.42
32:a:738:U:H2'	32:a:739:A:O4'	2.19	0.42
32:a:815:U:H2'	32:a:816:A:H8	1.84	0.42
32:a:1136:G:N2	32:a:1138:A:H62	2.17	0.42
34:d:31:TYR:N	34:d:32:PRO:HD3	2.34	0.42
37:g:93:PRO:O	37:g:97:THR:HG23	2.18	0.42
43:m:51:GLU:O	43:m:54:ILE:HG22	2.19	0.42
5:4:27:CYS:SG	5:4:28:SER:N	2.93	0.42
5:4:33:LYS:NZ	7:A:2981:C:OP1	2.53	0.42
7:A:835:A:H2'	7:A:836:G:O4'	2.19	0.42
7:A:1011:G:N1	7:A:1024:U:H1'	2.35	0.42
25:T:20:SER:O	25:T:24:LEU:HD23	2.19	0.42
32:a:38:G:O2'	42:l:115:SER:O	2.33	0.42
34:d:119:ASN:ND2	34:d:141:ARG:HE	2.14	0.42
43:m:14:ARG:HD2	43:m:42:ASP:HA	2.02	0.42
47:q:121:SER:OG	47:q:122:ALA:N	2.52	0.42
49:s:81:LYS:HB2	49:s:81:LYS:HE2	1.77	0.42
52:y:63:C:H2'	52:y:64:G:C8	2.54	0.42
7:A:342:C:H2'	7:A:343:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:795:C:H2'	7:A:796:U:C6	2.55	0.42
7:A:1201:C:H5'	7:A:1203:G:OP2	2.20	0.42
7:A:1902:G:O2'	7:A:2229:U:O4	2.33	0.42
7:A:2887:U:H2'	7:A:2888:C:C6	2.54	0.42
15:J:99:ARG:HA	15:J:102:GLU:HG2	2.00	0.42
25:T:70:ARG:H	25:T:70:ARG:HD3	1.83	0.42
27:V:69:ILE:HG22	27:V:70:ALA:H	1.84	0.42
40:j:51:VAL:HB	44:n:41:ARG:HB2	2.02	0.42
7:A:530:U:H2'	7:A:531:G:C8	2.55	0.42
7:A:1204:C:H2'	7:A:1205:C:C6	2.54	0.42
7:A:1610:G:H2'	7:A:1611:U:C6	2.54	0.42
7:A:1915:U:H2'	7:A:1916:G:O4'	2.19	0.42
32:a:1405:C:H2'	32:a:1406:A:H8	1.84	0.42
34:d:134:GLN:NE2	34:d:135:TYR:CE2	2.88	0.42
40:j:67:MET:HE1	44:n:36:LYS:HD3	2.01	0.42
6:6:43:PRO:C	6:6:45:TYR:H	2.27	0.42
7:A:293:G:H8	7:A:338:G:H2'	1.85	0.42
7:A:1469:G:O2'	25:T:18:GLU:OE2	2.37	0.42
7:A:1825:A:H2'	7:A:1826:C:H6	1.84	0.42
7:A:2043:A:H2'	7:A:2044:A:C8	2.54	0.42
9:C:23:GLU:CD	9:C:23:GLU:H	2.27	0.42
17:L:21:VAL:HG23	17:L:28:LYS:HD2	2.02	0.42
19:N:65:GLU:O	19:N:68:LYS:HB2	2.19	0.42
32:a:156:A:H2'	32:a:157:A:O4'	2.18	0.42
32:a:668:U:H3	32:a:704:G:H22	1.68	0.42
32:a:735:C:H2'	32:a:736:A:C8	2.54	0.42
32:a:915:G:H2'	32:a:916:A:C8	2.55	0.42
32:a:1126:G:H2'	32:a:1126:G:N3	2.35	0.42
32:a:1171:A:H2'	32:a:1172:A:O4'	2.19	0.42
32:a:1395:4OC:H2'	32:a:1396:C:O4'	2.19	0.42
33:c:131:ARG:HG2	33:c:134:ARG:HH22	1.84	0.42
47:q:59:LYS:HD3	47:q:59:LYS:HA	1.79	0.42
50:t:30:THR:HA	50:t:33:ARG:HG2	2.01	0.42
7:A:2341:C:H2'	7:A:2342:G:H8	1.85	0.42
7:A:2775:U:H2'	7:A:2776:C:H6	1.83	0.42
32:a:78:U:C2	32:a:79:C:H5	2.38	0.42
32:a:466:C:H2'	32:a:467:G:N9	2.35	0.42
32:a:960:5MC:OP2	32:a:961:A:O2'	2.36	0.42
35:e:185:ALA:HB1	35:e:191:PRO:HA	2.02	0.42
7:A:285:G:C2	7:A:303:U:O2	2.73	0.42
7:A:1399:A:H2'	7:A:1400:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2338:G:C6	7:A:2425:U:N3	2.86	0.42
7:A:2351:A:O2'	7:A:2352:G:O4'	2.25	0.42
7:A:2393:G:C4	7:A:2394:G:H1'	2.55	0.42
7:A:2442:A:H2'	7:A:2443:A:C8	2.55	0.42
13:G:90:ILE:HD11	13:G:106:PHE:HE1	1.84	0.42
18:M:118:LEU:HD23	18:M:118:LEU:HA	1.90	0.42
31:Z:50:VAL:HG23	31:Z:53:LEU:HD12	2.02	0.42
32:a:1015:C:H2'	32:a:1016:G:C8	2.54	0.42
32:a:1435:G:OP2	32:a:1436:C:N4	2.30	0.42
35:e:117:GLN:OE1	35:e:126:LEU:HD13	2.20	0.42
42:l:114:ARG:HG3	42:l:119:ALA:HB3	2.01	0.42
2:1:40:LYS:HD3	7:A:2583:G:OP2	2.20	0.42
7:A:500:G:OP2	7:A:2644:A:O2'	2.33	0.42
7:A:581:G:H2'	7:A:582:G:O4'	2.19	0.42
7:A:1917:C:H2'	7:A:1918:C:H6	1.85	0.42
7:A:2049:A:OP2	9:C:54:LYS:NZ	2.53	0.42
12:F:101:ASP:OD1	12:F:102:ARG:N	2.53	0.42
26:U:86:ARG:HB2	26:U:97:ILE:HD13	2.02	0.42
32:a:1058:A:N1	32:a:1099:G:O2'	2.50	0.42
32:a:1512:MA6:H92	32:a:1513:G:O2'	2.20	0.42
34:d:118:PHE:CE1	34:d:140:VAL:HG22	2.55	0.42
34:d:183:ARG:HH12	34:d:189:PRO:HD2	1.84	0.42
35:e:106:PRO:HG2	35:e:178:LEU:HB3	2.01	0.42
35:e:106:PRO:HB3	35:e:180:ARG:HG2	2.02	0.42
41:k:104:GLU:OE1	41:k:104:GLU:N	2.53	0.42
7:A:780:G:N2	7:A:781:A:N1	2.44	0.42
7:A:913:G:H5'	7:A:914:G:OP1	2.20	0.42
7:A:962:G:H2'	7:A:963:C:C6	2.55	0.42
7:A:1049:G:H21	7:A:2507:A:H8	1.68	0.42
7:A:1185:G:H5'	7:A:1214:A:H2	1.85	0.42
7:A:1319:G:H5''	23:R:85:TYR:CE1	2.55	0.42
7:A:1720:G:H2'	7:A:1721:A:H8	1.85	0.42
7:A:2594:U:H2'	7:A:2595:U:O4'	2.20	0.42
11:E:30:LEU:HD23	11:E:118:ARG:HD3	2.02	0.42
23:R:37:SER:C	23:R:38:LEU:HD12	2.45	0.42
32:a:536:C:H5''	34:d:64:GLU:HG2	2.01	0.42
32:a:742:U:H2'	32:a:743:G:O4'	2.19	0.42
32:a:1233:G:H2'	32:a:1234:G:H8	1.85	0.42
33:c:67:ILE:HG23	33:c:102:ILE:HD13	2.02	0.42
33:c:90:LEU:HB3	33:c:98:VAL:HG21	2.01	0.42
34:d:94:ASP:OD1	34:d:95:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:107:LEU:HD21	35:e:151:VAL:HG22	2.00	0.42
35:e:119:GLU:OE1	35:e:124:VAL:HG22	2.19	0.42
46:p:70:VAL:O	46:p:74:LEU:HG	2.20	0.42
1:0:3:VAL:HG12	7:A:2253:A:N3	2.35	0.41
7:A:127:A:H5''	7:A:128:C:C6	2.54	0.41
7:A:285:G:O2'	7:A:288:U:H4'	2.20	0.41
7:A:308:G:O4'	14:H:41:ARG:NH1	2.53	0.41
7:A:403:G:H4'	7:A:405:A:N7	2.35	0.41
7:A:1580:A:N3	7:A:1623:G:H2'	2.35	0.41
7:A:1807:A:H2'	7:A:1808:A:C8	2.55	0.41
7:A:1978:G:H2'	7:A:1979:A:C8	2.55	0.41
7:A:2024:C:H2'	7:A:2025:A:C5	2.55	0.41
8:B:65:A:H61	8:B:103:A:H2'	1.85	0.41
16:K:8:LEU:HD13	16:K:84:ALA:HB2	2.02	0.41
26:U:79:LYS:HE2	26:U:79:LYS:HB2	1.88	0.41
30:Y:22:LEU:HD21	30:Y:58:TYR:CE1	2.55	0.41
32:a:453:G:H2'	32:a:454:U:C6	2.55	0.41
32:a:545:U:H2'	32:a:546:C:C6	2.55	0.41
32:a:901:A:H2'	32:a:902:A:H8	1.84	0.41
32:a:1398:G:O2'	32:a:1511:MA6:O2'	2.36	0.41
34:d:83:GLU:OE1	34:d:83:GLU:N	2.53	0.41
36:f:18:THR:C	36:f:21:PRO:HD2	2.45	0.41
46:p:74:LEU:HA	46:p:77:THR:HG22	2.02	0.41
7:A:219:G:H2'	7:A:220:G:C8	2.55	0.41
7:A:233:U:H2'	7:A:234:G:O4'	2.20	0.41
7:A:889:G:H2'	7:A:890:A:O4'	2.19	0.41
7:A:1349:A:H2'	7:A:1350:C:H6	1.85	0.41
7:A:1546:G:H2'	7:A:1547:C:C6	2.54	0.41
7:A:2340:A:N6	7:A:2424:A:C5	2.88	0.41
8:B:41:C:N4	12:F:95:ARG:HH12	2.17	0.41
32:a:108:G:H2'	32:a:109:U:C6	2.55	0.41
32:a:861:C:H2'	32:a:862:A:O4'	2.20	0.41
32:a:1297:G:H22	32:a:1323:G:H1'	1.85	0.41
32:a:1318:C:H2'	32:a:1319:C:H6	1.83	0.41
38:h:39:ILE:HG21	38:h:105:ILE:HD12	2.02	0.41
7:A:289:A:C5'	7:A:302:U:H3	2.33	0.41
7:A:1220:G:H2'	7:A:1221:C:H6	1.85	0.41
7:A:1548:G:O2'	7:A:1820:A:N1	2.34	0.41
7:A:2338:G:N1	7:A:2425:U:C2	2.87	0.41
7:A:2484:A:H2'	7:A:2485:A:C8	2.55	0.41
11:E:10:LYS:NZ	11:E:25:GLU:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:159:LYS:O	13:G:172:ARG:NH2	2.54	0.41
19:N:110:MET:HE3	19:N:110:MET:HB3	1.89	0.41
32:a:877:U:H4'	32:a:878:G:H5''	2.02	0.41
32:a:1051:U:H5	33:c:2:GLY:HA3	1.84	0.41
32:a:1109:U:H2'	32:a:1110:C:C6	2.55	0.41
32:a:1517:C:H2'	32:a:1518:G:C8	2.55	0.41
34:d:93:LEU:O	34:d:97:ILE:HG12	2.21	0.41
40:j:20:ALA:HA	40:j:23:ARG:HD3	2.03	0.41
5:4:12:ASP:OD2	5:4:13:LYS:N	2.54	0.41
7:A:582:G:H4'	24:S:16:LYS:HB2	2.01	0.41
7:A:1517:C:H2'	7:A:1518:G:H8	1.85	0.41
7:A:2252:A:H2'	7:A:2253:A:C8	2.54	0.41
7:A:2339:U:N3	7:A:2424:A:N6	2.68	0.41
12:F:8:GLN:NE2	12:F:13:GLU:OE2	2.49	0.41
12:F:142:GLN:NE2	12:F:156:VAL:HA	2.36	0.41
26:U:2:LYS:HD3	26:U:83:ILE:HB	2.02	0.41
32:a:44:G:H2'	32:a:45:G:H8	1.84	0.41
32:a:904:U:H2'	32:a:905:C:C6	2.55	0.41
32:a:1404:U:H2'	32:a:1405:C:H6	1.86	0.41
33:c:175:LEU:HD23	33:c:182:ILE:HD13	2.03	0.41
35:e:92:ALA:O	35:e:96:GLU:OE1	2.38	0.41
35:e:180:ARG:HB2	35:e:183:GLU:CD	2.44	0.41
42:l:71:GLY:O	42:l:99:ARG:NH2	2.40	0.41
46:p:71:LEU:HG	46:p:75:LYS:HE2	2.01	0.41
6:6:25:ARG:HH22	12:F:101:ASP:CG	2.28	0.41
7:A:683:C:H2'	7:A:684:U:C6	2.55	0.41
7:A:1027:U:H2'	7:A:1028:G:O4'	2.20	0.41
7:A:1818:C:H2'	7:A:1819:G:O4'	2.21	0.41
7:A:2036:A:H2'	7:A:2037:A:H8	1.82	0.41
7:A:2331:A:H5'	14:H:25:TYR:CD1	2.55	0.41
7:A:2335:U:H2'	7:A:2336:C:C6	2.56	0.41
7:A:2690:C:H2'	7:A:2691:A:C8	2.56	0.41
32:a:451:A:C8	46:p:46:PRO:HB2	2.55	0.41
32:a:713:G:O2'	32:a:714:U:H2'	2.20	0.41
32:a:836:C:H4'	32:a:837:U:O5'	2.21	0.41
32:a:894:A:C5	32:a:895:G:H1'	2.55	0.41
7:A:622:U:O2'	22:Q:49:ASP:OD2	2.32	0.41
7:A:1779:C:H2'	7:A:1780:G:O4'	2.20	0.41
7:A:2485:A:H2'	7:A:2486:C:H6	1.85	0.41
7:A:2551:C:O4'	12:F:44:ASN:ND2	2.54	0.41
9:C:125:ILE:HB	36:f:81:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:271:C:C2	32:a:272:A:C8	3.09	0.41
32:a:434:U:H2'	32:a:435:C:H6	1.86	0.41
32:a:653:C:H2'	32:a:654:A:C8	2.56	0.41
32:a:829:U:H2'	32:a:830:U:C6	2.54	0.41
32:a:1306:C:H2'	32:a:1307:U:H6	1.86	0.41
33:c:11:ARG:NH2	33:c:177:THR:O	2.50	0.41
35:e:50:ASN:OD1	35:e:65:THR:OG1	2.38	0.41
42:l:54:ARG:HA	42:l:54:ARG:HD2	1.92	0.41
52:y:1:C:H2'	52:y:2:G:C8	2.51	0.41
7:A:637:C:H2'	7:A:638:C:C5	2.56	0.41
7:A:731:A:H2'	17:L:76:ILE:HD11	2.03	0.41
7:A:858:G:H5'	7:A:859:C:H5''	2.03	0.41
7:A:1720:G:C6	7:A:1744:A:C6	3.08	0.41
7:A:1749:U:H2'	7:A:1750:C:C6	2.55	0.41
7:A:2302:C:H2'	7:A:2303:C:H6	1.84	0.41
7:A:2381:G:O2'	7:A:2383:C:OP2	2.27	0.41
7:A:2884:C:H2'	7:A:2885:U:O4'	2.20	0.41
8:B:86:C:H2'	8:B:87:C:O4'	2.20	0.41
32:a:44:G:H2'	32:a:45:G:C8	2.56	0.41
32:a:322:U:H2'	32:a:323:G:O4'	2.20	0.41
33:c:131:ARG:HG2	33:c:134:ARG:NH2	2.36	0.41
35:e:139:GLY:O	35:e:143:ARG:CB	2.68	0.41
42:l:107:VAL:CG2	42:l:117:TYR:HB3	2.51	0.41
42:l:116:ARG:C	42:l:118:GLY:H	2.28	0.41
49:s:10:PHE:O	49:s:39:THR:HG22	2.21	0.41
52:y:17:C:OP1	52:y:19:G:H5'	2.21	0.41
1:0:3:VAL:HG12	7:A:2253:A:C2	2.56	0.41
7:A:1221:C:H3'	7:A:1222:G:C8	2.54	0.41
7:A:1531:C:H2'	7:A:1532:G:C8	2.55	0.41
7:A:2366:C:H2'	7:A:2367:U:C2	2.56	0.41
7:A:2504:A:H4'	7:A:2505:A:N3	2.36	0.41
7:A:2915:G:H2'	7:A:2916:A:C8	2.55	0.41
26:U:43:LYS:HG2	26:U:44:HIS:H	1.86	0.41
26:U:89:GLU:CA	26:U:91:THR:H	2.33	0.41
32:a:500:A:H2'	32:a:501:A:C8	2.56	0.41
32:a:544:G:H2'	32:a:545:U:C6	2.56	0.41
32:a:1364:G:O3'	39:i:92:GLY:HA3	2.21	0.41
32:a:1457:G:H2'	32:a:1458:U:C6	2.54	0.41
34:d:80:LYS:HG2	34:d:81:THR:N	2.33	0.41
36:f:1:MET:HB2	36:f:66:LYS:NZ	2.36	0.41
48:r:35:THR:HG22	48:r:39:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:10:GLU:OE1	6:6:10:GLU:N	2.54	0.41
7:A:344:C:H2'	7:A:345:G:O4'	2.21	0.41
7:A:652:G:H2'	7:A:653:U:H5''	2.02	0.41
7:A:745:U:H2'	7:A:746:G:O4'	2.21	0.41
7:A:987:G:N3	7:A:2506:A:H2'	2.36	0.41
7:A:1165:G:C6	7:A:1249:G:C6	3.08	0.41
7:A:1193:C:N4	7:A:1198:A:H3'	2.33	0.41
7:A:2363:A:C5	7:A:2400:U:H1'	2.56	0.41
7:A:2474:C:H2'	7:A:2475:G:O4'	2.21	0.41
7:A:3048:C:H2'	7:A:3049:C:H6	1.84	0.41
8:B:24:A:H2'	8:B:25:A:C8	2.55	0.41
8:B:29:C:H2'	8:B:30:C:H5'	2.02	0.41
8:B:108:G:H2'	8:B:109:C:H6	1.85	0.41
20:O:13:ARG:HD2	20:O:102:TYR:CZ	2.56	0.41
27:V:68:ASP:HA	27:V:73:GLU:HA	2.03	0.41
28:W:46:HIS:HB2	28:W:77:THR:HG22	2.03	0.41
32:a:583:G:H2'	32:a:584:U:C6	2.55	0.41
32:a:631:A:O2'	38:h:109:SER:HB3	2.21	0.41
32:a:726:G:H2'	32:a:727:U:C6	2.56	0.41
32:a:991:G:H2'	32:a:992:C:H6	1.86	0.41
32:a:1062:C:H2'	32:a:1063:G:C8	2.55	0.41
32:a:1087:C:H2'	32:a:1088:C:H6	1.86	0.41
32:a:1307:U:H2'	32:a:1308:G:O4'	2.20	0.41
32:a:1395:4OC:H6	32:a:1395:4OC:O5'	2.21	0.41
32:a:1397:C:H2'	32:a:1398:G:C8	2.56	0.41
34:d:14:ARG:HA	34:d:14:ARG:HD3	1.96	0.41
34:d:32:PRO:HB3	34:d:38:ARG:HG3	2.03	0.41
34:d:145:LEU:HD22	34:d:172:ARG:NH1	2.35	0.41
37:g:18:TYR:O	37:g:20:SER:N	2.52	0.41
43:m:81:LYS:O	43:m:84:ILE:HG22	2.21	0.41
49:s:16:LEU:HA	49:s:16:LEU:HD12	1.86	0.41
50:t:59:ASP:OD1	50:t:76:LYS:NZ	2.48	0.41
7:A:272:A:OP2	7:A:315:G:N1	2.36	0.41
7:A:285:G:H3'	7:A:286:G:C5'	2.51	0.41
7:A:1623:G:H4'	7:A:1624:C:H6	1.86	0.41
7:A:2028:U:H2'	7:A:2029:C:H6	1.86	0.41
11:E:67:GLY:HA3	11:E:86:ARG:HG2	2.03	0.41
15:J:18:ILE:HD11	15:J:35:LEU:HD12	2.03	0.41
32:a:97:G:H2'	32:a:98:U:H6	1.86	0.41
32:a:670:C:H2'	32:a:671:C:H6	1.86	0.41
38:h:22:HIS:O	38:h:66:TYR:OH	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:40:VAL:O	40:j:72:ARG:HA	2.21	0.41
52:y:67:C:H2'	52:y:68:C:C6	2.55	0.41
7:A:871:U:H2'	7:A:872:A:H8	1.84	0.40
7:A:1577:C:H2'	7:A:1578:C:H6	1.85	0.40
7:A:1980:U:H2'	7:A:1981:C:H6	1.82	0.40
7:A:1981:C:H2'	7:A:1982:C:C6	2.56	0.40
7:A:2142:G:O2'	7:A:2166:A:N1	2.46	0.40
11:E:161:LEU:HB2	11:E:197:ALA:HB2	2.02	0.40
20:O:21:ARG:NH1	20:O:24:LEU:O	2.54	0.40
23:R:31:GLU:N	23:R:34:GLU:OE1	2.54	0.40
32:a:453:G:OP2	46:p:72:LYS:HE3	2.22	0.40
32:a:537:G:N7	34:d:63:MET:HE1	2.36	0.40
32:a:571:C:H2'	32:a:572:G:O4'	2.21	0.40
34:d:124:HIS:ND1	34:d:141:ARG:HD2	2.36	0.40
39:i:31:GLY:O	39:i:99:ALA:HB1	2.22	0.40
42:l:70:GLU:HG2	42:l:70:GLU:O	2.21	0.40
42:l:99:ARG:HB2	42:l:117:TYR:HA	2.02	0.40
7:A:199:A:N6	7:A:2668:A:H2'	2.36	0.40
7:A:320:G:H2'	7:A:321:G:C8	2.56	0.40
7:A:621:G:H2'	7:A:622:U:C6	2.56	0.40
7:A:857:G:H4'	9:C:13:ARG:HD2	2.03	0.40
7:A:957:U:H2'	7:A:958:A:C8	2.57	0.40
7:A:1076:C:H1'	7:A:1113:G:C8	2.56	0.40
7:A:2805:G:H2'	7:A:2806:C:C6	2.55	0.40
14:H:8:ASP:N	14:H:8:ASP:OD1	2.55	0.40
17:L:82:ILE:HD13	17:L:82:ILE:HA	1.91	0.40
19:N:38:GLU:OE2	19:N:42:ARG:NH2	2.43	0.40
21:P:52:GLY:O	21:P:55:ARG:HG2	2.20	0.40
22:Q:19:LYS:HD2	22:Q:22:ARG:NH2	2.36	0.40
26:U:41:ILE:HD13	26:U:41:ILE:HA	1.96	0.40
32:a:543:U:C2	32:a:544:G:C8	3.09	0.40
34:d:50:LEU:O	34:d:54:GLN:HG2	2.21	0.40
38:h:27:LEU:HD11	38:h:60:LEU:HD23	2.02	0.40
7:A:933:A:H5''	7:A:934:G:OP1	2.21	0.40
7:A:1567:U:C5	7:A:1632:G:H5''	2.56	0.40
7:A:1814:C:H2'	7:A:1815:U:C6	2.56	0.40
7:A:1959:A:H2	7:A:1970:G:N2	2.19	0.40
19:N:24:LEU:HB3	19:N:44:LEU:HD22	2.03	0.40
32:a:263:C:H2'	32:a:264:G:O4'	2.21	0.40
32:a:331:G:OP2	50:t:5:LYS:HD2	2.22	0.40
32:a:411:U:O3'	32:a:413:A:H4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:566:G:O2'	32:a:812:G:OP2	2.37	0.40
32:a:1306:C:OP2	49:s:4:SER:OG	2.39	0.40
32:a:1365:U:H2'	32:a:1366:G:O4'	2.22	0.40
39:i:47:GLY:H	39:i:83:ASP:HB3	1.86	0.40
52:y:52:C:C2	52:y:53:G:C8	3.09	0.40
4:3:28:ASN:ND2	7:A:2599:A:O3'	2.54	0.40
7:A:72:U:C6	30:Y:58:TYR:HD2	2.39	0.40
7:A:743:U:H2'	7:A:744:C:C6	2.57	0.40
7:A:1084:G:H5''	18:M:77:LYS:HE2	2.04	0.40
7:A:2345:U:H5	7:A:2417:U:H3	1.68	0.40
7:A:2371:A:H5''	7:A:2395:A:H4'	2.03	0.40
7:A:2886:G:H2'	7:A:2887:U:H6	1.85	0.40
9:C:146:GLU:HG2	9:C:152:GLY:C	2.46	0.40
21:P:51:GLY:HA2	21:P:56:GLU:HG3	2.03	0.40
32:a:570:U:H2'	32:a:571:C:C6	2.56	0.40
32:a:1440:A:P	32:a:1441:C:H41	2.45	0.40
33:c:175:LEU:HD23	33:c:175:LEU:HA	1.94	0.40
35:e:63:SER:OG	35:e:64:PHE:N	2.54	0.40
39:i:105:ALA:O	39:i:109:ILE:HG12	2.21	0.40
43:m:65:LYS:HB2	43:m:65:LYS:HE3	1.78	0.40
47:q:105:VAL:O	47:q:105:VAL:HG13	2.20	0.40
7:A:288:U:O2'	7:A:290:A:OP2	2.22	0.40
7:A:992:A:H2'	7:A:993:G:H8	1.83	0.40
7:A:1130:A:H2'	7:A:1131:G:O4'	2.21	0.40
7:A:1584:C:H2'	7:A:1585:G:O4'	2.21	0.40
7:A:2347:G:H4'	7:A:2384:A:N6	2.37	0.40
7:A:3045:A:H2'	7:A:3046:G:O4'	2.22	0.40
9:C:16:ALA:HB2	9:C:207:GLY:HA3	2.03	0.40
22:Q:76:TYR:CZ	22:Q:80:ILE:HG13	2.55	0.40
22:Q:80:ILE:HD13	22:Q:80:ILE:HA	1.94	0.40
30:Y:18:LEU:HD23	30:Y:18:LEU:HA	1.91	0.40
32:a:192:A:H2'	32:a:193:U:O4'	2.21	0.40
32:a:375:G:C2	32:a:388:A:C2	3.09	0.40
34:d:42:LYS:NZ	34:d:44:SER:HB3	2.37	0.40
37:g:65:ALA:O	37:g:69:VAL:HG22	2.22	0.40
44:n:27:CYS:SG	44:n:29:ARG:HB2	2.62	0.40
47:q:69:LYS:H	47:q:69:LYS:HG2	1.68	0.40
49:s:36:ARG:NH1	49:s:53:ASP:HA	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	52/57 (91%)	52 (100%)	0	0	100	100
2	1	46/55 (84%)	46 (100%)	0	0	100	100
3	2	40/47 (85%)	39 (98%)	1 (2%)	0	100	100
4	3	60/64 (94%)	60 (100%)	0	0	100	100
5	4	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
6	6	53/80 (66%)	46 (87%)	7 (13%)	0	100	100
9	C	270/280 (96%)	259 (96%)	11 (4%)	0	100	100
10	D	211/217 (97%)	198 (94%)	13 (6%)	0	100	100
11	E	205/223 (92%)	201 (98%)	4 (2%)	0	100	100
12	F	176/187 (94%)	162 (92%)	12 (7%)	2 (1%)	11	29
13	G	172/179 (96%)	162 (94%)	10 (6%)	0	100	100
14	H	45/152 (30%)	41 (91%)	4 (9%)	0	100	100
15	J	144/195 (74%)	141 (98%)	3 (2%)	0	100	100
16	K	119/122 (98%)	113 (95%)	6 (5%)	0	100	100
17	L	141/146 (97%)	127 (90%)	13 (9%)	1 (1%)	18	41
18	M	132/138 (96%)	122 (92%)	10 (8%)	0	100	100
19	N	114/180 (63%)	113 (99%)	1 (1%)	0	100	100
20	O	114/122 (93%)	107 (94%)	7 (6%)	0	100	100
21	P	110/113 (97%)	103 (94%)	7 (6%)	0	100	100
22	Q	120/129 (93%)	117 (98%)	3 (2%)	0	100	100
23	R	98/104 (94%)	87 (89%)	10 (10%)	1 (1%)	12	32
24	S	111/197 (56%)	108 (97%)	3 (3%)	0	100	100
25	T	96/100 (96%)	89 (93%)	7 (7%)	0	100	100
26	U	86/105 (82%)	74 (86%)	11 (13%)	1 (1%)	10	27
27	V	93/215 (43%)	85 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	W	69/86 (80%)	65 (94%)	4 (6%)	0	100	100
29	X	61/64 (95%)	56 (92%)	5 (8%)	0	100	100
30	Y	63/77 (82%)	60 (95%)	3 (5%)	0	100	100
31	Z	57/65 (88%)	55 (96%)	2 (4%)	0	100	100
33	c	205/274 (75%)	187 (91%)	18 (9%)	0	100	100
34	d	198/201 (98%)	174 (88%)	24 (12%)	0	100	100
35	e	158/220 (72%)	140 (89%)	18 (11%)	0	100	100
36	f	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
37	g	150/156 (96%)	144 (96%)	6 (4%)	0	100	100
38	h	128/132 (97%)	124 (97%)	4 (3%)	0	100	100
39	i	125/151 (83%)	107 (86%)	18 (14%)	0	100	100
40	j	97/101 (96%)	85 (88%)	12 (12%)	0	100	100
41	k	115/139 (83%)	110 (96%)	5 (4%)	0	100	100
42	l	120/124 (97%)	90 (75%)	29 (24%)	1 (1%)	16	37
43	m	114/124 (92%)	102 (90%)	12 (10%)	0	100	100
44	n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	o	85/89 (96%)	77 (91%)	7 (8%)	1 (1%)	10	27
46	p	89/162 (55%)	78 (88%)	10 (11%)	1 (1%)	11	29
47	q	91/135 (67%)	75 (82%)	16 (18%)	0	100	100
48	r	61/84 (73%)	56 (92%)	5 (8%)	0	100	100
49	s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	t	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
51	v	20/24 (83%)	20 (100%)	0	0	100	100
All	All	5161/6188 (83%)	4780 (93%)	373 (7%)	8 (0%)	44	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	F	144	VAL
23	R	51	THR
42	l	114	ARG
12	F	143	ALA
17	L	5	LEU
26	U	91	THR

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Mol	Chain	Res	Type
45	o	19	GLU
46	p	46	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	44/47 (94%)	44 (100%)	0	100	100
2	1	45/51 (88%)	45 (100%)	0	100	100
3	2	36/40 (90%)	36 (100%)	0	100	100
4	3	53/54 (98%)	53 (100%)	0	100	100
5	4	35/35 (100%)	35 (100%)	0	100	100
6	6	49/66 (74%)	49 (100%)	0	100	100
9	C	212/219 (97%)	212 (100%)	0	100	100
10	D	163/166 (98%)	163 (100%)	0	100	100
11	E	159/172 (92%)	159 (100%)	0	100	100
12	F	147/155 (95%)	147 (100%)	0	100	100
13	G	143/147 (97%)	143 (100%)	0	100	100
14	H	36/121 (30%)	36 (100%)	0	100	100
15	J	120/161 (74%)	120 (100%)	0	100	100
16	K	100/101 (99%)	100 (100%)	0	100	100
17	L	107/110 (97%)	107 (100%)	0	100	100
18	M	110/114 (96%)	110 (100%)	0	100	100
19	N	94/139 (68%)	94 (100%)	0	100	100
20	O	88/93 (95%)	88 (100%)	0	100	100
21	P	98/99 (99%)	98 (100%)	0	100	100
22	Q	95/99 (96%)	95 (100%)	0	100	100
23	R	81/83 (98%)	81 (100%)	0	100	100
24	S	87/140 (62%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	T	82/83 (99%)	82 (100%)	0	100	100
26	U	77/88 (88%)	77 (100%)	0	100	100
27	V	75/164 (46%)	75 (100%)	0	100	100
28	W	51/62 (82%)	51 (100%)	0	100	100
29	X	52/52 (100%)	52 (100%)	0	100	100
30	Y	58/66 (88%)	58 (100%)	0	100	100
31	Z	51/55 (93%)	51 (100%)	0	100	100
33	c	170/210 (81%)	170 (100%)	0	100	100
34	d	176/177 (99%)	175 (99%)	1 (1%)	78	91
35	e	114/159 (72%)	114 (100%)	0	100	100
36	f	84/85 (99%)	84 (100%)	0	100	100
37	g	127/131 (97%)	127 (100%)	0	100	100
38	h	106/108 (98%)	106 (100%)	0	100	100
39	i	102/120 (85%)	102 (100%)	0	100	100
40	j	89/90 (99%)	89 (100%)	0	100	100
41	k	90/107 (84%)	90 (100%)	0	100	100
42	l	104/105 (99%)	104 (100%)	0	100	100
43	m	99/104 (95%)	99 (100%)	0	100	100
44	n	46/47 (98%)	46 (100%)	0	100	100
45	o	77/79 (98%)	77 (100%)	0	100	100
46	p	75/125 (60%)	75 (100%)	0	100	100
47	q	84/105 (80%)	84 (100%)	0	100	100
48	r	53/72 (74%)	53 (100%)	0	100	100
49	s	75/85 (88%)	75 (100%)	0	100	100
50	t	62/65 (95%)	62 (100%)	0	100	100
51	v	18/20 (90%)	18 (100%)	0	100	100
All	All	4299/4976 (86%)	4298 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	d	126	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
6	6	20	ASN
9	C	53	HIS
9	C	87	ASN
9	C	96	HIS
10	D	34	ASN
10	D	130	HIS
11	E	97	HIS
11	E	190	ASN
11	E	214	ASN
12	F	34	GLN
17	L	126	HIS
18	M	9	HIS
18	M	39	HIS
19	N	17	GLN
19	N	54	HIS
20	O	48	ASN
20	O	118	ASN
21	P	2	ASN
22	Q	39	GLN
22	Q	72	ASN
24	S	51	GLN
25	T	41	GLN
27	V	7	ASN
27	V	8	GLN
33	c	6	ASN
33	c	99	GLN
33	c	152	GLN
33	c	176	HIS
34	d	95	ASN
34	d	126	ASN
34	d	173	GLN
34	d	193	GLN
41	k	79	ASN
42	l	112	GLN
45	o	7	GLN
45	o	28	GLN
45	o	48	HIS
45	o	50	HIS
46	p	41	HIS
46	p	65	GLN
49	s	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	a	1518/1537 (98%)	211 (13%)	0
52	y	76/77 (98%)	15 (19%)	0
7	A	3116/3138 (99%)	441 (14%)	2 (0%)
8	B	114/115 (99%)	13 (11%)	0
All	All	4824/4867 (99%)	680 (14%)	2 (0%)

All (680) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	13	A
7	A	35	G
7	A	44	A
7	A	51	G
7	A	63	A
7	A	71	A
7	A	74	U
7	A	75	G
7	A	94	C
7	A	118	A
7	A	119	A
7	A	120	U
7	A	125	A
7	A	143	G
7	A	167	A
7	A	176	G
7	A	183	A
7	A	198	A
7	A	201	A
7	A	217	G
7	A	218	A
7	A	224	A
7	A	225	A
7	A	231	U
7	A	232	G
7	A	250	G
7	A	269	G
7	A	274	A
7	A	279	A
7	A	284	U
7	A	286	G
7	A	287	G

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Mol	Chain	Res	Type
7	A	288	U
7	A	289	A
7	A	290	A
7	A	291	C
7	A	293	G
7	A	294	G
7	A	297	A
7	A	301	G
7	A	302	U
7	A	303	U
7	A	308	G
7	A	320	G
7	A	327	U
7	A	328	A
7	A	330	G
7	A	331	U
7	A	332	C
7	A	339	C
7	A	358	U
7	A	362	A
7	A	370	G
7	A	371	U
7	A	372	G
7	A	377	G
7	A	394	U
7	A	399	U
7	A	413	A
7	A	414	G
7	A	446	A
7	A	447	G
7	A	448	U
7	A	475	G
7	A	500	G
7	A	501	A
7	A	526	U
7	A	544	U
7	A	570	G
7	A	592	G
7	A	593	A
7	A	595	U
7	A	596	A
7	A	597	C

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Mol	Chain	Res	Type
7	A	616	A
7	A	618	U
7	A	619	C
7	A	620	C
7	A	621	G
7	A	636	U
7	A	637	C
7	A	639	U
7	A	641	U
7	A	642	C
7	A	643	C
7	A	645	G
7	A	646	A
7	A	653	U
7	A	665	G
7	A	673	A
7	A	675	G
7	A	677	A
7	A	689	G
7	A	693	G
7	A	694	G
7	A	706	A
7	A	738	G
7	A	741	A
7	A	750	A
7	A	758	C
7	A	759	C
7	A	760	A
7	A	770	A
7	A	772	G
7	A	773	C
7	A	776	G
7	A	779	U
7	A	780	G
7	A	781	A
7	A	782	A
7	A	783	U
7	A	784	A
7	A	799	A
7	A	815	U
7	A	824	G
7	A	843	U

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Mol	Chain	Res	Type
7	A	846	G
7	A	859	C
7	A	869	C
7	A	876	U
7	A	891	U
7	A	893	A
7	A	894	G
7	A	904	G
7	A	905	G
7	A	911	A
7	A	913	G
7	A	914	G
7	A	921	A
7	A	934	G
7	A	941	C
7	A	956	U
7	A	957	U
7	A	958	A
7	A	988	G
7	A	1007	G
7	A	1025	A
7	A	1039	A
7	A	1043	C
7	A	1059	A
7	A	1061	A
7	A	1069	A
7	A	1074	G
7	A	1086	U
7	A	1087	A
7	A	1089	G
7	A	1096	A
7	A	1103	A
7	A	1112	A
7	A	1114	C
7	A	1125	G
7	A	1138	A
7	A	1142	G
7	A	1155	G
7	A	1162	U
7	A	1168	G
7	A	1175	A
7	A	1177	A

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Mol	Chain	Res	Type
7	A	1187	G
7	A	1188	G
7	A	1189	U
7	A	1190	U
7	A	1191	G
7	A	1192	G
7	A	1193	C
7	A	1196	A
7	A	1198	A
7	A	1199	A
7	A	1200	G
7	A	1202	A
7	A	1206	A
7	A	1207	C
7	A	1208	C
7	A	1212	G
7	A	1216	G
7	A	1217	A
7	A	1223	U
7	A	1230	U
7	A	1232	A
7	A	1233	C
7	A	1239	A
7	A	1240	A
7	A	1249	G
7	A	1257	A
7	A	1259	U
7	A	1261	U
7	A	1262	A
7	A	1264	C
7	A	1271	C
7	A	1273	A
7	A	1301	A
7	A	1304	U
7	A	1305	U
7	A	1306	G
7	A	1308	G
7	A	1309	G
7	A	1342	C
7	A	1368	A
7	A	1378	A
7	A	1381	G

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Mol	Chain	Res	Type
7	A	1384	A
7	A	1387	G
7	A	1402	G
7	A	1403	A
7	A	1432	A
7	A	1452	C
7	A	1483	U
7	A	1491	G
7	A	1496	A
7	A	1499	G
7	A	1510	U
7	A	1515	A
7	A	1526	A
7	A	1551	C
7	A	1552	G
7	A	1560	U
7	A	1561	C
7	A	1562	A
7	A	1563	G
7	A	1567	U
7	A	1568	A
7	A	1572	A
7	A	1580	A
7	A	1581	A
7	A	1582	A
7	A	1588	U
7	A	1609	U
7	A	1610	G
7	A	1615	G
7	A	1622	G
7	A	1624	C
7	A	1626	G
7	A	1636	U
7	A	1646	G
7	A	1657	A
7	A	1658	A
7	A	1666	C
7	A	1690	A
7	A	1693	G
7	A	1696	A
7	A	1697	A
7	A	1698	C

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Mol	Chain	Res	Type
7	A	1699	A
7	A	1705	G
7	A	1720	G
7	A	1727	A
7	A	1730	C
7	A	1731	A
7	A	1746	U
7	A	1754	A
7	A	1772	G
7	A	1773	U
7	A	1774	U
7	A	1791	U
7	A	1803	A
7	A	1806	A
7	A	1821	G
7	A	1832	G
7	A	1842	C
7	A	1843	A
7	A	1845	A
7	A	1881	U
7	A	1883	C
7	A	1888	U
7	A	1889	A
7	A	1909	G
7	A	1949	U
7	A	1950	A
7	A	1959	A
7	A	1960	C
7	A	1961	C
7	A	1963	U
7	A	1964	U
7	A	1990	G
7	A	1992	A
7	A	1998	U
7	A	2007	A
7	A	2010	G
7	A	2016	U
7	A	2020	A
7	A	2034	C
7	A	2035	G
7	A	2050	U
7	A	2063	A

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Mol	Chain	Res	Type
7	A	2105	G
7	A	2107	A
7	A	2108	A
7	A	2109	G
7	A	2110	G
7	A	2124	U
7	A	2144	G
7	A	2152	C
7	A	2157	A
7	A	2161	U
7	A	2165	A
7	A	2167	G
7	A	2168	G
7	A	2175	A
7	A	2176	A
7	A	2193	U
7	A	2205	C
7	A	2208	A
7	A	2209	U
7	A	2210	G
7	A	2229	U
7	A	2231	U
7	A	2261	A
7	A	2269	A
7	A	2270	G
7	A	2271	A
7	A	2274	C
7	A	2281	C
7	A	2293	C
7	A	2294	G
7	A	2297	A
7	A	2298	A
7	A	2299	G
7	A	2300	A
7	A	2330	G
7	A	2340	A
7	A	2343	G
7	A	2344	U
7	A	2346	U
7	A	2348	U
7	A	2349	G
7	A	2352	G

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Mol	Chain	Res	Type
7	A	2353	G
7	A	2354	A
7	A	2355	U
7	A	2356	A
7	A	2360	G
7	A	2361	G
7	A	2362	G
7	A	2364	G
7	A	2366	C
7	A	2367	U
7	A	2368	G
7	A	2369	U
7	A	2370	G
7	A	2371	A
7	A	2377	C
7	A	2378	G
7	A	2381	G
7	A	2382	C
7	A	2384	A
7	A	2385	G
7	A	2387	U
7	A	2388	G
7	A	2389	G
7	A	2391	G
7	A	2393	G
7	A	2394	G
7	A	2395	A
7	A	2396	G
7	A	2398	C
7	A	2400	U
7	A	2401	U
7	A	2402	G
7	A	2403	U
7	A	2405	G
7	A	2408	A
7	A	2412	C
7	A	2413	A
7	A	2416	C
7	A	2417	U
7	A	2419	A
7	A	2424	A
7	A	2429	G

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Mol	Chain	Res	Type
7	A	2435	A
7	A	2448	G
7	A	2463	A
7	A	2476	G
7	A	2477	G
7	A	2489	OMG
7	A	2517	G
7	A	2520	G
7	A	2521	C
7	A	2524	A
7	A	2525	A
7	A	2526	A
7	A	2543	A
7	A	2546	G
7	A	2547	C
7	A	2558	C
7	A	2563	G
7	A	2573	A
7	A	2585	C
7	A	2588	C
7	A	2621	G
7	A	2623	A
7	A	2641	C
7	A	2644	A
7	A	2656	G
7	A	2661	U
7	A	2663	A
7	A	2667	G
7	A	2668	A
7	A	2679	C
7	A	2686	A
7	A	2712	C
7	A	2714	A
7	A	2743	G
7	A	2751	G
7	A	2756	A
7	A	2767	G
7	A	2773	G
7	A	2804	A
7	A	2805	G
7	A	2811	C
7	A	2840	A

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Mol	Chain	Res	Type
7	A	2847	U
7	A	2851	U
7	A	2853	U
7	A	2868	A
7	A	2884	C
7	A	2901	G
7	A	2908	G
7	A	2952	G
7	A	2962	C
7	A	2964	C
7	A	2967	U
7	A	2982	G
7	A	2986	A
7	A	2990	C
7	A	3003	A
7	A	3016	A
7	A	3018	C
7	A	3037	G
7	A	3038	U
7	A	3040	G
7	A	3047	G
7	A	3056	A
7	A	3070	A
7	A	3107	A
7	A	3114	G
7	A	3118	A
7	A	3119	C
7	A	3120	C
7	A	3127	A
7	A	3128	A
7	A	3129	A
8	B	2	U
8	B	4	C
8	B	29	C
8	B	41	C
8	B	44	A
8	B	55	U
8	B	56	A
8	B	65	A
8	B	86	C
8	B	88	G
8	B	101	G

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Mol	Chain	Res	Type
8	B	105	A
8	B	114	C
32	a	9	G
32	a	10	G
32	a	12	G
32	a	25	G
32	a	35	A
32	a	42	G
32	a	50	C
32	a	51	U
32	a	54	A
32	a	62	A
32	a	81	C
32	a	84	C
32	a	86	G
32	a	89	A
32	a	90	U
32	a	91	A
32	a	93	U
32	a	115	A
32	a	116	C
32	a	125	G
32	a	126	A
32	a	127	U
32	a	140	U
32	a	142	G
32	a	152	U
32	a	167	A
32	a	169	U
32	a	178	G
32	a	185	G
32	a	189	U
32	a	194	G
32	a	204	G
32	a	208	A
32	a	213	U
32	a	214	U
32	a	215	U
32	a	216	A
32	a	217	G
32	a	219	G
32	a	244	C

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Mol	Chain	Res	Type
32	a	246	G
32	a	247	C
32	a	250	G
32	a	265	G
32	a	266	C
32	a	279	C
32	a	288	G
32	a	320	A
32	a	328	A
32	a	346	G
32	a	350	G
32	a	351	C
32	a	353	G
32	a	362	A
32	a	366	U
32	a	371	C
32	a	387	G
32	a	391	C
32	a	396	A
32	a	397	C
32	a	405	G
32	a	409	G
32	a	410	A
32	a	411	U
32	a	412	G
32	a	413	A
32	a	414	C
32	a	420	U
32	a	421	C
32	a	428	U
32	a	437	U
32	a	451	A
32	a	452	G
32	a	453	G
32	a	455	C
32	a	456	C
32	a	459	G
32	a	460	U
32	a	461	U
32	a	463	U
32	a	465	U
32	a	467	G

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Mol	Chain	Res	Type
32	a	468	G
32	a	471	U
32	a	473	A
32	a	476	G
32	a	486	A
32	a	488	G
32	a	502	C
32	a	509	C
32	a	512	G
32	a	517	C
32	a	518	G7M
32	a	523	A
32	a	524	A
32	a	538	A
32	a	553	U
32	a	555	C
32	a	563	A
32	a	564	A
32	a	567	A
32	a	568	G
32	a	570	U
32	a	587	C
32	a	604	C
32	a	623	U
32	a	624	G
32	a	644	A
32	a	656	G
32	a	678	A
32	a	686	A
32	a	694	G
32	a	712	G
32	a	715	G
32	a	740	A
32	a	746	G
32	a	750	A
32	a	768	A
32	a	784	U
32	a	785	A
32	a	806	A
32	a	808	C
32	a	810	G
32	a	812	G

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Mol	Chain	Res	Type
32	a	830	U
32	a	833	U
32	a	835	C
32	a	836	C
32	a	837	U
32	a	838	U
32	a	883	G
32	a	895	G
32	a	900	A
32	a	907	A
32	a	915	G
32	a	919	G
32	a	927	C
32	a	928	A
32	a	953	U
32	a	959	2MG
32	a	962	A
32	a	964	G
32	a	968	A
32	a	969	G
32	a	970	A
32	a	985	U
32	a	986	G
32	a	993	A
32	a	997	G
32	a	1018	U
32	a	1019	C
32	a	1021	C
32	a	1022	U
32	a	1023	U
32	a	1024	G
32	a	1031	G
32	a	1033	G
32	a	1056	U
32	a	1085	G
32	a	1086	U
32	a	1092	A
32	a	1126	G
32	a	1129	A
32	a	1131	G
32	a	1132	G
32	a	1150	C

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Mol	Chain	Res	Type
32	a	1151	U
32	a	1159	U
32	a	1161	A
32	a	1174	G
32	a	1176	G
32	a	1188	A
32	a	1189	A
32	a	1199	C
32	a	1204	U
32	a	1205	A
32	a	1219	A
32	a	1230	A
32	a	1249	U
32	a	1250	G
32	a	1252	G
32	a	1270	G
32	a	1272	A
32	a	1274	C
32	a	1279	A
32	a	1292	G
32	a	1294	U
32	a	1297	G
32	a	1312	C
32	a	1332	G
32	a	1338	A
32	a	1355	A
32	a	1356	A
32	a	1357	C
32	a	1363	G
32	a	1390	C
32	a	1391	A
32	a	1435	G
32	a	1436	C
32	a	1439	A
32	a	1444	U
32	a	1480	G
32	a	1485	A
32	a	1486	A
32	a	1490	G
32	a	1502	C
32	a	1510	G
32	a	1512	MA6

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Mol	Chain	Res	Type
32	a	1522	G
32	a	1523	G
32	a	1524	A
52	y	5	G
52	y	13	C
52	y	17	C
52	y	18	U
52	y	20	G
52	y	21	U
52	y	22	A
52	y	44	A
52	y	47	G
52	y	48	U
52	y	49	C
52	y	53	G
52	y	74	A
52	y	75	C
52	y	77	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	913	G
7	A	3127	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	5MU	A	2177	7,55	19,22,23	2.38	8 (42%)	27,32,35	2.38	6 (22%)
32	MA6	a	1512	32	23,26,27	1.38	3 (13%)	33,38,41	2.17	11 (33%)
32	UR3	a	1491	32	19,22,23	2.70	6 (31%)	26,32,35	1.57	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	a	960	32	19,22,23	3.17	6 (31%)	26,32,35	1.21	4 (15%)
7	6MZ	A	2296	7	22,25,26	3.22	6 (27%)	29,36,39	2.13	10 (34%)
32	G7M	a	518	32	23,26,27	3.01	4 (17%)	34,39,42	1.85	7 (20%)
32	MA6	a	1511	32	23,26,27	1.40	3 (13%)	33,38,41	2.13	9 (27%)
7	OMG	A	2489	52,7	23,26,27	2.73	4 (17%)	32,38,41	1.92	8 (25%)
7	OMC	A	2736	7,55	19,22,23	1.95	6 (31%)	25,31,34	0.96	1 (4%)
32	2MG	a	1509	32	23,26,27	2.53	6 (26%)	33,38,41	2.20	12 (36%)
7	OMG	A	2791	7	23,26,27	2.74	4 (17%)	32,38,41	1.87	10 (31%)
32	2MG	a	959	32	23,26,27	2.51	6 (26%)	33,38,41	2.30	12 (36%)
7	6MZ	A	2268	7	22,25,26	3.05	8 (36%)	29,36,39	3.14	11 (37%)
32	4OC	a	1395	32	20,23,24	2.74	6 (30%)	25,32,35	1.17	3 (12%)

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
7	5MU	A	2177	7,55	-	0/7/25/26	0/2/2/2
32	MA6	a	1512	32	-	2/11/29/30	0/3/3/3
32	UR3	a	1491	32	-	0/7/25/26	0/2/2/2
32	5MC	a	960	32	-	0/7/25/26	0/2/2/2
7	6MZ	A	2296	7	-	2/9/27/28	0/3/3/3
32	G7M	a	518	32	-	1/7/25/26	0/3/3/3
32	MA6	a	1511	32	-	1/11/29/30	0/3/3/3
7	OMG	A	2489	52,7	-	3/9/27/28	0/3/3/3
7	OMC	A	2736	7,55	-	0/9/27/28	0/2/2/2
32	2MG	a	1509	32	-	0/9/27/28	0/3/3/3
7	OMG	A	2791	7	-	0/9/27/28	0/3/3/3
32	2MG	a	959	32	-	2/9/27/28	0/3/3/3
7	6MZ	A	2268	7	-	2/9/27/28	0/3/3/3
32	4OC	a	1395	32	-	2/9/29/30	0/2/2/2

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2296	6MZ	C6-N6	12.87	1.48	1.34
32	a	518	G7M	O6-C6	11.89	1.46	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	960	5MC	C5-C4	-11.51	1.35	1.44
7	A	2268	6MZ	C6-N6	11.41	1.47	1.34
7	A	2791	OMG	O6-C6	10.76	1.44	1.23
7	A	2489	OMG	O6-C6	10.54	1.43	1.23
32	a	1395	4OC	O2-C2	9.50	1.41	1.23
32	a	1509	2MG	O6-C6	8.71	1.40	1.23
32	a	959	2MG	O6-C6	8.71	1.40	1.23
32	a	1491	UR3	O4-C4	7.64	1.39	1.23
32	a	518	G7M	C2-N2	6.10	1.48	1.34
7	A	2791	OMG	C2-N2	5.63	1.47	1.34
7	A	2489	OMG	C2-N2	5.53	1.47	1.34
32	a	959	2MG	C2-N2	5.39	1.44	1.33
32	a	1509	2MG	C2-N2	5.30	1.44	1.33
32	a	1491	UR3	C2-N1	-5.18	1.31	1.38
7	A	2296	6MZ	C8-N9	-4.61	1.29	1.37
7	A	2177	5MU	C2-N1	-4.56	1.31	1.38
7	A	2736	OMC	C4-N4	4.45	1.44	1.33
7	A	2268	6MZ	C8-N9	-4.44	1.30	1.37
32	a	960	5MC	C2-N1	-4.29	1.31	1.40
7	A	2268	6MZ	C5-N7	-4.24	1.31	1.39
32	a	1491	UR3	C2-N3	-4.22	1.30	1.39
32	a	960	5MC	C4-N4	4.18	1.44	1.34
7	A	2177	5MU	C4-C5	-4.15	1.38	1.44
32	a	1395	4OC	C2-N1	-4.11	1.31	1.40
7	A	2177	5MU	C2-N3	-4.03	1.31	1.38
32	a	1395	4OC	C4-N4	4.02	1.44	1.36
7	A	2296	6MZ	C5-N7	-4.01	1.31	1.39
7	A	2736	OMC	C2-N1	-4.01	1.31	1.40
32	a	1511	MA6	C6-N6	4.00	1.47	1.36
7	A	2177	5MU	C4-N3	-3.98	1.31	1.38
32	a	1512	MA6	C6-N6	3.90	1.47	1.36
32	a	1509	2MG	C6-N1	-3.81	1.31	1.38
32	a	518	G7M	C5-N7	-3.76	1.34	1.39
32	a	1491	UR3	O2-C2	-3.68	1.15	1.22
32	a	959	2MG	C6-N1	-3.64	1.32	1.38
7	A	2177	5MU	C6-N1	-3.63	1.31	1.38
32	a	1512	MA6	C8-N9	-3.46	1.31	1.37
32	a	1511	MA6	C8-N9	-3.43	1.31	1.37
7	A	2736	OMC	O2-C2	-3.32	1.17	1.23
7	A	2489	OMG	C6-N1	-3.31	1.32	1.38
7	A	2177	5MU	O2-C2	-3.03	1.17	1.23
32	a	959	2MG	C2-N1	-3.01	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2791	OMG	C6-N1	-2.99	1.33	1.38
32	a	1509	2MG	C2-N1	-2.96	1.32	1.36
7	A	2177	5MU	O4-C4	-2.85	1.18	1.23
32	a	960	5MC	C2-N3	-2.82	1.30	1.36
7	A	2268	6MZ	C4-N9	-2.80	1.31	1.37
32	a	1395	4OC	CM4-N4	2.73	1.50	1.45
32	a	1512	MA6	C5-N7	-2.71	1.34	1.39
7	A	2736	OMC	C6-N1	-2.71	1.31	1.38
7	A	2489	OMG	C2-N1	-2.66	1.31	1.37
7	A	2736	OMC	C2-N3	-2.66	1.31	1.36
32	a	1511	MA6	C5-N7	-2.63	1.34	1.39
32	a	1491	UR3	C5-C4	-2.63	1.37	1.43
7	A	2268	6MZ	C6-N1	-2.61	1.30	1.35
32	a	1509	2MG	C5-N7	-2.59	1.33	1.39
32	a	1491	UR3	C4-N3	-2.56	1.35	1.40
32	a	1395	4OC	C6-N1	-2.54	1.32	1.38
32	a	1509	2MG	C8-N9	-2.53	1.31	1.37
32	a	959	2MG	C5-N7	-2.52	1.34	1.39
7	A	2791	OMG	C2-N1	-2.52	1.31	1.37
32	a	1395	4OC	C2-N3	-2.50	1.31	1.36
32	a	959	2MG	C8-N9	-2.48	1.32	1.37
7	A	2268	6MZ	C2-N3	-2.48	1.29	1.33
32	a	518	G7M	C6-N1	-2.42	1.34	1.38
7	A	2296	6MZ	C6-N1	-2.41	1.31	1.35
7	A	2177	5MU	C6-C5	2.38	1.38	1.34
7	A	2268	6MZ	C2-N1	-2.29	1.29	1.33
7	A	2296	6MZ	C4-N9	-2.22	1.33	1.37
7	A	2296	6MZ	C2-N3	-2.07	1.30	1.33
32	a	960	5MC	CM5-C5	2.06	1.55	1.50
32	a	960	5MC	C6-C5	2.05	1.38	1.34
7	A	2736	OMC	C5-C4	-2.03	1.38	1.42
7	A	2268	6MZ	C5-C6	-2.03	1.37	1.41

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2268	6MZ	C9-N6-C6	-12.20	111.53	122.85
32	a	959	2MG	C2-N3-C4	7.14	120.93	112.00
32	a	1509	2MG	C2-N3-C4	6.88	120.60	112.00
32	a	959	2MG	C5-C4-N3	-6.20	118.53	128.39
7	A	2489	OMG	C5-C4-N3	-5.89	119.01	128.39
32	a	1509	2MG	C5-C4-N3	-5.87	119.04	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2177	5MU	N3-C2-N1	5.74	122.36	114.89
7	A	2177	5MU	C4-N3-C2	-5.69	119.88	127.34
32	a	518	G7M	C2-N3-C4	5.64	122.02	112.30
7	A	2791	OMG	C5-C4-N3	-5.62	119.44	128.39
32	a	1512	MA6	C5-C4-N3	-5.36	119.33	126.72
7	A	2177	5MU	C5-C6-N1	-5.31	117.54	123.31
7	A	2268	6MZ	N1-C2-N3	-5.12	120.83	128.58
32	a	1511	MA6	C5-C4-N3	-5.01	119.82	126.72
32	a	518	G7M	C5-C4-N3	-4.98	118.75	128.15
7	A	2268	6MZ	C6-C5-N7	4.90	137.78	132.43
32	a	1511	MA6	N1-C2-N3	-4.89	121.17	128.58
7	A	2177	5MU	C5-C4-N3	4.86	119.54	115.32
32	a	1512	MA6	N1-C2-N3	-4.75	121.39	128.58
32	a	1491	UR3	C4-N3-C2	-4.64	120.84	124.58
7	A	2489	OMG	N9-C4-N3	4.55	135.04	125.95
7	A	2296	6MZ	N1-C2-N3	-4.43	121.88	128.58
32	a	959	2MG	N9-C4-N3	4.38	134.72	125.95
7	A	2296	6MZ	C5-C4-N3	-4.35	120.72	126.72
32	a	1512	MA6	C4-C5-N7	-4.27	105.70	110.58
7	A	2489	OMG	C2-N3-C4	4.26	119.63	112.30
7	A	2791	OMG	C2-N3-C4	4.23	119.59	112.30
7	A	2296	6MZ	C6-C5-N7	4.20	137.01	132.43
32	a	518	G7M	N9-C4-N3	4.09	134.13	125.95
32	a	1509	2MG	N9-C4-N3	4.07	134.09	125.95
7	A	2791	OMG	N9-C4-N3	4.01	133.98	125.95
32	a	1511	MA6	C4-C5-N7	-3.97	106.04	110.58
7	A	2296	6MZ	C4-C5-N7	-3.95	106.06	110.58
32	a	1511	MA6	C2-N1-C6	3.92	121.39	111.83
32	a	1512	MA6	C2-N3-C4	3.90	121.34	111.83
7	A	2177	5MU	O4-C4-C5	-3.80	120.56	124.92
32	a	959	2MG	C2-N1-C6	-3.80	119.96	124.55
32	a	1511	MA6	C2-N3-C4	3.77	121.03	111.83
32	a	1512	MA6	C2-N1-C6	3.73	120.95	111.83
7	A	2268	6MZ	C5-C4-N3	-3.72	121.59	126.72
32	a	518	G7M	C5-C6-N1	3.61	119.30	111.84
32	a	1512	MA6	C5-N7-C8	3.57	109.06	103.45
7	A	2268	6MZ	C2-N3-C4	3.47	120.31	111.83
32	a	1511	MA6	C5-N7-C8	3.44	108.86	103.45
7	A	2268	6MZ	N9-C8-N7	-3.42	109.09	113.94
32	a	1491	UR3	C5-C4-N3	3.40	119.52	115.04
32	a	1509	2MG	C2-N1-C6	-3.39	120.45	124.55
7	A	2296	6MZ	C5-N7-C8	3.39	108.78	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1511	MA6	N9-C8-N7	-3.37	109.16	113.94
7	A	2296	6MZ	C2-N3-C4	3.27	119.82	111.83
32	a	1512	MA6	N9-C8-N7	-3.26	109.31	113.94
7	A	2296	6MZ	N9-C8-N7	-3.22	109.37	113.94
32	a	518	G7M	O6-C6-C5	-3.20	120.86	128.01
32	a	1512	MA6	N3-C4-N9	3.18	132.58	127.17
7	A	2268	6MZ	C4-C5-N7	-3.12	107.01	110.58
32	a	1511	MA6	N3-C4-N9	3.09	132.42	127.17
7	A	2489	OMG	C2-N1-C6	-3.07	119.54	125.11
32	a	960	5MC	C5-C6-N1	-3.05	120.00	123.31
32	a	960	5MC	C5-C4-N3	-2.99	118.69	121.75
7	A	2791	OMG	C2-N1-C6	-2.98	119.70	125.11
7	A	2268	6MZ	C5-N7-C8	2.92	108.04	103.45
7	A	2736	OMC	O2-C2-N3	-2.86	117.82	122.33
32	a	1395	4OC	O2-C2-N3	-2.77	117.97	122.33
32	a	1395	4OC	C5-C4-N3	-2.75	118.29	122.60
7	A	2177	5MU	O2-C2-N1	-2.67	119.32	122.80
7	A	2268	6MZ	C4-N9-C8	2.65	108.52	105.74
7	A	2296	6MZ	N3-C4-N9	2.60	131.59	127.17
32	a	959	2MG	CM2-N2-C2	-2.60	118.07	123.65
32	a	1509	2MG	N1-C2-N2	2.60	119.21	116.56
32	a	959	2MG	N1-C2-N2	2.57	119.19	116.56
7	A	2268	6MZ	C5-C6-N1	2.48	120.81	118.15
7	A	2489	OMG	O6-C6-C5	-2.45	120.07	126.53
32	a	1491	UR3	C1'-N1-C2	2.43	121.01	117.04
32	a	959	2MG	C5-C6-N1	2.40	119.35	113.25
7	A	2489	OMG	C5-C6-N1	2.37	119.28	113.25
7	A	2791	OMG	N9-C8-N7	-2.34	109.05	113.40
32	a	1511	MA6	C4-N9-C8	2.32	108.18	105.74
32	a	1509	2MG	CM2-N2-C2	-2.32	118.67	123.65
32	a	1509	2MG	C5-C6-N1	2.30	119.10	113.25
32	a	1395	4OC	N1-C2-N3	2.29	122.78	118.80
7	A	2268	6MZ	N3-C4-N9	2.29	131.06	127.17
7	A	2791	OMG	O6-C6-C5	-2.27	120.55	126.53
32	a	959	2MG	O6-C6-C5	-2.26	120.57	126.53
32	a	1491	UR3	C6-N1-C2	-2.25	119.96	121.80
32	a	1509	2MG	C6-C5-N7	2.25	134.38	130.29
7	A	2296	6MZ	C4-N9-C8	2.24	108.09	105.74
32	a	518	G7M	C2-N1-C6	-2.24	121.05	125.11
32	a	1509	2MG	C4-C5-N7	-2.24	107.12	110.67
32	a	1509	2MG	N9-C8-N7	-2.23	109.27	113.40
32	a	960	5MC	O2-C2-N3	-2.22	118.83	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2296	6MZ	C9-N6-C6	-2.22	120.80	122.85
32	a	959	2MG	C4-C5-N7	-2.22	107.16	110.67
7	A	2791	OMG	C5-C6-N1	2.21	118.89	113.25
32	a	959	2MG	C8-N7-C5	2.19	108.16	104.26
32	a	518	G7M	C6-C5-N7	2.19	134.91	132.17
7	A	2791	OMG	C8-N7-C5	2.17	108.12	104.26
7	A	2791	OMG	C4-C5-N7	-2.15	107.27	110.67
32	a	1509	2MG	C8-N7-C5	2.14	108.07	104.26
32	a	959	2MG	N9-C8-N7	-2.14	109.44	113.40
7	A	2489	OMG	N9-C8-N7	-2.12	109.47	113.40
32	a	959	2MG	C6-C5-N7	2.11	134.13	130.29
32	a	960	5MC	N1-C2-N3	2.10	122.45	118.80
32	a	1512	MA6	C5-C4-N9	2.09	108.09	105.81
32	a	1509	2MG	O6-C6-C5	-2.08	121.04	126.53
7	A	2791	OMG	C6-C5-N7	2.05	134.03	130.29
7	A	2489	OMG	C8-N7-C5	2.04	107.90	104.26
32	a	1512	MA6	C6-C5-N7	2.02	136.66	133.43
32	a	1491	UR3	O2-C2-N3	-2.02	118.55	121.33
32	a	1512	MA6	C4-N9-C8	2.01	107.85	105.74

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2296	6MZ	C5-C6-N6-C9
7	A	2296	6MZ	N1-C6-N6-C9
7	A	2489	OMG	O4'-C4'-C5'-O5'
7	A	2489	OMG	C1'-C2'-O2'-CM2
32	a	959	2MG	O4'-C4'-C5'-O5'
32	a	1512	MA6	O4'-C4'-C5'-O5'
32	a	1395	4OC	O4'-C4'-C5'-O5'
7	A	2489	OMG	C3'-C4'-C5'-O5'
32	a	959	2MG	C3'-C4'-C5'-O5'
32	a	1512	MA6	C3'-C4'-C5'-O5'
32	a	1511	MA6	C5-C6-N6-C9
32	a	518	G7M	C3'-C4'-C5'-O5'
32	a	1395	4OC	C3'-C4'-C5'-O5'
7	A	2268	6MZ	O4'-C4'-C5'-O5'
7	A	2268	6MZ	C3'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	a	1512	MA6	2	0
32	a	960	5MC	1	0
7	A	2296	6MZ	1	0
32	a	518	G7M	1	0
32	a	1511	MA6	1	0
7	A	2489	OMG	2	0
32	a	1509	2MG	1	0
7	A	2268	6MZ	1	0
32	a	1395	4OC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 454 ligands modelled in this entry, 453 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
54	WDP	A	3201	-	84,90,90	5.19	30 (35%)	101,132,132	2.56	24 (23%)

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
54	WDP	A	3201	-	-	45/103/158/158	0/4/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A	3201	WDP	C04-N03	28.76	1.53	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A	3201	WDP	O28-S26	19.99	1.66	1.43
54	A	3201	WDP	O27-S26	18.74	1.65	1.43
54	A	3201	WDP	S26-N25	10.30	1.77	1.61
54	A	3201	WDP	C18-N20	9.82	1.52	1.35
54	A	3201	WDP	O08-C06	7.59	1.57	1.44
54	A	3201	WDP	C62-N61	-6.99	1.32	1.46
54	A	3201	WDP	O74-C75	5.68	1.57	1.44
54	A	3201	WDP	O17-C18	5.51	1.45	1.34
54	A	3201	WDP	C14-C12	5.03	1.61	1.54
54	A	3201	WDP	C24-C21	4.99	1.60	1.53
54	A	3201	WDP	C76-C75	-4.86	1.39	1.51
54	A	3201	WDP	O50-C51	4.71	1.45	1.34
54	A	3201	WDP	C29-S26	4.57	1.83	1.76
54	A	3201	WDP	O40-C41	4.56	1.47	1.34
54	A	3201	WDP	C59-N61	-3.38	1.37	1.48
54	A	3201	WDP	C71-C69	3.34	1.59	1.51
54	A	3201	WDP	C07-C06	-3.28	1.38	1.51
54	A	3201	WDP	C24-N25	3.18	1.51	1.47
54	A	3201	WDP	O56-C57	2.99	1.49	1.41
54	A	3201	WDP	O50-C49	-2.84	1.40	1.44
54	A	3201	WDP	C14-C15	2.59	1.58	1.53
54	A	3201	WDP	C05-C04	-2.54	1.47	1.50
54	A	3201	WDP	O72-C73	2.49	1.44	1.40
54	A	3201	WDP	C05-C06	2.44	1.56	1.51
54	A	3201	WDP	O40-C39	-2.40	1.41	1.44
54	A	3201	WDP	O74-C73	2.40	1.48	1.41
54	A	3201	WDP	C21-N20	2.29	1.52	1.48
54	A	3201	WDP	C43-C41	2.25	1.55	1.50
54	A	3201	WDP	O19-C18	-2.20	1.17	1.21

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A	3201	WDP	C05-C04-N03	-14.95	109.49	126.93
54	A	3201	WDP	O17-C18-N20	8.23	120.65	109.88
54	A	3201	WDP	O28-S26-O27	-7.98	109.83	119.52
54	A	3201	WDP	C24-N25-S26	-5.37	108.87	119.59
54	A	3201	WDP	O50-C51-C53	4.80	121.78	111.53
54	A	3201	WDP	O40-C41-C43	4.56	119.60	111.43
54	A	3201	WDP	C49-O50-C51	-4.40	110.46	117.76
54	A	3201	WDP	O36-C35-C15	-4.39	110.22	119.97
54	A	3201	WDP	O19-C18-N20	-4.13	118.50	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A	3201	WDP	O40-C39-C37	3.75	114.49	107.84
54	A	3201	WDP	C85-C04-N03	-3.37	108.22	118.24
54	A	3201	WDP	C71-C69-C49	-3.21	105.89	111.08
54	A	3201	WDP	C38-C37-C35	3.19	115.17	108.07
54	A	3201	WDP	O50-C49-C47	3.18	114.84	107.52
54	A	3201	WDP	C69-C49-C47	-3.05	106.16	114.29
54	A	3201	WDP	O50-C49-C69	2.86	112.11	108.15
54	A	3201	WDP	O17-C18-O19	-2.70	120.84	125.64
54	A	3201	WDP	O50-C51-O52	-2.42	119.58	123.95
54	A	3201	WDP	O10-C11-C67	2.29	110.93	108.23
54	A	3201	WDP	C12-C11-C67	-2.28	108.20	114.29
54	A	3201	WDP	O42-C41-C43	-2.11	119.76	124.65
54	A	3201	WDP	C53-C55-C67	-2.10	106.86	112.91
54	A	3201	WDP	O52-C51-C53	-2.10	118.64	124.11
54	A	3201	WDP	C38-C37-C39	-2.09	108.33	113.00

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	A	3201	WDP	C12-C14-C15-O17
54	A	3201	WDP	O17-C15-C35-O36
54	A	3201	WDP	C22-C21-N20-C18
54	A	3201	WDP	C24-C21-N20-C18
54	A	3201	WDP	C23-C21-N20-C18
54	A	3201	WDP	C05-C04-N03-O02
54	A	3201	WDP	C85-C04-N03-O02
54	A	3201	WDP	C67-C11-C12-C13
54	A	3201	WDP	C67-C11-C12-C14
54	A	3201	WDP	O10-C11-C12-C13
54	A	3201	WDP	O10-C11-C12-C14
54	A	3201	WDP	O17-C18-N20-C21
54	A	3201	WDP	O19-C18-N20-C21
54	A	3201	WDP	C15-C35-C37-C38
54	A	3201	WDP	O36-C35-C37-C38
54	A	3201	WDP	C35-C37-C39-O40
54	A	3201	WDP	O40-C39-C47-C48
54	A	3201	WDP	C47-C39-O40-C41
54	A	3201	WDP	C49-C69-C71-O72
54	A	3201	WDP	C70-C69-C71-O72
54	A	3201	WDP	C04-N03-O02-C01
54	A	3201	WDP	O19-C18-O17-C15

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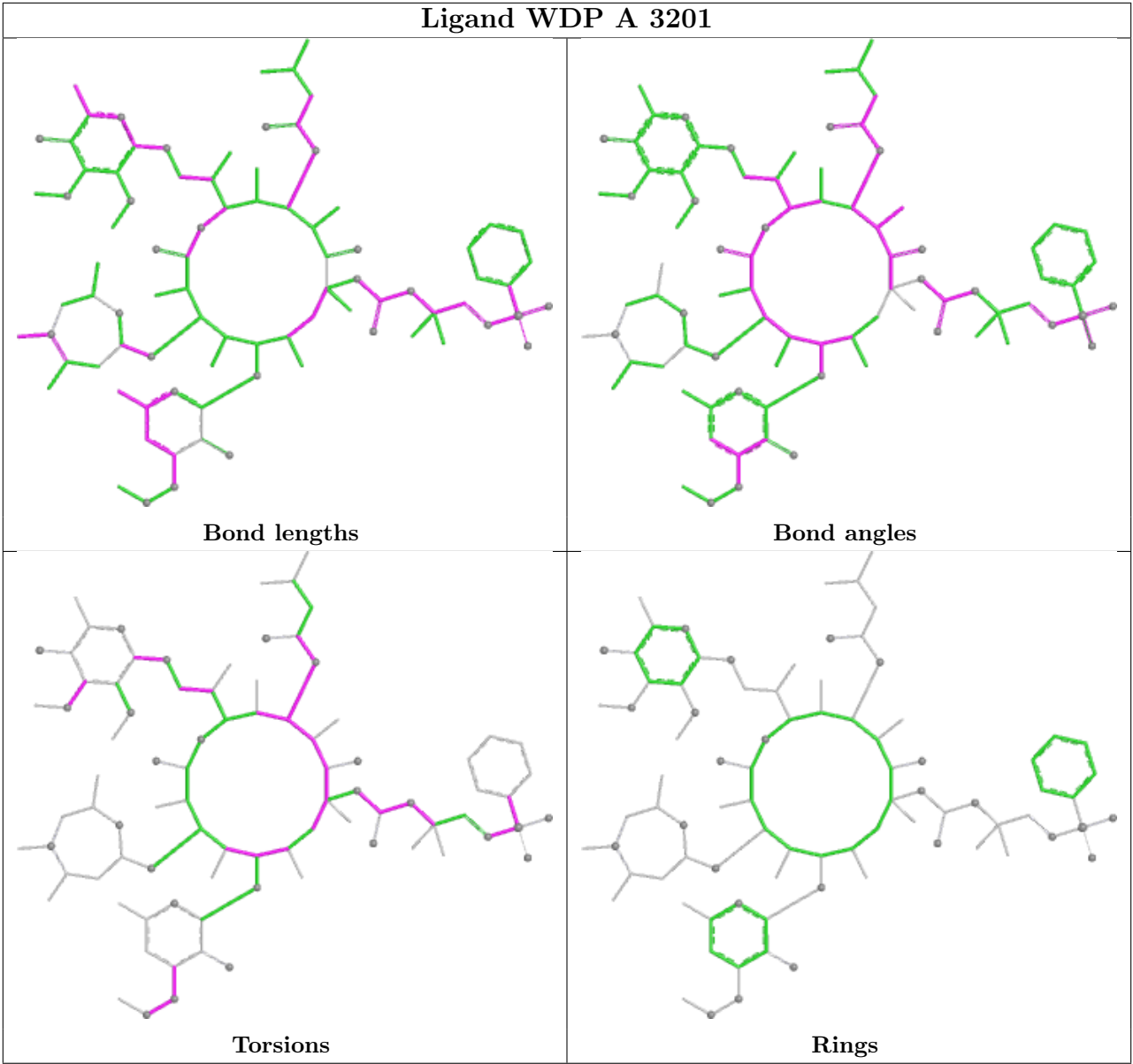
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Mol	Chain	Res	Type	Atoms
54	A	3201	WDP	N20-C18-O17-C15
54	A	3201	WDP	C24-N25-S26-O28
54	A	3201	WDP	C24-N25-S26-C29
54	A	3201	WDP	C82-C73-O72-C71
54	A	3201	WDP	C38-C37-C39-O40
54	A	3201	WDP	C43-C41-O40-C39
54	A	3201	WDP	O42-C41-O40-C39
54	A	3201	WDP	C34-C29-S26-O28
54	A	3201	WDP	C37-C39-O40-C41
54	A	3201	WDP	C30-C29-S26-O28
54	A	3201	WDP	C24-N25-S26-O27
54	A	3201	WDP	C12-C11-C67-C68
54	A	3201	WDP	C82-C79-O80-C81
54	A	3201	WDP	C30-C29-S26-N25
54	A	3201	WDP	C34-C29-S26-N25
54	A	3201	WDP	O10-C11-C67-C55
54	A	3201	WDP	C37-C39-C47-C49
54	A	3201	WDP	C12-C14-C15-C16
54	A	3201	WDP	C14-C15-C35-C37
54	A	3201	WDP	C16-C15-C35-C37
54	A	3201	WDP	O10-C11-C67-C68
54	A	3201	WDP	C16-C15-C35-O36
54	A	3201	WDP	C38-C37-C39-C47

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	43:LYS	C	44:GLY	N	6.14

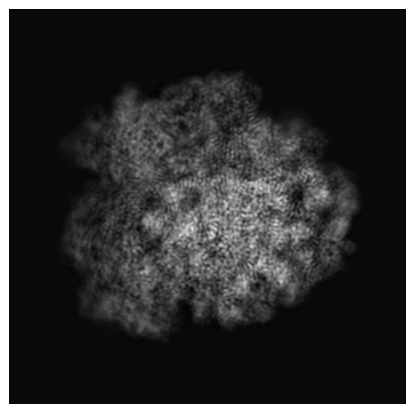
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22865. These allow visual inspection of the internal detail of the map and identification of artifacts.

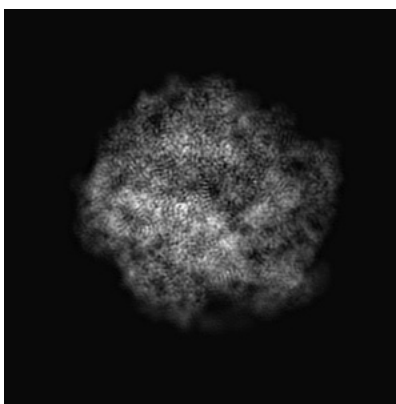
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

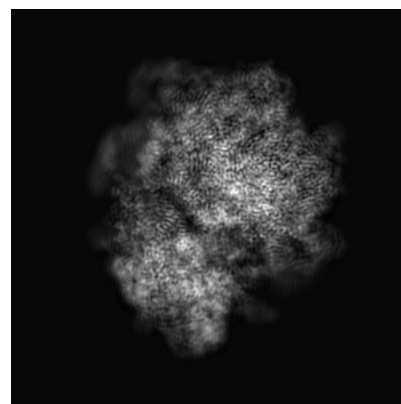
6.1.1 Primary map



X

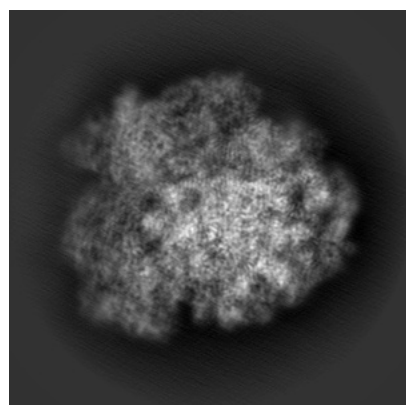


Y

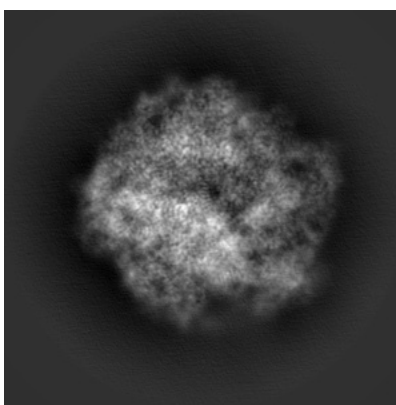


Z

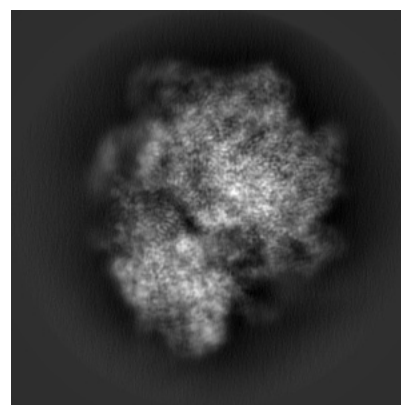
6.1.2 Raw map



X



Y

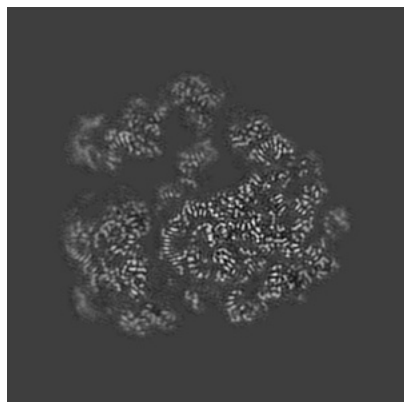


Z

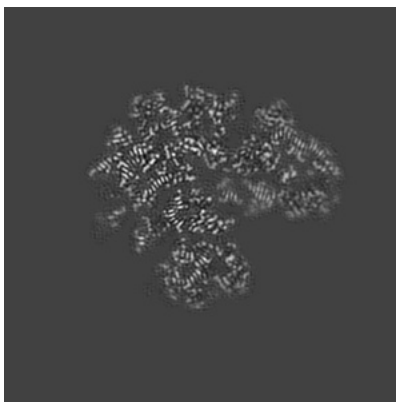
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

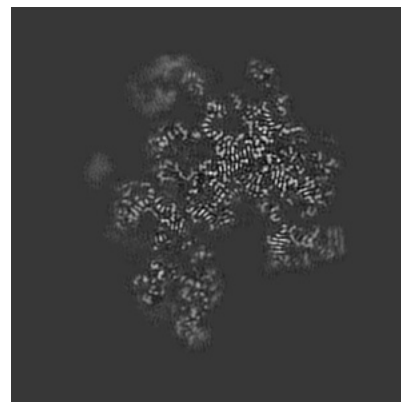
6.2.1 Primary map



X Index: 160

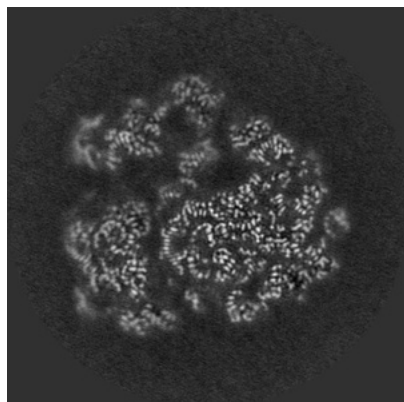


Y Index: 160

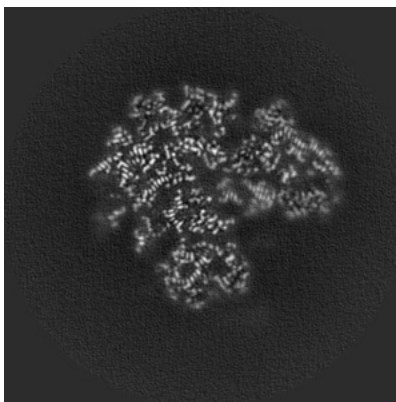


Z Index: 160

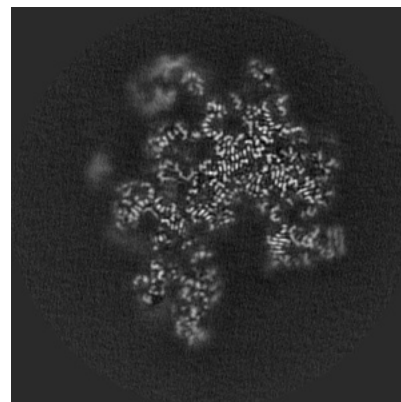
6.2.2 Raw map



X Index: 160



Y Index: 160

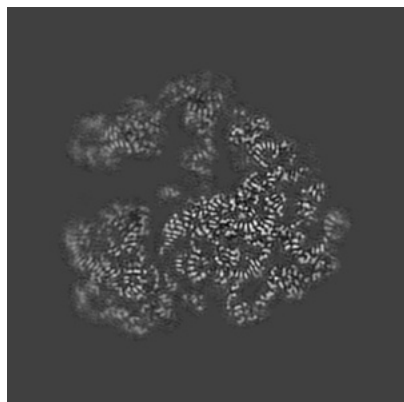


Z Index: 160

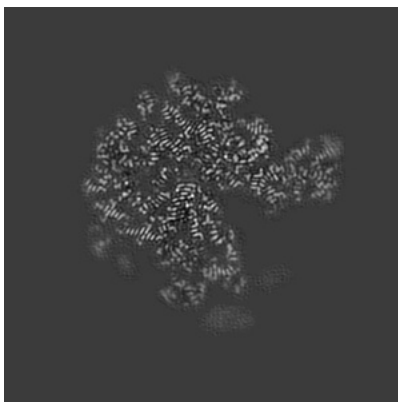
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

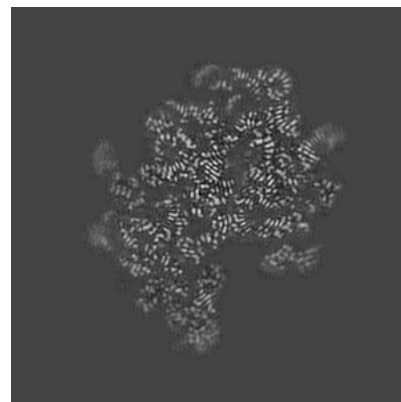
6.3.1 Primary map



X Index: 163

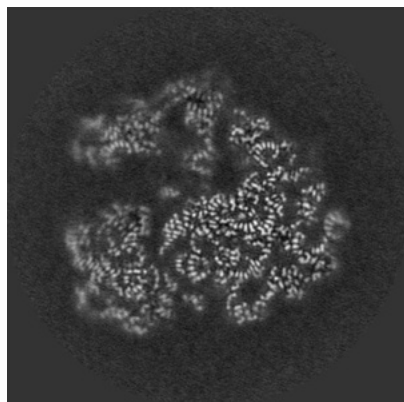


Y Index: 178

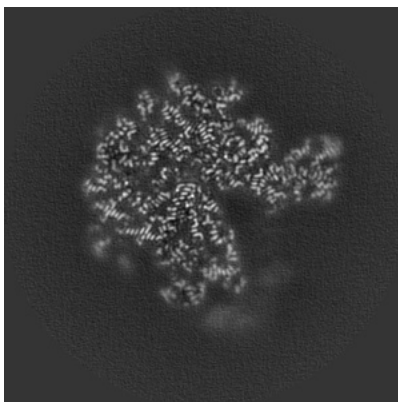


Z Index: 144

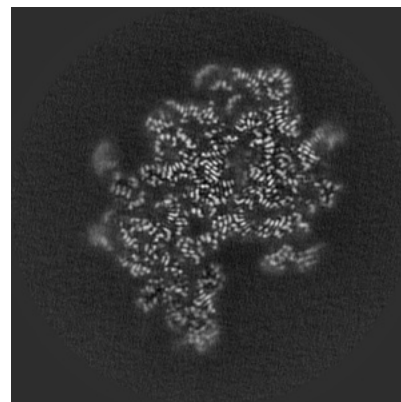
6.3.2 Raw map



X Index: 163



Y Index: 178

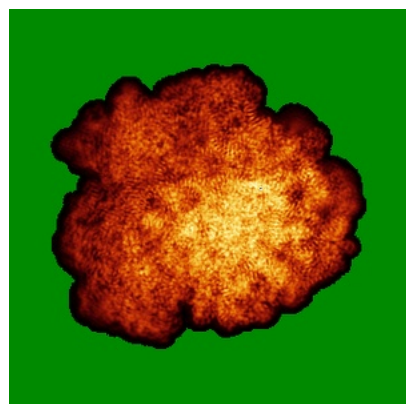


Z Index: 144

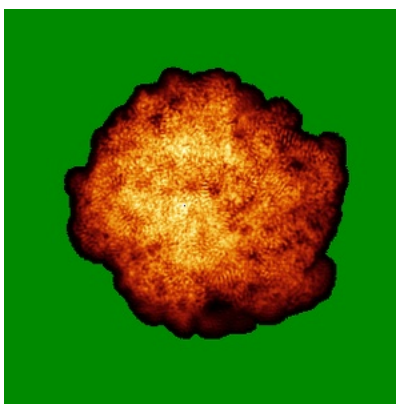
The images above show the largest variance slices of the map in three orthogonal directions.

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

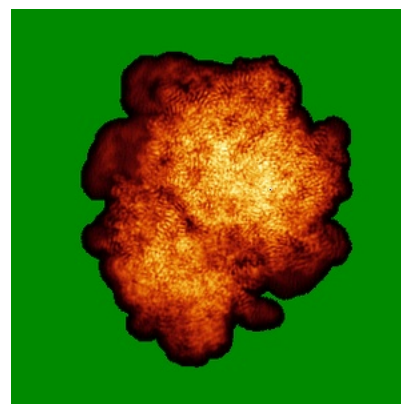
6.4.1 Primary map



X

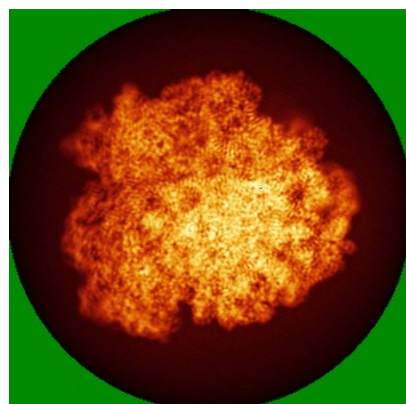


Y

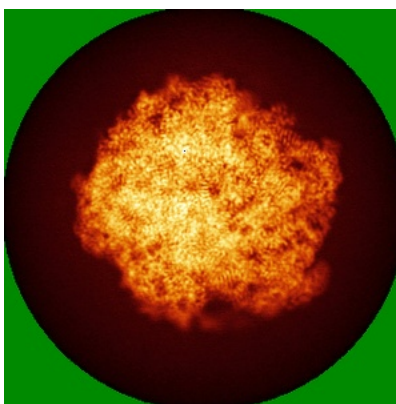


Z

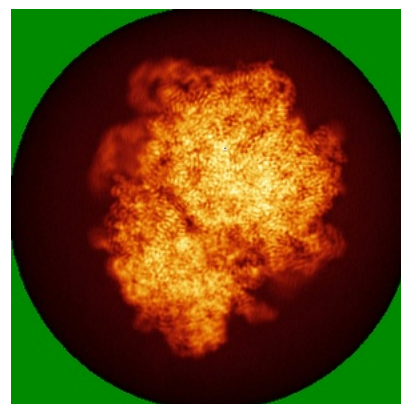
6.4.2 Raw map



X



Y

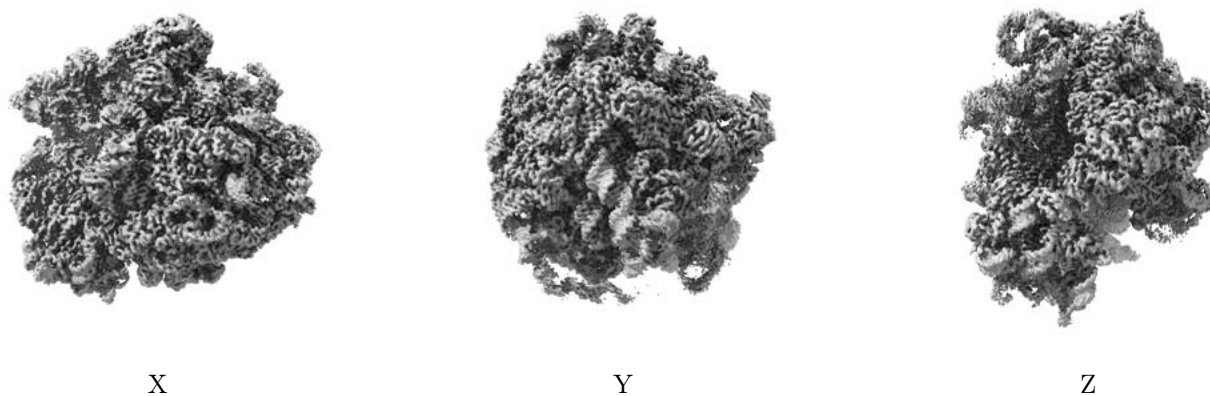


Z

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

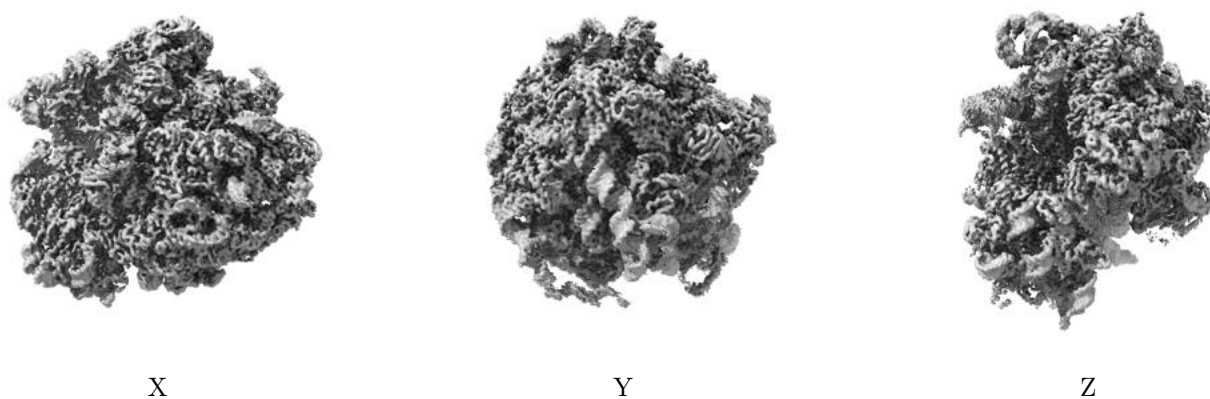
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

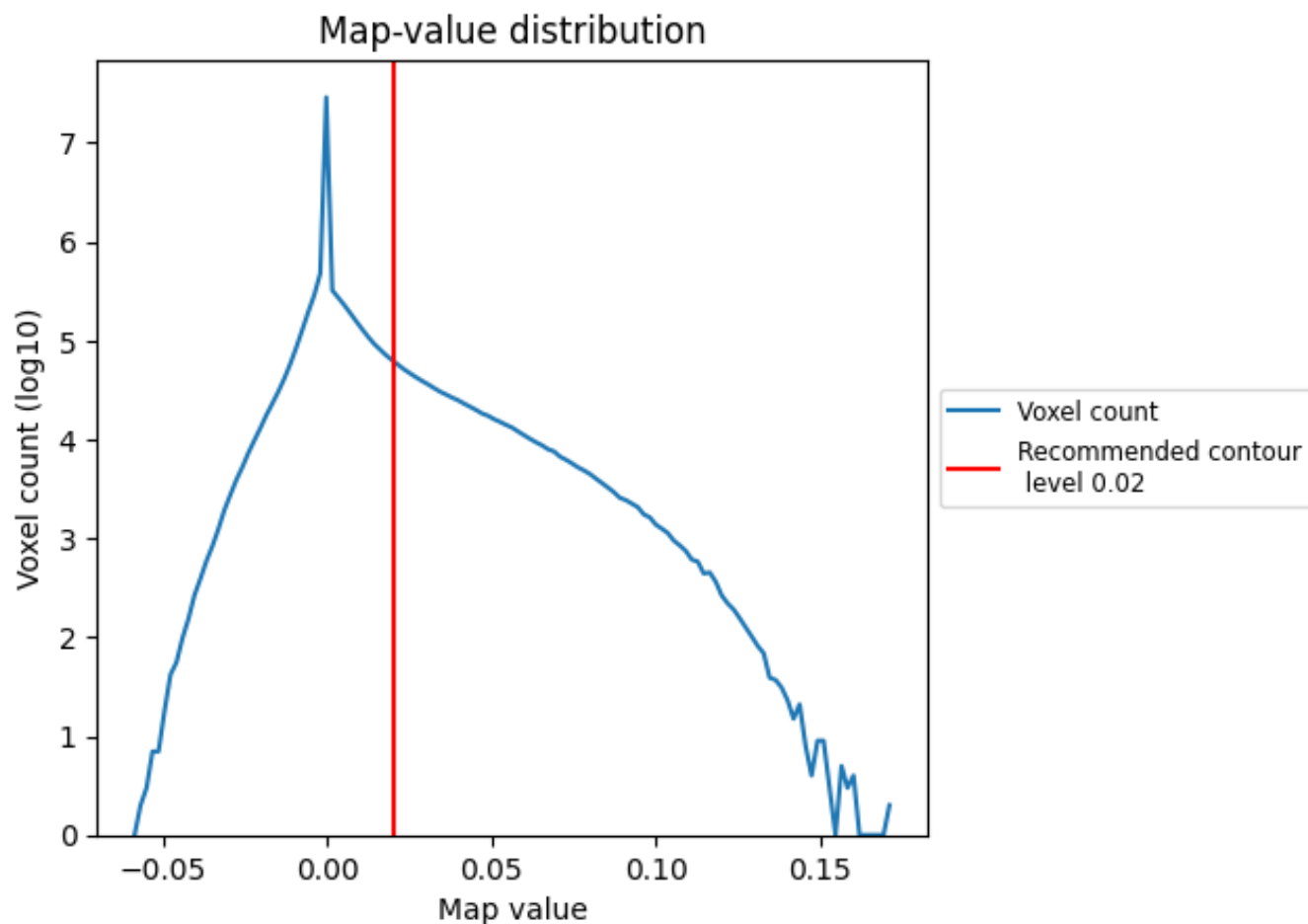
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

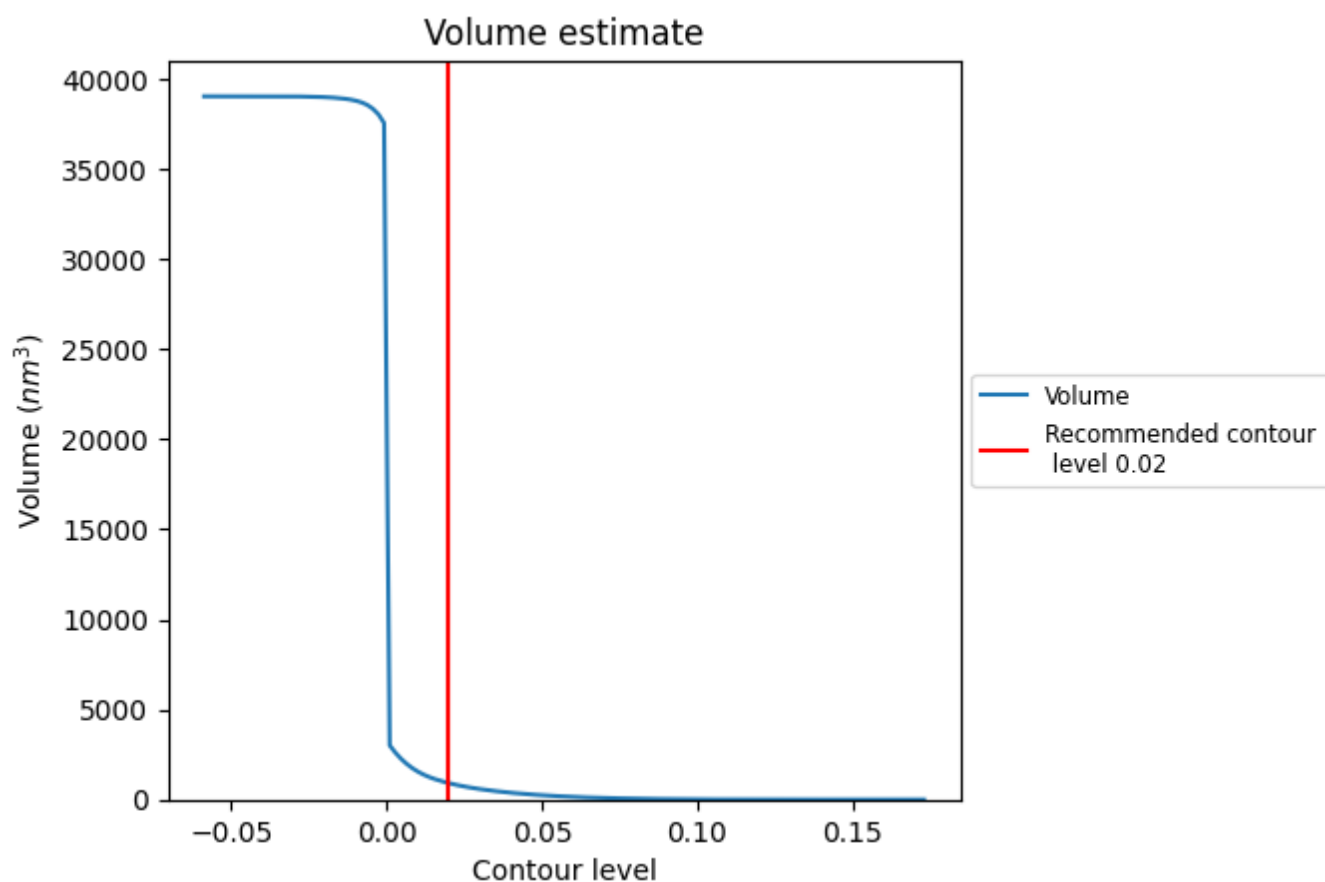
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

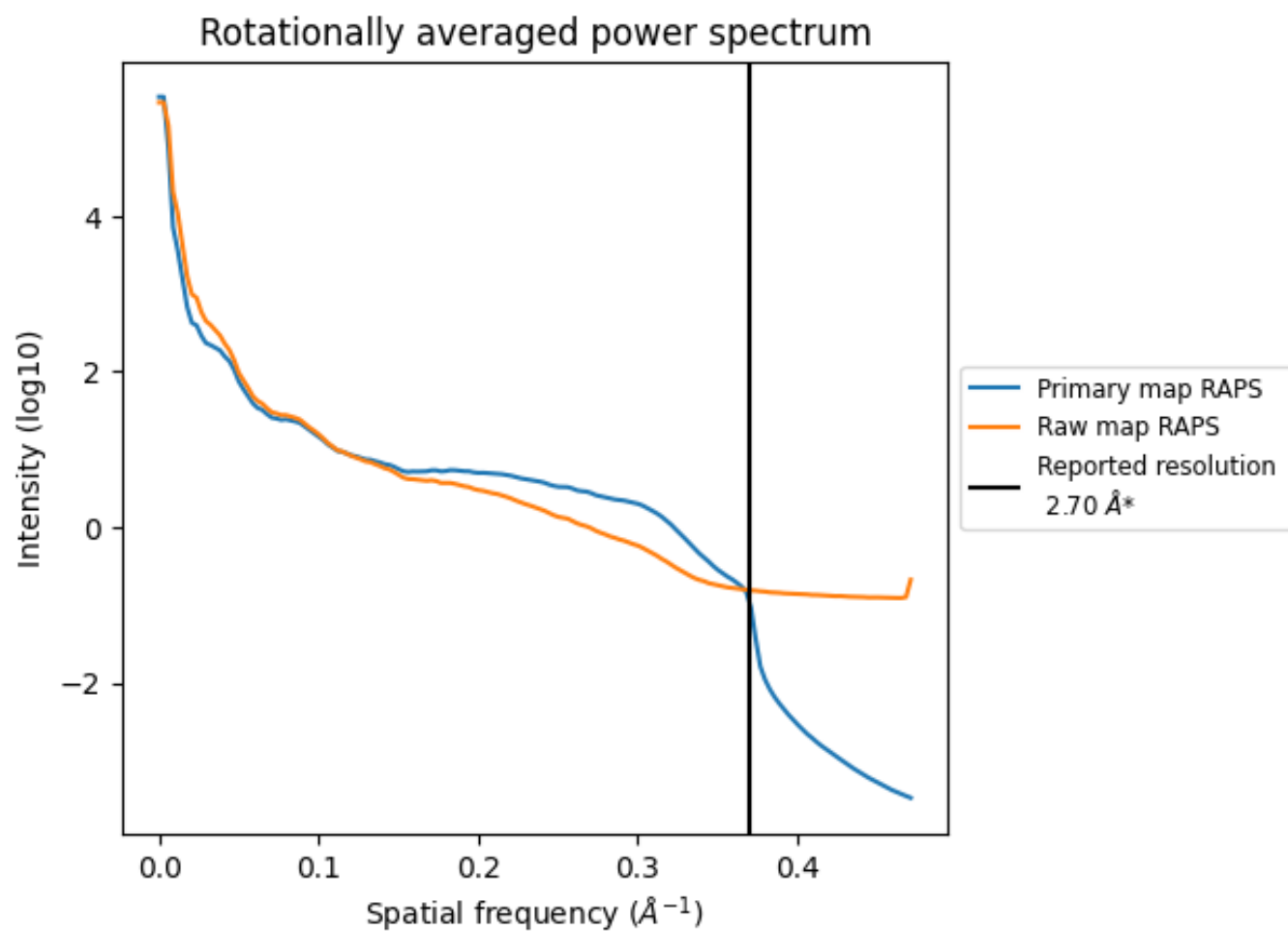
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 914 nm^3 ; this corresponds to an approximate mass of 826 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

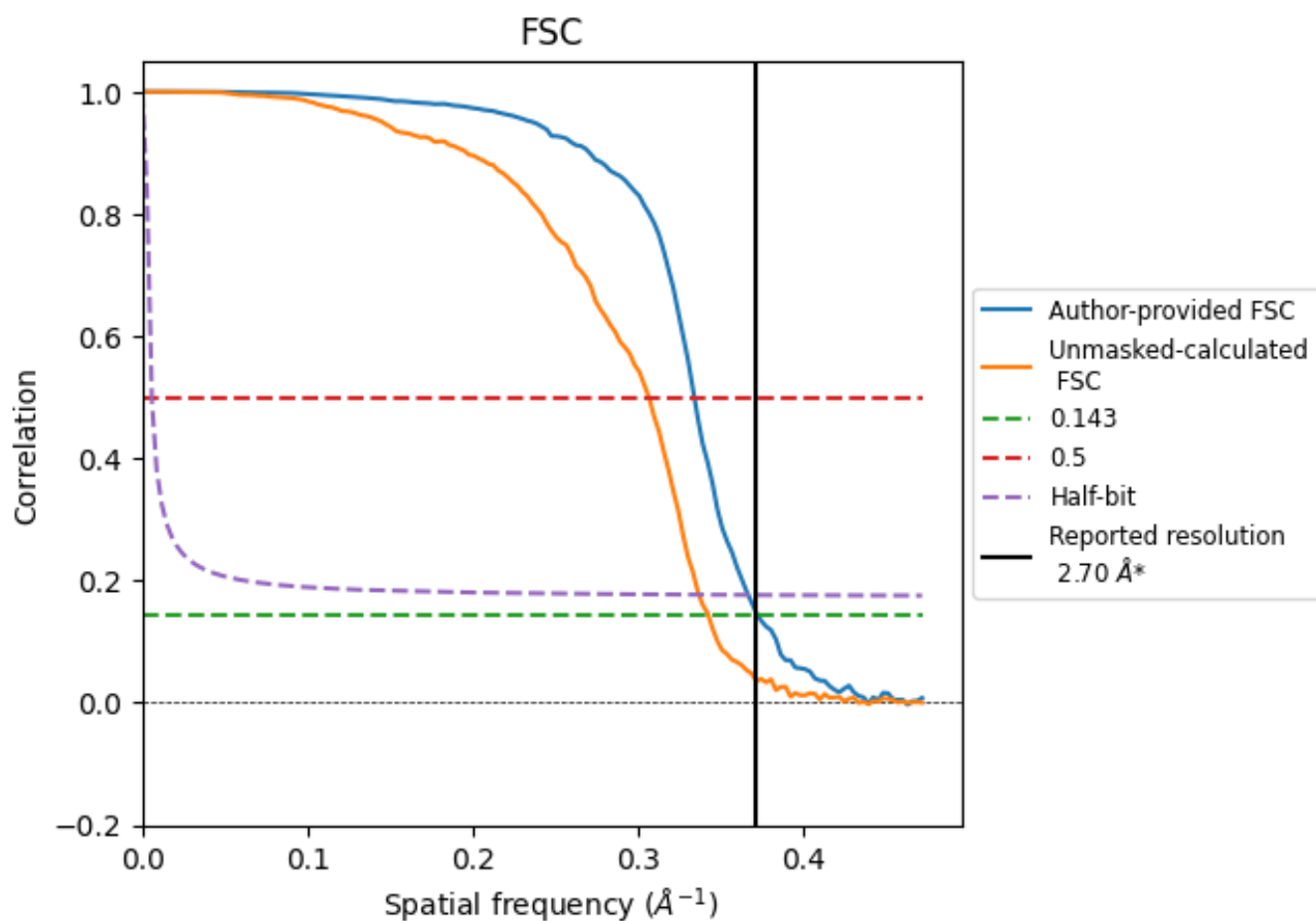


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.370 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

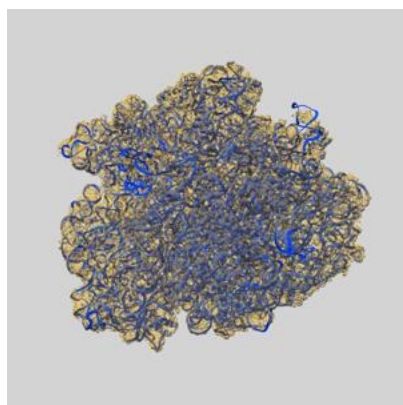
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	2.99	2.73
Unmasked-calculated*	2.92	3.26	2.97

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

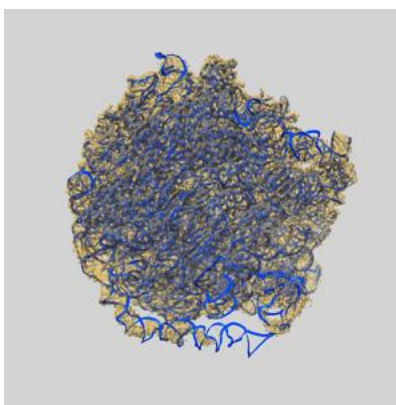
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22865 and PDB model 7KGB. Per-residue inclusion information can be found in section [3](#) on page [15](#).

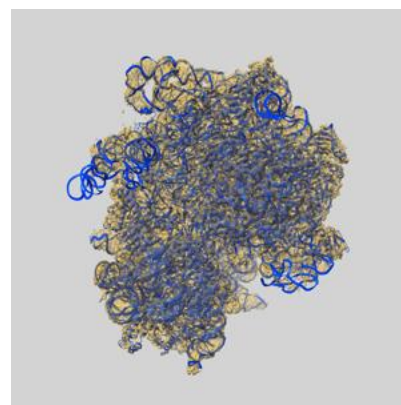
9.1 Map-model overlay [i](#)



X



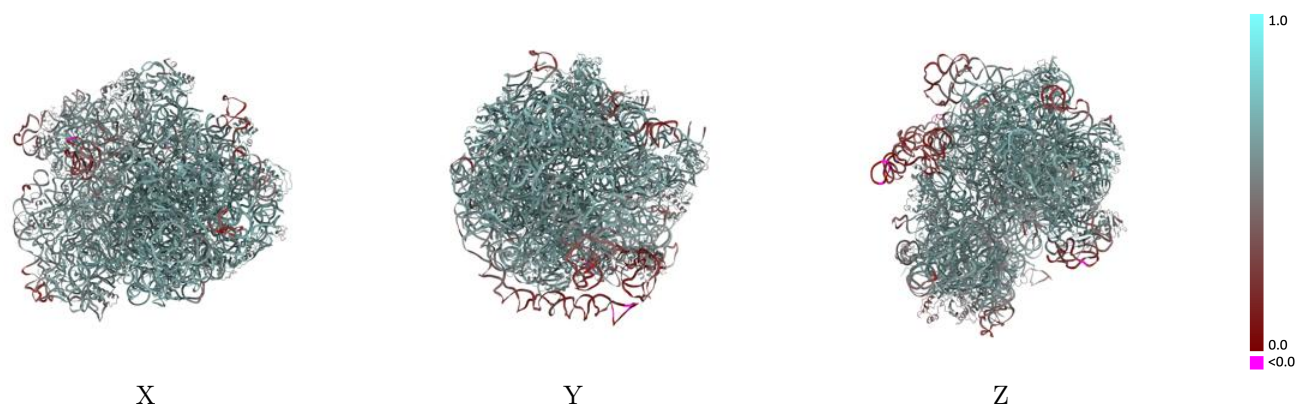
Y



Z

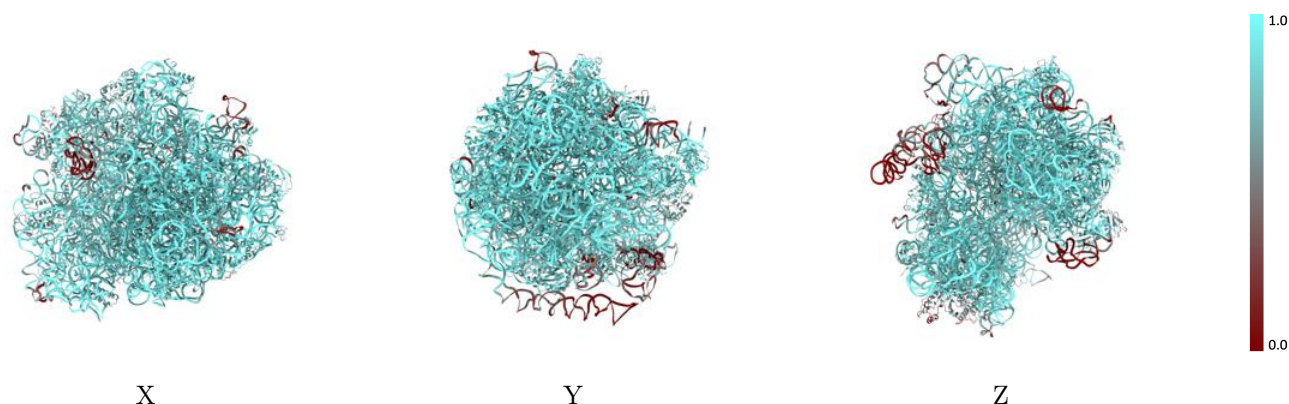
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



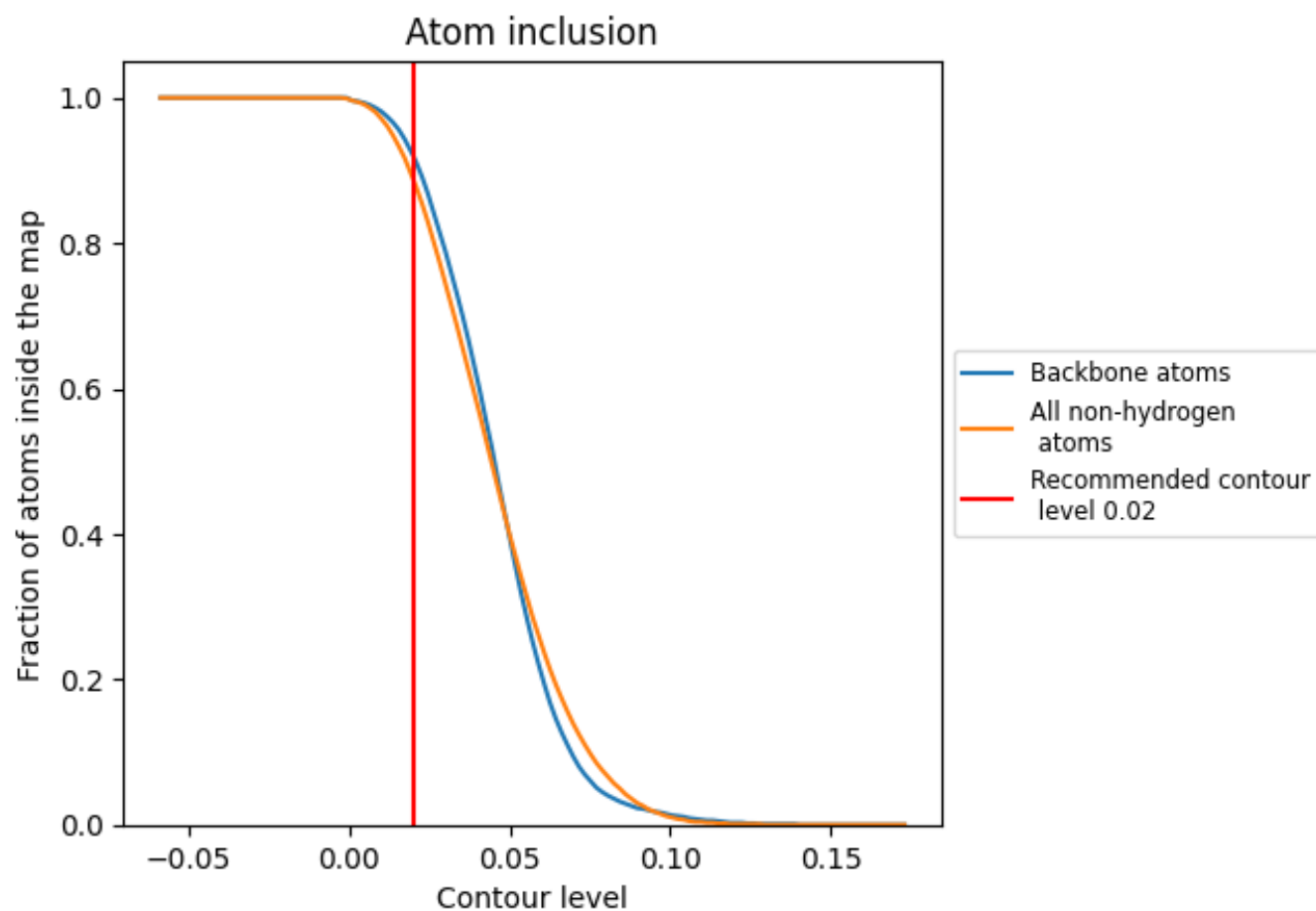
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.5760
0	 0.9020	 0.6260
1	 0.9100	 0.6200
2	 0.9540	 0.6530
3	 0.9360	 0.6400
4	 0.8960	 0.6060
6	 0.6700	 0.5070
A	 0.8950	 0.5760
B	 0.9520	 0.5860
C	 0.9250	 0.6380
D	 0.9110	 0.6170
E	 0.8920	 0.6040
F	 0.8040	 0.5420
G	 0.7370	 0.5270
H	 0.1110	 0.3090
J	 0.9070	 0.6130
K	 0.8880	 0.6180
L	 0.8930	 0.6100
M	 0.8870	 0.6100
N	 0.9330	 0.6290
O	 0.8480	 0.5660
P	 0.8530	 0.6040
Q	 0.9320	 0.6250
R	 0.8600	 0.6040
S	 0.9430	 0.6270
T	 0.8230	 0.5900
U	 0.7830	 0.5560
V	 0.7740	 0.5430
W	 0.9410	 0.6300
X	 0.9110	 0.6180
Y	 0.8340	 0.5660
Z	 0.8770	 0.6200
a	 0.9480	 0.5780
c	 0.6960	 0.5350
d	 0.6470	 0.4890



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Chain	Atom inclusion	Q-score
e	 0.8030	 0.5720
f	 0.7650	 0.5460
g	 0.8040	 0.5560
h	 0.8660	 0.5750
i	 0.7490	 0.5280
j	 0.5680	 0.4690
k	 0.8600	 0.5820
l	 0.7630	 0.5600
m	 0.7460	 0.5240
n	 0.8710	 0.5920
o	 0.8390	 0.5680
p	 0.8050	 0.5520
q	 0.7540	 0.5430
r	 0.8300	 0.5710
s	 0.7790	 0.5420
t	 0.7980	 0.5550
v	 0.8800	 0.6410
y	 0.8890	 0.5630