



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:48 PM UTC

PDB ID : 9O2X / pdb\_00009o2x  
EMDB ID : EMD-70050  
Title : Structure of WT E.coli ribosome 70S subunit with complexed with mRNA, P-site fMet-NH-tRNA<sup>fMet</sup> and A-site (S)-betahydroxyBocK charged NH-tRNA<sup>Pyl</sup>  
Authors : Majumdar, C.; Kent, A.; Hamlish, N.; Zhu, C.; Cate, J.  
Deposited on : 2025-04-04  
Resolution : 2.29 Å (reported)  
Based on initial model : 8EMM

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

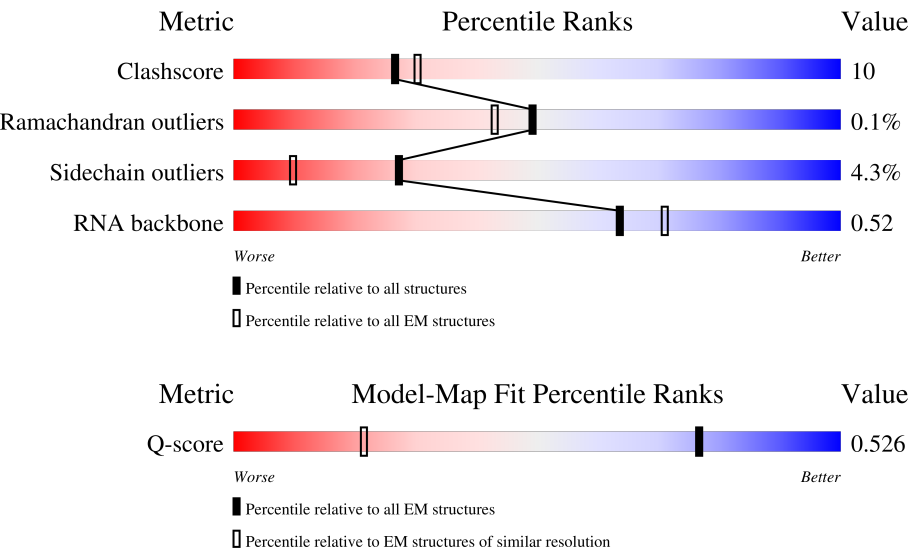
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.29 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	3699 ( 1.79 - 2.79 )

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  $\geq 3$ , 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	55	
2	1	46	

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Mol	Chain	Length	Quality of chain
3	2	65	
4	3	38	
5	B	241	
6	C	233	
7	D	206	
8	E	167	
9	F	135	
10	G	179	
11	H	130	
12	I	130	
13	J	103	
14	K	129	
15	L	124	
16	M	118	
17	N	101	
18	O	89	
19	P	82	
20	Q	84	
21	R	75	
22	S	92	
23	T	87	
24	U	71	
25	X	28	
26	Z	77	
27	b	120	

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Mol	Chain	Length	Quality of chain
28	c	273	
29	d	209	
30	e	201	
31	f	179	
32	g	177	
33	h	149	
34	i	142	
35	j	123	
36	k	144	
37	l	136	
38	m	127	
39	n	117	
40	o	115	
41	p	118	
42	q	103	
43	r	110	
44	s	100	
45	t	104	
46	u	94	
47	v	85	
48	w	78	
49	x	63	
50	y	59	
51	z	57	
52	A	1542	

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Mol	Chain	Length	Quality of chain
53	a	2904	<div><div>9%</div><div>57%</div><div>34%</div><div>5%</div></div>
54	4	70	<div><div>83%</div><div>53%</div><div>30%</div><div>14%</div></div>
55	Y	71	<div><div>72%</div><div>18%</div><div>41%</div><div>41%</div></div>

## 2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 145519 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 L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

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

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 9 is a protein called Small ribosomal subunit protein bS6.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP A0A0H3PWX2

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 19 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS17.



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

- Molecule 21 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 23 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 24 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	15	Total	C	N	O	P	0	0
			322	145	61	101	15		

- Molecule 26 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	76	Total	C	N	O	P	0	0
			1623	723	295	529	76		

- Molecule 27 is a RNA chain called 5S rRNA.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	173	Total	C	N	O	S	0	0
			1295	814	237	242	2		

- Molecule 33 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	138	MS6	MET	conflict	UNP P0ADY7

- Molecule 38 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	77	Total	C	N	O	S	0	0
			582	360	115	106	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a RNA chain called 16S rRNA.

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

- Molecule 53 is a RNA chain called 23S rRNA.

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

- Molecule 54 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 55 is a RNA chain called A-site tRNA<sup>Pyl</sup>.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Y	71	Total	C	N	O	P	0	0
			1518	675	276	496	71		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	C	1	Total	Mg	0
			1	1	
57	N	1	Total	Mg	0
			1	1	
57	Q	1	Total	Mg	0
			1	1	
57	Z	1	Total	Mg	0
			1	1	
57	b	5	Total	Mg	0
			5	5	
57	d	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	
57	A	90	Total	Mg	0
			90	90	
57	a	219	Total	Mg	0
			219	219	

- Molecule 58 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					AltConf
58	Z	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

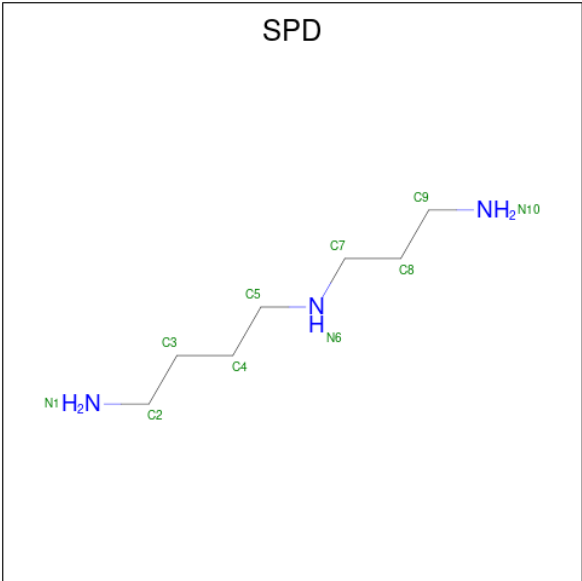
Mol	Chain	Residues	Atoms	AltConf
59	c	1	Total K 1 1	0
59	a	9	Total K 9 9	0

- Molecule 60 is PAROMOMYCIN (CCD ID: PAR) (formula:  $\text{C}_{23}\text{H}_{45}\text{N}_5\text{O}_{14}$ ).



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

- Molecule 61 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



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

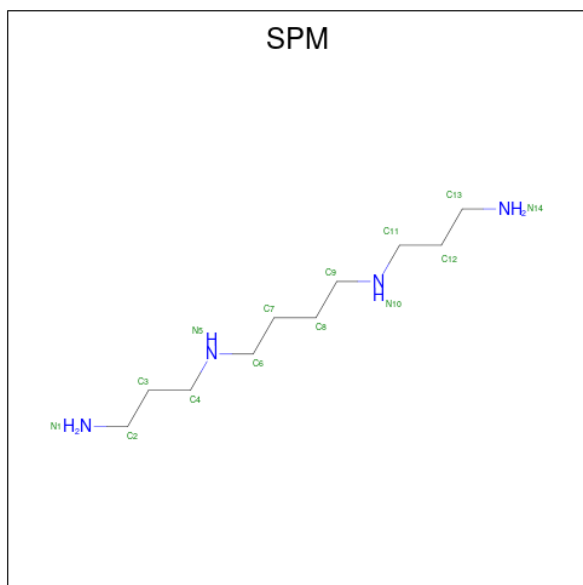
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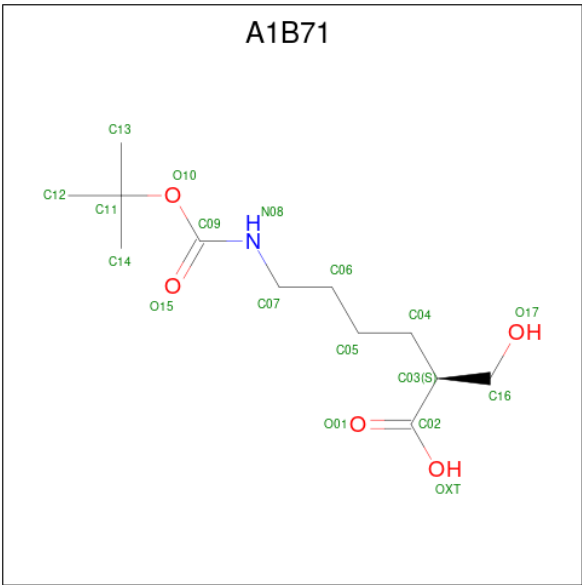
Mol	Chain	Residues	Atoms			AltConf
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	

- Molecule 62 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



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

- Molecule 63 is (2S)-6-[(tert-butoxycarbonyl)amino]-2-(hydroxymethyl)hexanoic acid (CCD ID: A1B71) (formula:  $C_{12}H_{23}NO_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
63	Y	1	Total	C	N	O	0
			17	12	1	4	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	0	2	Total	O	0
			2	2	
64	1	15	Total	O	0
			15	15	
64	2	19	Total	O	0
			19	19	
64	3	4	Total	O	0
			4	4	
64	Z	4	Total	O	0
			4	4	
64	b	41	Total	O	0
			41	41	
64	c	84	Total	O	0
			84	84	
64	d	36	Total	O	0
			36	36	
64	e	29	Total	O	0
			29	29	
64	h	1	Total	O	0
			1	1	
64	i	13	Total	O	0
			13	13	

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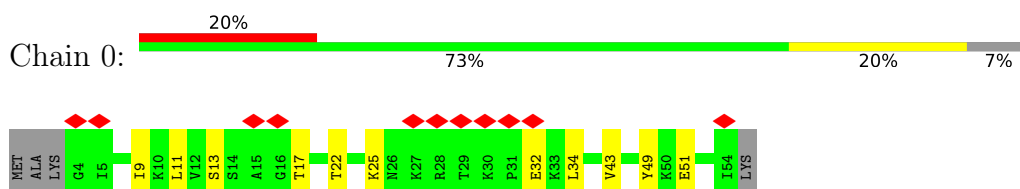
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Mol	Chain	Residues	Atoms		AltConf
64	j	14	Total 14	O 14	0
64	k	34	Total 34	O 34	0
64	l	25	Total 25	O 25	0
64	m	23	Total 23	O 23	0
64	o	13	Total 13	O 13	0
64	p	24	Total 24	O 24	0
64	q	13	Total 13	O 13	0
64	r	26	Total 26	O 26	0
64	s	5	Total 5	O 5	0
64	t	1	Total 1	O 1	0
64	u	3	Total 3	O 3	0
64	v	11	Total 11	O 11	0
64	w	12	Total 12	O 12	0
64	x	1	Total 1	O 1	0
64	z	24	Total 24	O 24	0
64	A	2	Total 2	O 2	0
64	a	2993	Total 2993	O 2993	0
64	Y	2	Total 2	O 2	0

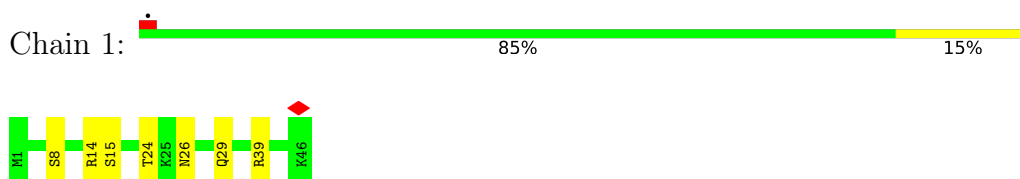
### 3 Residue-property plots

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

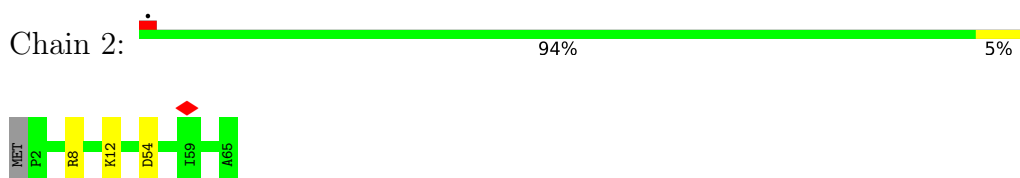
- Molecule 1: 50S ribosomal protein L33



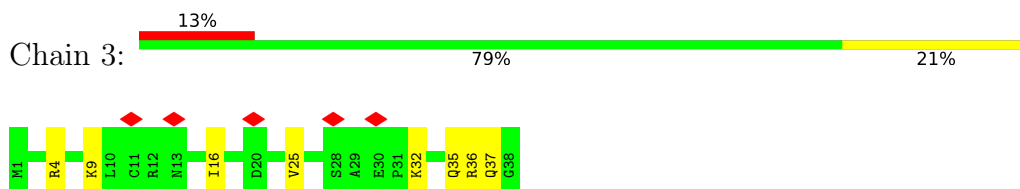
- Molecule 2: 50S ribosomal protein L34



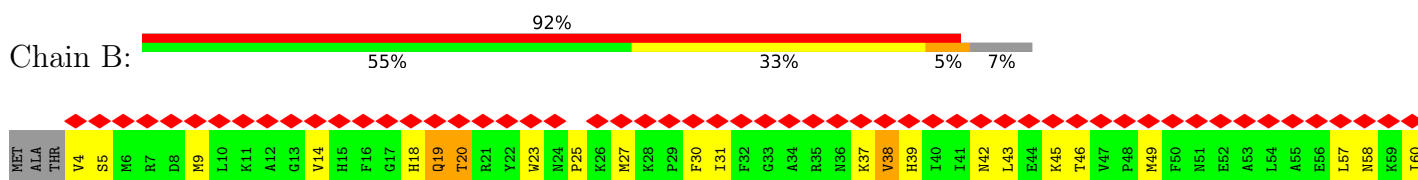
- Molecule 3: 50S ribosomal protein L35

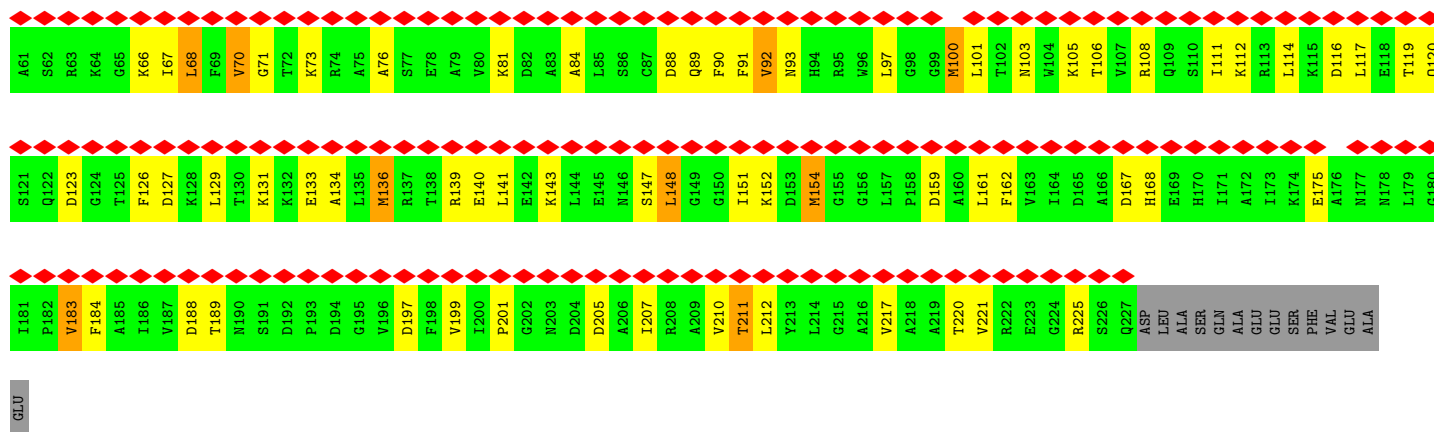


- Molecule 4: 50S ribosomal protein L36

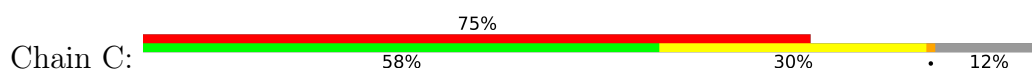


- Molecule 5: 30S ribosomal protein S2

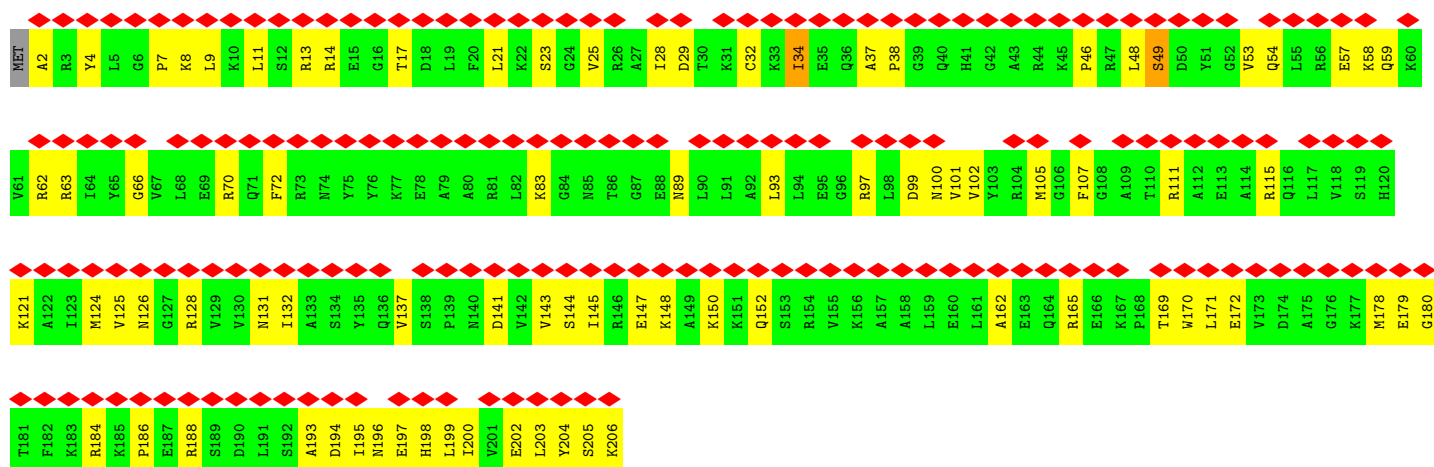
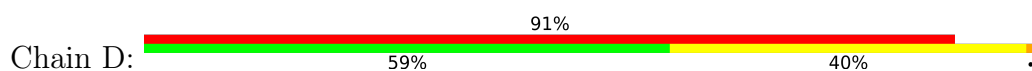


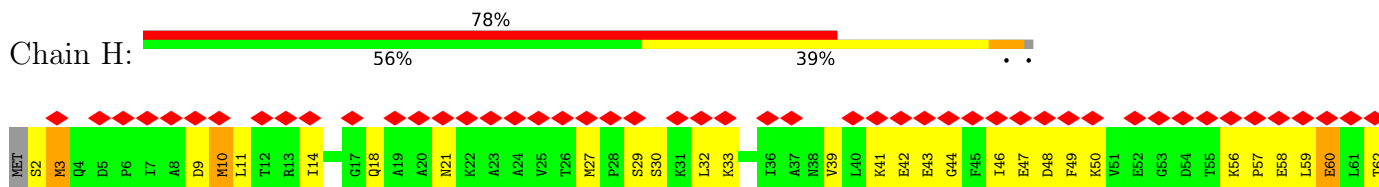


• Molecule 6: Small ribosomal subunit protein uS3



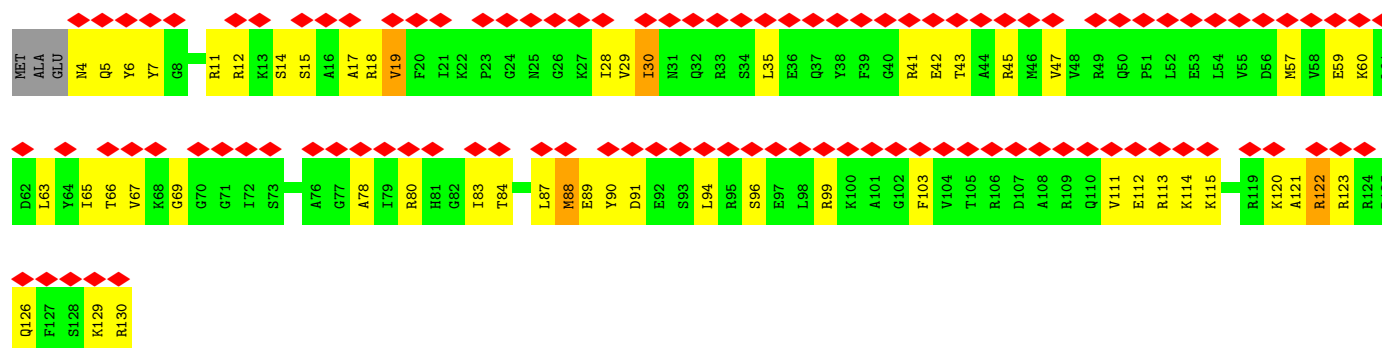
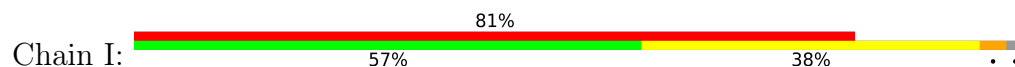
• Molecule 7: Small ribosomal subunit protein uS4



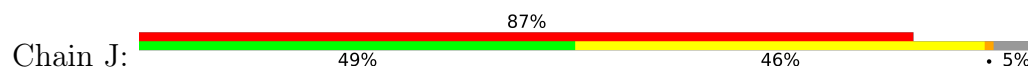




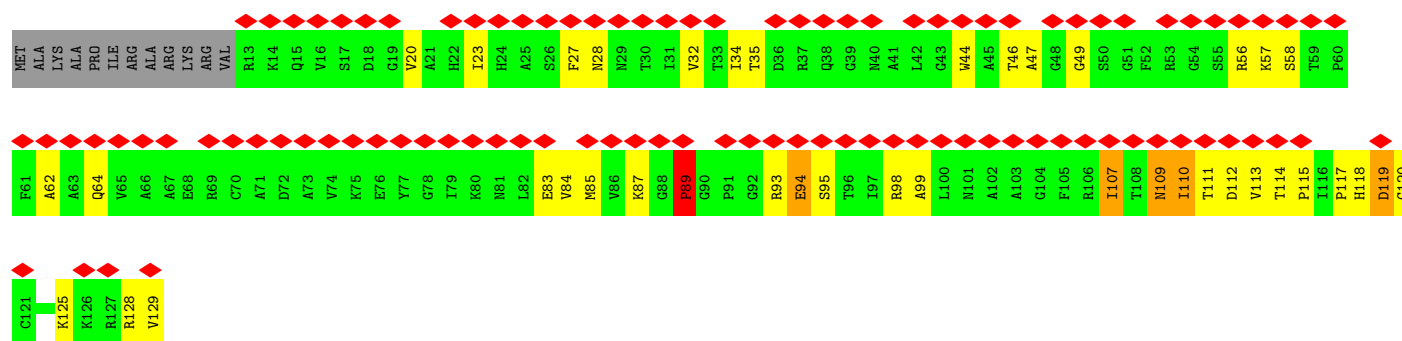
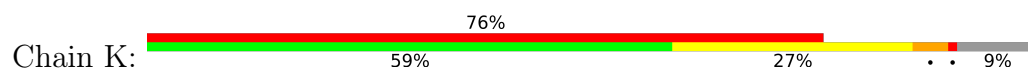
- Molecule 12: Small ribosomal subunit protein uS9



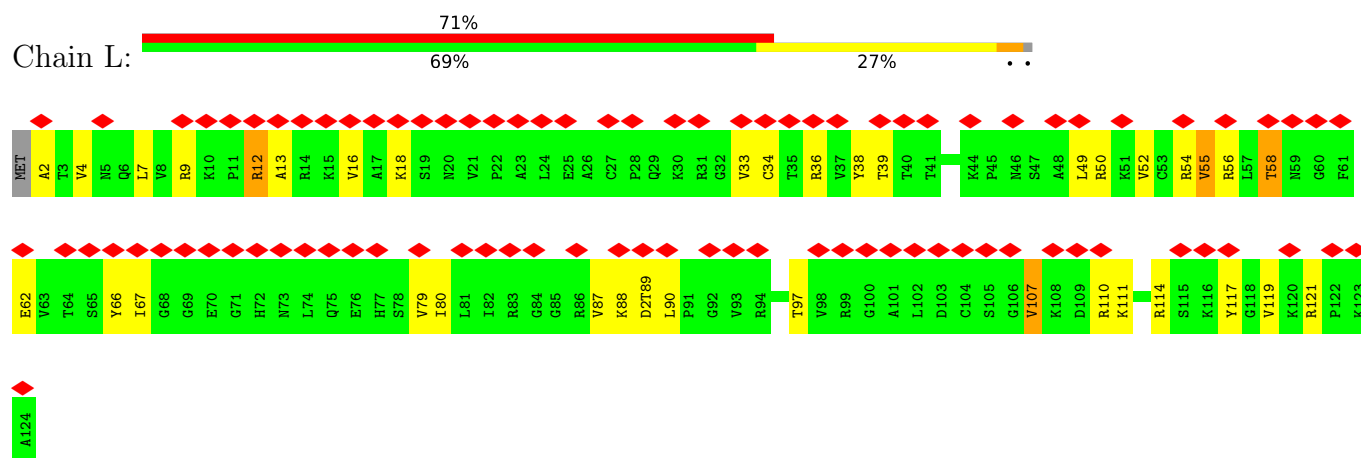
- Molecule 13: Small ribosomal subunit protein uS10



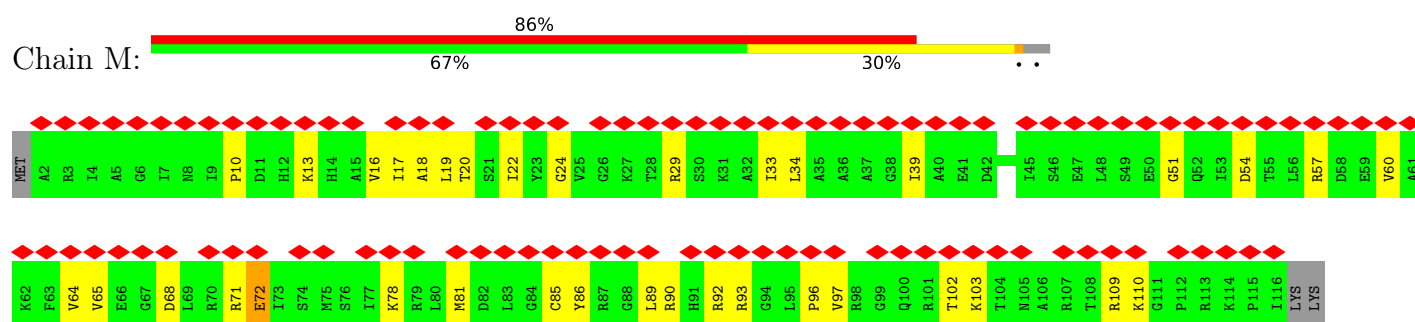
- Molecule 14: Small ribosomal subunit protein uS11



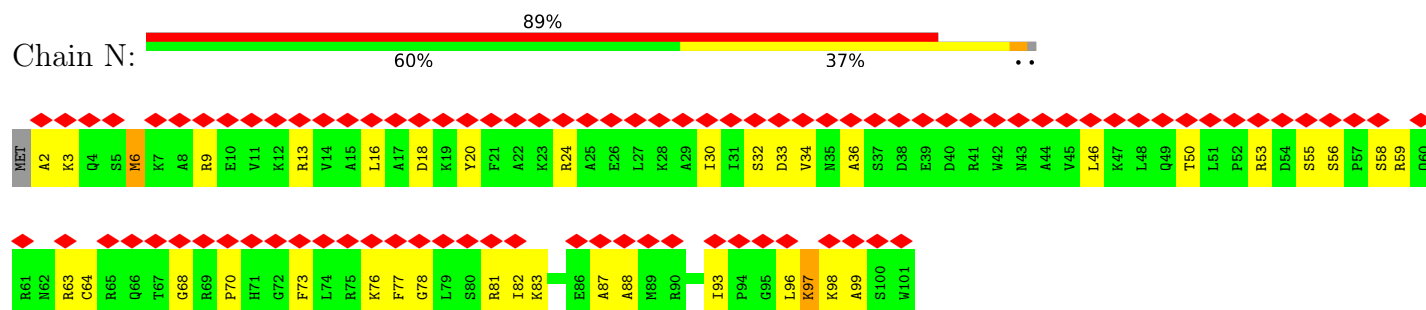
- Molecule 15: Small ribosomal subunit protein uS12



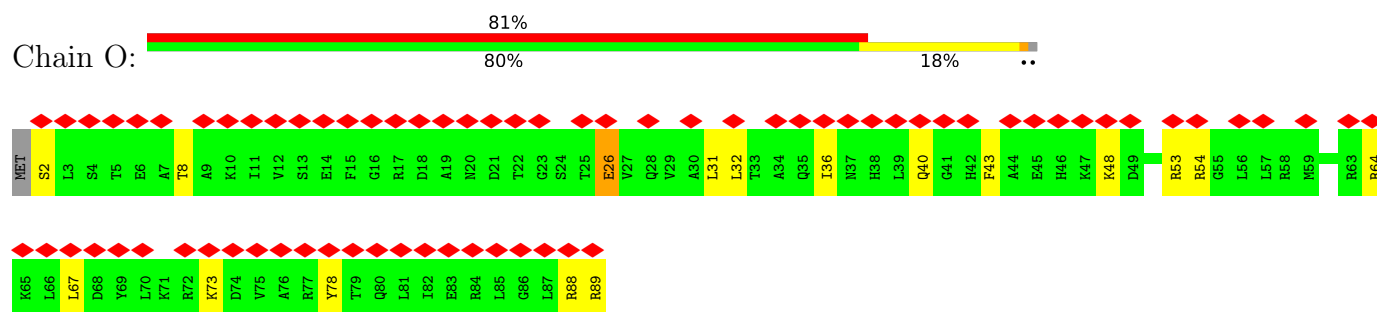
- Molecule 16: Small ribosomal subunit protein uS13



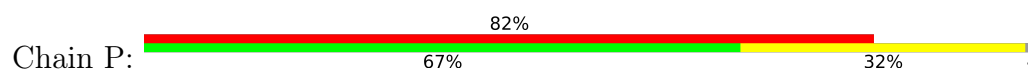
- Molecule 17: Small ribosomal subunit protein uS14



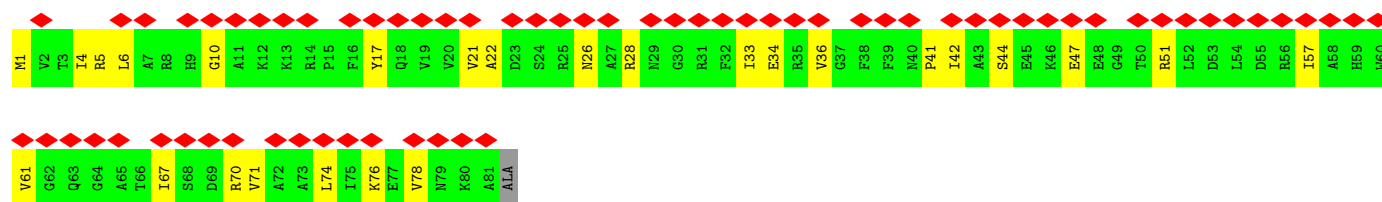
- Molecule 18: Small ribosomal subunit protein uS15



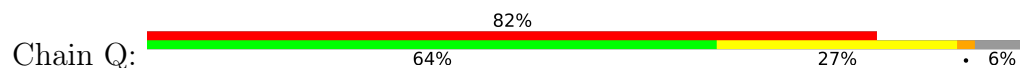
- Molecule 19: Small ribosomal subunit protein bS16



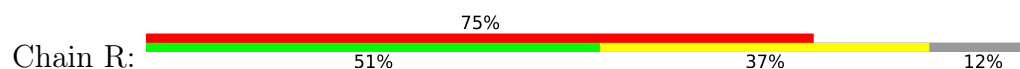




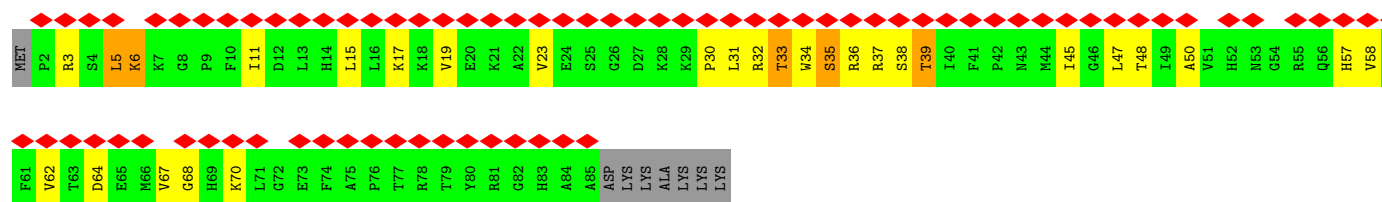
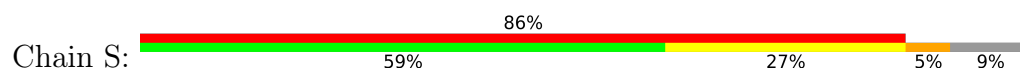
• Molecule 20: Small ribosomal subunit protein uS17



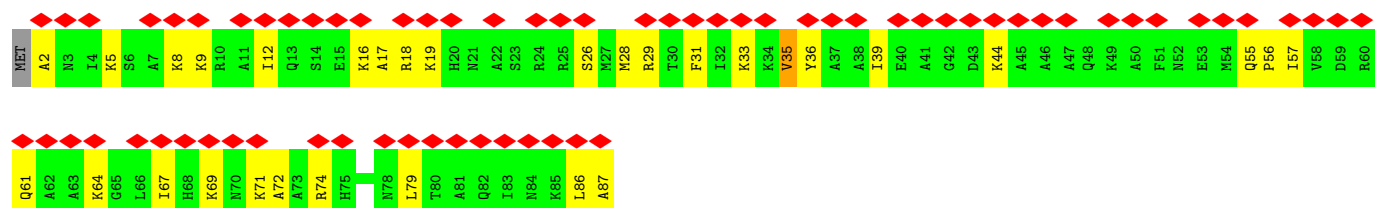
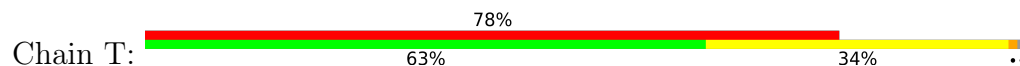
• Molecule 21: Small ribosomal subunit protein bS18



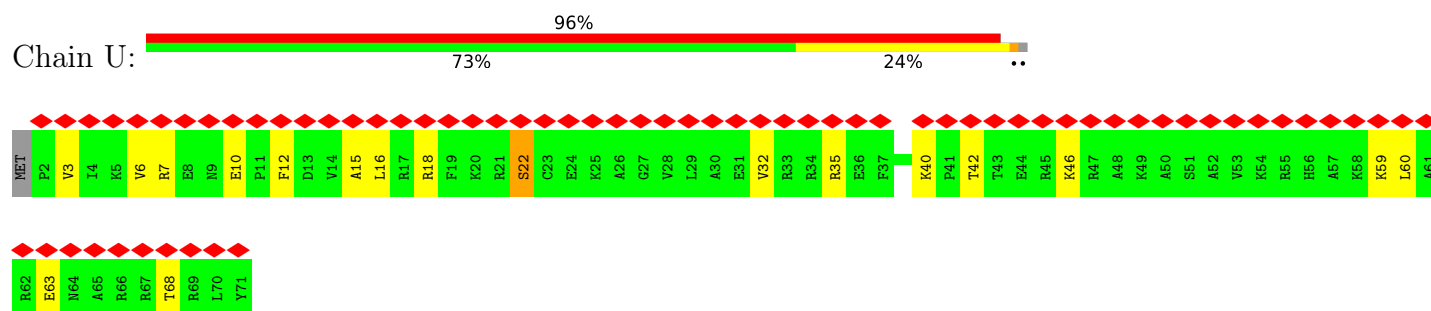
• Molecule 22: Small ribosomal subunit protein uS19



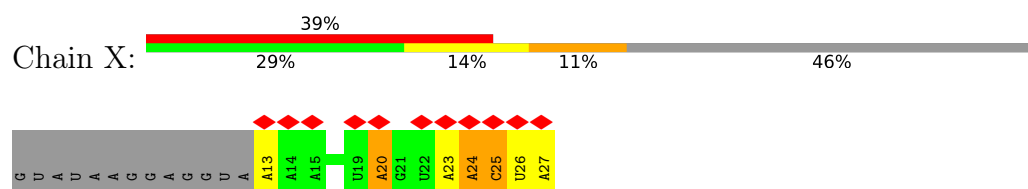
• Molecule 23: Small ribosomal subunit protein bS20



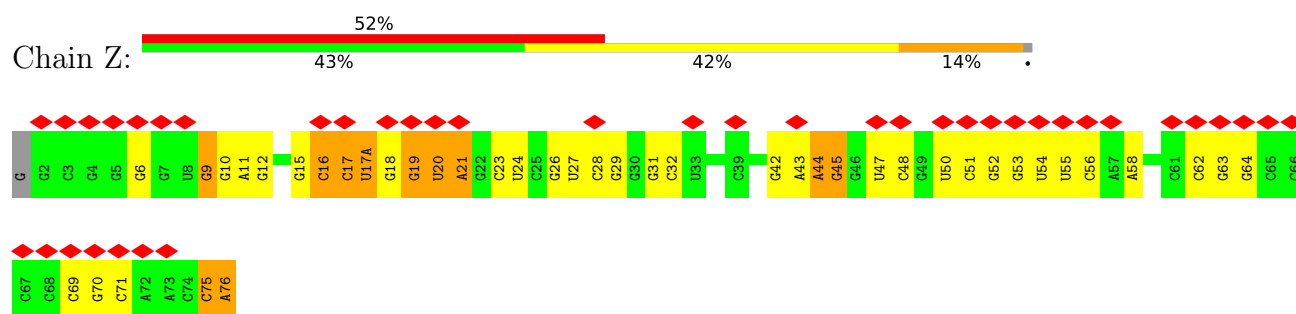
- Molecule 24: Small ribosomal subunit protein bS21



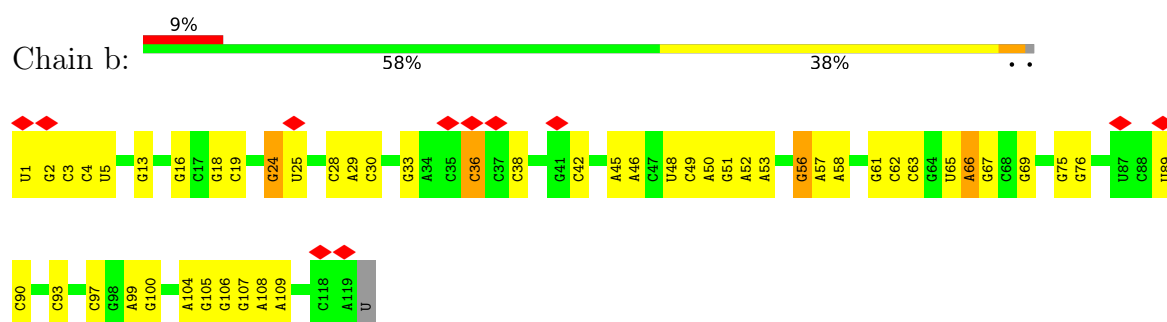
- Molecule 25: mRNA



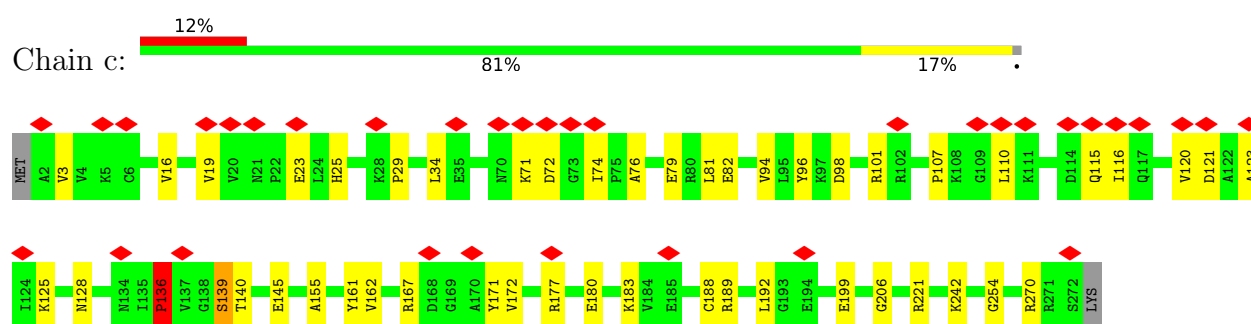
- Molecule 26: P-site tRNA fMet



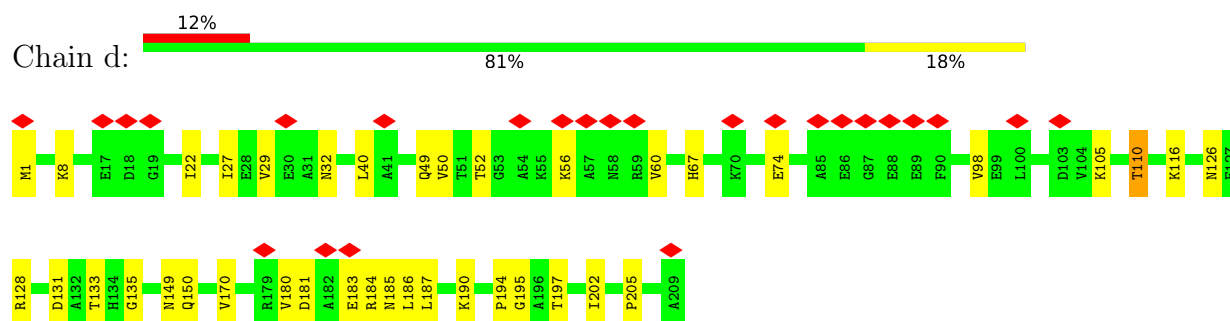
- Molecule 27: 5S rRNA



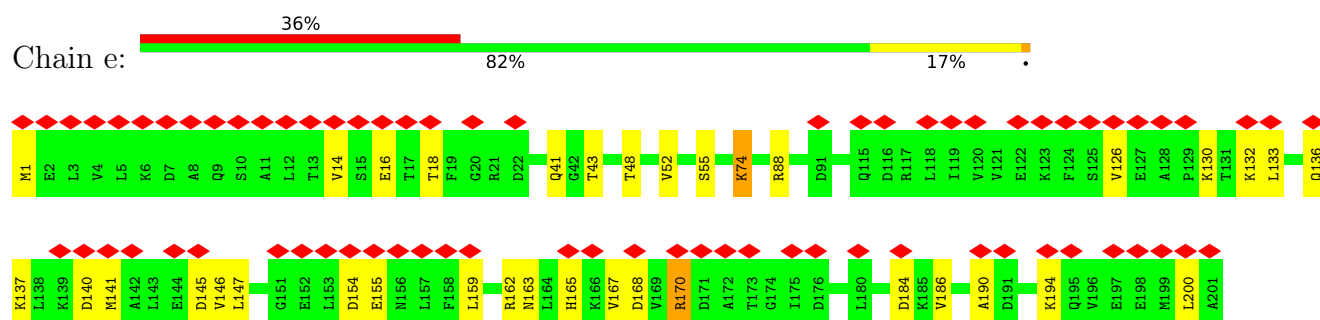
- Molecule 28: 50S ribosomal protein L2



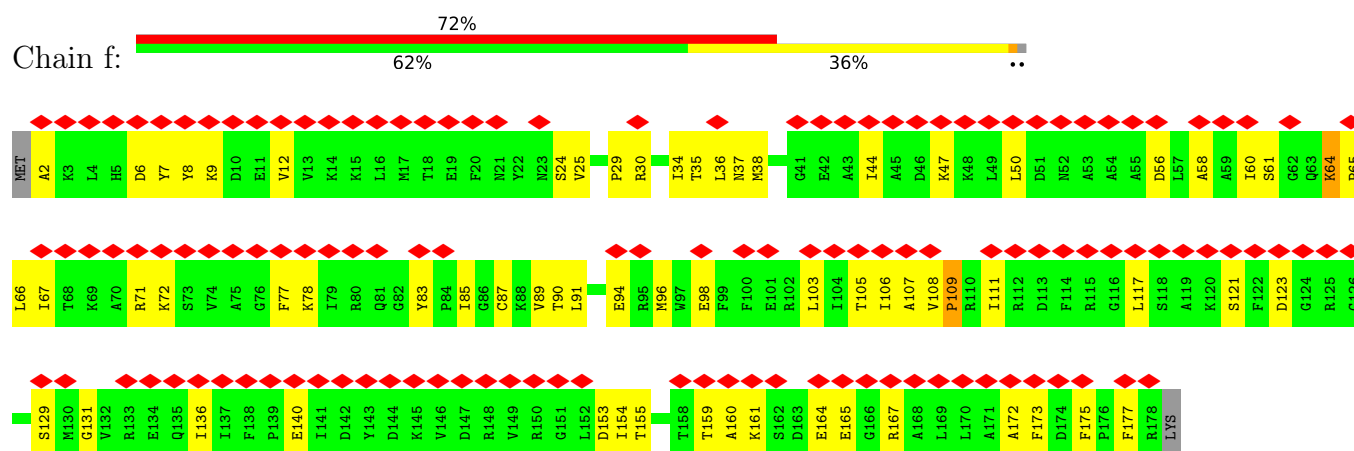
- Molecule 29: 50S ribosomal protein L3



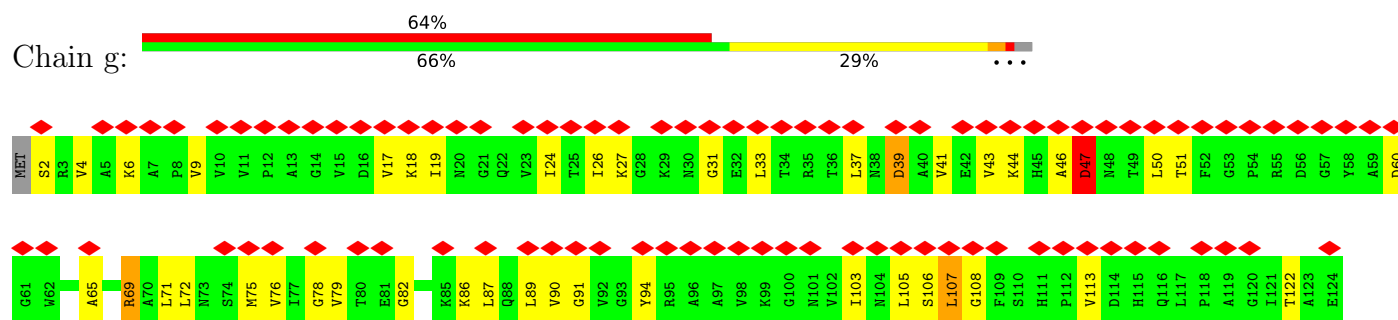
- Molecule 30: Large ribosomal subunit protein uL4

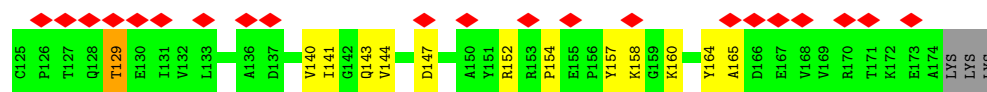


- Molecule 31: Large ribosomal subunit protein uL5

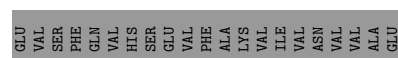
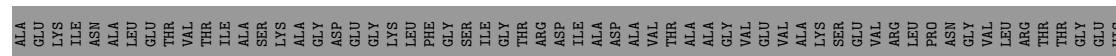


- Molecule 32: Large ribosomal subunit protein uL6

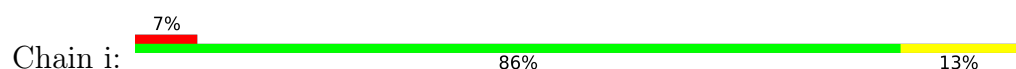




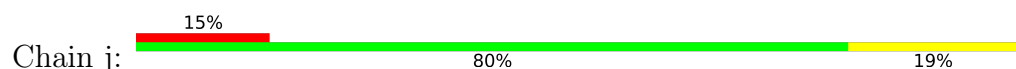
- Molecule 33: Large ribosomal subunit protein bL9



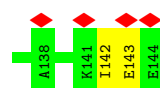
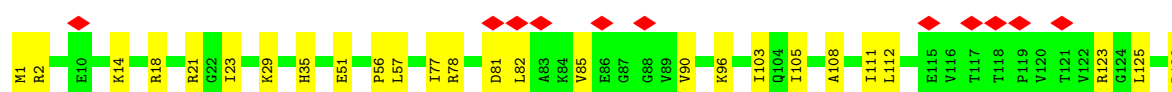
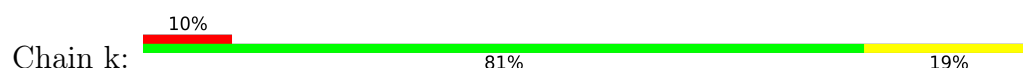
- Molecule 34: Large ribosomal subunit protein uL13



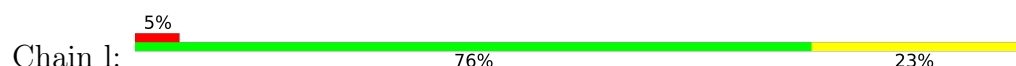
- Molecule 35: Large ribosomal subunit protein uL14

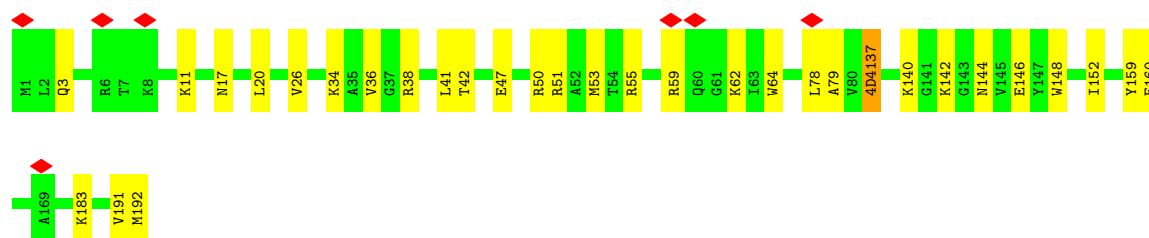


- Molecule 36: Large ribosomal subunit protein uL15

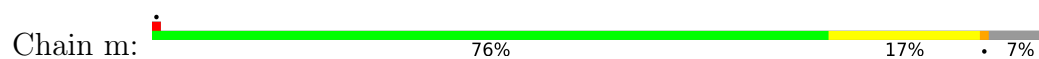


- Molecule 37: Large ribosomal subunit protein uL16

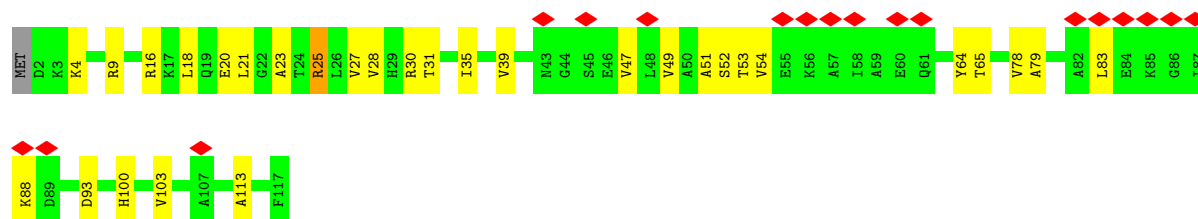




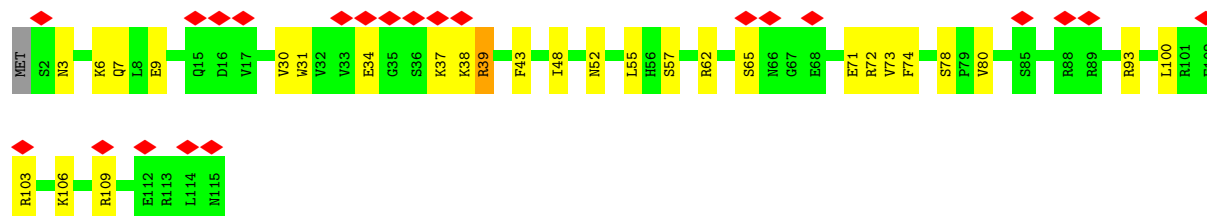
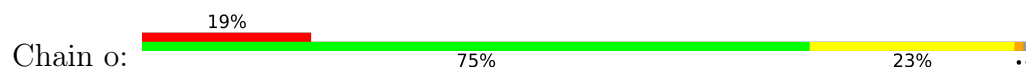
- Molecule 38: Large ribosomal subunit protein bL17



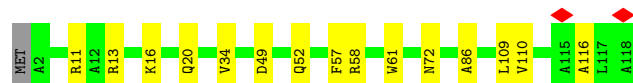
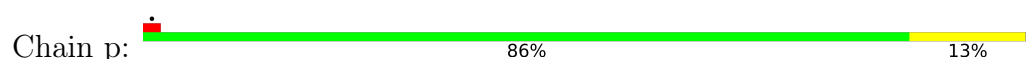
- Molecule 39: Large ribosomal subunit protein uL18



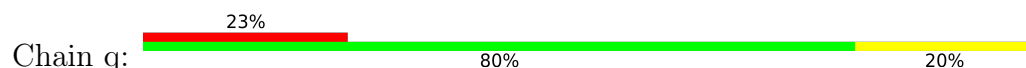
- Molecule 40: Large ribosomal subunit protein bL19

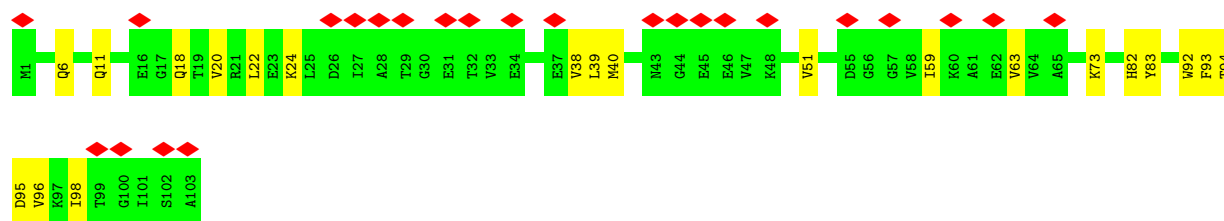


- Molecule 41: 50S ribosomal protein L20

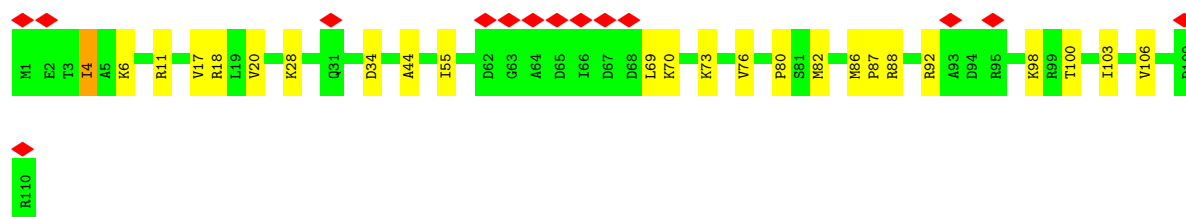
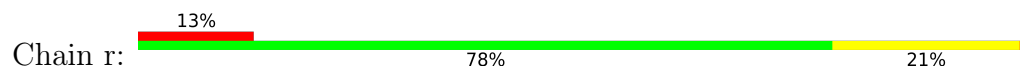


- Molecule 42: Large ribosomal subunit protein bL21

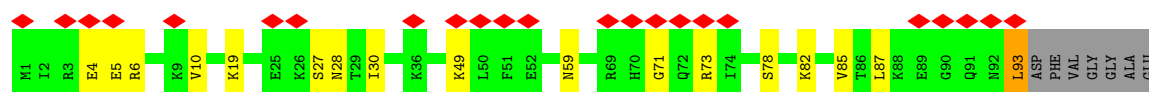
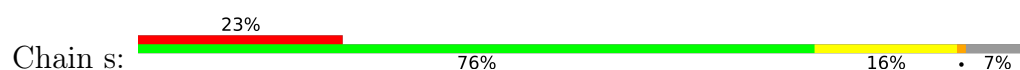




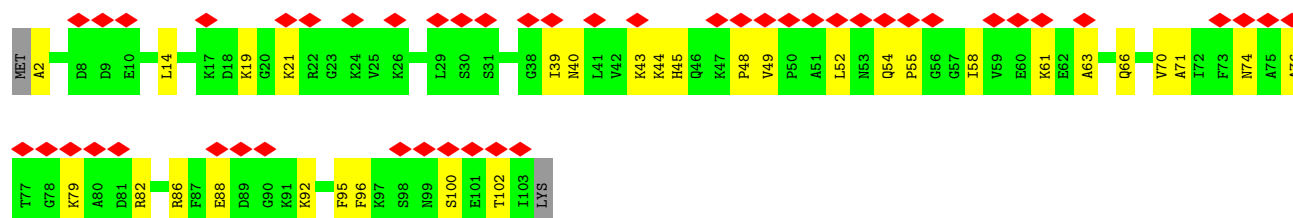
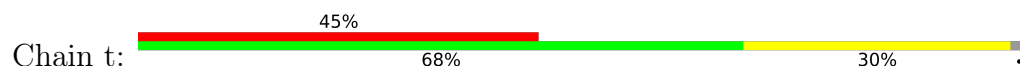
- Molecule 43: Large ribosomal subunit protein uL22



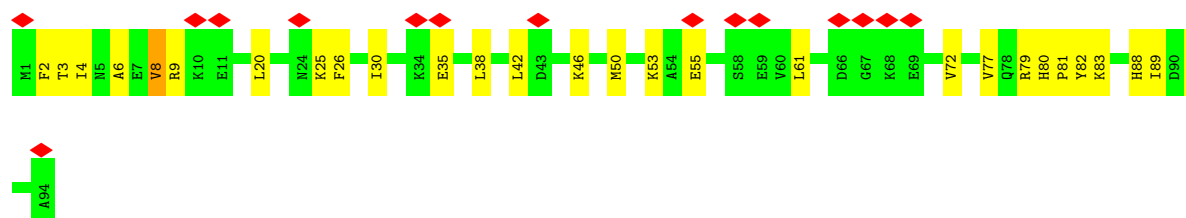
- Molecule 44: 50S ribosomal protein L23



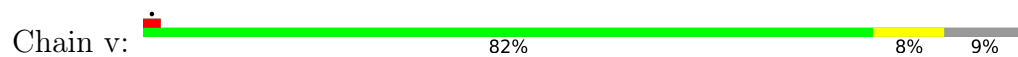
- Molecule 45: 50S ribosomal protein L24



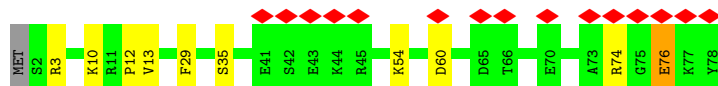
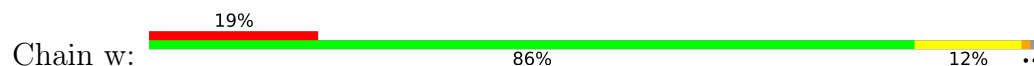
- Molecule 46: Large ribosomal subunit protein bL25



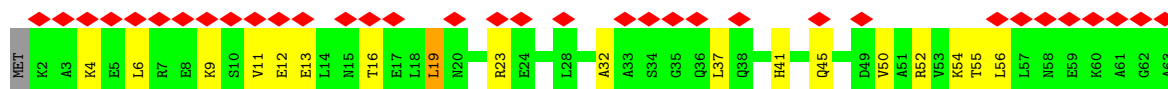
- Molecule 47: Large ribosomal subunit protein bL27



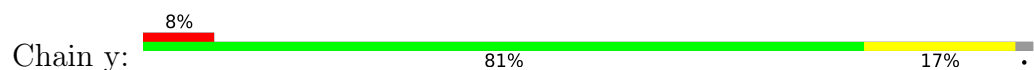
- Molecule 48: 50S ribosomal protein L28



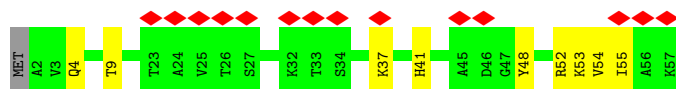
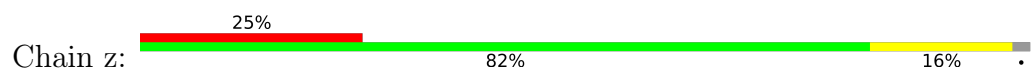
- Molecule 49: Large ribosomal subunit protein uL29



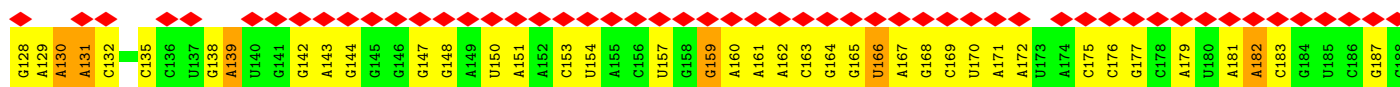
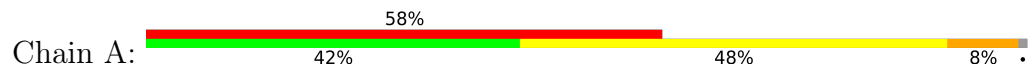
- Molecule 50: 50S ribosomal protein L30

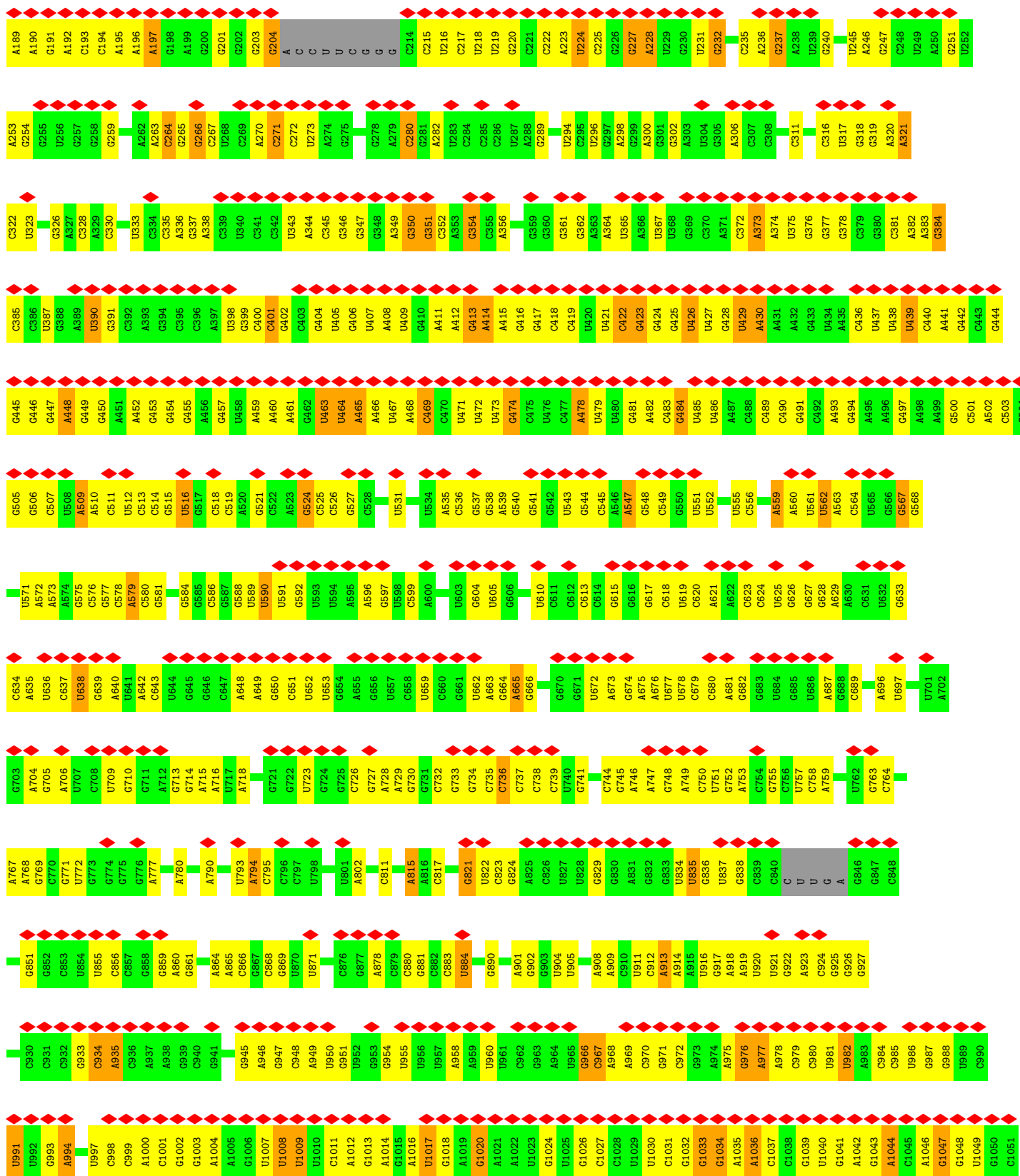


- Molecule 51: 50S ribosomal protein L32

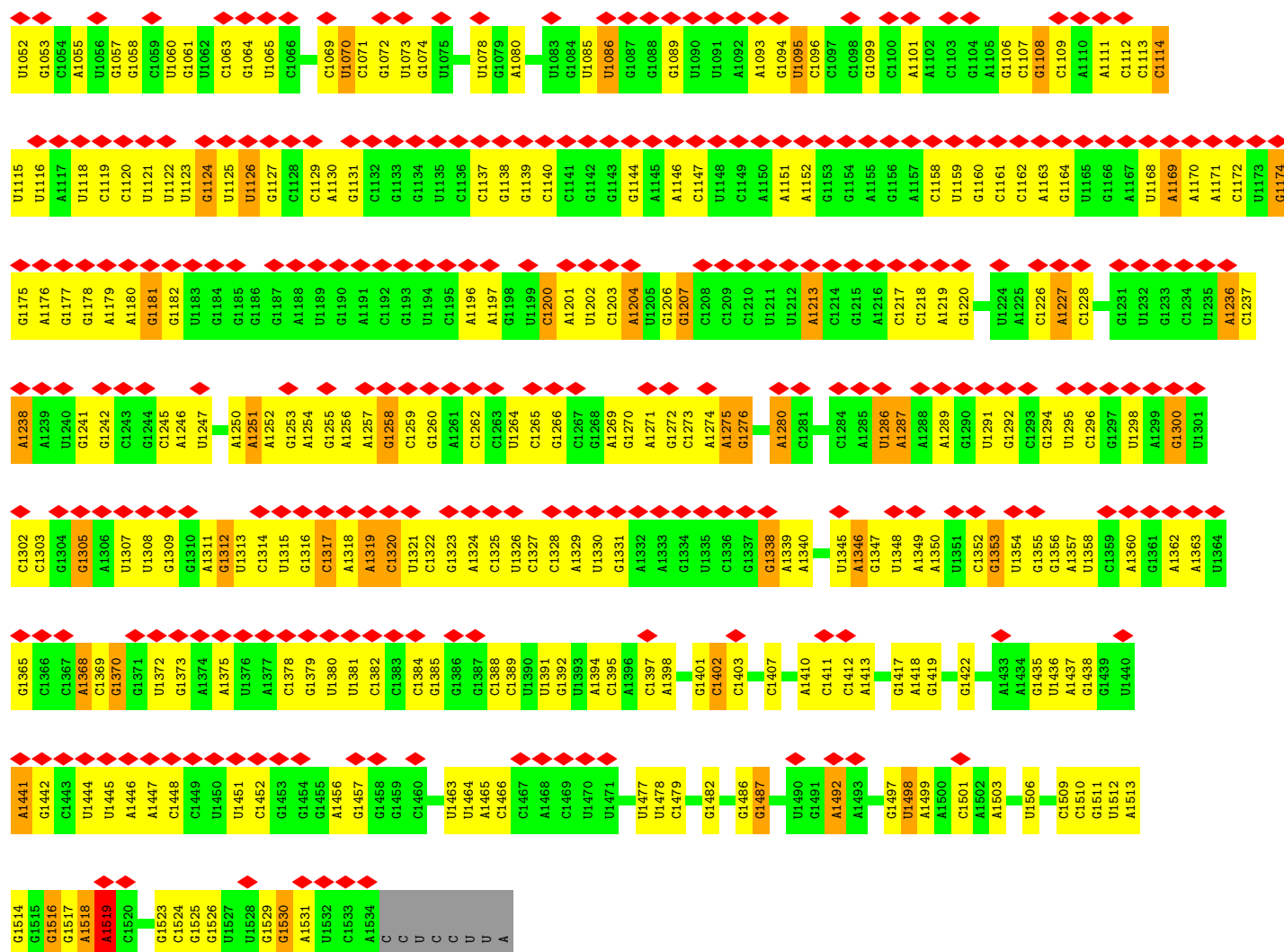


- Molecule 52: 16S rRNA

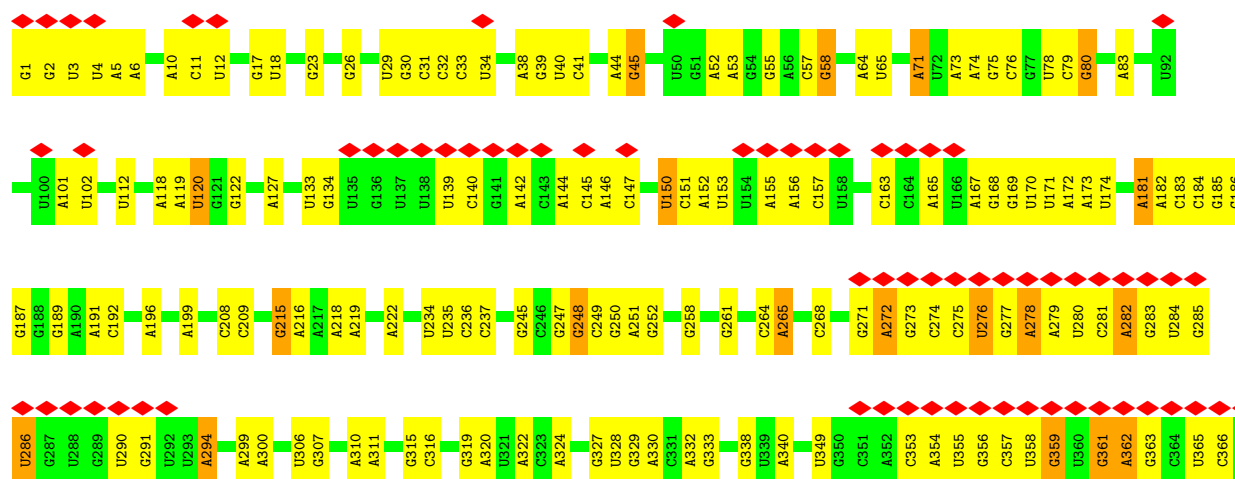








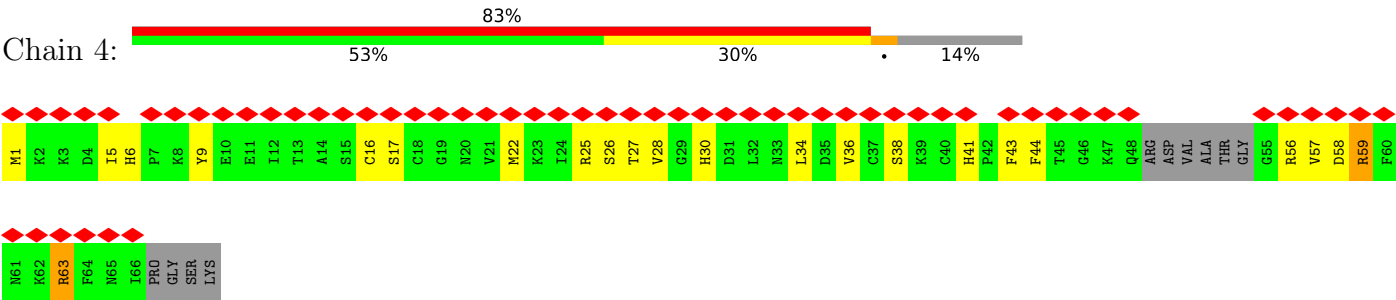
### • Molecule 53: 23S rRNA



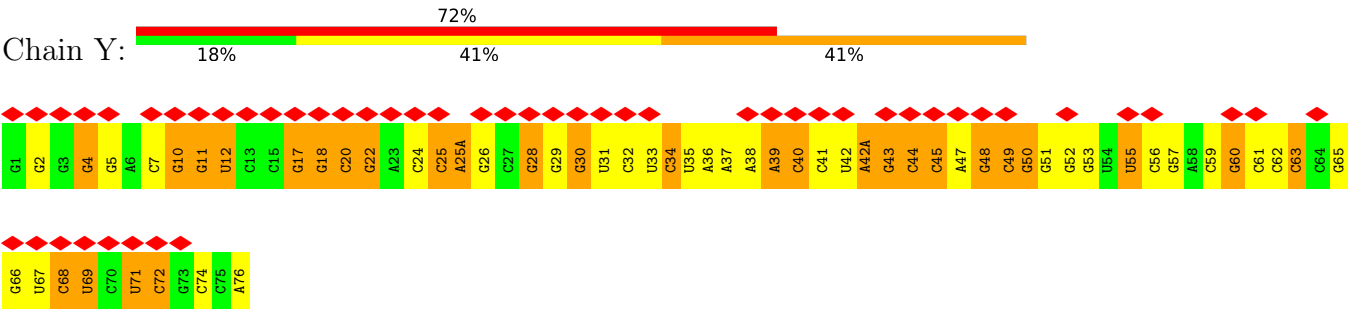




● Molecule 54: 50S ribosomal protein L31



● Molecule 55: A-site tRNA<sup>Pyl</sup>



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105571	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	15000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.192	Depositor
Minimum map value	-0.084	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0267	Depositor
Map size (Å)	422.1952, 422.1952, 422.1952	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8246, 0.8246, 0.8246	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, K, SPD, D2T, 2MA, UR3, IAS, OMC, SPM, PSU, 3TD, ZN, MS6, OMG, 4D4, 8AN, MA6, OMU, 2MG, MG, 1MG, FME, H2U, PAR, 5MU, G7M, 4OC, MEQ, A1B71, 6MZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.15	0/424	0.35	0/565
2	1	0.19	0/380	0.42	0/498
3	2	0.17	0/513	0.37	0/676
4	3	0.19	0/303	0.35	0/397
5	B	0.18	0/1784	0.42	0/2403
6	C	0.17	0/1651	0.40	0/2225
7	D	0.17	0/1665	0.38	0/2227
8	E	0.17	0/1165	0.40	0/1568
9	F	0.18	0/858	0.43	0/1160
10	G	0.17	0/1219	0.42	0/1635
11	H	0.17	0/989	0.43	0/1326
12	I	0.16	0/1034	0.38	0/1375
13	J	0.17	0/796	0.42	0/1077
14	K	0.20	0/884	0.49	1/1191 (0.1%)
15	L	0.16	0/960	0.38	0/1286
16	M	0.17	0/900	0.39	0/1204
17	N	0.16	0/817	0.38	0/1088
18	O	0.15	0/722	0.34	0/964
19	P	0.18	0/653	0.45	0/877
20	Q	0.16	0/650	0.38	0/871
21	R	0.19	0/553	0.46	0/742
22	S	0.15	0/685	0.38	0/922
23	T	0.20	0/676	0.37	0/895
24	U	0.16	0/597	0.34	0/792
25	X	0.29	0/361	0.43	0/560
26	Z	0.33	1/1788 (0.1%)	0.45	1/2786 (0.0%)
27	b	0.24	0/2850	0.33	0/4444
28	c	0.25	1/2121 (0.0%)	0.57	4/2852 (0.1%)
29	d	0.19	0/1576	0.37	0/2119
30	e	0.18	0/1571	0.38	0/2113
31	f	0.20	0/1434	0.47	1/1926 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	g	0.19	0/1315	0.48	0/1783
33	h	0.21	0/306	0.50	0/413
34	i	0.19	0/1152	0.38	0/1551
35	j	0.19	0/955	0.37	0/1279
36	k	0.20	0/1062	0.40	0/1413
37	l	0.21	0/1073	0.40	0/1433
38	m	0.20	0/958	0.43	0/1281
39	n	0.16	0/902	0.40	0/1209
40	o	0.19	0/929	0.40	0/1242
41	p	0.18	0/960	0.36	0/1278
42	q	0.20	0/829	0.51	0/1107
43	r	0.19	0/864	0.37	0/1156
44	s	0.17	0/744	0.38	0/994
45	t	0.19	0/787	0.48	0/1051
46	u	0.19	0/766	0.39	0/1025
47	v	0.17	0/589	0.39	0/780
48	w	0.16	0/635	0.37	0/848
49	x	0.19	0/502	0.38	0/667
50	y	0.18	0/453	0.38	0/605
51	z	0.15	0/450	0.33	0/599
52	A	0.26	1/36236 (0.0%)	0.34	0/56520
53	a	0.26	1/65651 (0.0%)	0.35	0/102413
54	4	0.17	0/488	0.39	0/649
55	Y	0.33	0/1665	0.62	0/2581
All	All	0.24	4/152850 (0.0%)	0.37	7/228641 (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
32	g	0	2
37	l	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	75	C	C2'-C1'	8.69	1.66	1.53
28	c	136	PRO	CG-CD	-8.02	1.23	1.50
53	a	2069	G7M	O3'-P	5.40	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A	527	G7M	O3'-P	5.20	1.61	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	136	PRO	N-CD-CG	-14.21	81.89	103.20
28	c	136	PRO	CA-CB-CG	-13.13	79.56	104.50
26	Z	75	C	C1'-C2'-O2'	7.70	119.96	108.40
28	c	136	PRO	CA-N-CD	-6.71	102.61	112.00
28	c	136	PRO	N-CA-CB	-6.00	97.97	103.31
31	f	109	PRO	CA-N-CD	-5.89	103.76	112.00
14	K	89	PRO	CA-CB-CG	-5.71	93.65	104.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	g	46	ALA	Peptide
32	g	47	ASP	Peptide
37	l	137	4D4	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	7	0
2	1	377	0	418	5	0
3	2	504	0	572	3	0
4	3	302	0	340	6	0
5	B	1753	0	1780	61	0
6	C	1624	0	1696	52	0
7	D	1643	0	1707	67	0
8	E	1152	0	1196	39	0
9	F	839	0	833	42	0
10	G	1203	0	1254	52	0
11	H	979	0	1031	39	0
12	I	1022	0	1070	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	J	786	0	828	48	0
14	K	877	0	882	32	0
15	L	957	0	1017	28	0
16	M	891	0	952	26	0
17	N	805	0	844	36	0
18	O	714	0	734	14	0
19	P	643	0	661	22	0
20	Q	641	0	682	16	0
21	R	544	0	565	23	0
22	S	668	0	693	24	0
23	T	670	0	719	21	0
24	U	589	0	629	17	0
25	X	322	0	162	5	0
26	Z	1623	0	825	28	0
27	b	2549	0	1291	33	0
28	c	2082	0	2154	33	0
29	d	1566	0	1618	22	0
30	e	1552	0	1619	21	0
31	f	1410	0	1444	41	0
32	g	1295	0	1332	41	0
33	h	303	0	327	6	0
34	i	1129	0	1162	12	0
35	j	946	0	1023	17	0
36	k	1053	0	1129	17	0
37	l	1075	0	1146	22	0
38	m	945	0	989	14	0
39	n	892	0	923	21	0
40	o	917	0	962	22	0
41	p	947	0	1019	12	0
42	q	816	0	839	13	0
43	r	857	0	922	19	0
44	s	738	0	807	10	0
45	t	779	0	831	21	0
46	u	753	0	780	21	0
47	v	582	0	593	5	0
48	w	625	0	652	5	0
49	x	501	0	531	11	0
50	y	449	0	488	6	0
51	z	444	0	458	7	0
52	A	32612	0	16432	647	0
53	a	59130	0	29763	677	0
54	4	480	0	478	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	Y	1518	0	776	45	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	90	0	0	0	0
57	C	1	0	0	0	0
57	N	1	0	0	0	0
57	Q	1	0	0	0	0
57	Z	1	0	0	0	0
57	a	219	0	0	0	0
57	b	5	0	0	0	0
57	d	1	0	0	0	0
57	z	1	0	0	0	0
58	Z	10	0	10	0	0
59	a	9	0	0	0	0
59	c	1	0	0	0	0
60	A	42	0	45	1	0
61	A	10	0	19	0	0
61	a	130	0	247	16	0
62	a	14	0	26	3	0
63	Y	17	0	0	0	0
64	0	2	0	0	0	0
64	1	15	0	0	1	0
64	2	19	0	0	0	0
64	3	4	0	0	0	0
64	A	2	0	0	0	0
64	Y	2	0	0	0	0
64	Z	4	0	0	1	0
64	a	2993	0	0	61	0
64	b	41	0	0	2	0
64	c	84	0	0	1	0
64	d	36	0	0	0	0
64	e	29	0	0	0	0
64	h	1	0	0	0	0
64	i	13	0	0	1	0
64	j	14	0	0	0	0
64	k	34	0	0	2	0
64	l	25	0	0	0	0
64	m	23	0	0	1	0
64	o	13	0	0	1	0
64	p	24	0	0	3	0
64	q	13	0	0	0	0
64	r	26	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	s	5	0	0	0	0
64	t	1	0	0	0	0
64	u	3	0	0	0	0
64	v	11	0	0	0	0
64	w	12	0	0	0	0
64	x	1	0	0	0	0
64	z	24	0	0	0	0
All	All	145519	0	95376	2328	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 10.

All (2328) 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)
21:R:9:LYS:HG3	21:R:10:PHE:H	1.17	1.04
11:H:2:SER:N	52:A:823:C:HO2'	1.67	0.93
52:A:1086:U:H3	52:A:1099:G:H22	1.14	0.91
55:Y:52:G:N2	55:Y:62:C:O2	2.05	0.90
26:Z:76:8AN:O2P	64:Z:201:HOH:O	1.91	0.88
7:D:46:PRO:HB2	7:D:48:LEU:HD23	1.55	0.86
31:f:30:ARG:H	31:f:159:THR:HG22	1.40	0.86
26:Z:52:G:N2	26:Z:62:C:O2	2.10	0.84
16:M:92:ARG:NH1	53:a:887:U:OP1	2.11	0.84
53:a:1912:A:N6	53:a:1917:PSU:O4	2.11	0.82
52:A:71:A:H61	52:A:99:C:H1'	1.44	0.82
30:e:168:ASP:OD2	30:e:170:ARG:NH1	2.13	0.82
52:A:673:A:H2'	52:A:674:G:C8	2.15	0.82
27:b:66:A:OP2	27:b:108:A:N6	2.13	0.82
53:a:283:G:N2	53:a:357:C:O2	2.11	0.82
6:C:129:MET:HB2	6:C:132:ARG:HG2	1.62	0.81
52:A:1032:G:H2'	52:A:1033:G:H4'	1.61	0.81
41:p:13:ARG:NH2	64:p:202:HOH:O	2.13	0.80
41:p:11:ARG:NH1	64:p:201:HOH:O	2.12	0.80
4:3:25:VAL:HB	4:3:35:GLN:HG2	1.64	0.79
27:b:36:C:H5''	27:b:38:C:H41	1.46	0.79
5:B:4:VAL:HG21	5:B:212:LEU:HD21	1.64	0.79
37:l:20:LEU:HD13	46:u:81:PRO:HG2	1.62	0.79
52:A:946:A:H2'	52:A:947:G:C8	2.17	0.78
53:a:291:G:O6	53:a:349:U:O2	2.02	0.78
19:P:5:ARG:NH2	19:P:26:ASN:O	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:83:GLU:HG2	14:K:109:ASN:HB2	1.63	0.77
28:c:167:ARG:HD3	28:c:172:VAL:HG12	1.67	0.77
52:A:664:G:H22	52:A:741:G:H1	1.33	0.77
31:f:85:ILE:HD11	53:a:2312:U:H5'	1.66	0.77
5:B:151:ILE:HB	5:B:154:MET:HE2	1.67	0.77
11:H:88:ARG:HG2	11:H:91:GLU:HG2	1.66	0.77
15:L:58:THR:HG21	52:A:362:G:H5''	1.67	0.77
42:q:6:GLN:HG3	42:q:39:LEU:HD21	1.66	0.77
52:A:203:G:N2	52:A:204:G:O6	2.18	0.77
3:2:8:ARG:NH2	53:a:245:G:N7	2.32	0.76
21:R:9:LYS:HG3	21:R:10:PHE:N	1.99	0.76
13:J:9:ARG:HH22	13:J:42:LEU:HD13	1.49	0.76
10:G:79:ARG:HH21	52:A:1382:C:H4'	1.48	0.76
29:d:184:ARG:HB3	29:d:186:LEU:HG	1.68	0.76
46:u:8:VAL:HG22	46:u:38:LEU:HD21	1.68	0.76
14:K:111:THR:HG23	24:U:3:VAL:HG12	1.68	0.75
32:g:107:LEU:O	32:g:152:ARG:NH2	2.20	0.75
22:S:50:ALA:HB1	22:S:57:HIS:HB3	1.67	0.74
9:F:26:THR:HG22	9:F:36:ILE:HG12	1.68	0.74
53:a:1802:A:H2'	53:a:1803:A:C8	2.22	0.74
52:A:197:A:N1	52:A:220:G:O2'	2.19	0.74
53:a:568:U:H1'	53:a:2030:6MZ:H9C1	1.68	0.74
24:U:10:GLU:OE2	24:U:18:ARG:NH2	2.21	0.74
52:A:75:G:H2'	52:A:76:G:H8	1.53	0.74
12:I:12:ARG:NH2	52:A:1347:G:O6	2.20	0.74
21:R:37:GLY:O	21:R:63:ARG:NH2	2.19	0.74
52:A:376:G:H2'	52:A:377:G:H8	1.52	0.73
29:d:110:THR:HG23	29:d:202:ILE:HB	1.70	0.73
32:g:31:GLY:HA3	32:g:79:VAL:HG12	1.70	0.73
53:a:1047:G:HO2'	53:a:1110:G:H1	0.73	0.73
1:0:25:LYS:NZ	1:0:32:GLU:O	2.22	0.73
7:D:131:ASN:OD1	52:A:619:U:N3	2.19	0.73
52:A:501:C:H2'	52:A:502:A:C8	2.24	0.72
22:S:31:LEU:HD11	22:S:47:LEU:HD22	1.71	0.72
55:Y:55:U:O2'	55:Y:57:G:N7	2.22	0.72
10:G:111:ARG:NH1	10:G:113:ASP:OD2	2.21	0.72
13:J:28:THR:HA	13:J:31:ARG:HE	1.55	0.72
52:A:490:C:H2'	52:A:491:G:H8	1.54	0.72
53:a:411:G:N7	61:a:3212:SPD:N10	2.35	0.72
19:P:4:ILE:HG12	19:P:21:VAL:HG22	1.72	0.72
52:A:181:A:N6	52:A:195:A:OP2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:38:VAL:HG11	8:E:114:VAL:HG12	1.72	0.72
7:D:59:GLN:OE1	7:D:62:ARG:NH1	2.22	0.72
52:A:665:A:H1'	52:A:733:G:H5'	1.72	0.72
31:f:64:LYS:HD3	54:4:5:ILE:HB	1.70	0.71
7:D:132:ILE:HG21	52:A:620:C:H1'	1.72	0.71
8:E:149:SER:OG	8:E:152:MET:SD	2.48	0.71
34:i:125:TYR:OH	34:i:132:HIS:NE2	2.21	0.71
9:F:95:ALA:HB1	9:F:97:THR:HG23	1.70	0.71
37:l:144:ASN:ND2	37:l:146:GLU:OE2	2.23	0.71
5:B:27:MET:HE1	5:B:201:PRO:HB3	1.71	0.71
13:J:66:GLU:HB2	17:N:99:ALA:HB2	1.73	0.71
53:a:1478:G:H1	53:a:1513:U:H3	1.39	0.71
10:G:114:LYS:NZ	52:A:1298:U:OP2	2.24	0.70
9:F:44:ARG:HD3	9:F:56:LYS:HD3	1.73	0.70
29:d:32:ASN:HB3	29:d:50:VAL:HG21	1.73	0.70
53:a:1469:A:H2'	53:a:1470:A:C8	2.27	0.70
7:D:105:MET:HG3	7:D:171:LEU:HD23	1.73	0.70
52:A:674:G:H2'	52:A:675:A:H8	1.56	0.70
13:J:9:ARG:NH1	52:A:1126:U:O4	2.24	0.70
52:A:28:A:O2'	52:A:296:U:OP1	2.10	0.70
9:F:37:HIS:HB3	9:F:97:THR:HG22	1.74	0.69
53:a:1434:A:H2'	53:a:1435:G:C8	2.27	0.69
5:B:68:LEU:HD22	5:B:90:PHE:HB2	1.73	0.69
27:b:100:G:N7	64:b:303:HOH:O	2.25	0.69
32:g:19:ILE:HG12	32:g:24:ILE:HD12	1.73	0.69
52:A:203:G:O2'	52:A:465:A:N1	2.24	0.69
14:K:28:ASN:O	14:K:57:LYS:NZ	2.25	0.69
7:D:2:ALA:N	52:A:405:U:O4	2.25	0.69
52:A:337:G:H2'	52:A:338:A:C8	2.27	0.69
28:c:136:PRO:O	28:c:139:SER:OG	2.10	0.69
45:t:86:ARG:NH1	45:t:100:SER:OG	2.24	0.69
12:I:112:GLU:OE2	12:I:115:LYS:NZ	2.20	0.69
5:B:9:MET:HG2	5:B:14:VAL:HG21	1.75	0.69
52:A:514:C:H2'	52:A:515:G:H8	1.57	0.68
53:a:1342:A:N3	64:a:3370:HOH:O	2.25	0.68
5:B:207:ILE:O	5:B:211:THR:OG1	2.11	0.68
32:g:4:VAL:HG21	53:a:2748:A:H5'	1.75	0.68
52:A:1266:G:N2	52:A:1269:A:OP2	2.24	0.68
10:G:93:PRO:HA	10:G:96:ARG:HG2	1.74	0.68
55:Y:4:G:H1	55:Y:69:U:H3	1.42	0.68
43:r:87:PRO:HD2	61:a:3217:SPD:H42	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:187:G:N7	64:a:3380:HOH:O	2.27	0.67
53:a:472:A:OP1	61:a:3216:SPD:N6	2.28	0.67
53:a:2351:G:OP2	64:a:3301:HOH:O	2.11	0.67
6:C:70:THR:HG21	6:C:76:VAL:HG21	1.77	0.67
28:c:79:GLU:OE2	28:c:101:ARG:NE	2.27	0.67
52:A:662:U:H2'	52:A:663:A:C8	2.28	0.67
26:Z:52:G:N1	26:Z:62:C:N3	2.33	0.67
52:A:203:G:H1'	52:A:465:A:H61	1.56	0.67
29:d:116:LYS:HA	38:m:1:MET:HE3	1.77	0.67
52:A:728:A:H2'	52:A:729:A:C8	2.29	0.67
52:A:1218:C:H2'	52:A:1219:A:C8	2.30	0.67
54:4:41:HIS:HB3	54:4:44:PHE:HB2	1.76	0.67
36:k:78:ARG:NH1	53:a:627:A:OP1	2.27	0.67
53:a:639:U:H2'	53:a:640:C:C6	2.30	0.67
53:a:764:A:O2'	64:a:3302:HOH:O	2.12	0.67
40:o:93:ARG:NH2	53:a:2849:U:OP1	2.25	0.67
7:D:125:VAL:HG22	7:D:143:VAL:HG22	1.76	0.67
29:d:1:MET:HB3	29:d:205:PRO:HG2	1.76	0.67
5:B:43:LEU:HA	5:B:46:THR:HG22	1.76	0.66
5:B:136:MET:SD	5:B:139:ARG:NH2	2.68	0.66
39:n:9:ARG:HG2	39:n:9:ARG:HH11	1.59	0.66
53:a:1386:C:H2'	53:a:1387:A:C8	2.30	0.66
52:A:113:G:H1'	52:A:354:G:H5'	1.75	0.66
53:a:1905:C:N4	64:a:3382:HOH:O	2.27	0.66
23:T:29:ARG:O	23:T:33:LYS:HG2	1.94	0.66
52:A:157:U:O2	52:A:164:G:O6	2.13	0.66
52:A:222:C:H2'	52:A:223:A:H8	1.59	0.66
16:M:24:GLY:O	16:M:29:ARG:NH1	2.27	0.66
14:K:87:LYS:HB2	14:K:113:VAL:HG23	1.75	0.66
53:a:1155:A:OP2	64:a:3303:HOH:O	2.13	0.66
9:F:38:ARG:HB3	9:F:63:ASN:HB2	1.77	0.65
7:D:99:ASP:OD1	7:D:100:ASN:N	2.29	0.65
17:N:24:ARG:NH1	17:N:55:SER:OG	2.30	0.65
34:i:9:GLU:HG2	34:i:10:THR:HG23	1.78	0.65
35:j:105:ARG:NH2	40:o:34:GLU:OE2	2.25	0.65
53:a:2096:C:O2	53:a:2193:G:N2	2.19	0.65
53:a:2243:U:H2'	53:a:2244:U:C6	2.31	0.65
9:F:63:ASN:ND2	9:F:96:VAL:HB	2.12	0.65
52:A:1001:C:H2'	52:A:1002:G:H8	1.62	0.65
52:A:1035:A:O2'	52:A:1036:A:O5'	2.15	0.65
28:c:29:PRO:HG2	28:c:34:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:493:A:H2'	52:A:494:G:C8	2.31	0.65
52:A:1162:C:H2'	52:A:1163:A:H8	1.60	0.65
12:I:11:ARG:NH1	52:A:1118:U:OP1	2.29	0.65
13:J:64:GLN:NE2	52:A:1368:A:OP1	2.30	0.65
52:A:77:A:H2'	52:A:78:A:C8	2.32	0.65
12:I:18:ARG:HH22	52:A:1129:C:H4'	1.61	0.65
53:a:252:G:N7	64:a:3391:HOH:O	2.28	0.65
54:4:9:TYR:HA	54:4:26:SER:O	1.97	0.65
6:C:57:ILE:HD12	6:C:64:ILE:HD11	1.78	0.64
55:Y:48:G:O2'	55:Y:49:C:OP2	2.15	0.64
31:f:105:THR:HA	54:4:38:SER:HB2	1.80	0.64
52:A:538:G:H2'	52:A:539:A:C8	2.32	0.64
53:a:1746:A:H2'	53:a:1747:U:C6	2.32	0.64
8:E:88:VAL:HG13	8:E:93:ARG:HG2	1.78	0.64
23:T:67:ILE:HB	23:T:71:LYS:HD3	1.79	0.64
53:a:2328:A:H2'	53:a:2329:U:C6	2.31	0.64
10:G:70:ARG:NH1	10:G:97:ASN:OD1	2.30	0.64
53:a:813:U:H2'	53:a:814:C:C6	2.32	0.64
53:a:1215:G:N7	64:a:3401:HOH:O	2.29	0.64
2:1:39:ARG:NH2	53:a:468:G:N7	2.44	0.64
20:Q:69:LYS:NZ	52:A:253:A:OP1	2.26	0.64
52:A:56:U:H2'	52:A:57:G:H8	1.63	0.64
5:B:183:VAL:HG23	5:B:197:ASP:H	1.61	0.64
9:F:6:ILE:HG12	9:F:89:VAL:HG22	1.78	0.64
48:w:74:ARG:NH1	48:w:76:GLU:OE2	2.30	0.64
52:A:460:A:H2'	52:A:461:A:C8	2.33	0.64
52:A:1124:G:H1'	52:A:1125:U:H5	1.63	0.64
53:a:370:G:OP2	64:a:3305:HOH:O	2.15	0.64
53:a:2431:U:OP1	64:a:3306:HOH:O	2.15	0.64
53:a:1178:C:H2'	53:a:1179:G:H8	1.61	0.64
53:a:2801:G:H2'	53:a:2802:G:H8	1.63	0.64
18:O:54:ARG:NH1	52:A:579:A:O2'	2.26	0.63
35:j:58:LEU:HD11	35:j:86:LEU:HD23	1.80	0.63
45:t:82:ARG:NH2	53:a:300:A:OP2	2.30	0.63
52:A:56:U:H2'	52:A:57:G:C8	2.32	0.63
52:A:490:C:H2'	52:A:491:G:C8	2.34	0.63
53:a:189:G:OP1	64:a:3304:HOH:O	2.14	0.63
6:C:138:VAL:HA	6:C:149:ILE:HD13	1.81	0.63
36:k:96:LYS:NZ	36:k:105:ILE:O	2.32	0.63
52:A:1169:A:H2'	52:A:1170:A:C8	2.34	0.63
53:a:1346:G:N7	64:a:3419:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:18:ARG:NH2	52:A:1130:A:OP1	2.32	0.63
53:a:2591:C:H2'	53:a:2592:G:C8	2.34	0.63
27:b:49:C:H2'	27:b:50:A:H8	1.63	0.63
52:A:538:G:H2'	52:A:539:A:H8	1.62	0.63
26:Z:76:8AN:N6	53:a:2451:A:H5'	2.14	0.63
34:i:37:ARG:NH1	53:a:1007:C:OP1	2.31	0.63
20:Q:69:LYS:HB2	52:A:266:G:H3'	1.81	0.63
53:a:3:U:H2'	53:a:4:U:C6	2.33	0.63
52:A:985:C:H2'	52:A:986:U:C6	2.34	0.63
52:A:1338:G:H2'	52:A:1339:A:C8	2.33	0.63
53:a:2291:U:H2'	53:a:2292:U:C6	2.34	0.63
15:L:33:VAL:HG22	15:L:79:VAL:HG22	1.81	0.63
52:A:335:C:H2'	52:A:336:A:H8	1.62	0.63
52:A:651:C:N4	52:A:753:A:OP2	2.32	0.63
20:Q:18:GLU:O	52:A:254:G:O2'	2.17	0.62
40:o:62:ARG:NH1	40:o:71:GLU:OE2	2.32	0.62
52:A:171:A:H2'	52:A:172:A:C8	2.34	0.62
52:A:216:U:H2'	52:A:217:C:C6	2.34	0.62
52:A:1049:U:H5'	52:A:1201:A:OP2	1.99	0.62
52:A:150:U:H2'	52:A:151:A:H8	1.64	0.62
53:a:2313:C:H2'	53:a:2314:A:H8	1.64	0.62
55:Y:68:C:H2'	55:Y:69:U:C6	2.33	0.62
17:N:2:ALA:N	52:A:1203:C:OP1	2.31	0.62
6:C:50:ALA:HB1	6:C:76:VAL:HG22	1.82	0.62
31:f:37:ASN:HB3	31:f:153:ASP:OD1	1.99	0.62
53:a:2801:G:H2'	53:a:2802:G:C8	2.35	0.62
23:T:67:ILE:HD12	23:T:71:LYS:HB3	1.82	0.62
52:A:815:A:N7	52:A:1509:C:O2'	2.28	0.62
9:F:26:THR:O	9:F:30:THR:OG1	2.18	0.62
52:A:294:U:OP1	52:A:610:U:O2'	2.13	0.62
53:a:277:G:H1'	53:a:278:A:C5	2.35	0.62
53:a:1405:U:H2'	53:a:1406:U:C6	2.35	0.62
7:D:28:ILE:HD13	7:D:34:ILE:HD11	1.81	0.62
41:p:49:ASP:HA	41:p:52:GLN:HB2	1.82	0.62
7:D:4:TYR:OH	7:D:7:PRO:O	2.11	0.62
52:A:1530:G:H2'	52:A:1531:A:H8	1.65	0.62
5:B:126:PHE:HA	5:B:129:LEU:HD13	1.82	0.61
53:a:5:A:H2'	53:a:6:A:H8	1.64	0.61
53:a:2864:G:OP2	61:a:3208:SPD:N1	2.33	0.61
46:u:35:GLU:N	46:u:35:GLU:OE1	2.31	0.61
52:A:415:A:N6	52:A:428:G:O6	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:105:VAL:O	10:G:109:ARG:HG2	2.01	0.61
52:A:1057:G:H2'	52:A:1058:G:O4'	2.00	0.61
10:G:146:GLU:HA	10:G:149:LYS:HE2	1.82	0.61
37:l:183:LYS:HE3	53:a:1029:A:H5''	1.82	0.61
52:A:1163:A:H2'	52:A:1164:G:H8	1.65	0.61
53:a:767:U:C4	62:a:3220:SPM:H132	2.35	0.61
11:H:89:LYS:HE3	11:H:120:GLY:HA2	1.83	0.61
52:A:73:C:O2'	52:A:74:A:H8	1.84	0.61
52:A:79:G:O6	52:A:80:A:N6	2.33	0.61
52:A:219:U:H2'	52:A:220:G:H8	1.66	0.61
52:A:945:G:C2	52:A:946:A:C8	2.89	0.61
6:C:108:LYS:HD2	6:C:111:LEU:HB2	1.82	0.61
8:E:81:LEU:HB3	8:E:147:MET:SD	2.40	0.61
52:A:738:C:H2'	52:A:739:C:H6	1.66	0.61
52:A:1241:G:H2'	52:A:1242:G:H8	1.66	0.61
8:E:159:LYS:NZ	11:H:42:GLU:O	2.31	0.61
52:A:714:G:H2'	52:A:715:A:C8	2.36	0.61
8:E:12:GLN:HB2	8:E:117:VAL:HG13	1.83	0.61
14:K:23:ILE:HG13	14:K:32:VAL:HG22	1.83	0.61
38:m:30:ARG:NH1	38:m:74:GLU:OE1	2.33	0.61
52:A:1163:A:H2'	52:A:1164:G:C8	2.36	0.61
43:r:92:ARG:NH1	64:r:202:HOH:O	2.34	0.60
53:a:5:A:H2'	53:a:6:A:C8	2.36	0.60
53:a:709:U:H2'	53:a:710:U:C6	2.36	0.60
53:a:2086:U:H2'	53:a:2087:G:C8	2.36	0.60
10:G:113:ASP:HB2	10:G:119:ARG:HB3	1.83	0.60
17:N:13:ARG:NH1	52:A:980:C:O2'	2.34	0.60
52:A:666:G:H5'	52:A:726:C:H1'	1.83	0.60
53:a:893:C:H2'	53:a:894:U:C6	2.36	0.60
53:a:1020:A:OP1	64:a:3309:HOH:O	2.17	0.60
52:A:21:G:H2'	52:A:22:G:C8	2.36	0.60
7:D:105:MET:HE1	7:D:143:VAL:HB	1.84	0.60
53:a:1:G:H2'	53:a:2:G:C8	2.36	0.60
53:a:1158:C:OP2	64:a:3307:HOH:O	2.16	0.60
53:a:1386:C:H2'	53:a:1387:A:H8	1.66	0.60
17:N:88:ALA:HB2	17:N:96:LEU:HD23	1.84	0.60
52:A:320:A:H2'	52:A:321:A:C8	2.37	0.60
52:A:738:C:H2'	52:A:739:C:C6	2.36	0.60
9:F:102:MET:HE1	21:R:26:ILE:HD12	1.83	0.60
13:J:53:ILE:HD11	13:J:61:ALA:HB1	1.82	0.60
22:S:45:ILE:HA	22:S:62:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:11:A:H2'	26:Z:12:G:C8	2.37	0.60
52:A:559:A:H4'	52:A:560:A:H3'	1.84	0.60
52:A:977:A:O2'	52:A:979:C:OP2	2.20	0.60
52:A:1032:G:N1	52:A:1033:G:N3	2.50	0.60
52:A:1144:G:H21	52:A:1146:A:H62	1.50	0.60
53:a:721:A:H2'	53:a:722:A:C8	2.36	0.60
7:D:54:GLN:HB3	7:D:203:LEU:HD22	1.83	0.60
33:h:17:ASP:OD1	33:h:17:ASP:N	2.34	0.60
43:r:28:LYS:HG2	43:r:70:LYS:HE3	1.83	0.60
52:A:1001:C:H2'	52:A:1002:G:C8	2.37	0.60
53:a:1794:A:H2'	53:a:1795:C:C6	2.37	0.60
53:a:1968:G:OP1	64:a:3310:HOH:O	2.17	0.60
52:A:994:A:H61	52:A:1047:G:H4'	1.65	0.60
53:a:1434:A:H2'	53:a:1435:G:H8	1.64	0.60
52:A:376:G:H2'	52:A:377:G:C8	2.35	0.60
53:a:856:G:H2'	53:a:857:G:C8	2.37	0.60
55:Y:38:A:H3'	55:Y:39:A:H8	1.67	0.60
5:B:119:THR:O	5:B:123:ASP:HB2	2.01	0.59
24:U:7:ARG:HE	24:U:18:ARG:HH21	1.50	0.59
36:k:18:ARG:NH1	64:k:202:HOH:O	2.18	0.59
54:4:26:SER:OG	54:4:27:THR:N	2.35	0.59
6:C:24:ALA:HB1	6:C:28:GLU:HB2	1.84	0.59
14:K:94:GLU:OE1	24:U:16:LEU:HD21	2.03	0.59
26:Z:16:C:OP1	26:Z:17:C:N4	2.35	0.59
26:Z:44:A:H2'	26:Z:45:G:C8	2.37	0.59
31:f:29:PRO:HB3	31:f:160:ALA:HB2	1.84	0.59
53:a:1746:A:H2'	53:a:1747:U:H6	1.64	0.59
11:H:49:PHE:HA	11:H:60:GLU:O	2.01	0.59
33:h:4:ILE:O	33:h:36:ALA:HA	2.02	0.59
52:A:235:C:H2'	52:A:236:A:H8	1.66	0.59
52:A:635:A:H2'	52:A:636:U:C6	2.37	0.59
6:C:111:LEU:O	6:C:204:LYS:NZ	2.35	0.59
52:A:501:C:H2'	52:A:502:A:H8	1.62	0.59
53:a:172:A:H2'	53:a:173:A:C8	2.38	0.59
36:k:35:HIS:O	64:k:201:HOH:O	2.17	0.59
52:A:235:C:H2'	52:A:236:A:C8	2.37	0.59
53:a:1475:G:O2'	53:a:1514:G:O6	2.18	0.59
27:b:49:C:H2'	27:b:50:A:C8	2.37	0.59
52:A:591:U:H2'	52:A:592:G:C8	2.38	0.59
53:a:659:G:OP2	64:a:3311:HOH:O	2.17	0.59
53:a:1715:G:O2'	53:a:1743:G:O6	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:140:GLU:HG2	5:B:143:LYS:HE3	1.85	0.59
15:L:55:VAL:HG21	15:L:80:ILE:HD11	1.84	0.59
52:A:16:A:N3	52:A:1080:A:O2'	2.32	0.59
52:A:987:G:H2'	52:A:988:G:H8	1.68	0.59
52:A:1086:U:O4	52:A:1099:G:N1	2.20	0.59
5:B:27:MET:HG3	5:B:189:THR:HA	1.85	0.59
8:E:142:ASP:O	8:E:146:ASN:ND2	2.27	0.59
12:I:113:ARG:NH2	52:A:1368:A:OP1	2.36	0.59
13:J:10:LEU:HD13	13:J:22:THR:HG22	1.84	0.59
35:j:28:SER:OG	53:a:2566:A:N1	2.31	0.59
25:X:23:A:H4'	25:X:24:A:O4'	2.03	0.59
53:a:1469:A:H2'	53:a:1470:A:H8	1.66	0.59
23:T:36:TYR:OH	52:A:259:G:OP1	2.20	0.59
52:A:1060:U:H2'	52:A:1061:G:H8	1.66	0.59
53:a:892:A:H2'	53:a:893:C:C6	2.38	0.59
20:Q:25:ILE:HB	20:Q:42:THR:HG23	1.86	0.58
45:t:58:ILE:HD11	53:a:483:A:C4	2.37	0.58
52:A:398:U:H2'	52:A:399:G:H8	1.67	0.58
52:A:673:A:H2'	52:A:674:G:H8	1.67	0.58
9:F:1:MET:HE3	9:F:67:PRO:HD3	1.83	0.58
34:i:120:ARG:NH2	64:i:202:HOH:O	2.35	0.58
37:l:53:MET:HE1	37:l:159:TYR:CD1	2.38	0.58
47:v:37:ILE:HG21	47:v:80:ILE:HG21	1.85	0.58
53:a:851:C:H2'	53:a:852:U:C6	2.38	0.58
26:Z:62:C:H2'	26:Z:63:G:C8	2.38	0.58
37:l:34:LYS:NZ	46:u:81:PRO:O	2.31	0.58
53:a:1028:A:N6	53:a:1125:G:H2'	2.18	0.58
53:a:2898:U:H2'	53:a:2899:A:H8	1.68	0.58
8:E:56:VAL:HG13	8:E:57:PRO:HD3	1.85	0.58
28:c:115:GLN:O	28:c:125:LYS:NZ	2.32	0.58
25:X:24:A:H4'	25:X:25:C:OP2	2.01	0.58
52:A:1356:G:H2'	52:A:1357:A:C8	2.38	0.58
52:A:1513:A:H2'	52:A:1514:G:C8	2.38	0.58
7:D:126:ASN:ND2	7:D:141:ASP:OD1	2.36	0.58
22:S:15:LEU:O	22:S:19:VAL:HG23	2.04	0.58
24:U:18:ARG:O	24:U:22:SER:OG	2.22	0.58
52:A:390:U:H2'	52:A:391:G:C8	2.38	0.58
53:a:813:U:H2'	53:a:814:C:H6	1.67	0.58
5:B:97:LEU:HD21	5:B:147:SER:HB2	1.86	0.58
52:A:1524:C:H2'	52:A:1525:G:C8	2.39	0.58
11:H:103:VAL:HG12	11:H:126:ILE:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:47:LEU:HG	10:G:58:GLU:HB3	1.86	0.58
13:J:68:ARG:HB3	13:J:68:ARG:HH11	1.68	0.58
18:O:8:THR:HG23	18:O:31:LEU:HD11	1.86	0.58
45:t:88:GLU:OE2	45:t:102:THR:OG1	2.19	0.58
53:a:581:C:H2'	53:a:582:A:C8	2.39	0.58
53:a:608:A:H2'	53:a:609:A:C8	2.38	0.58
53:a:2547:A:H2'	53:a:2548:U:C6	2.39	0.58
55:Y:39:A:H3'	55:Y:40:C:H6	1.69	0.58
6:C:33:LEU:HD11	17:N:93:ILE:HG23	1.85	0.58
31:f:6:ASP:HA	31:f:9:LYS:HE3	1.84	0.58
51:z:54:VAL:HG23	51:z:55:ILE:HG23	1.86	0.58
53:a:151:C:H2'	53:a:152:A:H8	1.68	0.58
5:B:73:LYS:NZ	5:B:205:ASP:OD1	2.37	0.57
35:j:43:ILE:HD12	35:j:56:ASP:HB2	1.85	0.57
41:p:72:ASN:HB3	41:p:110:VAL:HG11	1.84	0.57
45:t:49:VAL:HG12	45:t:52:LEU:H	1.68	0.57
55:Y:48:G:H5'	55:Y:49:C:H5'	1.86	0.57
10:G:138:ARG:HD3	10:G:142:HIS:CE1	2.39	0.57
11:H:41:LYS:HD2	11:H:48:ASP:HA	1.84	0.57
17:N:64:CYS:O	17:N:68:GLY:N	2.32	0.57
52:A:41:G:H2'	52:A:42:G:H8	1.68	0.57
52:A:1412:C:H2'	52:A:1413:A:C8	2.38	0.57
53:a:1590:A:H2'	53:a:1591:A:C8	2.39	0.57
16:M:57:ARG:NH1	54:4:17:SER:OG	2.37	0.57
21:R:9:LYS:CG	21:R:10:PHE:H	2.02	0.57
26:Z:75:C:P	26:Z:76:8AN:O2P	2.62	0.57
30:e:137:LYS:HE3	30:e:141:MET:HE3	1.85	0.57
54:4:16:CYS:HA	54:4:34:LEU:HB2	1.85	0.57
14:K:87:LYS:HG3	14:K:114:THR:HA	1.85	0.57
37:l:55:ARG:CD	53:a:2469:A:H4'	2.34	0.57
52:A:167:A:H2'	52:A:168:G:H8	1.69	0.57
52:A:1218:C:H2'	52:A:1219:A:H8	1.69	0.57
53:a:681:G:O6	64:a:3308:HOH:O	2.16	0.57
53:a:898:C:H2'	53:a:899:A:O4'	2.03	0.57
53:a:2064:C:H2'	53:a:2065:C:C6	2.39	0.57
11:H:47:GLU:HB3	11:H:62:THR:HB	1.86	0.57
52:A:51:A:N7	52:A:114:U:O2'	2.36	0.57
52:A:159:G:N2	52:A:161:A:H3'	2.18	0.57
52:A:489:C:H2'	52:A:490:C:C6	2.39	0.57
53:a:333:G:H4'	61:a:3214:SPD:H22	1.87	0.57
55:Y:42:U:H4'	55:Y:42(A):A:OP2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:116:ASP:O	5:B:119:THR:OG1	2.21	0.57
12:I:120:LYS:NZ	52:A:1350:A:OP2	2.33	0.57
44:s:30:ILE:HG13	44:s:85:VAL:HB	1.85	0.57
52:A:187:G:N2	52:A:190:A:OP2	2.35	0.57
52:A:834:U:H2'	52:A:835:U:C6	2.40	0.57
53:a:2074:U:H2'	53:a:2075:U:C6	2.38	0.57
13:J:42:LEU:HB2	13:J:71:LEU:HG	1.85	0.57
33:h:34:GLY:O	33:h:36:ALA:N	2.38	0.57
53:a:1734:G:H2'	53:a:1735:A:H8	1.68	0.57
53:a:2007:U:OP1	64:a:3312:HOH:O	2.17	0.57
52:A:920:U:H2'	52:A:921:U:C6	2.39	0.57
52:A:1014:A:N3	52:A:1219:A:H1'	2.20	0.57
52:A:1017:U:H2'	52:A:1018:G:C8	2.40	0.57
53:a:172:A:H2'	53:a:173:A:H8	1.70	0.57
53:a:182:A:H2'	53:a:183:C:H6	1.70	0.57
53:a:1028:A:H2'	53:a:1029:A:C8	2.39	0.57
15:L:12:ARG:NE	52:A:564:C:OP1	2.38	0.57
30:e:136:GLN:NE2	30:e:140:ASP:OD1	2.37	0.57
38:m:4:ARG:NH1	64:m:202:HOH:O	2.38	0.57
53:a:803:U:OP2	64:a:3314:HOH:O	2.17	0.57
53:a:2469:A:H2'	53:a:2470:G:O4'	2.05	0.57
13:J:32:THR:HB	13:J:83:THR:HG22	1.87	0.57
13:J:53:ILE:HD12	52:A:1060:U:H5''	1.86	0.57
35:j:7:MET:HE1	35:j:44:LYS:HG3	1.86	0.57
43:r:11:ARG:NH1	53:a:1322:A:OP1	2.37	0.57
52:A:17:U:H2'	52:A:18:C:C6	2.40	0.57
52:A:674:G:H2'	52:A:675:A:C8	2.38	0.57
52:A:1035:A:O2'	52:A:1036:A:N3	2.36	0.57
53:a:2469:A:N6	53:a:2481:G:O2'	2.38	0.57
53:a:2699:C:OP2	64:a:3313:HOH:O	2.17	0.57
9:F:29:ILE:HD12	9:F:36:ILE:HD11	1.86	0.56
26:Z:15:G:N2	26:Z:21:A:N3	2.53	0.56
28:c:177:ARG:NE	53:a:1820:U:OP1	2.36	0.56
32:g:89:LEU:H	32:g:129:THR:HG23	1.69	0.56
46:u:30:ILE:HG12	46:u:91:PHE:HB2	1.87	0.56
13:J:15:HIS:HB3	13:J:70:HIS:CE1	2.40	0.56
26:Z:23:C:H2'	26:Z:24:U:C6	2.39	0.56
52:A:73:C:H42	52:A:97:G:H1	1.53	0.56
52:A:626:G:H2'	52:A:627:G:C8	2.40	0.56
53:a:258:G:N7	64:a:3444:HOH:O	2.33	0.56
53:a:882:G:O2'	53:a:896:A:N1	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:1720:U:H2'	53:a:1721:G:O4'	2.05	0.56
53:a:2592:G:OP1	64:a:3310:HOH:O	2.17	0.56
53:a:2740:A:H2'	53:a:2741:A:C8	2.40	0.56
54:4:38:SER:HA	54:4:44:PHE:HD2	1.70	0.56
55:Y:38:A:C4	55:Y:39:A:C8	2.93	0.56
8:E:21:VAL:HG23	8:E:32:SER:HB3	1.87	0.56
9:F:38:ARG:HH21	9:F:61:LEU:HD21	1.69	0.56
10:G:87:VAL:HG22	10:G:151:PHE:HB3	1.87	0.56
11:H:105:SER:HB3	11:H:124:GLU:HB3	1.87	0.56
12:I:28:ILE:HG12	12:I:63:LEU:HD22	1.85	0.56
31:f:36:LEU:HD22	31:f:154:ILE:HG12	1.87	0.56
32:g:39:ASP:N	32:g:39:ASP:OD1	2.39	0.56
52:A:987:G:H2'	52:A:988:G:C8	2.40	0.56
52:A:1013:G:N2	52:A:1016:A:OP2	2.27	0.56
52:A:1053:G:N7	52:A:1200:C:H5'	2.20	0.56
52:A:1125:U:O2	52:A:1126:U:O2'	2.21	0.56
52:A:1237:C:OP1	52:A:1303:C:O2'	2.24	0.56
53:a:581:C:H2'	53:a:582:A:H8	1.71	0.56
53:a:1534:U:O2'	53:a:1537:G:O6	2.14	0.56
53:a:2082:A:OP2	64:a:3316:HOH:O	2.18	0.56
53:a:2788:C:H2'	53:a:2789:C:C6	2.40	0.56
7:D:206:LYS:NZ	52:A:8:A:O2'	2.38	0.56
16:M:78:LYS:HA	16:M:81:MET:HE2	1.87	0.56
43:r:55:ILE:HG23	43:r:69:LEU:HD12	1.86	0.56
45:t:86:ARG:HG3	45:t:95:PHE:CD1	2.41	0.56
52:A:263:A:H2'	52:A:264:C:C6	2.40	0.56
53:a:414:C:H2'	53:a:415:A:C8	2.41	0.56
23:T:2:ALA:HB1	23:T:8:LYS:HG3	1.88	0.56
40:o:106:LYS:HB3	40:o:109:ARG:HH21	1.70	0.56
52:A:950:U:H2'	52:A:951:G:C8	2.41	0.56
6:C:152:GLU:HG3	6:C:167:TRP:HB3	1.87	0.56
10:G:33:ASP:OD1	52:A:1350:A:O2'	2.19	0.56
11:H:101:ILE:HG13	11:H:129:VAL:HB	1.88	0.56
14:K:115:PRO:HB3	52:A:676:A:H5''	1.88	0.56
19:P:17:TYR:HE2	19:P:41:PRO:HG3	1.70	0.56
53:a:279:A:OP2	53:a:361:G:N2	2.39	0.56
53:a:2246:G:H2'	53:a:2247:A:C8	2.40	0.56
8:E:100:SER:OG	8:E:101:GLU:N	2.39	0.56
11:H:10:MET:HE3	11:H:14:ILE:HD11	1.88	0.56
34:i:65:THR:O	34:i:68:LYS:HG3	2.06	0.56
41:p:16:LYS:O	41:p:20:GLN:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:285:G:H2'	53:a:286:U:C6	2.39	0.56
53:a:851:C:H2'	53:a:852:U:H6	1.71	0.56
53:a:1484:U:H2'	53:a:1485:U:C6	2.41	0.56
53:a:1796:U:H2'	53:a:1797:G:C8	2.41	0.56
20:Q:12:VAL:HG22	20:Q:23:VAL:HG22	1.87	0.56
32:g:94:TYR:HA	32:g:106:SER:O	2.05	0.56
52:A:681:A:H2'	52:A:682:G:H8	1.69	0.56
52:A:1071:C:H2'	52:A:1072:G:H8	1.70	0.56
22:S:68:GLY:HA3	54:4:56:ARG:HH21	1.71	0.56
52:A:429:U:O4'	52:A:430:A:H8	1.89	0.56
52:A:580:C:H2'	52:A:581:G:O4'	2.06	0.56
12:I:113:ARG:HH22	13:J:64:GLN:HE22	1.52	0.56
52:A:591:U:H2'	52:A:592:G:H8	1.71	0.56
53:a:593:U:H2'	53:a:594:U:C6	2.41	0.56
53:a:858:G:N3	53:a:2268:A:H2'	2.21	0.56
53:a:1177:G:H2'	53:a:1178:C:C6	2.41	0.56
12:I:63:LEU:HD21	12:I:83:ILE:HD11	1.87	0.55
42:q:38:VAL:HG22	42:q:59:ILE:HD12	1.88	0.55
53:a:29:U:H2'	53:a:30:G:C8	2.41	0.55
53:a:151:C:H2'	53:a:152:A:C8	2.41	0.55
53:a:171:U:H2'	53:a:172:A:C8	2.41	0.55
53:a:848:C:H2'	53:a:849:A:H8	1.71	0.55
11:H:87:LYS:HB2	11:H:125:ILE:HD11	1.86	0.55
15:L:34:CYS:HA	15:L:55:VAL:HG22	1.86	0.55
17:N:30:ILE:O	17:N:33:ASP:HB2	2.07	0.55
31:f:8:TYR:HB2	31:f:173:PHE:HZ	1.70	0.55
50:y:25:LEU:HD11	53:a:930:G:H1'	1.87	0.55
53:a:284:U:H3	53:a:356:G:H1	1.54	0.55
53:a:1796:U:H2'	53:a:1797:G:H8	1.70	0.55
55:Y:20:C:H3'	55:Y:22:G:O4'	2.05	0.55
6:C:58:GLU:OE2	13:J:94:ALA:HB3	2.05	0.55
7:D:198:HIS:O	7:D:202:GLU:HG2	2.06	0.55
52:A:1151:A:HO2'	52:A:1152:A:H8	1.53	0.55
53:a:2070:A:H2'	53:a:2071:A:C8	2.41	0.55
5:B:20:THR:HA	5:B:39:HIS:CD2	2.41	0.55
8:E:72:ILE:HD13	8:E:145:GLU:HB2	1.86	0.55
37:l:53:MET:HE1	37:l:159:TYR:CG	2.41	0.55
52:A:75:G:H2'	52:A:76:G:C8	2.37	0.55
52:A:1530:G:H2'	52:A:1531:A:C8	2.40	0.55
53:a:1407:G:H2'	53:a:1408:G:H8	1.71	0.55
53:a:1734:G:H2'	53:a:1735:A:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:5:LYS:HA	23:T:8:LYS:HE2	1.88	0.55
27:b:65:U:H3'	27:b:108:A:H61	1.70	0.55
10:G:106:GLU:OE1	10:G:137:LYS:NZ	2.39	0.55
14:K:44:TRP:HZ3	14:K:46:THR:HG22	1.72	0.55
17:N:58:SER:HB2	52:A:1360:A:C8	2.42	0.55
21:R:22:ASP:OD1	21:R:24:LYS:NZ	2.39	0.55
38:m:103:ARG:HD3	38:m:110:MET:HE2	1.88	0.55
52:A:1095:U:OP2	52:A:1108:G:N1	2.28	0.55
53:a:64:A:H2'	53:a:65:U:C6	2.41	0.55
53:a:1847:A:N1	64:a:3436:HOH:O	2.32	0.55
10:G:15:ASP:OD1	10:G:44:TYR:OH	2.20	0.55
52:A:985:C:H2'	52:A:986:U:H6	1.69	0.55
53:a:848:C:H2'	53:a:849:A:C8	2.41	0.55
15:L:54:ARG:HE	15:L:62:GLU:HG2	1.71	0.55
27:b:65:U:H3'	27:b:108:A:N6	2.22	0.55
52:A:408:A:H2'	52:A:409:U:C6	2.41	0.55
52:A:1095:U:H2'	52:A:1096:C:C6	2.42	0.55
53:a:150:U:H2'	53:a:151:C:C6	2.41	0.55
53:a:549:G:H2'	53:a:550:C:C6	2.42	0.55
27:b:24:G:H4'	27:b:25:U:H5	1.71	0.55
32:g:158:LYS:NZ	53:a:2659:G:OP2	2.40	0.55
52:A:316:C:OP2	52:A:351:G:O2'	2.21	0.55
53:a:291:G:O6	53:a:349:U:C2	2.60	0.55
11:H:107:SER:HA	52:A:642:A:C5	2.41	0.55
53:a:1000:A:H2'	53:a:1001:A:C8	2.42	0.55
53:a:2799:A:O2'	53:a:2800:A:H5''	2.06	0.55
22:S:30:PRO:HB3	22:S:48:THR:HG23	1.89	0.54
22:S:32:ARG:HA	22:S:50:ALA:HB3	1.89	0.54
37:l:41:LEU:HG	37:l:152:ILE:HG13	1.89	0.54
52:A:407:U:H2'	52:A:408:A:C8	2.42	0.54
53:a:1710:G:H4'	53:a:2858:C:O2	2.07	0.54
10:G:23:LEU:O	10:G:27:VAL:HG23	2.07	0.54
12:I:111:VAL:HG11	52:A:1370:G:H5''	1.89	0.54
30:e:52:VAL:O	30:e:74:LYS:NZ	2.31	0.54
52:A:1127:G:H5'	52:A:1280:A:O2'	2.07	0.54
53:a:2647:U:OP2	64:a:3315:HOH:O	2.18	0.54
1:0:13:SER:HB2	1:0:49:TYR:CZ	2.42	0.54
52:A:343:U:H2'	52:A:345:C:H5	1.73	0.54
52:A:512:U:H2'	52:A:513:C:C6	2.42	0.54
53:a:11:C:H2'	53:a:12:U:H5'	1.88	0.54
53:a:1199:U:H2'	53:a:1200:C:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:1853:A:N1	53:a:2087:G:H1'	2.23	0.54
7:D:8:LYS:HG3	7:D:21:LEU:HD13	1.89	0.54
8:E:30:ILE:HD12	8:E:54:ARG:HH22	1.73	0.54
9:F:2:ARG:NH1	9:F:68:GLN:OE1	2.41	0.54
32:g:71:LEU:O	32:g:75:MET:HG2	2.07	0.54
52:A:454:G:H2'	52:A:455:G:H8	1.71	0.54
53:a:155:A:H2'	53:a:156:A:C8	2.41	0.54
53:a:276:U:H2'	53:a:277:G:C8	2.42	0.54
53:a:878:A:H2'	53:a:879:G:O4'	2.07	0.54
55:Y:17:G:H1'	55:Y:18:G:O5'	2.08	0.54
21:R:62:ALA:HB3	21:R:68:LEU:HD12	1.90	0.54
26:Z:10:G:N2	26:Z:26:G:H1'	2.23	0.54
31:f:34:ILE:HG12	31:f:96:MET:HG3	1.88	0.54
52:A:1380:U:O2	52:A:1382:C:N4	2.40	0.54
53:a:833:A:H2'	53:a:834:G:C8	2.42	0.54
15:L:66:TYR:HB2	15:L:87:VAL:HG21	1.90	0.54
19:P:5:ARG:HD2	52:A:376:G:H5''	1.90	0.54
39:n:18:LEU:HD22	39:n:23:ALA:HB3	1.90	0.54
45:t:66:GLN:HG3	53:a:328:U:O3'	2.08	0.54
52:A:1307:U:H2'	52:A:1308:U:C6	2.43	0.54
52:A:1437:A:H2'	52:A:1438:G:H8	1.72	0.54
53:a:582:A:H2'	53:a:583:G:C8	2.43	0.54
19:P:6:LEU:HD22	19:P:17:TYR:HB3	1.89	0.54
21:R:38:LYS:HG2	52:A:718:A:C2	2.42	0.54
52:A:440:C:C2	52:A:441:A:C8	2.96	0.54
52:A:672:U:H2'	52:A:673:A:C8	2.43	0.54
22:S:11:ILE:HA	22:S:38:SER:HB3	1.89	0.54
53:a:1747:U:H2'	53:a:1748:C:C6	2.43	0.54
55:Y:68:C:H2'	55:Y:69:U:H6	1.72	0.54
12:I:14:SER:O	12:I:14:SER:OG	2.25	0.54
15:L:9:ARG:HH22	52:A:881:G:P	2.30	0.54
39:n:9:ARG:HG2	39:n:9:ARG:NH1	2.23	0.54
55:Y:71:U:O2'	55:Y:72:C:OP1	2.21	0.54
5:B:103:ASN:ND2	52:A:1073:U:O2	2.34	0.54
5:B:131:LYS:HA	5:B:134:ALA:HB3	1.89	0.54
10:G:111:ARG:NH1	10:G:122:ASN:HB2	2.23	0.54
23:T:2:ALA:N	52:A:333:U:OP1	2.41	0.54
29:d:150:MEQ:OE1	53:a:2032:G:O2'	2.23	0.54
40:o:39:ARG:NH1	52:A:346:G:OP1	2.30	0.54
52:A:472:U:H2'	52:A:473:U:C6	2.43	0.54
53:a:1441:G:H2'	53:a:1442:U:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:16:VAL:O	16:M:20:THR:HG23	2.07	0.53
17:N:16:LEU:HD22	17:N:20:TYR:HE2	1.73	0.53
52:A:215:C:H2'	52:A:216:U:C6	2.43	0.53
52:A:501:C:H1'	52:A:549:C:H1'	1.91	0.53
53:a:1794:A:H2'	53:a:1795:C:H6	1.71	0.53
7:D:62:ARG:HG2	7:D:72:PHE:CD2	2.44	0.53
17:N:9:ARG:NH2	52:A:1217:C:OP2	2.42	0.53
52:A:143:A:H5'	52:A:144:G:H5'	1.89	0.53
52:A:1017:U:H2'	52:A:1018:G:H8	1.72	0.53
52:A:1250:A:H2'	52:A:1251:A:C8	2.44	0.53
52:A:1477:U:H2'	52:A:1478:U:C6	2.44	0.53
53:a:1178:C:H2'	53:a:1179:G:C8	2.41	0.53
53:a:2898:U:H2'	53:a:2899:A:C8	2.43	0.53
53:a:2900:A:H2'	53:a:2901:C:C6	2.43	0.53
8:E:157:ARG:NH1	11:H:99:LEU:O	2.41	0.53
34:i:114:LEU:HG	34:i:118:MET:HE3	1.89	0.53
52:A:87:C:H2'	52:A:88:U:H6	1.72	0.53
53:a:274:C:H2'	53:a:275:C:C6	2.43	0.53
53:a:2273:A:H2'	53:a:2274:A:C8	2.44	0.53
53:a:2327:A:H2'	53:a:2328:A:C8	2.43	0.53
5:B:42:ASN:HB3	5:B:45:LYS:HB2	1.90	0.53
6:C:72:ARG:HB3	6:C:75:ILE:HD12	1.88	0.53
12:I:7:TYR:CE2	52:A:1147:C:H4'	2.44	0.53
16:M:10:PRO:HB2	16:M:13:LYS:HG3	1.90	0.53
52:A:41:G:H2'	52:A:42:G:C8	2.43	0.53
52:A:581:G:N1	52:A:759:A:OP2	2.28	0.53
14:K:128:ARG:O	52:A:795:C:O2'	2.20	0.53
46:u:4:ILE:HG21	46:u:42:LEU:HD22	1.90	0.53
52:A:321:A:H2'	52:A:322:C:H6	1.73	0.53
52:A:868:C:H2'	52:A:869:G:O4'	2.08	0.53
52:A:1251:A:H2'	52:A:1252:A:C8	2.44	0.53
52:A:1456:A:H2'	52:A:1457:G:O4'	2.07	0.53
7:D:11:LEU:HB3	7:D:63:ARG:HD3	1.91	0.53
11:H:11:LEU:HD22	11:H:75:ILE:HD11	1.90	0.53
12:I:59:GLU:OE1	12:I:59:GLU:N	2.41	0.53
13:J:45:ARG:HB3	13:J:69:THR:HB	1.91	0.53
22:S:17:LYS:NZ	52:A:1012:A:OP2	2.40	0.53
23:T:67:ILE:HD11	23:T:72:ALA:HB2	1.91	0.53
37:l:26:VAL:HA	37:l:160:GLU:OE2	2.08	0.53
52:A:555:U:H2'	52:A:556:C:C6	2.44	0.53
53:a:40:U:H2'	53:a:41:C:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:1141:U:H4'	53:a:1142:A:O4'	2.09	0.53
53:a:1198:U:H2'	53:a:1199:U:C6	2.44	0.53
53:a:1946:U:H2'	53:a:1947:C:C6	2.43	0.53
5:B:84:ALA:HB3	5:B:91:PHE:HD2	1.74	0.53
5:B:129:LEU:HD23	5:B:133:GLU:HG2	1.91	0.53
12:I:19:VAL:HG13	12:I:65:ILE:HG12	1.91	0.53
13:J:10:LEU:HB3	13:J:18:ILE:HD11	1.89	0.53
37:l:140:LYS:NZ	53:a:2250:G:OP1	2.42	0.53
43:r:6:LYS:HB2	53:a:494:G:H4'	1.90	0.53
52:A:1510:C:H2'	52:A:1511:G:C8	2.43	0.53
53:a:569:U:O2'	53:a:983:A:N1	2.42	0.53
53:a:839:U:H2'	53:a:840:C:C6	2.44	0.53
13:J:52:LEU:O	17:N:81:ARG:NH1	2.42	0.53
22:S:67:VAL:HG21	54:4:57:VAL:HG22	1.90	0.53
27:b:24:G:H4'	27:b:25:U:C5	2.44	0.53
39:n:21:LEU:HD11	53:a:2379:G:H4'	1.91	0.53
53:a:1047:G:O2'	53:a:1109:C:N4	2.42	0.53
53:a:1181:U:H2'	53:a:1182:G:C8	2.44	0.53
53:a:1182:G:H2'	53:a:1183:U:O4'	2.08	0.53
23:T:18:ARG:HH21	23:T:19:LYS:HG2	1.72	0.53
28:c:23:GLU:OE2	28:c:81:LEU:HD22	2.09	0.53
52:A:1130:A:H2'	52:A:1131:G:H8	1.74	0.53
53:a:1570:A:H2'	53:a:1571:A:C8	2.44	0.53
55:Y:43:G:P	55:Y:43:G:H8	2.30	0.53
55:Y:44:C:H4'	55:Y:45:C:OP1	2.09	0.53
2:1:29:GLN:NE2	64:1:102:HOH:O	2.34	0.52
13:J:47:GLU:OE1	17:N:76:LYS:NZ	2.30	0.52
22:S:32:ARG:HD3	22:S:34:TRP:CH2	2.42	0.52
32:g:60:ASP:OD1	32:g:60:ASP:N	2.38	0.52
52:A:224:U:H2'	52:A:225:C:C6	2.45	0.52
52:A:1349:A:H3'	52:A:1350:A:H8	1.74	0.52
53:a:1594:U:H2'	53:a:1595:C:C6	2.44	0.52
6:C:179:ARG:HH11	6:C:179:ARG:HG3	1.74	0.52
7:D:83:LYS:O	7:D:89:ASN:ND2	2.42	0.52
10:G:53:ARG:NH1	10:G:125:SER:OG	2.42	0.52
19:P:4:ILE:HG22	19:P:71:VAL:HG11	1.90	0.52
22:S:5:LEU:HD22	52:A:1312:G:H5'	1.90	0.52
52:A:398:U:H2'	52:A:399:G:C8	2.43	0.52
52:A:1000:A:H2'	52:A:1001:C:C6	2.44	0.52
53:a:169:G:H2'	53:a:170:U:C6	2.43	0.52
54:4:38:SER:HA	54:4:44:PHE:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:39:ALA:O	10:G:43:VAL:HG23	2.09	0.52
24:U:46:LYS:NZ	52:A:1530:G:N7	2.58	0.52
40:o:93:ARG:NH1	64:o:201:HOH:O	2.42	0.52
46:u:55:GLU:N	46:u:55:GLU:OE1	2.41	0.52
52:A:62:U:H2'	52:A:63:C:C6	2.44	0.52
52:A:1033:G:C8	52:A:1034:G:C8	2.97	0.52
53:a:742:A:H2'	53:a:743:A:C8	2.44	0.52
53:a:2480:C:H2'	53:a:2481:G:O4'	2.09	0.52
21:R:12:ARG:NE	21:R:32:TYR:OH	2.43	0.52
39:n:27:VAL:HA	39:n:93:ASP:HB3	1.92	0.52
39:n:28:VAL:HG21	39:n:103:VAL:HG13	1.92	0.52
52:A:128:G:H2'	52:A:129:A:C8	2.44	0.52
53:a:635:C:O2'	53:a:639:U:OP1	2.25	0.52
53:a:1808:A:H3'	53:a:1809:A:C8	2.43	0.52
6:C:184:TYR:HA	6:C:200:VAL:O	2.08	0.52
19:P:61:VAL:HG22	19:P:67:ILE:HD11	1.91	0.52
52:A:757:U:H2'	52:A:758:C:O4'	2.09	0.52
52:A:1238:A:H2	52:A:1241:G:N3	2.08	0.52
53:a:1197:G:H2'	53:a:1198:U:H6	1.74	0.52
53:a:1790:C:H2'	53:a:1791:A:C5	2.45	0.52
53:a:2393:U:OP2	64:a:3317:HOH:O	2.18	0.52
5:B:37:LYS:O	5:B:37:LYS:HG2	2.09	0.52
11:H:64:LYS:HG3	11:H:71:VAL:HG21	1.91	0.52
23:T:71:LYS:HG3	23:T:74:ARG:HH22	1.74	0.52
28:c:16:VAL:HG22	28:c:206:GLY:HA3	1.92	0.52
52:A:634:C:H2'	52:A:635:A:H8	1.75	0.52
52:A:639:G:O6	52:A:640:A:N6	2.42	0.52
52:A:1175:G:H2'	52:A:1176:A:H8	1.74	0.52
52:A:1295:U:H2'	52:A:1296:C:C6	2.45	0.52
53:a:1802:A:H2'	53:a:1803:A:H8	1.72	0.52
55:Y:11:G:H2'	55:Y:12:U:C6	2.45	0.52
10:G:130:ASN:HA	10:G:135:VAL:HG11	1.91	0.52
28:c:254:GLY:O	64:c:401:HOH:O	2.19	0.52
49:x:55:THR:HG21	53:a:76:C:O2'	2.10	0.52
52:A:662:U:H2'	52:A:663:A:H8	1.72	0.52
1:O:11:LEU:HD21	1:O:34:LEU:HD23	1.92	0.52
5:B:116:ASP:O	5:B:120:GLN:HG3	2.09	0.52
6:C:14:ILE:HD12	52:A:1113:C:H4'	1.91	0.52
9:F:32:ALA:HB2	9:F:70:VAL:HG11	1.92	0.52
53:a:743:A:O2'	53:a:1659:G:OP1	2.24	0.52
53:a:1027:A:N3	64:a:3474:HOH:O	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:49:TYR:HB3	21:R:74:HIS:CD2	2.45	0.52
31:f:50:LEU:HD11	31:f:67:ILE:HD12	1.92	0.52
35:j:121:GLU:OE1	40:o:65:SER:OG	2.28	0.52
53:a:181:A:H2'	53:a:182:A:C8	2.44	0.52
53:a:1585:C:H3'	53:a:1586:A:H8	1.74	0.52
53:a:1892:C:H2'	53:a:1893:C:H6	1.74	0.52
6:C:42:TYR:CZ	6:C:90:VAL:HG11	2.44	0.52
6:C:70:THR:HG22	6:C:72:ARG:H	1.75	0.52
14:K:118:HIS:HB3	52:A:718:A:C8	2.45	0.52
15:L:56:ARG:HH11	15:L:62:GLU:HB2	1.75	0.52
17:N:63:ARG:HH22	52:A:981:U:H5''	1.74	0.52
19:P:76:LYS:NZ	52:A:473:U:H5''	2.25	0.52
20:Q:41:THR:OG1	52:A:280:C:N3	2.30	0.52
26:Z:31:G:H2'	26:Z:32:C:H6	1.74	0.52
41:p:109:LEU:HD11	42:q:40:MET:HE1	1.91	0.52
49:x:6:LEU:HB3	49:x:56:LEU:HD12	1.92	0.52
52:A:1513:A:H2'	52:A:1514:G:H8	1.75	0.52
53:a:354:A:H2'	53:a:355:U:O4'	2.09	0.52
53:a:607:U:N3	53:a:608:A:N7	2.57	0.52
53:a:1413:A:H2'	53:a:1414:C:C6	2.45	0.52
53:a:1539:U:H2'	53:a:1540:G:H8	1.74	0.52
8:E:152:MET:O	8:E:156:LYS:HG2	2.09	0.51
11:H:95:VAL:HG23	11:H:102:ALA:HB2	1.92	0.51
13:J:18:ILE:O	13:J:22:THR:HG23	2.09	0.51
14:K:84:VAL:HB	14:K:110:ILE:HG12	1.91	0.51
36:k:21:ARG:HA	53:a:811:U:H2'	1.92	0.51
52:A:362:G:N2	52:A:365:U:OP2	2.43	0.51
52:A:1162:C:H2'	52:A:1163:A:C8	2.42	0.51
53:a:594:U:H2'	53:a:595:C:C6	2.45	0.51
53:a:2430:A:OP1	64:a:3321:HOH:O	2.19	0.51
9:F:67:PRO:HG2	9:F:70:VAL:HG22	1.92	0.51
31:f:56:ASP:O	31:f:60:ILE:HG13	2.10	0.51
37:l:59:ARG:NH1	55:Y:56:C:OP2	2.44	0.51
52:A:151:A:OP2	52:A:169:C:N4	2.42	0.51
52:A:984:C:H2'	52:A:985:C:H6	1.75	0.51
53:a:299:A:N3	53:a:319:G:O2'	2.34	0.51
53:a:1357:C:H2'	53:a:1358:G:O4'	2.10	0.51
53:a:2249:U:OP2	64:a:3320:HOH:O	2.19	0.51
7:D:121:LYS:HG2	7:D:131:ASN:HB3	1.91	0.51
10:G:121:ALA:HA	10:G:124:LEU:HD12	1.93	0.51
13:J:24:GLU:O	13:J:28:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:47:LYS:HD2	31:f:83:TYR:OH	2.09	0.51
52:A:918:A:H2'	52:A:919:A:C8	2.45	0.51
52:A:1354:U:H2'	52:A:1355:G:H8	1.74	0.51
53:a:784:G:H5'	53:a:785:G:OP1	2.11	0.51
53:a:1153:C:H2'	53:a:1154:G:O4'	2.11	0.51
7:D:2:ALA:HB3	52:A:404:G:N7	2.25	0.51
7:D:188:ARG:HH22	7:D:193:ALA:HA	1.74	0.51
9:F:49:TYR:OH	21:R:63:ARG:O	2.09	0.51
9:F:88:MET:HE3	21:R:64:TYR:CD2	2.46	0.51
12:I:80:ARG:O	12:I:83:ILE:HG22	2.10	0.51
27:b:75:G:O2'	46:u:88:HIS:NE2	2.42	0.51
43:r:4:ILE:HD13	43:r:106:VAL:HG13	1.92	0.51
53:a:191:A:H2'	53:a:192:C:C6	2.46	0.51
53:a:265:A:N1	53:a:427:U:O2'	2.39	0.51
53:a:2002:G:O6	64:a:3319:HOH:O	2.19	0.51
9:F:37:HIS:N	9:F:63:ASN:O	2.43	0.51
12:I:122:ARG:NH2	52:A:1346:A:OP1	2.44	0.51
23:T:31:PHE:O	23:T:35:VAL:HG23	2.11	0.51
26:Z:9:G:H21	26:Z:45:G:H3'	1.75	0.51
28:c:3:VAL:HG23	28:c:199:GLU:OE2	2.10	0.51
32:g:26:ILE:HD11	32:g:72:LEU:HD22	1.93	0.51
34:i:110:PRO:O	34:i:115:GLY:HA3	2.10	0.51
52:A:977:A:H2'	52:A:978:A:H5''	1.91	0.51
52:A:1040:U:H2'	52:A:1041:G:C8	2.45	0.51
53:a:1014:A:H2'	53:a:1015:U:C6	2.46	0.51
53:a:2514:U:H2'	53:a:2515:C:C6	2.45	0.51
7:D:13:ARG:HB2	7:D:38:PRO:HD3	1.92	0.51
36:k:51:GLU:OE1	36:k:56:PRO:HA	2.10	0.51
6:C:179:ARG:NH1	6:C:207:ILE:HG12	2.25	0.51
10:G:51:ALA:HB2	10:G:58:GLU:HG3	1.92	0.51
13:J:52:LEU:HD12	13:J:62:ARG:HD3	1.91	0.51
19:P:47:GLU:HG2	52:A:617:G:H5'	1.92	0.51
44:s:19:LYS:NZ	53:a:1340:U:OP1	2.38	0.51
52:A:222:C:H2'	52:A:223:A:C8	2.42	0.51
52:A:1043:G:O2'	52:A:1044:A:H8	1.93	0.51
52:A:1272:G:H2'	52:A:1273:C:C6	2.44	0.51
53:a:277:G:H21	53:a:361:G:H2'	1.76	0.51
53:a:1378:A:O2'	53:a:1380:G:N7	2.44	0.51
53:a:2567:G:H2'	53:a:2568:U:C6	2.45	0.51
53:a:2698:U:H2'	53:a:2699:C:C6	2.46	0.51
8:E:77:ASN:HD22	8:E:82:GLN:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:95:ARG:HD2	10:G:99:LEU:HD12	1.93	0.51
53:a:1619:G:N7	64:a:3475:HOH:O	2.34	0.51
53:a:2246:G:H2'	53:a:2247:A:H8	1.75	0.51
53:a:2300:C:H2'	53:a:2301:C:H6	1.76	0.51
53:a:2306:C:H3'	53:a:2307:G:H2'	1.93	0.51
31:f:131:GLY:HA3	53:a:2305:U:H5''	1.93	0.51
52:A:713:G:H2'	52:A:714:G:C8	2.46	0.51
52:A:933:G:N2	52:A:935:A:O4'	2.43	0.51
53:a:476:G:H4'	53:a:502:A:N1	2.26	0.51
53:a:927:A:H2'	53:a:928:A:C8	2.45	0.51
53:a:2636:C:H2'	53:a:2637:U:C6	2.46	0.51
53:a:2747:G:O6	53:a:2755:C:H5''	2.11	0.51
24:U:40:LYS:NZ	52:A:1526:G:N7	2.58	0.51
24:U:46:LYS:NZ	52:A:1530:G:O6	2.43	0.51
28:c:72:ASP:OD2	28:c:189:ARG:NH2	2.39	0.51
36:k:23:ILE:HG12	42:q:82:HIS:CD2	2.45	0.51
52:A:182:A:N1	52:A:223:A:O2'	2.44	0.51
52:A:709:U:H2'	52:A:710:G:H8	1.75	0.51
53:a:279:A:H1'	53:a:362:A:H4'	1.92	0.51
53:a:414:C:H2'	53:a:415:A:H8	1.74	0.51
53:a:590:A:H2'	53:a:591:U:C6	2.46	0.51
53:a:843:G:H2'	53:a:844:A:C8	2.46	0.51
53:a:1682:G:H2'	53:a:1683:U:C6	2.46	0.51
53:a:2566:A:H4'	53:a:2567:G:H5''	1.93	0.51
5:B:19:GLN:HA	5:B:38:VAL:HA	1.92	0.50
6:C:14:ILE:HG22	6:C:15:VAL:HG13	1.93	0.50
11:H:2:SER:N	52:A:823:C:O2'	2.38	0.50
12:I:18:ARG:HG3	12:I:66:THR:HB	1.94	0.50
13:J:9:ARG:HG2	13:J:9:ARG:HH11	1.75	0.50
13:J:12:ALA:HB2	13:J:18:ILE:HD13	1.93	0.50
20:Q:62:ARG:HG2	20:Q:76:VAL:HG22	1.93	0.50
29:d:184:ARG:NH1	40:o:7:GLN:OE1	2.43	0.50
32:g:86:LYS:HB2	32:g:165:ALA:HB2	1.93	0.50
52:A:165:G:H2'	52:A:166:U:C6	2.45	0.50
52:A:976:G:OP2	52:A:1358:U:O2'	2.30	0.50
53:a:155:A:H2'	53:a:156:A:H8	1.76	0.50
53:a:171:U:H2'	53:a:172:A:H8	1.76	0.50
53:a:279:A:H3'	53:a:280:U:C6	2.46	0.50
53:a:849:A:H2'	53:a:850:U:C6	2.46	0.50
53:a:979:A:H2'	53:a:982:C:H42	1.76	0.50
5:B:27:MET:O	5:B:31:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:172:ARG:HG2	52:A:1106:G:H5''	1.93	0.50
8:E:41:ASP:OD1	8:E:42:GLY:N	2.44	0.50
9:F:9:MET:SD	9:F:86:ARG:HB3	2.51	0.50
10:G:53:ARG:NH2	10:G:122:ASN:OD1	2.37	0.50
16:M:68:ASP:HA	16:M:71:ARG:HG2	1.92	0.50
52:A:317:U:H2'	52:A:318:G:H8	1.76	0.50
53:a:78:U:H2'	53:a:79:C:C6	2.45	0.50
53:a:277:G:O2'	53:a:278:A:O5'	2.25	0.50
53:a:315:G:H2'	53:a:316:C:C6	2.46	0.50
10:G:35:LYS:HE3	52:A:1289:A:O2'	2.11	0.50
16:M:13:LYS:HB2	16:M:18:ALA:HB2	1.93	0.50
23:T:57:ILE:O	23:T:61:GLN:HG2	2.11	0.50
38:m:22:ARG:HG3	38:m:70:THR:HA	1.93	0.50
52:A:562:U:H5'	52:A:563:A:C5	2.47	0.50
52:A:672:U:H2'	52:A:673:A:H8	1.75	0.50
53:a:1849:G:H2'	53:a:1850:G:C8	2.46	0.50
53:a:2300:C:H2'	53:a:2301:C:C6	2.46	0.50
53:a:2533:U:H2'	53:a:2534:A:O4'	2.11	0.50
10:G:42:ILE:HG21	10:G:116:MET:HG3	1.93	0.50
28:c:121:ASP:OD1	28:c:121:ASP:N	2.36	0.50
28:c:123:ALA:O	28:c:128:ASN:ND2	2.42	0.50
36:k:29:LYS:O	36:k:29:LYS:HG2	2.10	0.50
37:l:11:LYS:HD3	37:l:142:LYS:HD3	1.93	0.50
52:A:1009:U:H3	52:A:1020:G:H1	1.58	0.50
53:a:1486:U:H2'	53:a:1487:U:C6	2.47	0.50
53:a:2557:G:H2'	53:a:2558:C:C6	2.47	0.50
55:Y:66:G:H2'	55:Y:67:U:C6	2.46	0.50
15:L:107:VAL:HG23	15:L:117:TYR:HB3	1.92	0.50
15:L:110:ARG:HB3	15:L:119:VAL:HG21	1.93	0.50
17:N:6:MET:HE2	52:A:982:U:H5''	1.93	0.50
53:a:1296:G:OP1	53:a:2709:G:O2'	2.26	0.50
53:a:1594:U:H2'	53:a:1595:C:H6	1.77	0.50
5:B:81:LYS:HG3	5:B:91:PHE:CZ	2.47	0.50
7:D:105:MET:HG3	7:D:171:LEU:CD2	2.41	0.50
8:E:77:ASN:ND2	8:E:82:GLN:OE1	2.44	0.50
52:A:343:U:H2'	52:A:345:C:C5	2.46	0.50
52:A:350:G:H2'	52:A:351:G:C8	2.46	0.50
52:A:696:A:H2'	52:A:697:U:H6	1.76	0.50
52:A:1093:A:N3	52:A:1109:C:O2'	2.42	0.50
53:a:2014:A:H2'	53:a:2015:A:C8	2.46	0.50
6:C:116:VAL:O	6:C:120:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:29:SER:HB3	11:H:57:PRO:HB2	1.94	0.50
12:I:122:ARG:HD3	52:A:1348:U:H4'	1.94	0.50
15:L:13:ALA:O	52:A:562:U:O2'	2.19	0.50
19:P:5:ARG:HD2	52:A:376:G:H4'	1.94	0.50
22:S:3:ARG:NH1	52:A:1318:A:H5''	2.27	0.50
27:b:5:U:OP1	27:b:61:G:O2'	2.21	0.50
32:g:108:GLY:O	53:a:2666:C:N4	2.45	0.50
53:a:639:U:H2'	53:a:640:C:H6	1.74	0.50
53:a:755:U:H2'	53:a:756:A:C8	2.47	0.50
53:a:1028:A:H61	53:a:1125:G:H2'	1.76	0.50
53:a:1270:C:OP2	64:a:3324:HOH:O	2.20	0.50
53:a:2025:C:H2'	53:a:2026:U:C6	2.47	0.50
14:K:125:LYS:HD3	52:A:780:A:H5''	1.94	0.50
52:A:215:C:H2'	52:A:216:U:H6	1.77	0.50
52:A:300:A:O2'	52:A:564:C:N3	2.37	0.50
52:A:444:G:H2'	52:A:445:G:C8	2.46	0.50
52:A:514:C:H2'	52:A:515:G:C8	2.42	0.50
52:A:628:G:H2'	52:A:629:A:C8	2.46	0.50
53:a:290:U:H2'	53:a:291:G:O4'	2.11	0.50
53:a:320:A:H4'	53:a:322:A:N7	2.27	0.50
53:a:1306:C:H2'	53:a:1307:A:H8	1.76	0.50
32:g:2:SER:OG	53:a:2749:A:OP1	2.28	0.50
52:A:407:U:H2'	52:A:408:A:H8	1.76	0.50
52:A:1264:U:H2'	52:A:1265:C:C6	2.47	0.50
53:a:1040:A:H61	53:a:1115:G:H1	1.60	0.50
53:a:2895:G:H2'	53:a:2896:C:C6	2.46	0.50
5:B:66:LYS:H	5:B:159:ASP:HB2	1.77	0.49
34:i:68:LYS:HB3	34:i:72:LYS:HB2	1.94	0.49
48:w:3:ARG:O	48:w:12:PRO:HD3	2.12	0.49
52:A:399:G:H2'	52:A:400:C:C6	2.47	0.49
52:A:751:U:H2'	52:A:752:G:O4'	2.12	0.49
52:A:1273:C:H2'	52:A:1274:A:O4'	2.11	0.49
4:3:32:LYS:HE2	53:a:2478:A:H5'	1.93	0.49
13:J:9:ARG:HH12	13:J:73:LEU:HD22	1.76	0.49
17:N:6:MET:HE1	17:N:9:ARG:HH11	1.77	0.49
43:r:28:LYS:HA	43:r:70:LYS:HG3	1.94	0.49
52:A:153:C:H2'	52:A:154:U:C6	2.46	0.49
52:A:735:C:H2'	52:A:736:C:C6	2.47	0.49
52:A:1464:U:H2'	52:A:1465:A:H8	1.77	0.49
52:A:1516:2MG:N2	52:A:1519:MA6:OP2	2.44	0.49
52:A:1518:MA6:H8	52:A:1518:MA6:O5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:89:PRO:HD3	24:U:32:VAL:HG11	1.95	0.49
23:T:12:ILE:O	23:T:16:LYS:HG3	2.11	0.49
34:i:134:ALA:HB1	53:a:2898:U:O2	2.12	0.49
52:A:1391:U:H2'	52:A:1392:G:C8	2.47	0.49
53:a:1199:U:H2'	53:a:1200:C:H6	1.77	0.49
53:a:1439:A:OP2	64:a:3322:HOH:O	2.19	0.49
6:C:47:LEU:HB3	6:C:50:ALA:HB3	1.94	0.49
7:D:102:VAL:HG13	7:D:107:PHE:HB2	1.94	0.49
10:G:116:MET:HA	10:G:119:ARG:HH11	1.75	0.49
16:M:24:GLY:HA3	16:M:65:VAL:HG12	1.93	0.49
39:n:83:LEU:HD22	39:n:88:LYS:HD3	1.93	0.49
40:o:3:ASN:HA	40:o:6:LYS:HE2	1.94	0.49
52:A:1478:U:H2'	52:A:1479:C:C6	2.48	0.49
53:a:1338:G:O2'	53:a:1393:A:N1	2.40	0.49
53:a:1892:C:H2'	53:a:1893:C:C6	2.47	0.49
53:a:2233:U:H2'	53:a:2234:G:C8	2.47	0.49
53:a:2426:A:OP2	64:a:3326:HOH:O	2.20	0.49
53:a:2820:A:N3	53:a:2820:A:H2'	2.27	0.49
13:J:20:GLN:O	13:J:24:GLU:HG2	2.13	0.49
52:A:384:G:H2'	52:A:385:C:C6	2.47	0.49
52:A:471:U:H2'	52:A:472:U:C6	2.47	0.49
52:A:652:U:O2'	52:A:752:G:N2	2.45	0.49
52:A:811:C:O2'	52:A:901:A:N1	2.40	0.49
53:a:1026:G:H8	53:a:1026:G:OP2	1.95	0.49
53:a:1672:A:C2	53:a:2582:G:H5'	2.47	0.49
53:a:2305:U:H2'	53:a:2306:C:O4'	2.12	0.49
53:a:2396:G:N7	64:a:3479:HOH:O	2.35	0.49
12:I:84:THR:HG21	12:I:103:PHE:HB2	1.93	0.49
21:R:48:ARG:HB2	21:R:51:TYR:HD2	1.77	0.49
28:c:125:LYS:H	28:c:192:LEU:HD13	1.78	0.49
31:f:71:ARG:HD2	53:a:2298:A:OP1	2.12	0.49
52:A:1174:G:H2'	52:A:1175:G:O4'	2.13	0.49
52:A:1270:G:H2'	52:A:1271:A:C8	2.48	0.49
52:A:1380:U:H1'	52:A:1382:C:H41	1.77	0.49
53:a:285:G:H2'	53:a:286:U:H6	1.77	0.49
53:a:1496:A:H2'	53:a:1498:C:C4	2.47	0.49
53:a:1539:U:H2'	53:a:1540:G:C8	2.48	0.49
5:B:68:LEU:HD11	5:B:92:VAL:HG23	1.94	0.49
17:N:73:PHE:CZ	17:N:78:GLY:HA2	2.48	0.49
48:w:10:LYS:HE3	48:w:54:LYS:HD3	1.94	0.49
52:A:604:G:H2'	52:A:605:U:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:2591:C:H2'	53:a:2592:G:H8	1.77	0.49
5:B:23:TRP:CZ3	5:B:25:PRO:HA	2.48	0.49
6:C:53:SER:HA	6:C:114:LYS:HD2	1.95	0.49
11:H:30:SER:HB3	52:A:589:U:H5''	1.95	0.49
11:H:41:LYS:HB2	11:H:46:ILE:HG13	1.95	0.49
18:O:43:PHE:HB3	18:O:53:ARG:HH22	1.78	0.49
24:U:59:LYS:O	24:U:63:GLU:HG2	2.12	0.49
27:b:106:G:H2'	27:b:107:G:O4'	2.12	0.49
46:u:2:PHE:HZ	46:u:53:LYS:HD3	1.77	0.49
52:A:1356:G:H2'	52:A:1357:A:H8	1.78	0.49
53:a:2068:U:OP2	64:a:3325:HOH:O	2.20	0.49
9:F:45:ARG:O	9:F:56:LYS:HA	2.13	0.49
28:c:3:VAL:HG22	28:c:19:VAL:HG12	1.95	0.49
34:i:28:LEU:HD12	34:i:142:ILE:HG21	1.93	0.49
42:q:51:VAL:HG23	42:q:51:VAL:O	2.13	0.49
52:A:201:G:HO2'	52:A:469:C:HO2'	1.57	0.49
52:A:1171:A:H2'	52:A:1172:C:H6	1.78	0.49
53:a:586:A:N1	53:a:809:G:O2'	2.44	0.49
53:a:947:A:H2'	53:a:948:C:C6	2.48	0.49
53:a:948:C:H2'	53:a:949:G:H8	1.78	0.49
53:a:2859:G:H2'	53:a:2860:A:C8	2.48	0.49
5:B:111:ILE:HG23	5:B:152:LYS:HA	1.95	0.49
6:C:176:HIS:O	52:A:1111:A:N6	2.46	0.49
8:E:153:VAL:HG12	8:E:157:ARG:HD3	1.94	0.49
9:F:7:VAL:HG22	9:F:61:LEU:HD12	1.95	0.49
11:H:10:MET:HB2	11:H:33:LYS:HD3	1.95	0.49
11:H:18:GLN:NE2	11:H:65:TYR:CZ	2.80	0.49
13:J:6:ILE:HB	13:J:76:ILE:HG23	1.95	0.49
16:M:89:LEU:O	16:M:92:ARG:HB2	2.13	0.49
23:T:44:LYS:HD3	23:T:87:ALA:HA	1.94	0.49
24:U:7:ARG:HH21	24:U:18:ARG:NE	2.11	0.49
29:d:32:ASN:HB3	29:d:50:VAL:CG2	2.43	0.49
40:o:52:ASN:O	53:a:2845:U:H5''	2.13	0.49
40:o:103:ARG:HH22	53:a:1754:A:H4'	1.77	0.49
42:q:83:TYR:CE1	53:a:1187:G:H5''	2.47	0.49
52:A:390:U:H2'	52:A:391:G:H8	1.76	0.49
52:A:769:G:H4'	52:A:1513:A:H4'	1.94	0.49
52:A:771:G:H2'	52:A:772:U:C6	2.48	0.49
52:A:923:A:H2'	52:A:924:C:C6	2.48	0.49
52:A:1011:C:H2'	52:A:1012:A:C8	2.47	0.49
52:A:1114:C:H2'	52:A:1115:U:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:1656:C:H2'	53:a:1657:U:H6	1.77	0.49
53:a:2783:U:H2'	53:a:2784:U:C6	2.47	0.49
6:C:15:VAL:HG23	6:C:16:LYS:HE3	1.95	0.48
8:E:100:SER:N	52:A:6:G:O6	2.43	0.48
52:A:34:C:H2'	52:A:35:G:C8	2.48	0.48
52:A:1305:G:O2'	52:A:1331:G:N2	2.46	0.48
52:A:1311:A:OP1	54:4:59:ARG:NH1	2.45	0.48
53:a:30:G:H2'	53:a:31:C:C6	2.48	0.48
53:a:419:U:H2'	53:a:420:C:C6	2.48	0.48
53:a:2241:A:H2'	53:a:2242:G:C8	2.48	0.48
6:C:88:ARG:HD2	6:C:99:ALA:HB3	1.95	0.48
7:D:202:GLU:O	52:A:8:A:N6	2.46	0.48
10:G:82:GLY:HA3	25:X:13:A:C8	2.47	0.48
11:H:32:LEU:HD22	52:A:643:C:H5''	1.94	0.48
29:d:181:ASP:OD2	29:d:184:ARG:HB2	2.13	0.48
52:A:147:G:H2'	52:A:148:G:C8	2.48	0.48
53:a:570:G:H2'	53:a:2030:6MZ:N7	2.28	0.48
53:a:1667:G:O2'	53:a:1991:U:O4	2.26	0.48
6:C:111:LEU:HD22	6:C:202:ILE:HD11	1.95	0.48
8:E:149:SER:O	8:E:153:VAL:HG23	2.13	0.48
12:I:114:LYS:HB3	52:A:1368:A:H5''	1.94	0.48
17:N:82:ILE:HG21	52:A:1202:U:N3	2.27	0.48
19:P:1:MET:N	52:A:135:C:O2	2.37	0.48
22:S:11:ILE:HG13	22:S:38:SER:HB3	1.94	0.48
40:o:78:SER:OG	40:o:80:VAL:HG12	2.13	0.48
52:A:727:G:N2	52:A:730:G:OP2	2.40	0.48
52:A:855:U:H2'	52:A:856:C:C6	2.48	0.48
52:A:1444:U:H2'	52:A:1445:U:C6	2.48	0.48
53:a:52:A:H2'	53:a:53:A:C8	2.48	0.48
5:B:18:HIS:NE2	5:B:188:ASP:OD2	2.46	0.48
7:D:57:GLU:HG3	7:D:199:LEU:HD12	1.95	0.48
8:E:15:LEU:HD13	8:E:37:THR:HG22	1.95	0.48
12:I:113:ARG:HH22	13:J:64:GLN:NE2	2.11	0.48
31:f:65:PRO:HA	31:f:89:VAL:HG12	1.96	0.48
31:f:106:ILE:C	31:f:109:PRO:HG2	2.38	0.48
43:r:20:VAL:HG11	43:r:44:ALA:HA	1.96	0.48
46:u:72:VAL:HB	46:u:91:PHE:HB3	1.96	0.48
49:x:50:VAL:O	49:x:54:LYS:HG2	2.13	0.48
52:A:1043:G:O2'	52:A:1044:A:O5'	2.28	0.48
8:E:55:GLU:HB3	8:E:57:PRO:HD2	1.96	0.48
9:F:91:ARG:NH1	52:A:738:C:OP2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:64:VAL:HG11	16:M:72:GLU:OE2	2.12	0.48
32:g:47:ASP:N	32:g:47:ASP:OD1	2.45	0.48
52:A:335:C:H2'	52:A:336:A:C8	2.45	0.48
52:A:1118:U:H1'	52:A:1179:A:C5	2.49	0.48
53:a:39:G:H2'	53:a:40:U:C6	2.48	0.48
53:a:247:G:H4'	53:a:386:G:C5	2.49	0.48
53:a:668:A:H2'	53:a:670:A:H62	1.79	0.48
7:D:152:GLN:HG2	52:A:437:U:H5''	1.96	0.48
13:J:28:THR:O	13:J:32:THR:OG1	2.27	0.48
15:L:56:ARG:NH1	15:L:62:GLU:HB2	2.28	0.48
15:L:114:ARG:HH22	15:L:121:ARG:HD2	1.78	0.48
37:l:55:ARG:HD3	53:a:2469:A:H4'	1.94	0.48
50:y:7:ILE:O	50:y:35:THR:HA	2.14	0.48
52:A:78:A:H2'	52:A:79:G:O4'	2.13	0.48
52:A:579:A:H2'	52:A:580:C:C6	2.48	0.48
53:a:332:A:H2'	61:a:3214:SPD:H72	1.96	0.48
53:a:391:A:H1'	53:a:411:G:O4'	2.14	0.48
53:a:686:U:OP1	64:a:3327:HOH:O	2.20	0.48
53:a:933:A:H5'	53:a:934:U:OP2	2.14	0.48
55:Y:42(A):A:H2'	55:Y:43:G:H5'	1.94	0.48
9:F:99:ALA:HB1	9:F:103:VAL:HG22	1.94	0.48
12:I:83:ILE:O	12:I:87:LEU:HG	2.13	0.48
42:q:93:PHE:HE1	42:q:95:ASP:OD2	1.97	0.48
46:u:77:VAL:HG23	46:u:89:ILE:HG12	1.94	0.48
52:A:1014:A:C2	52:A:1219:A:H1'	2.49	0.48
52:A:1465:A:H2'	52:A:1466:C:C6	2.49	0.48
53:a:152:A:H2'	53:a:153:U:C6	2.48	0.48
53:a:1007:C:OP2	64:a:3328:HOH:O	2.20	0.48
7:D:172:GLU:O	7:D:180:GLY:HA2	2.14	0.48
30:e:145:ASP:HB3	30:e:184:ASP:HB2	1.96	0.48
37:l:3:GLN:HG3	37:l:148:TRP:CD1	2.49	0.48
45:t:54:GLN:NE2	45:t:55:PRO:HD3	2.29	0.48
52:A:272:C:H2'	52:A:273:U:C6	2.49	0.48
52:A:1151:A:O2'	52:A:1152:A:H8	1.97	0.48
52:A:1312:G:H2'	52:A:1313:U:C6	2.48	0.48
53:a:909:A:H2'	53:a:912:C:H5	1.79	0.48
5:B:117:LEU:HB3	5:B:141:LEU:HG	1.96	0.48
7:D:11:LEU:HD13	7:D:63:ARG:HD3	1.96	0.48
7:D:13:ARG:HB3	7:D:37:ALA:HA	1.96	0.48
23:T:28:MET:HE2	23:T:29:ARG:HG2	1.96	0.48
32:g:87:LEU:HD22	32:g:164:TYR:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:18:LEU:HD13	39:n:25:ARG:HG3	1.96	0.48
52:A:22:G:O2'	52:A:913:A:N1	2.39	0.48
52:A:634:C:H2'	52:A:635:A:C8	2.49	0.48
52:A:855:U:H2'	52:A:856:C:H6	1.78	0.48
5:B:76:ALA:HB1	5:B:210:VAL:HG11	1.96	0.48
11:H:86:TYR:OH	52:A:597:G:N2	2.45	0.48
13:J:65:TYR:HE1	17:N:98:LYS:HG2	1.78	0.48
19:P:41:PRO:HB2	52:A:450:G:H4'	1.96	0.48
27:b:3:C:H2'	27:b:4:C:H6	1.79	0.48
36:k:77:ILE:CD1	36:k:108:ALA:HB1	2.44	0.48
38:m:28:LEU:HD23	38:m:48:VAL:HG21	1.94	0.48
42:q:6:GLN:HG2	42:q:11:GLN:HG2	1.96	0.48
52:A:821:G:H2'	52:A:822:U:C6	2.48	0.48
52:A:1314:C:H2'	52:A:1315:U:H6	1.78	0.48
53:a:372:G:O2'	53:a:400:G:O6	2.28	0.48
53:a:546:U:H5''	53:a:548:G:N2	2.28	0.48
53:a:634:C:H2'	53:a:635:C:C6	2.49	0.48
53:a:832:U:H2'	53:a:833:A:C8	2.49	0.48
53:a:2590:A:H2'	53:a:2591:C:H6	1.78	0.48
7:D:11:LEU:HD22	7:D:63:ARG:HH11	1.79	0.47
9:F:50:PRO:HA	9:F:54:LEU:O	2.14	0.47
34:i:2:LYS:HD2	53:a:995:C:N4	2.29	0.47
52:A:161:A:H2'	52:A:162:A:C8	2.49	0.47
52:A:417:G:N2	52:A:541:G:H5'	2.30	0.47
52:A:1175:G:H2'	52:A:1176:A:C8	2.49	0.47
53:a:1683:U:H2'	53:a:1684:G:C8	2.48	0.47
53:a:1717:A:N6	53:a:1743:G:O2'	2.45	0.47
53:a:2391:G:O6	53:a:2425:A:H8	1.97	0.47
7:D:58:LYS:NZ	52:A:545:C:OP1	2.47	0.47
9:F:38:ARG:NH2	9:F:61:LEU:HD21	2.28	0.47
15:L:50:ARG:HG3	15:L:90:LEU:HD21	1.96	0.47
20:Q:28:PHE:CE2	20:Q:37:PHE:HB3	2.49	0.47
24:U:7:ARG:HH21	24:U:18:ARG:CZ	2.27	0.47
29:d:98:VAL:HG22	29:d:180:VAL:HG13	1.96	0.47
39:n:16:ARG:HH12	39:n:20:GLU:CG	2.27	0.47
51:z:52:ARG:HH21	51:z:54:VAL:HG12	1.79	0.47
53:a:80:G:O2'	53:a:294:A:N1	2.47	0.47
53:a:181:A:H2'	53:a:182:A:H8	1.79	0.47
53:a:588:U:H2'	53:a:589:U:C6	2.49	0.47
5:B:167:ASP:OD1	5:B:168:HIS:N	2.47	0.47
6:C:15:VAL:HG11	6:C:179:ARG:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:147:GLU:OE1	7:D:147:GLU:N	2.46	0.47
10:G:3:ARG:NH1	52:A:933:G:N7	2.62	0.47
20:Q:27:ARG:NH2	52:A:237:G:OP1	2.48	0.47
40:o:9:GLU:HB3	40:o:55:LEU:HB2	1.95	0.47
46:u:6:ALA:HB2	46:u:42:LEU:HD23	1.95	0.47
52:A:417:G:N2	52:A:540:G:O2'	2.47	0.47
52:A:1245:C:H2'	52:A:1246:A:O4'	2.14	0.47
53:a:472:A:OP1	61:a:3216:SPD:H91	2.13	0.47
53:a:1041:G:C2	53:a:1042:G:C8	3.02	0.47
53:a:1269:A:H2'	53:a:1270:C:C6	2.49	0.47
53:a:1353:A:H2'	53:a:1354:A:C8	2.49	0.47
53:a:2284:A:O2'	53:a:2288:A:N1	2.46	0.47
53:a:2597:G:N2	64:a:3409:HOH:O	2.30	0.47
55:Y:18:G:H4'	55:Y:18:G:OP1	2.14	0.47
11:H:112:THR:HG22	11:H:113:ASP:N	2.30	0.47
12:I:41:ARG:NH2	52:A:1373:G:OP1	2.37	0.47
17:N:3:LYS:HD2	52:A:1048:G:H5''	1.95	0.47
18:O:36:ILE:O	18:O:40:GLN:HG2	2.15	0.47
52:A:579:A:H2'	52:A:580:C:H6	1.80	0.47
53:a:248:G:H5'	53:a:250:G:N7	2.29	0.47
53:a:1418:G:O2'	53:a:1580:A:N6	2.42	0.47
53:a:1427:A:H4'	53:a:1428:C:O4'	2.14	0.47
53:a:1591:A:H2'	53:a:1592:C:C6	2.50	0.47
53:a:2809:A:H2'	53:a:2810:A:C8	2.49	0.47
7:D:188:ARG:NH1	7:D:188:ARG:O	2.47	0.47
14:K:93:ARG:NH2	14:K:112:ASP:OD2	2.46	0.47
32:g:27:LYS:HA	32:g:31:GLY:O	2.15	0.47
51:z:48:TYR:CZ	51:z:53:LYS:HG2	2.50	0.47
52:A:201:G:H1	52:A:216:U:H3	1.62	0.47
52:A:1052:U:O2'	52:A:1055:A:OP2	2.16	0.47
53:a:703:U:H2'	53:a:704:G:O4'	2.14	0.47
53:a:1870:C:O2'	53:a:1871:A:O5'	2.21	0.47
55:Y:71:U:H2'	55:Y:72:C:C6	2.49	0.47
5:B:101:LEU:HD12	5:B:175:GLU:HB2	1.97	0.47
11:H:39:VAL:HG11	11:H:103:VAL:HG22	1.95	0.47
14:K:120:GLY:N	52:A:716:A:N3	2.63	0.47
27:b:76:G:OP1	46:u:9:ARG:NH1	2.46	0.47
38:m:56:LYS:NZ	38:m:90:ARG:O	2.44	0.47
45:t:44:LYS:HD3	45:t:61:LYS:HE2	1.95	0.47
52:A:623:C:H2'	52:A:624:C:C6	2.50	0.47
52:A:623:C:H2'	52:A:624:C:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:1319:A:C8	52:A:1323:G:C6	3.02	0.47
53:a:1721:G:H1'	53:a:1739:A:H61	1.79	0.47
53:a:2813:A:H2'	53:a:2814:A:H8	1.78	0.47
53:a:2820:A:O2'	53:a:2821:A:OP1	2.31	0.47
55:Y:35:U:H2'	55:Y:36:A:O4'	2.15	0.47
6:C:33:LEU:HD23	6:C:33:LEU:HA	1.78	0.47
16:M:97:VAL:HG12	52:A:1308:U:OP1	2.13	0.47
19:P:74:LEU:O	19:P:78:VAL:HG22	2.15	0.47
26:Z:11:A:H2'	26:Z:12:G:H8	1.78	0.47
31:f:108:VAL:HA	31:f:111:ILE:HD12	1.96	0.47
32:g:4:VAL:O	32:g:69:ARG:HG2	2.14	0.47
40:o:48:ILE:HG22	40:o:100:LEU:HD12	1.96	0.47
52:A:438:U:C4	52:A:494:G:C5	3.02	0.47
52:A:455:G:C2	52:A:478:A:C2	3.02	0.47
52:A:1115:U:H2'	52:A:1116:U:C6	2.49	0.47
52:A:1305:G:N2	52:A:1331:G:O2'	2.44	0.47
53:a:250:G:H2'	53:a:251:A:C8	2.49	0.47
53:a:285:G:H1	53:a:355:U:H3	1.62	0.47
53:a:417:C:H2'	53:a:418:C:C6	2.50	0.47
53:a:576:U:H2'	53:a:577:G:C8	2.50	0.47
53:a:645:C:H2'	53:a:647:G:N7	2.29	0.47
53:a:1492:G:H5''	53:a:1493:C:H5''	1.96	0.47
53:a:1662:U:OP2	64:a:3329:HOH:O	2.20	0.47
53:a:1710:G:H2'	53:a:1711:A:C8	2.49	0.47
53:a:2292:U:H2'	53:a:2293:G:H8	1.80	0.47
1:O:22:THR:HG21	53:a:2419:U:H4'	1.97	0.47
8:E:41:ASP:CG	8:E:43:ASN:H	2.22	0.47
8:E:113:ALA:O	8:E:117:VAL:HG23	2.14	0.47
29:d:126:ASN:O	29:d:128:ARG:NH1	2.48	0.47
30:e:41:GLN:NE2	30:e:43:THR:OG1	2.45	0.47
31:f:140:GLU:HA	54:4:28:VAL:HB	1.96	0.47
32:g:17:VAL:O	32:g:17:VAL:HG23	2.15	0.47
52:A:61:G:H2'	52:A:62:U:O4'	2.14	0.47
52:A:426:U:O5'	52:A:426:U:H6	1.97	0.47
52:A:637:C:O2'	52:A:638:U:H5'	2.14	0.47
52:A:958:A:H1'	52:A:985:C:O2'	2.15	0.47
52:A:1314:C:H2'	52:A:1315:U:C6	2.50	0.47
53:a:184:C:H2'	53:a:185:G:C8	2.49	0.47
53:a:322:A:H5'	53:a:340:A:H1'	1.97	0.47
53:a:1149:G:H2'	53:a:1150:C:C6	2.50	0.47
53:a:1874:C:H2'	53:a:1875:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:88:ASP:OD2	5:B:225:ARG:NH2	2.48	0.47
7:D:14:ARG:HD2	7:D:37:ALA:HB1	1.97	0.47
10:G:60:GLU:O	10:G:63:GLU:HG3	2.15	0.47
12:I:30:ILE:HG12	12:I:65:ILE:HD12	1.96	0.47
17:N:59:ARG:NH1	52:A:979:C:O2	2.48	0.47
18:O:64:ARG:NH2	18:O:67:LEU:HB3	2.30	0.47
52:A:246:A:C2	52:A:282:A:C5	3.03	0.47
52:A:984:C:H2'	52:A:985:C:C6	2.49	0.47
52:A:999:C:H2'	52:A:1000:A:C8	2.50	0.47
53:a:580:U:H2'	53:a:581:C:C6	2.50	0.47
53:a:861:A:OP2	61:a:3218:SPD:N1	2.47	0.47
53:a:1709:U:O2'	53:a:2859:G:H1'	2.15	0.47
5:B:20:THR:OG1	5:B:37:LYS:O	2.26	0.47
7:D:148:LYS:HE3	7:D:148:LYS:HB3	1.60	0.47
10:G:99:LEU:HG	10:G:102:ARG:HH21	1.80	0.47
11:H:43:GLU:HG3	11:H:101:ILE:HG21	1.97	0.47
17:N:20:TYR:HB2	17:N:55:SER:HB2	1.97	0.47
17:N:46:LEU:O	17:N:50:THR:HG23	2.15	0.47
19:P:22:ALA:HA	19:P:33:ILE:HD12	1.97	0.47
39:n:25:ARG:O	39:n:39:VAL:HA	2.15	0.47
52:A:794:A:H2'	52:A:795:C:C6	2.50	0.47
52:A:1270:G:H2'	52:A:1271:A:H8	1.79	0.47
52:A:1325:C:H2'	52:A:1326:U:H6	1.79	0.47
53:a:1:G:H2'	53:a:2:G:H8	1.80	0.47
53:a:55:G:O2'	53:a:127:A:N1	2.40	0.47
53:a:888:C:H2'	53:a:889:C:C6	2.49	0.47
7:D:196:ASN:HB3	7:D:198:HIS:CD2	2.50	0.46
10:G:116:MET:SD	10:G:119:ARG:HD2	2.55	0.46
10:G:150:ALA:HB3	14:K:56:ARG:HG2	1.97	0.46
15:L:39:THR:HA	15:L:50:ARG:O	2.14	0.46
31:f:106:ILE:O	31:f:109:PRO:HG2	2.14	0.46
32:g:140:VAL:O	32:g:144:VAL:HG23	2.15	0.46
52:A:860:A:H2'	52:A:861:G:O4'	2.15	0.46
52:A:1327:C:H2'	52:A:1328:C:H6	1.79	0.46
53:a:845:A:H3'	53:a:845:A:N3	2.29	0.46
53:a:1442:U:H2'	53:a:1443:U:C6	2.50	0.46
7:D:169:THR:O	7:D:184:ARG:NH2	2.34	0.46
40:o:37:LYS:HD3	40:o:37:LYS:HA	1.70	0.46
43:r:80:PRO:O	43:r:100:THR:OG1	2.29	0.46
52:A:40:C:H2'	52:A:41:G:C8	2.50	0.46
52:A:665:A:N3	52:A:732:C:H2'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:1013:C:H2'	53:a:1014:A:H8	1.79	0.46
53:a:1704:C:H2'	53:a:1705:A:C8	2.51	0.46
53:a:2243:U:H2'	53:a:2244:U:H6	1.79	0.46
9:F:86:ARG:NH1	52:A:673:A:H4'	2.30	0.46
15:L:36:ARG:HD3	15:L:38:TYR:CD1	2.50	0.46
45:t:92:LYS:NZ	53:a:83:A:OP1	2.47	0.46
52:A:59:A:H5''	52:A:387:U:H5''	1.97	0.46
52:A:441:A:C5	52:A:442:G:C8	3.03	0.46
52:A:1123:U:O2'	52:A:1124:G:H5'	2.15	0.46
53:a:78:U:H2'	53:a:79:C:H6	1.79	0.46
53:a:1266:G:O2'	53:a:2012:G:O6	2.20	0.46
53:a:1322:A:N1	53:a:1333:G:O2'	2.38	0.46
55:Y:33:U:H2'	55:Y:35:U:H5	1.79	0.46
10:G:108:ALA:O	10:G:119:ARG:HD3	2.15	0.46
15:L:18:LYS:HE2	15:L:18:LYS:HB3	1.78	0.46
51:z:4:GLN:HA	53:a:2615:U:C2	2.50	0.46
52:A:317:U:H2'	52:A:318:G:C8	2.50	0.46
52:A:482:A:H2'	52:A:483:C:O4'	2.15	0.46
52:A:1418:A:H2	53:a:1948:G:N3	2.13	0.46
53:a:271:G:HO2'	53:a:272:A:H8	1.62	0.46
53:a:859:G:O2'	53:a:916:G:O6	2.33	0.46
53:a:1019:U:OP1	53:a:1035:U:O2'	2.26	0.46
53:a:1589:U:H2'	53:a:1590:A:C8	2.51	0.46
53:a:2331:G:O2'	53:a:2336:A:N1	2.42	0.46
8:E:155:ALA:HB3	8:E:156:LYS:HE2	1.98	0.46
12:I:57:MET:HE1	12:I:90:TYR:HE2	1.80	0.46
19:P:42:ILE:O	19:P:42:ILE:HG12	2.15	0.46
26:Z:54:U:H2'	26:Z:55:U:O4'	2.16	0.46
27:b:16:G:N2	27:b:69:G:H1'	2.31	0.46
52:A:1251:A:H2'	52:A:1252:A:H8	1.79	0.46
53:a:4:U:H2'	53:a:5:A:H8	1.81	0.46
53:a:30:G:H2'	53:a:31:C:H6	1.81	0.46
53:a:632:A:H2'	53:a:633:A:C8	2.51	0.46
53:a:886:A:H2'	53:a:887:U:O4'	2.15	0.46
53:a:1882:U:H2'	53:a:1883:U:C6	2.51	0.46
6:C:70:THR:HG21	6:C:76:VAL:CG2	2.44	0.46
7:D:144:SER:HB3	7:D:179:GLU:OE1	2.16	0.46
10:G:18:PHE:CE2	10:G:47:LEU:HD23	2.50	0.46
14:K:64:GLN:HG3	14:K:99:ALA:HB2	1.98	0.46
21:R:43:ARG:NH1	21:R:44:ILE:HG12	2.31	0.46
22:S:19:VAL:O	22:S:23:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:50:ARG:NH1	55:Y:55:U:OP1	2.48	0.46
39:n:51:ALA:HB3	39:n:78:VAL:HB	1.98	0.46
45:t:54:GLN:CD	45:t:55:PRO:HD3	2.40	0.46
52:A:16:A:N1	52:A:919:A:H2	2.14	0.46
52:A:113:G:H2'	52:A:114:U:C6	2.50	0.46
52:A:382:A:H2'	52:A:383:A:C8	2.51	0.46
53:a:12:U:O2	53:a:2626:C:H4'	2.16	0.46
53:a:307:G:N1	53:a:310:A:OP2	2.47	0.46
53:a:358:U:H2'	53:a:359:G:H8	1.81	0.46
53:a:657:U:H2'	53:a:658:U:C6	2.50	0.46
53:a:1582:C:C2	53:a:1583:A:H1'	2.51	0.46
53:a:2037:A:H2'	53:a:2038:G:C8	2.51	0.46
53:a:2377:A:H2'	53:a:2378:A:C8	2.50	0.46
5:B:57:LEU:HA	5:B:60:ILE:HG22	1.96	0.46
5:B:127:ASP:OD1	5:B:127:ASP:N	2.48	0.46
7:D:9:LEU:HD13	7:D:32:CYS:HB3	1.98	0.46
9:F:47:LEU:HD21	9:F:57:ALA:HB3	1.98	0.46
14:K:46:THR:HG23	14:K:49:GLY:H	1.81	0.46
28:c:72:ASP:CG	28:c:189:ARG:HH22	2.23	0.46
29:d:22:ILE:HG23	29:d:190:LYS:HD2	1.97	0.46
47:v:29:GLU:OE2	53:a:922:C:O2'	2.28	0.46
48:w:13:VAL:HG22	48:w:29:PHE:HB2	1.97	0.46
52:A:219:U:H2'	52:A:220:G:C8	2.49	0.46
52:A:428:G:OP1	52:A:430:A:H1'	2.15	0.46
52:A:681:A:H2'	52:A:682:G:C8	2.49	0.46
52:A:967:5MC:H2'	52:A:968:A:C8	2.51	0.46
52:A:1000:A:H2'	52:A:1001:C:H6	1.80	0.46
53:a:1278:C:H2'	53:a:1279:G:H8	1.80	0.46
53:a:1622:G:O6	64:a:3323:HOH:O	2.20	0.46
53:a:2070:A:H2'	53:a:2071:A:H8	1.79	0.46
6:C:77:ILE:HA	6:C:84:VAL:CG2	2.46	0.46
9:F:63:ASN:HD22	9:F:96:VAL:HB	1.80	0.46
17:N:88:ALA:HB2	17:N:93:ILE:HD12	1.98	0.46
20:Q:25:ILE:N	20:Q:42:THR:O	2.33	0.46
28:c:180:GLU:OE1	53:a:1799:G:O2'	2.27	0.46
29:d:8:LYS:NZ	29:d:195:GLY:O	2.44	0.46
31:f:98:GLU:OE1	54:4:25:ARG:HD2	2.16	0.46
31:f:164:GLU:HA	31:f:167:ARG:HG2	1.98	0.46
32:g:19:ILE:HG21	32:g:43:VAL:HG21	1.98	0.46
52:A:401:C:H2'	52:A:402:G:C8	2.51	0.46
52:A:821:G:H2'	52:A:822:U:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:1440:U:O4	64:a:3322:HOH:O	2.21	0.46
53:a:1581:G:H2'	53:a:1582:C:C6	2.51	0.46
10:G:68:ASN:ND2	10:G:127:ALA:O	2.41	0.46
14:K:113:VAL:HA	21:R:73:ARG:NE	2.31	0.46
31:f:77:PHE:CE2	53:a:2310:C:H2'	2.51	0.46
31:f:103:LEU:HA	31:f:107:ALA:HB3	1.98	0.46
44:s:71:GLY:C	44:s:73:ARG:H	2.24	0.46
52:A:514:C:C2	52:A:515:G:C8	3.04	0.46
53:a:1581:G:H2'	53:a:1582:C:H6	1.80	0.46
53:a:2071:A:H2'	53:a:2072:C:C6	2.51	0.46
53:a:2230:G:H2'	53:a:2231:U:C6	2.51	0.46
53:a:2247:A:OP1	61:a:3221:SPD:H42	2.16	0.46
53:a:2526:G:N2	64:a:3747:HOH:O	2.49	0.46
54:4:1:MET:HB3	54:4:6:HIS:HE2	1.81	0.46
55:Y:18:G:O4'	55:Y:57:G:N2	2.48	0.46
8:E:81:LEU:HD11	8:E:96:MET:HB3	1.98	0.46
27:b:48:U:H4'	39:n:100:HIS:HD2	1.81	0.46
30:e:190:ALA:O	30:e:194:LYS:HG2	2.16	0.46
49:x:41:HIS:O	49:x:45:GLN:HG3	2.16	0.46
52:A:2:A:H1'	52:A:613:C:O2'	2.16	0.46
52:A:513:C:H2'	52:A:514:C:C6	2.51	0.46
52:A:946:A:H2'	52:A:947:G:H8	1.71	0.46
53:a:184:C:H2'	53:a:185:G:H8	1.81	0.46
53:a:2421:G:O6	64:a:3318:HOH:O	2.19	0.46
9:F:47:LEU:HD11	9:F:57:ALA:HB2	1.97	0.45
12:I:112:GLU:HB3	12:I:121:ALA:HB1	1.98	0.45
13:J:9:ARG:HH21	13:J:71:LEU:HD21	1.81	0.45
25:X:20:A:O2'	52:A:1492:A:N3	2.38	0.45
41:p:11:ARG:NH2	64:p:205:HOH:O	2.50	0.45
45:t:48:PRO:HB3	45:t:55:PRO:C	2.40	0.45
52:A:167:A:H2'	52:A:168:G:C8	2.51	0.45
52:A:509:A:H2'	52:A:510:A:C8	2.51	0.45
52:A:551:U:H2'	52:A:552:U:C6	2.51	0.45
52:A:916:U:H2'	52:A:917:G:H8	1.80	0.45
53:a:838:C:OP2	64:a:3330:HOH:O	2.21	0.45
53:a:2599:G:OP1	64:a:3331:HOH:O	2.21	0.45
7:D:72:PHE:CE1	7:D:204:TYR:HE2	2.34	0.45
12:I:113:ARG:NH2	13:J:64:GLN:HE22	2.14	0.45
12:I:123:ARG:HG3	52:A:1350:A:P	2.56	0.45
22:S:39:THR:HA	22:S:70:LYS:HD3	1.97	0.45
52:A:911:U:H2'	52:A:912:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:922:G:H2'	52:A:923:A:C8	2.51	0.45
53:a:852:U:H2'	53:a:853:C:C6	2.51	0.45
9:F:88:MET:HE3	21:R:64:TYR:HD2	1.80	0.45
11:H:27:MET:HE2	11:H:27:MET:HB3	1.79	0.45
26:Z:62:C:H2'	26:Z:63:G:H8	1.79	0.45
38:m:38:LEU:HB3	38:m:39:PRO:HD3	1.98	0.45
49:x:12:GLU:O	49:x:16:THR:HG22	2.16	0.45
52:A:448:A:H3'	52:A:449:G:H8	1.81	0.45
52:A:536:C:H2'	52:A:537:G:C8	2.51	0.45
52:A:1323:G:H2'	52:A:1324:A:C8	2.51	0.45
53:a:272:A:H2'	53:a:273:G:H8	1.82	0.45
53:a:841:G:H2'	53:a:842:U:C6	2.52	0.45
53:a:1180:U:H2'	53:a:1181:U:O4'	2.17	0.45
53:a:1878:G:H2'	53:a:1879:C:C6	2.52	0.45
53:a:2813:A:H2'	53:a:2814:A:C8	2.51	0.45
6:C:14:ILE:CD1	52:A:1113:C:H4'	2.47	0.45
6:C:179:ARG:HG3	6:C:179:ARG:NH1	2.30	0.45
10:G:35:LYS:HA	10:G:35:LYS:HD2	1.85	0.45
14:K:117:PRO:HB3	52:A:676:A:H1'	1.99	0.45
35:j:15:GLY:O	35:j:47:ILE:HG12	2.16	0.45
39:n:53:THR:HB	39:n:65:THR:HB	1.97	0.45
52:A:89:U:H2'	52:A:90:C:C6	2.51	0.45
52:A:216:U:H1'	52:A:466:A:H61	1.81	0.45
52:A:516:PSU:O2'	52:A:519:C:N3	2.50	0.45
52:A:709:U:H2'	52:A:710:G:C8	2.51	0.45
52:A:1118:U:H2'	52:A:1119:C:H6	1.81	0.45
52:A:1308:U:H2'	52:A:1309:G:H8	1.81	0.45
52:A:1347:G:O2'	52:A:1373:G:O6	2.28	0.45
53:a:1853:A:H2'	53:a:1854:A:C8	2.51	0.45
53:a:2783:U:H2'	53:a:2784:U:H6	1.81	0.45
9:F:91:ARG:HG2	52:A:737:C:H5''	1.99	0.45
16:M:103:LYS:HG3	52:A:1226:C:N4	2.31	0.45
20:Q:27:ARG:HE	20:Q:42:THR:HG22	1.81	0.45
26:Z:19:G:H4'	26:Z:20:U:OP2	2.13	0.45
30:e:159:LEU:HD23	30:e:162:ARG:NH1	2.31	0.45
36:k:82:LEU:HD22	36:k:90:VAL:HG21	1.97	0.45
37:l:79:ALA:HA	53:a:2494:G:O2'	2.16	0.45
42:q:94:THR:HG22	42:q:96:VAL:HG23	1.99	0.45
45:t:2:ALA:HB2	53:a:83:A:OP1	2.17	0.45
52:A:109:A:H4'	52:A:110:C:OP2	2.16	0.45
52:A:321:A:H2'	52:A:322:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:383:A:H8	52:A:383:A:O5'	1.99	0.45
52:A:422:C:O2	52:A:423:G:N1	2.49	0.45
52:A:502:A:H2'	52:A:503:C:O4'	2.17	0.45
53:a:1599:U:H2'	53:a:1600:C:C6	2.52	0.45
8:E:150:PRO:HG3	11:H:99:LEU:HD21	1.98	0.45
10:G:153:HIS:ND1	10:G:154:TYR:O	2.50	0.45
27:b:3:C:H2'	27:b:4:C:C6	2.51	0.45
35:j:77:ILE:HG12	40:o:72:ARG:HG3	1.97	0.45
52:A:160:A:H1'	52:A:344:A:N7	2.32	0.45
52:A:865:A:H2'	52:A:866:C:C6	2.51	0.45
52:A:950:U:H2'	52:A:951:G:H8	1.82	0.45
52:A:1073:U:C2	52:A:1074:G:C8	3.04	0.45
52:A:1171:A:H2'	52:A:1172:C:C6	2.52	0.45
52:A:1238:A:C2	52:A:1241:G:H1'	2.52	0.45
52:A:1435:G:H2'	52:A:1436:U:C6	2.52	0.45
53:a:987:C:H2'	53:a:988:A:O4'	2.17	0.45
53:a:1946:U:H2'	53:a:1947:C:H6	1.80	0.45
53:a:2292:U:H2'	53:a:2293:G:C8	2.50	0.45
55:Y:71:U:HO2'	55:Y:72:C:P	2.36	0.45
6:C:123:GLN:HB3	6:C:128:VAL:HB	1.97	0.45
16:M:93:ARG:HD2	16:M:93:ARG:N	2.30	0.45
18:O:78:TYR:OH	18:O:89:ARG:O	2.23	0.45
20:Q:19:LYS:HA	20:Q:48:ASP:O	2.16	0.45
37:l:47:GLU:OE2	37:l:51:ARG:HG3	2.17	0.45
52:A:459:A:H2'	52:A:460:A:C8	2.51	0.45
52:A:1287:A:H2	52:A:1353:G:H1'	1.81	0.45
53:a:1668:A:O2'	53:a:1674:G:N7	2.43	0.45
53:a:1786:A:H1'	53:a:1938:A:N6	2.32	0.45
1:O:9:ILE:HD12	1:O:51:GLU:HG3	1.99	0.45
9:F:81:ASN:OD1	9:F:83:ALA:HB3	2.17	0.45
12:I:15:SER:OG	12:I:69:GLY:O	2.20	0.45
24:U:12:PHE:CZ	24:U:16:LEU:HD22	2.52	0.45
27:b:1:U:H2'	27:b:2:G:H8	1.82	0.45
29:d:135:GLY:HA2	53:a:743:A:OP1	2.17	0.45
35:j:40:LYS:NZ	53:a:2562:U:OP1	2.30	0.45
35:j:48:PRO:HG3	52:A:1422:G:H5'	1.99	0.45
40:o:31:TRP:CE3	40:o:38:LYS:HE2	2.52	0.45
52:A:264:C:H2'	52:A:265:G:O4'	2.16	0.45
52:A:384:G:H2'	52:A:385:C:H6	1.82	0.45
52:A:635:A:H2'	52:A:636:U:H6	1.80	0.45
52:A:837:U:H2'	52:A:838:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:948:C:H2'	52:A:949:A:H8	1.82	0.45
52:A:1036:A:H2'	52:A:1037:C:H5'	1.99	0.45
52:A:1410:A:H2'	52:A:1411:C:C6	2.52	0.45
53:a:500:G:N1	53:a:503:A:OP2	2.49	0.45
53:a:645:C:H2'	53:a:647:G:C8	2.52	0.45
53:a:1292:G:H2'	53:a:1293:C:C6	2.52	0.45
53:a:1411:U:H2'	53:a:1412:U:C6	2.52	0.45
53:a:1478:G:N7	64:a:3399:HOH:O	2.36	0.45
6:C:152:GLU:CG	6:C:167:TRP:HB3	2.47	0.45
10:G:48:GLU:HG3	10:G:49:THR:N	2.32	0.45
52:A:1144:G:N2	52:A:1146:A:H62	2.14	0.45
52:A:1410:A:H2'	52:A:1411:C:H6	1.81	0.45
60:A:1601:PAR:N64	60:A:1601:PAR:O44	2.48	0.45
53:a:493:G:N7	64:a:3488:HOH:O	2.36	0.45
53:a:883:G:H2'	53:a:884:U:C6	2.52	0.45
54:4:58:ASP:OD1	54:4:58:ASP:N	2.50	0.45
55:Y:7:C:H4'	55:Y:10:G:H3'	1.99	0.45
7:D:206:LYS:HA	7:D:206:LYS:HD2	1.68	0.45
8:E:26:LYS:HD3	52:A:923:A:H5''	1.98	0.45
16:M:86:TYR:CZ	52:A:1321:U:H4'	2.51	0.45
19:P:57:ILE:O	19:P:61:VAL:HG23	2.16	0.45
22:S:70:LYS:NZ	52:A:1320:C:OP1	2.51	0.45
32:g:143:GLN:NE2	32:g:147:ASP:OD1	2.49	0.45
32:g:158:LYS:HD3	32:g:160:LYS:HD2	1.99	0.45
52:A:181:A:H1'	52:A:194:C:N4	2.32	0.45
53:a:144:A:H2'	53:a:145:C:O4'	2.17	0.45
53:a:598:U:H2'	53:a:599:A:H8	1.82	0.45
53:a:910:A:H2'	53:a:911:A:C8	2.51	0.45
53:a:1641:A:H2'	53:a:1642:G:O4'	2.17	0.45
53:a:1889:A:H2'	53:a:1890:A:C8	2.52	0.45
53:a:2837:A:H2'	53:a:2838:G:H8	1.82	0.45
53:a:2853:C:H2'	53:a:2854:G:H8	1.82	0.45
55:Y:45:C:H2'	55:Y:47:A:P	2.57	0.45
10:G:65:ALA:O	10:G:69:VAL:HG23	2.16	0.44
19:P:5:ARG:HB2	52:A:376:G:H5''	1.98	0.44
26:Z:76:8AN:C5	53:a:2451:A:H4'	2.47	0.44
28:c:125:LYS:N	28:c:192:LEU:HD13	2.33	0.44
28:c:155:ALA:HB2	28:c:162:VAL:HG23	1.99	0.44
53:a:236:C:H2'	53:a:237:C:H6	1.82	0.44
53:a:1849:G:H2'	53:a:1850:G:H8	1.82	0.44
53:a:2483:C:OP1	55:Y:63:C:H5'	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:2556:C:H2'	53:a:2557:G:O4'	2.18	0.44
9:F:10:VAL:HG21	9:F:18:VAL:HG22	1.98	0.44
12:I:4:ASN:OD1	12:I:5:GLN:N	2.48	0.44
21:R:13:PHE:HD1	21:R:18:VAL:HG21	1.82	0.44
30:e:48:THR:CG2	30:e:88:ARG:HH22	2.29	0.44
31:f:38:MET:HB2	31:f:87:CYS:SG	2.57	0.44
43:r:82:MET:HB2	43:r:98:LYS:HB2	1.99	0.44
52:A:790:A:H61	52:A:1498:UR3:P	2.41	0.44
52:A:1413:A:H2	52:A:1487:G:H22	1.65	0.44
53:a:365:U:H2'	53:a:366:C:C6	2.52	0.44
12:I:129:LYS:HD3	12:I:130:ARG:NH2	2.33	0.44
14:K:64:GLN:HB2	14:K:95:SER:OG	2.17	0.44
30:e:1:MET:HG2	30:e:14:VAL:HG23	1.98	0.44
32:g:78:GLY:HA2	32:g:82:GLY:HA2	2.00	0.44
36:k:132:ARG:HG3	36:k:142:ILE:HD12	1.99	0.44
44:s:59:ASN:ND2	53:a:1341:G:O2'	2.50	0.44
45:t:21:LYS:HB3	45:t:39:ILE:CD1	2.48	0.44
47:v:18:ALA:HB1	53:a:2271:G:OP1	2.17	0.44
52:A:71:A:N1	52:A:99:C:O2'	2.42	0.44
52:A:123:U:OP1	52:A:311:C:O2'	2.30	0.44
52:A:1072:G:H2'	52:A:1073:U:C6	2.51	0.44
53:a:278:A:N6	53:a:362:A:N7	2.66	0.44
53:a:642:U:O2'	53:a:644:A:N7	2.31	0.44
53:a:2221:G:H2'	53:a:2222:C:O4'	2.17	0.44
55:Y:49:C:H5'	55:Y:50:G:OP2	2.18	0.44
7:D:197:GLU:OE1	7:D:200:ILE:HD12	2.17	0.44
12:I:42:GLU:HA	12:I:45:ARG:HG3	1.99	0.44
13:J:15:HIS:O	13:J:18:ILE:HG22	2.17	0.44
14:K:47:ALA:HB1	14:K:62:ALA:HB1	1.98	0.44
17:N:9:ARG:HH21	52:A:1217:C:P	2.39	0.44
27:b:18:G:H2'	27:b:19:C:C6	2.53	0.44
29:d:131:ASP:HB3	29:d:133:THR:O	2.17	0.44
31:f:2:ALA:HB2	31:f:94:GLU:OE2	2.17	0.44
50:y:8:THR:HA	50:y:34:HIS:O	2.17	0.44
52:A:5:U:H6	52:A:5:U:P	2.41	0.44
52:A:925:G:C2	52:A:927:G:C8	3.05	0.44
52:A:1352:C:H2'	52:A:1353:G:C8	2.52	0.44
53:a:145:C:H2'	53:a:146:A:C8	2.53	0.44
53:a:1447:C:H2'	53:a:1448:G:H8	1.82	0.44
3:2:54:ASP:HB3	36:k:57:LEU:HD22	1.98	0.44
7:D:29:ASP:HA	7:D:32:CYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:100:ASN:OD1	7:D:111:ARG:NH2	2.44	0.44
10:G:4:ARG:HB3	10:G:6:VAL:HG23	1.99	0.44
15:L:67:ILE:HG13	15:L:97:THR:HG21	1.99	0.44
23:T:55:GLN:HB3	23:T:56:PRO:HD3	1.99	0.44
28:c:221:ARG:HD3	53:a:1828:G:O6	2.17	0.44
32:g:37:LEU:HD13	32:g:41:VAL:HG11	2.00	0.44
49:x:19:LEU:HD23	49:x:23:ARG:NH2	2.32	0.44
52:A:625:U:H2'	52:A:626:G:C8	2.53	0.44
52:A:1315:U:H2'	52:A:1316:G:O4'	2.17	0.44
53:a:2636:C:H2'	53:a:2637:U:H6	1.82	0.44
55:Y:28:G:C2	55:Y:43:G:C6	3.05	0.44
5:B:84:ALA:HB3	5:B:91:PHE:CD2	2.51	0.44
6:C:80:LYS:HG3	6:C:80:LYS:O	2.16	0.44
6:C:117:ALA:O	6:C:121:THR:HG22	2.17	0.44
8:E:91:GLY:C	8:E:130:SER:HB3	2.42	0.44
9:F:74:LEU:HD12	9:F:74:LEU:HA	1.86	0.44
22:S:36:ARG:HB2	52:A:1320:C:H42	1.82	0.44
28:c:140:THR:HG23	28:c:161:TYR:HB2	2.00	0.44
44:s:4:GLU:OE1	44:s:49:LYS:HD3	2.18	0.44
45:t:74:ASN:HA	45:t:96:PHE:CZ	2.53	0.44
52:A:1120:C:H2'	52:A:1121:U:C6	2.53	0.44
52:A:1158:C:C5	52:A:1160:G:H1'	2.52	0.44
52:A:1246:A:H2'	52:A:1247:U:H6	1.83	0.44
53:a:219:A:N3	53:a:234:U:O2'	2.40	0.44
53:a:319:G:H2'	53:a:320:A:O4'	2.18	0.44
53:a:358:U:N3	53:a:359:G:N7	2.65	0.44
1:O:17:THR:HG21	1:O:43:VAL:HG13	2.00	0.44
6:C:190:HIS:ND1	6:C:195:VAL:HG22	2.33	0.44
6:C:199:LYS:HE3	52:A:1058:G:H5''	2.00	0.44
7:D:170:TRP:CD1	7:D:186:PRO:HD3	2.53	0.44
18:O:67:LEU:HG	18:O:78:TYR:HE1	1.83	0.44
21:R:43:ARG:HH11	21:R:43:ARG:HG3	1.82	0.44
23:T:9:LYS:HB3	23:T:9:LYS:HE2	1.69	0.44
41:p:58:ARG:HA	41:p:61:TRP:CE3	2.52	0.44
52:A:113:G:H2'	52:A:114:U:H6	1.83	0.44
52:A:1246:A:H2'	52:A:1247:U:C6	2.52	0.44
53:a:182:A:H2'	53:a:183:C:C6	2.52	0.44
53:a:754:U:H2'	53:a:755:U:C6	2.52	0.44
53:a:1480:C:H2'	53:a:1481:U:O4'	2.17	0.44
53:a:1681:G:N3	53:a:1762:A:H2'	2.32	0.44
53:a:2065:C:H2'	53:a:2066:C:H6	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:105:LYS:O	5:B:108:ARG:HG2	2.17	0.44
6:C:5:VAL:HG11	6:C:10:ILE:HD12	2.00	0.44
8:E:110:ALA:O	8:E:114:VAL:HG13	2.18	0.44
16:M:17:ILE:O	16:M:20:THR:OG1	2.28	0.44
20:Q:59:VAL:HG23	20:Q:78:VAL:HA	2.00	0.44
32:g:94:TYR:CD1	32:g:107:LEU:HA	2.53	0.44
38:m:1:MET:HE2	38:m:3:HIS:CE1	2.53	0.44
52:A:192:A:H2'	52:A:193:C:H6	1.83	0.44
52:A:648:A:H2'	52:A:649:A:C8	2.53	0.44
53:a:120:U:H5''	53:a:122:G:OP2	2.18	0.44
53:a:1447:C:H2'	53:a:1448:G:C8	2.52	0.44
53:a:1548:A:H2'	53:a:1549:A:C8	2.53	0.44
53:a:1563:U:H2'	53:a:1564:C:C6	2.52	0.44
53:a:2229:U:H2'	53:a:2230:G:H8	1.81	0.44
53:a:2345:G:N3	53:a:2381:A:H2'	2.33	0.44
6:C:27:LYS:HE3	6:C:27:LYS:HB2	1.78	0.44
6:C:40:ARG:HG2	6:C:55:ILE:HD12	1.99	0.44
10:G:78:ARG:HH21	10:G:87:VAL:CG1	2.31	0.44
12:I:43:THR:O	12:I:47:VAL:HG23	2.17	0.44
13:J:30:LYS:HB3	13:J:30:LYS:HE3	1.68	0.44
39:n:4:LYS:HB2	39:n:4:LYS:HE3	1.82	0.44
51:z:9:THR:CG2	53:a:2020:A:H5'	2.47	0.44
52:A:60:A:N7	52:A:108:G:H4'	2.33	0.44
52:A:1120:C:H2'	52:A:1121:U:H6	1.82	0.44
52:A:1307:U:H2'	52:A:1308:U:H6	1.81	0.44
53:a:57:C:H2'	53:a:58:G:O4'	2.18	0.44
53:a:1932:A:H2'	53:a:1933:G:O4'	2.18	0.44
5:B:106:THR:HG21	52:A:1072:G:N2	2.32	0.43
8:E:114:VAL:HG11	8:E:137:VAL:HG13	1.99	0.43
10:G:146:GLU:O	10:G:149:LYS:HG3	2.18	0.43
17:N:76:LYS:HG2	17:N:77:PHE:CE1	2.53	0.43
19:P:76:LYS:HZ1	52:A:473:U:H5''	1.82	0.43
28:c:23:GLU:HG2	28:c:23:GLU:O	2.18	0.43
31:f:61:SER:HB2	31:f:91:LEU:HD21	2.00	0.43
31:f:121:SER:HB3	31:f:129:SER:O	2.18	0.43
49:x:9:LYS:HG3	49:x:13:GLU:OE1	2.18	0.43
52:A:92:U:H2'	52:A:93:U:C6	2.53	0.43
52:A:426:U:H2'	52:A:427:U:C6	2.53	0.43
52:A:1176:A:H2'	52:A:1177:G:C8	2.53	0.43
52:A:1402:4OC:HM22	52:A:1403:C:H5'	2.00	0.43
52:A:1441:A:C8	52:A:1442:G:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:306:U:H2'	53:a:307:G:O4'	2.17	0.43
53:a:2216:G:H2'	53:a:2217:G:C8	2.53	0.43
53:a:2316:G:H2'	53:a:2317:A:H8	1.82	0.43
55:Y:25(A):A:H2'	55:Y:26:G:H8	1.83	0.43
5:B:19:GLN:H	5:B:19:GLN:HG3	1.55	0.43
7:D:49:SER:O	7:D:53:VAL:HG22	2.19	0.43
17:N:53:ARG:HD3	52:A:1317:C:N4	2.33	0.43
19:P:70:ARG:HA	19:P:70:ARG:HD2	1.81	0.43
28:c:76:ALA:HB3	28:c:116:ILE:HD11	1.99	0.43
43:r:17:VAL:HG11	43:r:103:ILE:HG12	2.00	0.43
52:A:1437:A:H2'	52:A:1438:G:C8	2.53	0.43
53:a:133:U:H2'	53:a:134:G:C8	2.53	0.43
53:a:741:U:H2'	53:a:742:A:C8	2.53	0.43
53:a:1636:U:H2'	53:a:1637:A:C8	2.53	0.43
53:a:1857:G:N2	53:a:1884:G:H1'	2.33	0.43
53:a:1913:A:N1	55:Y:37:A:O2'	2.49	0.43
53:a:2680:U:O2'	53:a:2681:C:H5'	2.18	0.43
54:4:59:ARG:HG3	54:4:63:ARG:HD2	1.99	0.43
4:3:16:ILE:HG13	4:3:25:VAL:HG22	2.01	0.43
9:F:51:ILE:O	9:F:54:LEU:HB2	2.17	0.43
13:J:9:ARG:NH2	13:J:71:LEU:HD21	2.32	0.43
22:S:33:THR:HG23	22:S:35:SER:H	1.82	0.43
26:Z:50:U:H2'	26:Z:51:C:C6	2.54	0.43
35:j:75:SER:HB2	40:o:73:VAL:O	2.18	0.43
41:p:49:ASP:OD2	53:a:534:U:O2'	2.25	0.43
42:q:73:LYS:NZ	53:a:1225:G:OP1	2.51	0.43
52:A:25:C:H2'	52:A:26:A:C8	2.53	0.43
52:A:954:G:H2'	52:A:955:U:C6	2.53	0.43
52:A:1095:U:P	52:A:1108:G:H1	2.37	0.43
53:a:208:C:H2'	53:a:209:C:H6	1.83	0.43
53:a:626:A:N7	64:a:3494:HOH:O	2.36	0.43
53:a:1809:A:H2'	53:a:1810:A:C8	2.53	0.43
53:a:2247:A:H2'	53:a:2248:C:H6	1.84	0.43
4:3:32:LYS:NZ	53:a:2529:G:O6	2.51	0.43
5:B:100:MET:HE2	5:B:100:MET:HB2	1.73	0.43
12:I:91:ASP:HB3	12:I:94:LEU:HD12	2.00	0.43
14:K:27:PHE:O	14:K:58:SER:OG	2.31	0.43
14:K:46:THR:HG23	14:K:49:GLY:N	2.33	0.43
16:M:85:CYS:O	16:M:89:LEU:HG	2.19	0.43
17:N:53:ARG:HH22	52:A:1220:G:P	2.39	0.43
29:d:29:VAL:O	29:d:185:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:57:PHE:HB3	41:p:61:TRP:CZ2	2.53	0.43
43:r:73:LYS:HB3	43:r:106:VAL:HB	1.99	0.43
52:A:97:G:H8	52:A:97:G:O5'	2.00	0.43
52:A:337:G:H2'	52:A:338:A:H8	1.80	0.43
52:A:524:G:H2'	52:A:525:C:C6	2.54	0.43
52:A:744:C:H2'	52:A:745:G:C8	2.53	0.43
52:A:1032:G:C5	52:A:1033:G:H1'	2.53	0.43
52:A:1170:A:H2'	52:A:1171:A:O4'	2.18	0.43
52:A:1178:G:N2	52:A:1180:A:H3'	2.33	0.43
53:a:146:A:H2'	53:a:147:C:C6	2.52	0.43
53:a:215:G:OP2	64:a:3332:HOH:O	2.21	0.43
53:a:412:A:N7	53:a:2411:A:H2	2.17	0.43
53:a:1680:U:H2'	53:a:1681:G:O4'	2.19	0.43
53:a:1913:A:H4'	53:a:1914:C:H5''	2.00	0.43
55:Y:49:C:O2	55:Y:49:C:H2'	2.18	0.43
6:C:128:VAL:HG13	6:C:132:ARG:HD2	2.01	0.43
7:D:23:SER:HB2	7:D:25:VAL:HG23	2.00	0.43
8:E:136:VAL:O	8:E:140:THR:OG1	2.33	0.43
13:J:59:LYS:HD3	52:A:972:C:O3'	2.18	0.43
28:c:242:LYS:O	53:a:1902:C:H4'	2.18	0.43
32:g:9:VAL:HG11	32:g:50:LEU:HD12	2.00	0.43
36:k:108:ALA:HB3	36:k:125:LEU:HD22	2.00	0.43
52:A:745:G:H2'	52:A:746:A:H8	1.83	0.43
52:A:768:A:H4'	52:A:1523:G:N2	2.33	0.43
52:A:1118:U:H2'	52:A:1119:C:C6	2.53	0.43
53:a:17:G:H2'	53:a:18:U:C6	2.54	0.43
53:a:373:U:H2'	53:a:374:A:H8	1.83	0.43
53:a:820:A:H2'	53:a:821:A:O4'	2.18	0.43
53:a:1591:A:H2'	53:a:1592:C:H6	1.82	0.43
53:a:2796:U:H3	53:a:2799:A:N6	2.17	0.43
2:1:26:ASN:CG	53:a:682:G:H5'	2.43	0.43
8:E:160:SER:OG	8:E:163:GLU:OE1	2.29	0.43
12:I:99:ARG:HH12	52:A:1180:A:P	2.42	0.43
14:K:119:IAS:O	24:U:35:ARG:NH2	2.41	0.43
43:r:86:MET:SD	61:a:3217:SPD:H31	2.58	0.43
49:x:4:LYS:HD3	49:x:4:LYS:HA	1.82	0.43
52:A:543:U:H2'	52:A:544:G:C8	2.54	0.43
52:A:620:C:H2'	52:A:621:A:C8	2.54	0.43
52:A:705:G:C5	52:A:706:A:C8	3.07	0.43
52:A:908:A:H2'	52:A:909:A:C8	2.54	0.43
52:A:1286:U:H2'	52:A:1287:A:H5'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:1329:A:C5	52:A:1330:U:C5	3.06	0.43
53:a:1736:U:H2'	53:a:1737:G:O4'	2.19	0.43
53:a:2649:C:H2'	53:a:2650:U:H6	1.84	0.43
7:D:70:ARG:HA	7:D:70:ARG:HD3	1.87	0.43
19:P:28:ARG:NH1	52:A:390:U:H4'	2.33	0.43
27:b:93:C:N4	64:b:312:HOH:O	2.48	0.43
30:e:130:LYS:HE3	30:e:132:LYS:HD2	2.01	0.43
31:f:105:THR:HB	54:4:22:MET:HE1	2.01	0.43
31:f:123:ASP:OD1	31:f:123:ASP:N	2.40	0.43
52:A:349:A:O2'	52:A:350:G:H5'	2.19	0.43
52:A:444:G:C6	52:A:491:G:C6	3.06	0.43
52:A:596:A:H2'	52:A:597:G:H8	1.83	0.43
53:a:320:A:H4'	53:a:322:A:C8	2.53	0.43
53:a:1361:G:H2'	53:a:1362:C:C6	2.53	0.43
53:a:2291:U:OP1	53:a:2380:C:O2'	2.35	0.43
5:B:71:GLY:O	5:B:93:ASN:HA	2.19	0.43
5:B:97:LEU:H	5:B:100:MET:HE1	1.84	0.43
9:F:29:ILE:HG22	9:F:34:GLY:O	2.19	0.43
12:I:17:ALA:HB2	12:I:67:VAL:HG23	2.00	0.43
15:L:66:TYR:O	15:L:97:THR:HG23	2.18	0.43
18:O:67:LEU:HG	18:O:78:TYR:CE1	2.54	0.43
23:T:17:ALA:HB3	52:A:323:U:H4'	2.00	0.43
30:e:1:MET:HB2	30:e:16:GLU:OE1	2.18	0.43
32:g:41:VAL:HG23	32:g:65:ALA:HA	2.01	0.43
35:j:58:LEU:HA	35:j:89:ASN:OD1	2.19	0.43
49:x:32:ALA:HB2	49:x:37:LEU:HD23	2.00	0.43
50:y:5:ILE:HG23	50:y:40:ASP:HB2	2.01	0.43
52:A:381:C:H2'	52:A:382:A:O4'	2.19	0.43
52:A:908:A:H2'	52:A:909:A:H8	1.83	0.43
52:A:1181:G:O2'	52:A:1182:G:N7	2.46	0.43
52:A:1486:G:H2'	52:A:1487:G:O4'	2.18	0.43
53:a:362:A:C4	53:a:363:G:C8	3.06	0.43
53:a:415:A:H2'	53:a:416:U:C6	2.52	0.43
53:a:2193:G:H2'	53:a:2194:U:H6	1.83	0.43
53:a:2228:G:H2'	53:a:2229:U:C6	2.53	0.43
53:a:2646:C:O5'	53:a:2646:C:H6	2.01	0.43
5:B:18:HIS:O	5:B:39:HIS:HB2	2.19	0.43
17:N:33:ASP:HB3	17:N:36:ALA:HB2	2.01	0.43
19:P:10:GLY:C	52:A:624:C:H4'	2.44	0.43
24:U:10:GLU:CD	24:U:15:ALA:HB2	2.44	0.43
31:f:175:PHE:HB3	31:f:177:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:157:TYR:CE2	53:a:2531:A:H5'	2.54	0.43
41:p:86:ALA:HB2	41:p:116:ALA:HB2	2.01	0.43
50:y:13:ALA:O	50:y:16:ARG:HG2	2.19	0.43
52:A:66:A:C2	52:A:104:G:H1'	2.53	0.43
52:A:150:U:C4	52:A:170:U:C4	3.07	0.43
52:A:1007:U:H2'	52:A:1008:U:C6	2.53	0.43
52:A:1275:A:H3'	52:A:1276:G:H8	1.84	0.43
52:A:1327:C:C2	52:A:1328:C:C5	3.07	0.43
53:a:185:G:H4'	53:a:218:A:H4'	2.01	0.43
53:a:543:G:C6	53:a:551:G:C6	3.07	0.43
53:a:594:U:H2'	53:a:595:C:H6	1.84	0.43
53:a:1637:A:H5'	53:a:1760:C:O2'	2.19	0.43
53:a:1683:U:H2'	53:a:1684:G:H8	1.84	0.43
55:Y:47:A:H2'	55:Y:48:G:C8	2.54	0.43
4:3:36:ARG:HD3	53:a:2742:G:OP1	2.18	0.43
7:D:107:PHE:CG	7:D:145:ILE:HD11	2.53	0.43
7:D:150:LYS:HG2	7:D:178:MET:HE3	2.01	0.43
14:K:87:LYS:HG3	14:K:115:PRO:HD3	2.01	0.43
27:b:45:A:C4	27:b:46:A:C8	3.07	0.43
30:e:163:ASN:ND2	53:a:320:A:N3	2.52	0.43
37:l:78:LEU:HD12	37:l:78:LEU:HA	1.87	0.43
39:n:52:SER:OG	39:n:54:VAL:HG22	2.19	0.43
46:u:20:LEU:HD22	46:u:25:LYS:HB2	2.00	0.43
52:A:179:A:H61	52:A:196:A:H62	1.66	0.43
52:A:191:G:H8	52:A:191:G:OP2	2.02	0.43
52:A:481:G:O2'	52:A:483:C:N4	2.48	0.43
52:A:679:C:H2'	52:A:680:C:C6	2.54	0.43
53:a:828:U:H4'	53:a:831:G:N1	2.34	0.43
53:a:860:U:P	61:a:3218:SPD:H32	2.59	0.43
53:a:1704:C:H2'	53:a:1705:A:H8	1.84	0.43
53:a:2405:G:H1'	53:a:2412:A:N6	2.34	0.43
53:a:2515:C:H2'	53:a:2516:A:H8	1.83	0.43
26:Z:10:G:C2	26:Z:26:G:H1'	2.54	0.42
27:b:51:G:O2'	27:b:52:A:H5'	2.19	0.42
39:n:52:SER:OG	39:n:53:THR:N	2.52	0.42
44:s:30:ILE:HD13	44:s:93:LEU:HD13	2.01	0.42
52:A:373:A:C2	52:A:482:A:C6	3.06	0.42
52:A:513:C:H2'	52:A:514:C:H6	1.83	0.42
52:A:652:U:O4	52:A:752:G:O2'	2.31	0.42
52:A:1107:C:C4	52:A:1108:G:C8	3.07	0.42
53:a:277:G:H1'	53:a:278:A:C4	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:481:G:O2'	53:a:507:A:N1	2.46	0.42
53:a:493:G:H2'	53:a:494:G:O4'	2.18	0.42
53:a:1545:A:H2'	53:a:1546:G:O4'	2.19	0.42
6:C:177:THR:HG23	52:A:1111:A:C2	2.54	0.42
7:D:194:ASP:OD1	7:D:194:ASP:N	2.52	0.42
13:J:68:ARG:HB3	13:J:68:ARG:NH1	2.33	0.42
15:L:9:ARG:NH1	52:A:880:C:OP1	2.52	0.42
15:L:111:LYS:HG2	52:A:538:G:H5''	2.01	0.42
16:M:96:PRO:HG3	16:M:109:ARG:HG3	2.00	0.42
18:O:32:LEU:HD23	18:O:32:LEU:HA	1.90	0.42
18:O:54:ARG:HH22	52:A:579:A:H4'	1.84	0.42
21:R:41:PRO:HD2	21:R:44:ILE:HB	2.01	0.42
29:d:170:VAL:HG11	53:a:2679:A:H4'	2.01	0.42
36:k:1:MET:C	36:k:2:ARG:HD2	2.44	0.42
40:o:72:ARG:HD3	40:o:74:PHE:CE1	2.54	0.42
45:t:86:ARG:O	45:t:92:LYS:HA	2.18	0.42
52:A:109:A:H2'	52:A:326:G:N2	2.34	0.42
52:A:218:U:H2'	52:A:219:U:C6	2.53	0.42
52:A:446:G:H2'	52:A:447:G:O4'	2.20	0.42
52:A:547:A:H4'	52:A:548:G:O5'	2.19	0.42
52:A:883:C:O2'	52:A:884:U:H5'	2.18	0.42
52:A:934:C:N4	52:A:1345:U:C4	2.87	0.42
52:A:1162:C:C2	52:A:1163:A:C8	3.07	0.42
52:A:1412:C:H2'	52:A:1413:A:H8	1.84	0.42
53:a:1327:A:H2'	53:a:1328:A:O4'	2.19	0.42
53:a:1428:C:N4	53:a:1570:A:OP2	2.47	0.42
53:a:2047:C:H2'	53:a:2048:G:H8	1.84	0.42
7:D:124:MET:N	7:D:144:SER:O	2.50	0.42
7:D:195:ILE:H	7:D:195:ILE:HG13	1.59	0.42
11:H:96:MET:SD	11:H:130:ALA:HB1	2.60	0.42
16:M:110:LYS:HE3	52:A:1227:A:OP2	2.19	0.42
21:R:56:ALA:O	21:R:60:LYS:HD2	2.19	0.42
26:Z:43:A:H2'	26:Z:44:A:C8	2.54	0.42
52:A:130:A:H1'	52:A:263:A:O2'	2.19	0.42
52:A:270:A:H2'	52:A:271:C:C6	2.54	0.42
52:A:590:U:H2'	52:A:591:U:O4'	2.19	0.42
52:A:1320:C:H2'	52:A:1321:U:C6	2.55	0.42
52:A:1401:G:H2'	52:A:1402:4OC:O4'	2.19	0.42
53:a:235:U:H2'	53:a:236:C:C6	2.54	0.42
53:a:766:U:O4	62:a:3220:SPM:H71	2.19	0.42
53:a:1437:C:H2'	53:a:1438:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:1504:A:H2'	53:a:1505:A:C8	2.55	0.42
53:a:1985:C:OP1	64:a:3333:HOH:O	2.21	0.42
53:a:2196:C:H2'	53:a:2197:U:C6	2.54	0.42
53:a:2853:C:H2'	53:a:2854:G:C8	2.55	0.42
54:4:36:VAL:HG21	54:4:41:HIS:ND1	2.34	0.42
4:3:4:ARG:O	4:3:37:GLN:HA	2.20	0.42
5:B:140:GLU:HA	5:B:143:LYS:HG2	2.01	0.42
27:b:57:A:H2'	27:b:58:A:H8	1.84	0.42
31:f:30:ARG:NH1	31:f:159:THR:HG21	2.34	0.42
42:q:63:VAL:HA	42:q:96:VAL:HG22	2.01	0.42
43:r:86:MET:HE2	43:r:86:MET:HB2	1.90	0.42
46:u:46:LYS:O	46:u:50:MET:HG3	2.19	0.42
52:A:1093:A:O2'	52:A:1095:U:OP1	2.34	0.42
52:A:1388:C:H2'	52:A:1389:C:C6	2.54	0.42
52:A:1447:A:P	52:A:1448:C:H5	2.42	0.42
53:a:387:U:OP1	61:a:3213:SPD:H92	2.18	0.42
53:a:722:A:H2'	53:a:723:C:O4'	2.20	0.42
53:a:886:A:C2	53:a:891:G:C6	3.07	0.42
53:a:2002:G:OP2	64:a:3336:HOH:O	2.22	0.42
53:a:2751:G:N3	53:a:2751:G:H2'	2.34	0.42
5:B:221:VAL:HG12	5:B:225:ARG:HD2	2.00	0.42
10:G:15:ASP:O	10:G:19:GLY:N	2.39	0.42
12:I:6:TYR:CD2	12:I:90:TYR:HB2	2.54	0.42
13:J:38:GLY:HA2	52:A:1123:U:O2'	2.19	0.42
31:f:12:VAL:HG13	31:f:172:ALA:CB	2.50	0.42
38:m:5:LYS:NZ	53:a:2000:C:OP1	2.43	0.42
38:m:53:THR:OG1	53:a:2840:C:H5''	2.19	0.42
40:o:6:LYS:HE2	40:o:6:LYS:HB2	1.82	0.42
52:A:192:A:H2'	52:A:193:C:C6	2.54	0.42
52:A:414:A:H2'	52:A:415:A:O4'	2.20	0.42
52:A:418:C:H2'	52:A:419:C:C6	2.55	0.42
53:a:26:G:H1'	53:a:514:A:N6	2.34	0.42
53:a:740:C:O5'	53:a:740:C:H6	2.03	0.42
53:a:896:A:C8	55:Y:17:G:C6	3.07	0.42
53:a:2267:A:H5''	53:a:2268:A:H5'	2.01	0.42
53:a:2439:A:O2'	53:a:2600:A:OP1	2.28	0.42
53:a:2491:U:H5''	53:a:2570:G:H5'	2.01	0.42
6:C:143:ARG:NE	6:C:143:ARG:O	2.52	0.42
11:H:29:SER:HB2	11:H:59:LEU:HB2	2.01	0.42
18:O:88:ARG:NH1	53:a:714:U:OP2	2.52	0.42
20:Q:68:SER:OG	20:Q:71:LYS:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:r:88:ARG:HD2	43:r:88:ARG:HA	1.87	0.42
52:A:18:C:H4'	52:A:1078:U:O2	2.19	0.42
52:A:79:G:H1	52:A:90:C:H42	1.68	0.42
52:A:439:U:C2	52:A:440:C:C6	3.08	0.42
52:A:1160:G:C2	52:A:1161:C:C6	3.07	0.42
52:A:1372:U:H2'	52:A:1373:G:O4'	2.19	0.42
53:a:766:U:H2'	53:a:767:U:C6	2.55	0.42
53:a:841:G:H2'	53:a:842:U:H6	1.84	0.42
53:a:2408:U:H2'	53:a:2409:G:C8	2.54	0.42
53:a:2646:C:H2'	53:a:2647:U:O4'	2.20	0.42
6:C:7:PRO:O	6:C:11:ARG:HB2	2.18	0.42
6:C:151:VAL:HG22	6:C:200:VAL:HG22	2.01	0.42
13:J:24:GLU:HB2	13:J:90:LEU:HD21	2.01	0.42
14:K:107:ILE:HD12	24:U:6:VAL:HG11	2.01	0.42
31:f:58:ALA:HB2	31:f:65:PRO:HD3	2.02	0.42
32:g:90:VAL:HG22	32:g:91:GLY:H	1.84	0.42
36:k:77:ILE:HG23	36:k:81:ASP:HB2	2.01	0.42
38:m:14:SER:OG	53:a:2690:U:OP1	2.31	0.42
51:z:41:HIS:ND1	53:a:2815:C:O2'	2.47	0.42
52:A:3:A:N3	52:A:613:C:H1'	2.35	0.42
52:A:119:A:H4'	52:A:120:A:C4	2.55	0.42
52:A:160:A:H2'	52:A:161:A:O4'	2.19	0.42
52:A:165:G:H2'	52:A:166:U:H6	1.85	0.42
52:A:994:A:H61	52:A:1047:G:C4'	2.32	0.42
52:A:1206:G:H2'	52:A:1207:2MG:H8	1.83	0.42
53:a:261:G:N3	64:a:3504:HOH:O	2.37	0.42
53:a:1503:A:H2'	53:a:1504:A:O4'	2.20	0.42
53:a:2741:A:H2'	53:a:2742:G:O4'	2.20	0.42
53:a:2804:U:H2'	53:a:2805:C:H6	1.84	0.42
8:E:36:LEU:HD21	8:E:137:VAL:HG21	2.02	0.42
13:J:12:ALA:HB3	13:J:18:ILE:HB	2.02	0.42
15:L:58:THR:CG2	52:A:362:G:H5''	2.44	0.42
23:T:36:TYR:CE2	23:T:79:LEU:HD21	2.55	0.42
27:b:52:A:N7	39:n:64:TYR:OH	2.48	0.42
37:l:192:MET:O	46:u:79:ARG:NH1	2.52	0.42
41:p:34:VAL:HG21	53:a:2019:A:H4'	2.01	0.42
50:y:12:SER:OG	53:a:989:G:OP2	2.34	0.42
52:A:62:U:H2'	52:A:63:C:H6	1.83	0.42
52:A:87:C:H2'	52:A:88:U:C6	2.51	0.42
52:A:575:G:O2'	52:A:821:G:H5'	2.19	0.42
52:A:586:C:O2'	52:A:878:A:H4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:836:G:C5	52:A:851:G:C6	3.08	0.42
52:A:970:C:H5''	52:A:971:G:OP1	2.20	0.42
52:A:1120:C:C2	52:A:1121:U:C5	3.07	0.42
52:A:1313:U:H2'	52:A:1314:C:H6	1.85	0.42
53:a:479:A:N3	53:a:481:G:H5''	2.35	0.42
53:a:542:C:H2'	53:a:543:G:H8	1.85	0.42
55:Y:18:G:N3	55:Y:18:G:H2'	2.34	0.42
7:D:196:ASN:HB2	7:D:199:LEU:HG	2.01	0.42
10:G:36:LYS:HB3	12:I:41:ARG:NH2	2.35	0.42
10:G:132:GLY:O	10:G:135:VAL:HG22	2.20	0.42
15:L:39:THR:HB	15:L:49:LEU:HD22	2.02	0.42
22:S:5:LEU:HA	22:S:5:LEU:HD12	1.79	0.42
25:X:25:C:H3'	25:X:26:U:H6	1.84	0.42
26:Z:76:8AN:N7	53:a:2451:A:H4'	2.34	0.42
30:e:41:GLN:HG2	30:e:43:THR:HG23	2.00	0.42
32:g:27:LYS:HE3	32:g:27:LYS:HB3	1.92	0.42
35:j:23:LYS:HB2	35:j:23:LYS:HE2	1.85	0.42
36:k:123:ARG:HG3	36:k:143:GLU:HB2	2.01	0.42
42:q:24:LYS:HD3	42:q:92:TRP:HB3	2.02	0.42
43:r:34:ASP:OD2	51:z:37:LYS:HE3	2.20	0.42
44:s:6:ARG:O	44:s:10:VAL:HG13	2.19	0.42
49:x:52:ARG:O	49:x:56:LEU:HG	2.20	0.42
52:A:425:G:H2'	52:A:426:U:C6	2.55	0.42
52:A:429:U:H1'	52:A:430:A:H5''	2.01	0.42
52:A:1270:G:C2	52:A:1271:A:C5	3.07	0.42
52:A:1417:G:N2	52:A:1482:G:H2'	2.35	0.42
53:a:1039:A:H2	53:a:1116:G:H22	1.66	0.42
53:a:1586:A:H3'	53:a:1587:G:H8	1.85	0.42
53:a:2078:C:H2'	53:a:2079:U:C6	2.55	0.42
53:a:2314:A:H2'	53:a:2315:G:C8	2.55	0.42
53:a:2443:C:H2'	53:a:2444:G:H8	1.84	0.42
8:E:132:ASN:O	8:E:136:VAL:HG23	2.19	0.42
9:F:8:PHE:HB2	9:F:84:VAL:HG13	2.01	0.42
11:H:89:LYS:HD2	11:H:117:ARG:HG3	2.00	0.42
16:M:51:GLY:HA2	16:M:54:ASP:OD2	2.19	0.42
27:b:28:C:H5''	39:n:31:THR:HG21	2.01	0.42
28:c:76:ALA:HB2	28:c:96:TYR:CD2	2.54	0.42
38:m:2:ARG:HA	38:m:5:LYS:HD2	2.02	0.42
52:A:436:C:H2'	52:A:437:U:C6	2.55	0.42
52:A:463:U:O3'	52:A:464:U:O4'	2.38	0.42
52:A:536:C:H2'	52:A:537:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:745:G:H2'	52:A:746:A:C8	2.55	0.42
52:A:749:A:H2'	52:A:750:C:O4'	2.20	0.42
53:a:465:G:H2'	53:a:466:A:C8	2.55	0.42
53:a:680:C:H2'	53:a:681:G:C8	2.55	0.42
53:a:967:U:H2'	53:a:968:C:C6	2.55	0.42
53:a:1656:C:H2'	53:a:1657:U:C6	2.54	0.42
53:a:2492:U:H2'	53:a:2493:U:C6	2.54	0.42
53:a:2537:U:H2'	53:a:2538:C:C6	2.55	0.42
53:a:2597:G:H2'	53:a:2598:A:C8	2.54	0.42
5:B:67:ILE:O	5:B:89:GLN:HB3	2.20	0.41
6:C:57:ILE:HG23	6:C:64:ILE:HD11	2.02	0.41
6:C:153:VAL:CG1	6:C:157:LEU:HD21	2.49	0.41
12:I:63:LEU:CD2	12:I:83:ILE:HD11	2.48	0.41
12:I:112:GLU:OE1	12:I:122:ARG:HD2	2.20	0.41
16:M:19:LEU:O	16:M:22:ILE:HD12	2.19	0.41
16:M:90:ARG:HD3	16:M:96:PRO:O	2.19	0.41
26:Z:43:A:O2'	26:Z:44:A:H5'	2.20	0.41
27:b:104:A:H2'	27:b:105:G:O4'	2.20	0.41
30:e:18:THR:HG23	30:e:200:LEU:HD12	2.02	0.41
44:s:28:ASN:OD1	44:s:87:LEU:HB2	2.20	0.41
45:t:74:ASN:C	45:t:76:ALA:H	2.27	0.41
52:A:227:G:H2'	52:A:228:A:C8	2.54	0.41
52:A:696:A:H2'	52:A:697:U:C6	2.54	0.41
52:A:997:U:H2'	52:A:998:C:O4'	2.19	0.41
52:A:1130:A:C8	52:A:1146:A:N1	2.88	0.41
52:A:1206:G:C4	52:A:1207:2MG:C8	3.09	0.41
52:A:1313:U:H2'	52:A:1314:C:C6	2.54	0.41
52:A:1463:U:H2'	52:A:1464:U:C6	2.55	0.41
53:a:173:A:H2'	53:a:174:U:C6	2.55	0.41
53:a:272:A:H2'	53:a:273:G:C8	2.55	0.41
53:a:1114:C:O2'	53:a:1115:G:OP1	2.35	0.41
53:a:1136:G:N7	64:a:3506:HOH:O	2.37	0.41
53:a:1340:U:OP2	64:a:3337:HOH:O	2.22	0.41
53:a:1870:C:O2'	53:a:1871:A:O4'	2.38	0.41
53:a:1965:C:H5''	53:a:1966:A:H2'	2.01	0.41
53:a:2229:U:H2'	53:a:2230:G:C8	2.54	0.41
53:a:2329:U:H2'	53:a:2330:G:C8	2.55	0.41
2:1:26:ASN:ND2	53:a:682:G:H5'	2.35	0.41
10:G:70:ARG:HA	10:G:100:ALA:HB2	2.02	0.41
17:N:32:SER:O	17:N:33:ASP:C	2.64	0.41
18:O:73:LYS:HD3	18:O:73:LYS:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:29:A:H2'	27:b:30:C:O4'	2.20	0.41
30:e:146:VAL:HG13	30:e:167:VAL:HG13	2.01	0.41
35:j:98:ARG:HH21	52:A:338:A:H3'	1.86	0.41
38:m:55:ALA:HA	38:m:80:PHE:CE1	2.55	0.41
52:A:626:G:H2'	52:A:627:G:H8	1.85	0.41
52:A:763:G:H2'	52:A:764:C:C6	2.54	0.41
53:a:208:C:H2'	53:a:209:C:C6	2.54	0.41
53:a:577:G:H2'	53:a:578:G:C8	2.56	0.41
53:a:675:A:N3	53:a:2443:C:O2'	2.45	0.41
53:a:861:A:H2'	53:a:862:G:O4'	2.20	0.41
53:a:872:U:H2'	53:a:873:C:C6	2.55	0.41
53:a:1196:C:H2'	53:a:1197:G:C8	2.55	0.41
53:a:1841:U:H2'	53:a:1842:G:O4'	2.19	0.41
53:a:1992:G:N2	53:a:1996:C:O2'	2.54	0.41
53:a:2088:A:H2'	53:a:2089:C:C6	2.55	0.41
53:a:2407:A:H2'	53:a:2408:U:C6	2.55	0.41
53:a:2443:C:H2'	53:a:2444:G:C8	2.55	0.41
53:a:2590:A:H2'	53:a:2591:C:C6	2.55	0.41
53:a:2810:A:H2'	53:a:2811:G:O4'	2.19	0.41
53:a:2851:A:OP2	61:a:3208:SPD:H92	2.20	0.41
1:0:11:LEU:HB3	1:0:49:TYR:HB3	2.02	0.41
12:I:12:ARG:HB3	12:I:78:ALA:N	2.36	0.41
12:I:120:LYS:HB3	12:I:120:LYS:HE2	1.88	0.41
13:J:18:ILE:HD12	13:J:18:ILE:HA	1.82	0.41
13:J:90:LEU:HB3	13:J:92:LEU:HD12	2.01	0.41
14:K:20:VAL:HB	14:K:35:THR:HG22	2.02	0.41
15:L:88:LYS:HE3	52:A:526:C:OP2	2.20	0.41
23:T:64:LYS:NZ	52:A:196:A:OP1	2.53	0.41
28:c:171:TYR:HB3	28:c:183:LYS:HG2	2.01	0.41
30:e:154:ASP:OD1	30:e:155:GLU:N	2.53	0.41
35:j:70:ARG:HD2	35:j:76:VAL:HB	2.02	0.41
44:s:5:GLU:HG2	44:s:6:ARG:N	2.36	0.41
45:t:40:ASN:HB3	45:t:63:ALA:O	2.20	0.41
47:v:75:LYS:HE3	47:v:77:ARG:CZ	2.51	0.41
47:v:83:GLU:OE1	47:v:83:GLU:HA	2.19	0.41
52:A:1510:C:H2'	52:A:1511:G:H8	1.82	0.41
53:a:71:A:OP1	53:a:112:U:O2'	2.35	0.41
53:a:727:A:OP2	61:a:3215:SPD:N6	2.53	0.41
53:a:1321:A:C4	53:a:1322:A:C8	3.08	0.41
53:a:1526:C:H2'	53:a:1527:G:O4'	2.20	0.41
2:1:14:ARG:NH1	53:a:770:G:O3'	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:147:SER:OG	5:B:148:LEU:N	2.52	0.41
5:B:217:VAL:O	5:B:220:THR:HG22	2.20	0.41
7:D:202:GLU:HA	7:D:205:SER:HB2	2.03	0.41
11:H:3:MET:HE1	11:H:9:ASP:HB2	2.03	0.41
13:J:45:ARG:NH2	52:A:1255:G:OP2	2.53	0.41
15:L:2:ALA:N	52:A:568:G:O6	2.53	0.41
17:N:70:PRO:HG3	52:A:982:U:P	2.60	0.41
22:S:48:THR:HA	22:S:60:VAL:O	2.20	0.41
30:e:162:ARG:NH2	53:a:340:A:O2'	2.54	0.41
32:g:33:LEU:HD13	32:g:75:MET:HB3	2.01	0.41
52:A:272:C:H2'	52:A:273:U:H6	1.86	0.41
52:A:505:G:OP2	52:A:535:A:H5'	2.21	0.41
52:A:506:G:H2'	52:A:507:C:O4'	2.20	0.41
52:A:1057:G:C6	52:A:1204:A:C6	3.08	0.41
52:A:1237:C:O2'	52:A:1300:G:N1	2.46	0.41
52:A:1318:A:H8	52:A:1318:A:O5'	2.03	0.41
52:A:1436:U:H2'	52:A:1437:A:C8	2.55	0.41
53:a:167:A:H2'	53:a:168:G:O4'	2.19	0.41
53:a:634:C:H2'	53:a:635:C:H6	1.85	0.41
53:a:1438:U:H2'	53:a:1439:A:H8	1.86	0.41
53:a:1703:G:H2'	53:a:1704:C:C6	2.55	0.41
53:a:2219:U:H2'	53:a:2220:U:O4'	2.21	0.41
53:a:2514:U:H2'	53:a:2515:C:H6	1.84	0.41
55:Y:25:C:C2	55:Y:25(A):A:C8	3.09	0.41
55:Y:59:C:N4	55:Y:60:G:O6	2.53	0.41
11:H:21:ASN:HA	11:H:65:TYR:OH	2.20	0.41
15:L:110:ARG:HA	15:L:110:ARG:HD2	1.92	0.41
29:d:194:PRO:HA	53:a:2680:U:H5'	2.01	0.41
52:A:459:A:C6	52:A:474:G:C6	3.09	0.41
52:A:1063:C:H2'	52:A:1064:G:C8	2.55	0.41
53:a:169:G:H2'	53:a:170:U:H6	1.83	0.41
53:a:538:A:H2'	53:a:539:G:O4'	2.21	0.41
53:a:792:A:OP2	64:a:3335:HOH:O	2.22	0.41
53:a:1401:G:H2'	53:a:1402:U:O4'	2.20	0.41
54:4:41:HIS:CD2	54:4:43:PHE:H	2.38	0.41
5:B:30:PHE:HB3	5:B:201:PRO:HG3	2.02	0.41
5:B:161:LEU:HD23	5:B:161:LEU:HA	1.87	0.41
6:C:123:GLN:OE1	6:C:128:VAL:HG11	2.20	0.41
9:F:79:ARG:HB2	9:F:79:ARG:HH11	1.84	0.41
17:N:97:LYS:HB3	17:N:97:LYS:HE3	1.64	0.41
21:R:38:LYS:HG2	52:A:718:A:N1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:97:C:O2'	53:a:918:A:H5''	2.20	0.41
29:d:74:GLU:OE1	29:d:74:GLU:N	2.43	0.41
31:f:94:GLU:O	31:f:98:GLU:HG3	2.21	0.41
31:f:117:LEU:O	31:f:177:PHE:HA	2.20	0.41
37:l:17:ASN:O	37:l:38:ARG:HD3	2.21	0.41
45:t:14:LEU:HD11	45:t:71:ALA:HB2	2.01	0.41
52:A:823:C:H2'	52:A:824:G:H8	1.86	0.41
53:a:261:G:N7	64:a:3507:HOH:O	2.37	0.41
53:a:281:C:C2	53:a:282:A:C8	3.08	0.41
53:a:794:A:H2'	53:a:795:C:C6	2.55	0.41
53:a:843:G:H2'	53:a:844:A:H8	1.86	0.41
53:a:936:A:H2'	53:a:937:C:C6	2.56	0.41
53:a:978:G:O4'	53:a:1001:A:H2	2.04	0.41
55:Y:47:A:O2'	55:Y:48:G:O5'	2.35	0.41
55:Y:67:U:C2'	55:Y:68:C:H5'	2.51	0.41
6:C:130:PHE:O	6:C:134:MET:HG3	2.21	0.41
7:D:72:PHE:CD1	7:D:72:PHE:C	2.99	0.41
7:D:101:VAL:HG21	7:D:137:VAL:HG21	2.02	0.41
8:E:41:ASP:CG	8:E:45:ARG:HB2	2.46	0.41
10:G:99:LEU:HD22	10:G:103:TRP:NE1	2.35	0.41
11:H:88:ARG:HA	52:A:599:C:H5''	2.02	0.41
12:I:60:LYS:HD3	12:I:60:LYS:N	2.35	0.41
13:J:8:ILE:HG12	13:J:100:ILE:HG13	2.03	0.41
17:N:56:SER:OG	52:A:1317:C:OP1	2.33	0.41
19:P:34:GLU:HG2	19:P:36:VAL:HG13	2.01	0.41
24:U:40:LYS:HE3	24:U:42:THR:CG2	2.51	0.41
27:b:51:G:H2'	27:b:52:A:C8	2.55	0.41
28:c:221:ARG:NH1	53:a:1827:U:OP2	2.49	0.41
43:r:18:ARG:HG3	43:r:76:VAL:HB	2.03	0.41
52:A:231:U:O2'	52:A:232:G:H5'	2.20	0.41
52:A:916:U:H2'	52:A:917:G:C8	2.55	0.41
52:A:1254:A:H2'	52:A:1255:G:C8	2.55	0.41
53:a:457:A:N1	53:a:470:A:H5''	2.36	0.41
53:a:1725:U:H2'	53:a:1726:C:C6	2.55	0.41
55:Y:34:C:H2'	55:Y:35:U:C6	2.56	0.41
5:B:119:THR:O	5:B:123:ASP:CB	2.69	0.41
7:D:2:ALA:HA	52:A:547:A:OP2	2.20	0.41
7:D:162:ALA:HA	7:D:165:ARG:NH1	2.36	0.41
7:D:188:ARG:HA	7:D:188:ARG:HD2	1.60	0.41
16:M:34:LEU:HD22	16:M:39:ILE:HB	2.02	0.41
27:b:62:C:H2'	27:b:63:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:147:LEU:HB3	30:e:186:VAL:HG22	2.03	0.41
33:h:34:GLY:C	33:h:36:ALA:H	2.28	0.41
37:l:62:LYS:HD3	37:l:64:TRP:CZ2	2.55	0.41
42:q:18:GLN:O	42:q:98:ILE:HG12	2.20	0.41
46:u:2:PHE:HB3	46:u:61:LEU:HD23	2.02	0.41
52:A:112:G:HO2'	52:A:354:G:HO2'	1.69	0.41
52:A:441:A:H2'	52:A:442:G:O4'	2.20	0.41
52:A:512:U:H2'	52:A:513:C:H6	1.84	0.41
52:A:971:G:H1'	52:A:1365:G:O2'	2.21	0.41
52:A:976:G:H2'	52:A:1362:A:C2	2.55	0.41
52:A:1130:A:H61	52:A:1144:G:H1'	1.85	0.41
52:A:1308:U:H2'	52:A:1309:G:C8	2.56	0.41
52:A:1395:C:O2'	52:A:1401:G:O2'	2.35	0.41
53:a:150:U:H2'	53:a:151:C:H6	1.83	0.41
53:a:948:C:H2'	53:a:949:G:C8	2.56	0.41
53:a:1496:A:H2'	53:a:1498:C:C5	2.55	0.41
53:a:1505:A:H2'	53:a:1506:U:C6	2.56	0.41
61:a:3209:SPD:H21	61:a:3209:SPD:H52	1.77	0.41
5:B:18:HIS:CD2	5:B:18:HIS:H	2.38	0.41
7:D:57:GLU:OE1	7:D:57:GLU:HA	2.21	0.41
7:D:59:GLN:O	7:D:63:ARG:HG3	2.21	0.41
7:D:93:LEU:HD12	7:D:93:LEU:HA	1.91	0.41
7:D:147:GLU:H	7:D:147:GLU:CD	2.29	0.41
9:F:2:ARG:HD3	9:F:91:ARG:CZ	2.51	0.41
10:G:28:ASN:ND2	52:A:1375:A:OP1	2.54	0.41
10:G:50:LEU:HD22	10:G:124:LEU:HB3	2.03	0.41
10:G:95:ARG:HD2	10:G:99:LEU:CD1	2.50	0.41
11:H:103:VAL:HB	11:H:127:CYS:SG	2.61	0.41
12:I:88:MET:HB2	12:I:88:MET:HE2	1.87	0.41
13:J:40:ILE:HB	13:J:73:LEU:HB3	2.02	0.41
13:J:63:ASP:OD2	17:N:98:LYS:HE3	2.20	0.41
14:K:46:THR:OG1	52:A:689:C:OP1	2.24	0.41
17:N:87:ALA:HB3	17:N:93:ILE:HD11	2.03	0.41
20:Q:61:ILE:HD12	20:Q:73:TRP:CE3	2.55	0.41
22:S:37:ARG:HA	52:A:1320:C:C5	2.56	0.41
26:Z:45:G:OP2	26:Z:45:G:H8	2.04	0.41
27:b:13:G:O5'	27:b:13:G:H8	2.04	0.41
30:e:55:SER:HB3	53:a:468:G:H5''	2.02	0.41
30:e:130:LYS:HB2	30:e:133:LEU:HD12	2.02	0.41
31:f:12:VAL:HG13	31:f:172:ALA:HB3	2.03	0.41
32:g:6:LYS:HA	32:g:6:LYS:HD2	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:44:LYS:HA	32:g:44:LYS:HD3	1.90	0.41
32:g:86:LYS:O	32:g:165:ALA:N	2.51	0.41
36:k:14:LYS:HE2	53:a:1193:G:OP1	2.20	0.41
37:l:36:VAL:HG22	46:u:82:TYR:HB2	2.02	0.41
44:s:82:LYS:NZ	53:a:1340:U:OP2	2.54	0.41
52:A:96:U:H2'	52:A:97:G:C8	2.56	0.41
52:A:175:C:H2'	52:A:176:C:C6	2.56	0.41
52:A:374:A:C6	52:A:375:U:C4	3.09	0.41
52:A:484:G:H4'	52:A:485:U:H3'	2.02	0.41
52:A:677:U:H3	52:A:713:G:H22	1.69	0.41
52:A:768:A:N3	52:A:1512:U:O2'	2.53	0.41
52:A:904:U:H2'	52:A:905:U:C6	2.56	0.41
52:A:913:A:H8	52:A:913:A:OP2	2.04	0.41
52:A:1032:G:H3'	52:A:1032:G:N3	2.36	0.41
52:A:1071:C:H2'	52:A:1072:G:C8	2.52	0.41
52:A:1258:G:H2'	52:A:1259:C:C6	2.56	0.41
52:A:1291:U:H2'	52:A:1292:G:C8	2.56	0.41
53:a:38:A:H2'	53:a:39:G:O4'	2.21	0.41
53:a:71:A:H5''	53:a:73:A:C8	2.56	0.41
53:a:447:A:OP2	64:a:3338:HOH:O	2.22	0.41
53:a:572:A:H5''	53:a:573:U:OP2	2.20	0.41
53:a:645:C:O2'	53:a:646:U:H5''	2.21	0.41
53:a:744:U:H2'	53:a:745:1MG:O4'	2.21	0.41
53:a:969:G:H2'	53:a:970:U:C6	2.56	0.41
53:a:1027:A:C6	53:a:1126:A:C4	3.08	0.41
53:a:1319:C:O2'	53:a:1320:C:H5'	2.21	0.41
53:a:1385:A:N3	64:a:3502:HOH:O	2.37	0.41
53:a:1869:G:N2	53:a:1871:A:H3'	2.36	0.41
53:a:1937:A:H1'	53:a:1939:5MU:H72	2.03	0.41
53:a:2745:C:H2'	53:a:2746:U:C6	2.56	0.41
53:a:2819:G:H2'	53:a:2821:A:N7	2.36	0.41
53:a:2837:A:H2'	53:a:2838:G:C8	2.55	0.41
54:4:28:VAL:HG22	54:4:30:HIS:CD2	2.55	0.41
55:Y:18:G:H5''	55:Y:57:G:N3	2.36	0.41
5:B:9:MET:HB3	5:B:43:LEU:HD21	2.03	0.41
9:F:79:ARG:HB2	9:F:79:ARG:NH1	2.36	0.41
14:K:94:GLU:OE2	14:K:98:ARG:NH2	2.53	0.41
16:M:109:ARG:HD3	52:A:1307:U:O3'	2.21	0.41
21:R:47:THR:HG22	21:R:48:ARG:O	2.20	0.41
31:f:6:ASP:OD1	31:f:7:TYR:N	2.54	0.41
33:h:9:VAL:HG23	33:h:11:ASN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:23:LYS:HB3	35:j:40:LYS:HB3	2.02	0.41
45:t:45:HIS:HD2	53:a:483:A:C8	2.39	0.41
46:u:80:HIS:CE1	46:u:83:LYS:HG3	2.56	0.41
52:A:346:G:H3'	52:A:346:G:N3	2.36	0.41
52:A:401:C:O2'	52:A:621:A:N3	2.53	0.41
52:A:413:G:N2	52:A:428:G:H1'	2.35	0.41
52:A:1069:C:H2'	52:A:1070:U:O4'	2.20	0.41
52:A:1327:C:H2'	52:A:1328:C:C6	2.56	0.41
53:a:884:U:H3'	53:a:885:C:H6	1.86	0.41
53:a:1916:A:H2'	53:a:1917:PSU:O4'	2.21	0.41
53:a:2313:C:H2'	53:a:2314:A:C8	2.50	0.41
53:a:2528:U:H2'	53:a:2530:A:O5'	2.22	0.41
8:E:77:ASN:N	8:E:80:THR:O	2.44	0.40
9:F:98:GLU:HG2	9:F:99:ALA:H	1.86	0.40
11:H:44:GLY:O	11:H:64:LYS:HD2	2.21	0.40
13:J:19:ASP:OD1	13:J:72:ARG:NH2	2.44	0.40
14:K:113:VAL:HG12	21:R:73:ARG:HD3	2.02	0.40
15:L:7:LEU:HD23	20:Q:34:TYR:CE1	2.56	0.40
18:O:26:GLU:H	18:O:26:GLU:HG2	1.53	0.40
23:T:39:ILE:HG23	23:T:86:LEU:HD12	2.02	0.40
26:Z:16:C:H3'	26:Z:17:C:C5	2.56	0.40
26:Z:26:G:N2	26:Z:27:U:H1'	2.35	0.40
28:c:25:HIS:HB3	28:c:82:GLU:HG2	2.03	0.40
32:g:44:LYS:HG3	32:g:51:THR:N	2.36	0.40
32:g:90:VAL:HG13	32:g:160:LYS:HA	2.03	0.40
34:i:39:LYS:HB3	34:i:39:LYS:HE2	1.90	0.40
35:j:63:VAL:HG12	35:j:107:LEU:HD11	2.02	0.40
39:n:30:ARG:HG3	39:n:35:ILE:HD12	2.02	0.40
39:n:79:ALA:HB3	39:n:113:ALA:HB3	2.03	0.40
48:w:29:PHE:HB3	53:a:396:G:H1'	2.03	0.40
52:A:138:G:H2'	52:A:139:A:C8	2.56	0.40
52:A:413:G:H21	52:A:428:G:H1'	1.85	0.40
52:A:687:A:C2	52:A:704:A:C5	3.09	0.40
53:a:156:A:H2'	53:a:157:C:O4'	2.20	0.40
53:a:753:A:H2'	53:a:754:U:H6	1.86	0.40
53:a:1354:A:H2'	53:a:1355:G:O4'	2.21	0.40
53:a:1634:A:OP1	64:a:3340:HOH:O	2.22	0.40
53:a:2460:U:C2	53:a:2461:A:C8	3.09	0.40
53:a:2650:U:H2'	53:a:2651:C:H6	1.86	0.40
53:a:2812:G:H2'	53:a:2813:A:C8	2.56	0.40
5:B:162:PHE:HA	5:B:184:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:138:ARG:NH1	10:G:139:GLU:OE2	2.54	0.40
16:M:109:ARG:HD3	52:A:1307:U:H4'	2.04	0.40
28:c:145:GLU:HB2	28:c:188:CYS:HB3	2.01	0.40
28:c:180:GLU:OE2	28:c:270:ARG:NH1	2.54	0.40
29:d:49:GLN:OE1	29:d:67:HIS:NE2	2.42	0.40
32:g:154:PRO:HA	32:g:160:LYS:O	2.21	0.40
40:o:43:PHE:CD2	40:o:72:ARG:HD2	2.57	0.40
40:o:93:ARG:HH21	53:a:2849:U:P	2.40	0.40
46:u:80:HIS:HE1	46:u:82:TYR:CZ	2.40	0.40
49:x:19:LEU:O	49:x:23:ARG:HG3	2.21	0.40
52:A:193:C:H2'	52:A:194:C:H6	1.86	0.40
52:A:563:A:H2'	52:A:567:G:C8	2.56	0.40
52:A:991:U:O2	52:A:1213:A:N7	2.55	0.40
52:A:1179:A:H2'	52:A:1180:A:O4'	2.21	0.40
53:a:32:C:H2'	53:a:33:C:C6	2.56	0.40
53:a:463:G:N2	53:a:466:A:OP2	2.48	0.40
53:a:688:U:H2'	53:a:689:A:H8	1.86	0.40
53:a:1443:U:H2'	53:a:1444:G:H8	1.85	0.40
53:a:2756:U:H1'	53:a:2757:A:H5''	2.04	0.40
53:a:2813:A:C4	53:a:2814:A:C8	3.09	0.40
5:B:70:VAL:HG12	5:B:161:LEU:HD22	2.04	0.40
7:D:66:GLY:O	7:D:115:ARG:NH1	2.54	0.40
10:G:47:LEU:HD12	10:G:47:LEU:HA	1.88	0.40
27:b:48:U:H2'	27:b:49:C:C6	2.56	0.40
31:f:44:ILE:HG13	31:f:78:LYS:O	2.20	0.40
32:g:103:ILE:HG22	32:g:105:LEU:HD22	2.03	0.40
43:r:88:ARG:HA	61:a:3217:SPD:H92	2.03	0.40
52:A:175:C:O2'	52:A:1447:A:N1	2.43	0.40
52:A:678:U:H2'	52:A:679:C:H6	1.86	0.40
52:A:1236:A:H2'	52:A:1237:C:C6	2.57	0.40
52:A:1384:C:H2'	52:A:1385:G:O4'	2.22	0.40
53:a:327:G:N3	64:a:3511:HOH:O	2.37	0.40
53:a:1914:C:H2'	53:a:1915:3TD:H6	2.04	0.40
53:a:2615:U:H2'	53:a:2616:C:H6	1.86	0.40
3:2:12:LYS:NZ	53:a:249:C:O2	2.40	0.40
5:B:45:LYS:HD2	5:B:45:LYS:HA	1.59	0.40
6:C:42:TYR:CE1	6:C:90:VAL:HG11	2.57	0.40
8:E:157:ARG:CZ	8:E:164:ILE:HD12	2.52	0.40
11:H:56:LYS:O	11:H:58:GLU:HG3	2.21	0.40
13:J:51:VAL:HG21	13:J:65:TYR:CE2	2.56	0.40
16:M:96:PRO:HD2	16:M:102:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:83:LYS:HD2	17:N:83:LYS:HA	1.71	0.40
18:O:48:LYS:HB2	18:O:48:LYS:HE2	1.82	0.40
22:S:6:LYS:HB3	22:S:6:LYS:HE2	1.87	0.40
26:Z:17:C:H2'	26:Z:17(A):U:C6	2.57	0.40
27:b:24:G:N7	27:b:56:G:H2'	2.36	0.40
28:c:98:ASP:OD2	53:a:1490:A:O2'	2.33	0.40
28:c:107:PRO:HD2	28:c:110:LEU:HD22	2.03	0.40
29:d:27:ILE:HB	29:d:187:LEU:HB3	2.04	0.40
29:d:56:LYS:O	29:d:60:VAL:HG23	2.22	0.40
31:f:108:VAL:HG13	31:f:109:PRO:HD2	2.02	0.40
32:g:72:LEU:HD23	32:g:72:LEU:HA	1.80	0.40
32:g:105:LEU:HB2	32:g:113:VAL:HB	2.03	0.40
39:n:16:ARG:HG3	53:a:2334:U:C4	2.57	0.40
46:u:26:PHE:HE2	46:u:89:ILE:HG13	1.86	0.40
52:A:578:C:O2'	52:A:728:A:N3	2.45	0.40
52:A:864:A:H2'	52:A:865:A:C8	2.57	0.40
52:A:1251:A:N3	52:A:1369:C:O2'	2.49	0.40
53:a:4:U:H2'	53:a:5:A:C8	2.57	0.40
53:a:852:U:H2'	53:a:853:C:H6	1.85	0.40
53:a:971:G:H2'	53:a:972:A:O4'	2.22	0.40
53:a:1042:G:C4	53:a:1043:C:C5	3.09	0.40
53:a:2454:G:C4	53:a:2455:G:C8	3.09	0.40
53:a:2543:G:H2'	53:a:2544:G:C8	2.56	0.40
53:a:2644:G:O2'	53:a:2645:G:H5'	2.22	0.40
53:a:2700:A:H2'	53:a:2701:U:C6	2.56	0.40
53:a:2895:G:H2'	53:a:2896:C:H6	1.83	0.40
62:a:3220:SPM:H62	62:a:3220:SPM:H31	1.77	0.40
55:Y:30:G:H5''	55:Y:31:U:OP2	2.21	0.40
8:E:105:ILE:HD11	8:E:120:VAL:O	2.22	0.40
13:J:28:THR:HG21	13:J:90:LEU:HD22	2.03	0.40
22:S:36:ARG:NH2	52:A:1321:U:O2	2.53	0.40
28:c:71:LYS:HE3	28:c:74:ILE:HD12	2.03	0.40
31:f:161:LYS:HB2	31:f:165:GLU:OE1	2.21	0.40
33:h:6:LEU:C	33:h:15:LEU:HD12	2.46	0.40
45:t:43:LYS:HD2	45:t:58:ILE:CG2	2.51	0.40
52:A:131:A:H2'	52:A:132:C:C6	2.55	0.40
52:A:150:U:H2'	52:A:151:A:C8	2.51	0.40
52:A:728:A:H2'	52:A:729:A:H8	1.78	0.40
52:A:767:A:H2'	52:A:768:A:O4'	2.22	0.40
52:A:1169:A:H2'	52:A:1170:A:H8	1.84	0.40
52:A:1394:A:C5	52:A:1501:C:H4'	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:44:A:H2'	53:a:45:G:O4'	2.22	0.40
53:a:324:A:N6	53:a:338:G:O2'	2.50	0.40
53:a:608:A:H2'	53:a:609:A:H8	1.86	0.40
53:a:1042:G:C6	53:a:1043:C:C4	3.09	0.40
53:a:1876:A:H2'	53:a:1877:A:C8	2.56	0.40
53:a:2796:U:H3	53:a:2799:A:H61	1.67	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	B	222/241 (92%)	204 (92%)	18 (8%)	0	100	100
6	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
7	D	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
8	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
9	F	101/135 (75%)	91 (90%)	10 (10%)	0	100	100
10	G	151/179 (84%)	138 (91%)	13 (9%)	0	100	100
11	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
12	I	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
13	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	15
14	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
15	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	M	113/118 (96%)	104 (92%)	9 (8%)	0	100	100
17	N	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
18	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
19	P	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
20	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
21	R	64/75 (85%)	57 (89%)	7 (11%)	0	100	100
22	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
23	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
24	U	68/71 (96%)	68 (100%)	0	0	100	100
28	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
29	d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	31
30	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
31	f	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
32	g	171/177 (97%)	146 (85%)	24 (14%)	1 (1%)	21	27
33	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
34	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
35	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
36	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
37	l	132/136 (97%)	126 (96%)	6 (4%)	0	100	100
38	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
39	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
40	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
41	p	115/118 (98%)	115 (100%)	0	0	100	100
42	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
43	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
44	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
45	t	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
46	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
47	v	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
48	w	75/78 (96%)	75 (100%)	0	0	100	100
49	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
51	z	54/57 (95%)	54 (100%)	0	0	100	100
54	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
All	All	5477/5913 (93%)	5222 (95%)	252 (5%)	3 (0%)	49	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	J	57	VAL
32	g	47	ASP
29	d	149	ASN

### 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	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	35 (92%)	3 (8%)	11	15
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	55
5	B	186/199 (94%)	168 (90%)	18 (10%)	8	10
6	C	170/190 (90%)	159 (94%)	11 (6%)	15	22
7	D	172/173 (99%)	167 (97%)	5 (3%)	37	55
8	E	119/126 (94%)	115 (97%)	4 (3%)	32	49
9	F	90/116 (78%)	81 (90%)	9 (10%)	7	9
10	G	126/147 (86%)	122 (97%)	4 (3%)	34	51
11	H	104/105 (99%)	98 (94%)	6 (6%)	18	26
12	I	105/107 (98%)	96 (91%)	9 (9%)	10	13
13	J	86/90 (96%)	80 (93%)	6 (7%)	14	19
14	K	89/98 (91%)	81 (91%)	8 (9%)	9	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	L	102/103 (99%)	95 (93%)	7 (7%)	14	20
16	M	93/96 (97%)	90 (97%)	3 (3%)	34	51
17	N	83/84 (99%)	79 (95%)	4 (5%)	23	35
18	O	76/77 (99%)	74 (97%)	2 (3%)	40	59
19	P	65/65 (100%)	63 (97%)	2 (3%)	35	52
20	Q	73/78 (94%)	67 (92%)	6 (8%)	10	14
21	R	57/65 (88%)	54 (95%)	3 (5%)	20	30
22	S	72/79 (91%)	65 (90%)	7 (10%)	8	10
23	T	65/66 (98%)	62 (95%)	3 (5%)	24	36
24	U	60/61 (98%)	57 (95%)	3 (5%)	22	33
28	c	216/218 (99%)	212 (98%)	4 (2%)	50	69
29	d	163/163 (100%)	157 (96%)	6 (4%)	30	45
30	e	165/165 (100%)	161 (98%)	4 (2%)	43	62
31	f	148/150 (99%)	139 (94%)	9 (6%)	17	24
32	g	134/138 (97%)	126 (94%)	8 (6%)	17	25
33	h	32/114 (28%)	30 (94%)	2 (6%)	16	23
34	i	116/116 (100%)	113 (97%)	3 (3%)	40	59
35	j	104/104 (100%)	101 (97%)	3 (3%)	37	55
36	k	103/103 (100%)	99 (96%)	4 (4%)	28	43
37	l	107/107 (100%)	105 (98%)	2 (2%)	50	69
38	m	98/103 (95%)	96 (98%)	2 (2%)	48	67
39	n	86/87 (99%)	83 (96%)	3 (4%)	32	48
40	o	99/100 (99%)	96 (97%)	3 (3%)	36	53
41	p	89/90 (99%)	89 (100%)	0	100	100
42	q	84/84 (100%)	82 (98%)	2 (2%)	43	62
43	r	93/93 (100%)	92 (99%)	1 (1%)	65	81
44	s	80/84 (95%)	77 (96%)	3 (4%)	29	44
45	t	83/85 (98%)	80 (96%)	3 (4%)	31	47
46	u	78/78 (100%)	76 (97%)	2 (3%)	40	59
47	v	58/63 (92%)	58 (100%)	0	100	100
48	w	67/68 (98%)	64 (96%)	3 (4%)	24	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	x	54/55 (98%)	52 (96%)	2 (4%)	30	45
50	y	48/49 (98%)	48 (100%)	0	100	100
51	z	47/48 (98%)	47 (100%)	0	100	100
54	4	55/62 (89%)	53 (96%)	2 (4%)	31	47
All	All	4569/4825 (95%)	4374 (96%)	195 (4%)	27	39

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	8	SER
2	1	15	SER
2	1	24	THR
4	3	9	LYS
5	B	5	SER
5	B	19	GLN
5	B	20	THR
5	B	38	VAL
5	B	49	MET
5	B	58	ASN
5	B	68	LEU
5	B	70	VAL
5	B	92	VAL
5	B	100	MET
5	B	112	LYS
5	B	114	LEU
5	B	136	MET
5	B	148	LEU
5	B	154	MET
5	B	183	VAL
5	B	199	VAL
5	B	211	THR
6	C	4	LYS
6	C	31	ASP
6	C	66	VAL
6	C	97	VAL
6	C	107	ARG
6	C	142	MET
6	C	149	ILE
6	C	166	GLU
6	C	186	THR
6	C	191	THR

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Mol	Chain	Res	Type
6	C	207	ILE
7	D	17	THR
7	D	34	ILE
7	D	49	SER
7	D	97	ARG
7	D	128	ARG
8	E	11	LEU
8	E	56	VAL
8	E	72	ILE
8	E	100	SER
9	F	14	GLN
9	F	15	SER
9	F	30	THR
9	F	35	LYS
9	F	64	VAL
9	F	87	SER
9	F	88	MET
9	F	102	MET
9	F	103	VAL
10	G	11	LYS
10	G	38	THR
10	G	84	THR
10	G	109	ARG
11	H	3	MET
11	H	10	MET
11	H	50	LYS
11	H	60	GLU
11	H	89	LYS
11	H	96	MET
12	I	19	VAL
12	I	29	VAL
12	I	30	ILE
12	I	35	LEU
12	I	88	MET
12	I	89	GLU
12	I	96	SER
12	I	122	ARG
12	I	126	GLN
13	J	25	ILE
13	J	32	THR
13	J	44	THR
13	J	67	ILE

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Mol	Chain	Res	Type
13	J	80	THR
13	J	88	MET
14	K	34	ILE
14	K	85	MET
14	K	89	PRO
14	K	94	GLU
14	K	107	ILE
14	K	109	ASN
14	K	110	ILE
14	K	129	VAL
15	L	4	VAL
15	L	12	ARG
15	L	16	VAL
15	L	52	VAL
15	L	55	VAL
15	L	58	THR
15	L	107	VAL
16	M	33	ILE
16	M	60	VAL
16	M	72	GLU
17	N	6	MET
17	N	18	ASP
17	N	34	VAL
17	N	97	LYS
18	O	2	SER
18	O	26	GLU
19	P	44	SER
19	P	51	ARG
20	Q	13	VAL
20	Q	29	VAL
20	Q	38	ILE
20	Q	42	THR
20	Q	59	VAL
20	Q	81	LYS
21	R	40	VAL
21	R	42	SER
21	R	45	THR
22	S	5	LEU
22	S	6	LYS
22	S	33	THR
22	S	35	SER
22	S	39	THR

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Mol	Chain	Res	Type
22	S	58	VAL
22	S	64	ASP
23	T	26	SER
23	T	35	VAL
23	T	69	LYS
24	U	22	SER
24	U	60	LEU
24	U	68	THR
28	c	94	VAL
28	c	120	VAL
28	c	136	PRO
28	c	139	SER
29	d	40	LEU
29	d	52	THR
29	d	105	LYS
29	d	110	THR
29	d	183	GLU
29	d	197	THR
30	e	74	LYS
30	e	126	VAL
30	e	165	HIS
30	e	170	ARG
31	f	24	SER
31	f	25	VAL
31	f	35	THR
31	f	64	LYS
31	f	66	LEU
31	f	72	LYS
31	f	90	THR
31	f	136	ILE
31	f	155	THR
32	g	18	LYS
32	g	39	ASP
32	g	69	ARG
32	g	76	VAL
32	g	107	LEU
32	g	122	THR
32	g	129	THR
32	g	141	ILE
33	h	12	LEU
33	h	21	VAL
34	i	11	VAL

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Mol	Chain	Res	Type
34	i	64	VAL
34	i	142	ILE
35	j	29	HIS
35	j	76	VAL
35	j	95	ILE
36	k	85	VAL
36	k	103	ILE
36	k	111	ILE
36	k	112	LEU
37	l	42	THR
37	l	191	VAL
38	m	70	THR
38	m	116	VAL
39	n	25	ARG
39	n	47	VAL
39	n	49	VAL
40	o	30	VAL
40	o	39	ARG
40	o	57	SER
42	q	20	VAL
42	q	22	LEU
43	r	4	ILE
44	s	27	SER
44	s	78	SER
44	s	93	LEU
45	t	19	LYS
45	t	70	VAL
45	t	79	LYS
46	u	3	THR
46	u	8	VAL
48	w	35	SER
48	w	60	ASP
48	w	76	GLU
49	x	11	VAL
49	x	19	LEU
54	4	59	ARG
54	4	63	ARG

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

Mol	Chain	Res	Type
5	B	39	HIS

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Mol	Chain	Res	Type
5	B	93	ASN
7	D	40	GLN
7	D	74	ASN
7	D	198	HIS
8	E	77	ASN
8	E	122	ASN
9	F	14	GLN
9	F	37	HIS
10	G	28	ASN
11	H	4	GLN
11	H	38	ASN
12	I	32	GLN
13	J	20	GLN
13	J	58	ASN
14	K	81	ASN
19	P	29	ASN
21	R	31	ASN
21	R	52	GLN
21	R	74	HIS
23	T	52	ASN
28	c	115	GLN
28	c	117	GLN
30	e	195	GLN
31	f	5	HIS
32	g	73	ASN
33	h	2	GLN
33	h	18	GLN
35	j	29	HIS
35	j	88	ASN
35	j	93	GLN
36	k	35	HIS
40	o	41	GLN
41	p	20	GLN
44	s	59	ASN
48	w	36	HIS
49	x	31	GLN
49	x	39	GLN
50	y	9	GLN
54	4	30	HIS
54	4	61	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	X	14/28 (50%)	4 (28%)	1 (7%)
26	Z	74/77 (96%)	23 (31%)	1 (1%)
27	b	118/120 (98%)	12 (10%)	0
52	A	1516/1542 (98%)	270 (17%)	5 (0%)
53	a	2749/2904 (94%)	334 (12%)	0
55	Y	66/71 (92%)	37 (56%)	8 (12%)
All	All	4537/4742 (95%)	680 (14%)	15 (0%)

All (680) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	X	20	A
25	X	24	A
25	X	25	C
25	X	27	A
26	Z	6	G
26	Z	9	G
26	Z	16	C
26	Z	17	C
26	Z	17(A)	U
26	Z	18	G
26	Z	19	G
26	Z	20	U
26	Z	21	A
26	Z	28	C
26	Z	29	G
26	Z	42	G
26	Z	44	A
26	Z	45	G
26	Z	47	U
26	Z	48	C
26	Z	53	G
26	Z	56	C
26	Z	58	A
26	Z	64	G
26	Z	69	C
26	Z	70	G
26	Z	71	C
27	b	24	G
27	b	33	G
27	b	36	C
27	b	42	C
27	b	53	A

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Mol	Chain	Res	Type
27	b	56	G
27	b	66	A
27	b	67	G
27	b	89	U
27	b	90	C
27	b	99	A
27	b	109	A
52	A	4	U
52	A	5	U
52	A	9	G
52	A	22	G
52	A	25	C
52	A	27	G
52	A	29	U
52	A	32	A
52	A	35	G
52	A	39	G
52	A	44	A
52	A	47	C
52	A	48	C
52	A	50	A
52	A	51	A
52	A	70	U
52	A	71	A
52	A	72	A
52	A	74	A
52	A	75	G
52	A	81	A
52	A	83	C
52	A	84	U
52	A	85	U
52	A	86	G
52	A	87	C
52	A	94	G
52	A	95	C
52	A	96	U
52	A	122	G
52	A	130	A
52	A	131	A
52	A	139	A
52	A	142	G
52	A	159	G

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Mol	Chain	Res	Type
52	A	163	C
52	A	166	U
52	A	177	G
52	A	182	A
52	A	183	C
52	A	189	A
52	A	197	A
52	A	204	G
52	A	224	U
52	A	227	G
52	A	228	A
52	A	232	G
52	A	237	G
52	A	240	G
52	A	245	U
52	A	247	G
52	A	251	G
52	A	264	C
52	A	266	G
52	A	267	C
52	A	271	C
52	A	280	C
52	A	289	G
52	A	298	A
52	A	302	G
52	A	306	A
52	A	319	G
52	A	321	A
52	A	328	C
52	A	330	C
52	A	347	G
52	A	350	G
52	A	351	G
52	A	352	C
52	A	354	G
52	A	356	A
52	A	361	G
52	A	364	A
52	A	367	U
52	A	372	C
52	A	373	A
52	A	378	G

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Mol	Chain	Res	Type
52	A	384	G
52	A	390	U
52	A	401	C
52	A	406	G
52	A	412	A
52	A	413	G
52	A	414	A
52	A	416	G
52	A	421	U
52	A	422	C
52	A	423	G
52	A	424	G
52	A	426	U
52	A	429	U
52	A	430	A
52	A	439	U
52	A	448	A
52	A	452	A
52	A	453	G
52	A	457	G
52	A	463	U
52	A	464	U
52	A	465	A
52	A	467	U
52	A	468	A
52	A	469	C
52	A	474	G
52	A	478	A
52	A	479	U
52	A	484	G
52	A	486	U
52	A	497	G
52	A	500	G
52	A	509	A
52	A	511	C
52	A	518	C
52	A	521	G
52	A	524	G
52	A	531	U
52	A	547	A
52	A	559	A
52	A	561	U

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Mol	Chain	Res	Type
52	A	562	U
52	A	567	G
52	A	571	U
52	A	572	A
52	A	573	A
52	A	576	C
52	A	577	G
52	A	579	A
52	A	584	G
52	A	588	G
52	A	590	U
52	A	615	G
52	A	618	C
52	A	633	G
52	A	638	U
52	A	650	G
52	A	653	U
52	A	659	U
52	A	665	A
52	A	723	U
52	A	734	G
52	A	736	C
52	A	747	A
52	A	748	G
52	A	755	G
52	A	777	A
52	A	793	U
52	A	794	A
52	A	802	A
52	A	815	A
52	A	817	C
52	A	821	G
52	A	829	G
52	A	835	U
52	A	859	G
52	A	871	U
52	A	884	U
52	A	890	G
52	A	902	G
52	A	913	A
52	A	914	A
52	A	926	G

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Mol	Chain	Res	Type
52	A	934	C
52	A	935	A
52	A	960	U
52	A	966	2MG
52	A	969	A
52	A	975	A
52	A	976	G
52	A	977	A
52	A	982	U
52	A	991	U
52	A	993	G
52	A	994	A
52	A	1003	G
52	A	1004	A
52	A	1008	U
52	A	1009	U
52	A	1017	U
52	A	1020	G
52	A	1024	G
52	A	1027	C
52	A	1030	U
52	A	1031	C
52	A	1033	G
52	A	1034	G
52	A	1036	A
52	A	1039	G
52	A	1042	A
52	A	1044	A
52	A	1046	A
52	A	1047	G
52	A	1065	U
52	A	1070	U
52	A	1085	U
52	A	1086	U
52	A	1089	G
52	A	1094	G
52	A	1095	U
52	A	1101	A
52	A	1108	G
52	A	1112	C
52	A	1122	U
52	A	1124	G

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Mol	Chain	Res	Type
52	A	1126	U
52	A	1137	C
52	A	1138	G
52	A	1139	G
52	A	1140	C
52	A	1159	U
52	A	1168	U
52	A	1169	A
52	A	1174	G
52	A	1181	G
52	A	1196	A
52	A	1197	A
52	A	1200	C
52	A	1204	A
52	A	1213	A
52	A	1227	A
52	A	1228	C
52	A	1236	A
52	A	1238	A
52	A	1251	A
52	A	1253	G
52	A	1256	A
52	A	1257	A
52	A	1258	G
52	A	1260	G
52	A	1262	C
52	A	1275	A
52	A	1276	G
52	A	1280	A
52	A	1286	U
52	A	1287	A
52	A	1294	G
52	A	1300	G
52	A	1302	C
52	A	1305	G
52	A	1312	G
52	A	1317	C
52	A	1319	A
52	A	1320	C
52	A	1322	C
52	A	1338	G
52	A	1340	A

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Mol	Chain	Res	Type
52	A	1346	A
52	A	1353	G
52	A	1363	A
52	A	1368	A
52	A	1370	G
52	A	1378	C
52	A	1379	G
52	A	1381	U
52	A	1397	C
52	A	1398	A
52	A	1419	G
52	A	1441	A
52	A	1446	A
52	A	1451	U
52	A	1452	C
52	A	1487	G
52	A	1492	A
52	A	1497	G
52	A	1499	A
52	A	1503	A
52	A	1506	U
52	A	1517	G
52	A	1519	MA6
52	A	1529	G
52	A	1530	G
53	a	10	A
53	a	23	G
53	a	34	U
53	a	45	G
53	a	58	G
53	a	71	A
53	a	74	A
53	a	75	G
53	a	80	G
53	a	101	A
53	a	102	U
53	a	118	A
53	a	119	A
53	a	120	U
53	a	139	U
53	a	140	C
53	a	142	A

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Mol	Chain	Res	Type
53	a	150	U
53	a	163	C
53	a	165	A
53	a	181	A
53	a	186	G
53	a	196	A
53	a	199	A
53	a	215	G
53	a	216	A
53	a	222	A
53	a	248	G
53	a	264	C
53	a	265	A
53	a	268	C
53	a	272	A
53	a	276	U
53	a	278	A
53	a	282	A
53	a	286	U
53	a	294	A
53	a	311	A
53	a	329	G
53	a	330	A
53	a	353	C
53	a	359	G
53	a	361	G
53	a	362	A
53	a	386	G
53	a	404	A
53	a	405	U
53	a	406	G
53	a	411	G
53	a	451	U
53	a	481	G
53	a	491	G
53	a	504	A
53	a	505	A
53	a	508	A
53	a	509	C
53	a	529	A
53	a	530	G
53	a	531	C

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Mol	Chain	Res	Type
53	a	532	A
53	a	543	G
53	a	544	C
53	a	545	U
53	a	546	U
53	a	547	A
53	a	548	G
53	a	549	G
53	a	563	A
53	a	573	U
53	a	575	A
53	a	603	A
53	a	613	A
53	a	615	U
53	a	627	A
53	a	637	A
53	a	645	C
53	a	646	U
53	a	647	G
53	a	654	A
53	a	655	A
53	a	686	U
53	a	717	C
53	a	721	A
53	a	730	A
53	a	738	G
53	a	740	C
53	a	747	5MU
53	a	775	G
53	a	776	G
53	a	782	A
53	a	784	G
53	a	785	G
53	a	789	A
53	a	805	G
53	a	812	C
53	a	827	U
53	a	828	U
53	a	845	A
53	a	846	U
53	a	847	U
53	a	859	G

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Mol	Chain	Res	Type
53	a	881	G
53	a	882	G
53	a	884	U
53	a	885	C
53	a	886	A
53	a	888	C
53	a	890	C
53	a	891	G
53	a	893	C
53	a	895	U
53	a	896	A
53	a	897	C
53	a	904	G
53	a	907	G
53	a	910	A
53	a	914	G
53	a	915	C
53	a	931	U
53	a	946	C
53	a	961	C
53	a	974	G
53	a	983	A
53	a	996	A
53	a	1012	U
53	a	1013	C
53	a	1022	G
53	a	1026	G
53	a	1033	U
53	a	1040	A
53	a	1041	G
53	a	1042	G
53	a	1044	C
53	a	1045	C
53	a	1046	A
53	a	1047	G
53	a	1108	U
53	a	1110	G
53	a	1111	A
53	a	1112	G
53	a	1115	G
53	a	1116	G
53	a	1132	U

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Mol	Chain	Res	Type
53	a	1133	A
53	a	1135	C
53	a	1142	A
53	a	1155	A
53	a	1171	G
53	a	1212	G
53	a	1250	G
53	a	1253	A
53	a	1256	G
53	a	1271	G
53	a	1272	A
53	a	1300	G
53	a	1301	A
53	a	1321	A
53	a	1329	U
53	a	1352	U
53	a	1365	A
53	a	1379	U
53	a	1383	A
53	a	1409	U
53	a	1415	U
53	a	1416	G
53	a	1421	G
53	a	1427	A
53	a	1428	C
53	a	1452	G
53	a	1453	A
53	a	1460	U
53	a	1476	U
53	a	1482	G
53	a	1493	C
53	a	1495	A
53	a	1497	U
53	a	1504	A
53	a	1509	A
53	a	1510	G
53	a	1515	A
53	a	1529	G
53	a	1536	C
53	a	1559	U
53	a	1560	G
53	a	1566	A

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Mol	Chain	Res	Type
53	a	1569	A
53	a	1578	U
53	a	1583	A
53	a	1584	U
53	a	1585	C
53	a	1586	A
53	a	1587	G
53	a	1608	A
53	a	1609	A
53	a	1647	U
53	a	1648	U
53	a	1649	G
53	a	1650	A
53	a	1674	G
53	a	1715	G
53	a	1726	C
53	a	1729	U
53	a	1730	C
53	a	1733	G
53	a	1738	G
53	a	1746	A
53	a	1764	C
53	a	1773	A
53	a	1782	U
53	a	1800	C
53	a	1801	A
53	a	1808	A
53	a	1816	C
53	a	1829	A
53	a	1842	G
53	a	1847	A
53	a	1848	A
53	a	1850	G
53	a	1858	A
53	a	1862	G
53	a	1869	G
53	a	1870	C
53	a	1871	A
53	a	1872	A
53	a	1873	G
53	a	1906	G
53	a	1907	G

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Mol	Chain	Res	Type
53	a	1913	A
53	a	1929	G
53	a	1930	G
53	a	1937	A
53	a	1938	A
53	a	1955	U
53	a	1964	G
53	a	1967	C
53	a	1970	A
53	a	1971	U
53	a	1972	G
53	a	1991	U
53	a	1993	U
53	a	1996	C
53	a	2023	C
53	a	2031	A
53	a	2033	A
53	a	2043	C
53	a	2055	C
53	a	2056	G
53	a	2060	A
53	a	2061	G
53	a	2062	A
53	a	2069	G7M
53	a	2192	U
53	a	2198	A
53	a	2204	G
53	a	2211	A
53	a	2225	A
53	a	2238	G
53	a	2239	G
53	a	2268	A
53	a	2279	G
53	a	2283	C
53	a	2287	A
53	a	2288	A
53	a	2305	U
53	a	2308	G
53	a	2311	A
53	a	2322	A
53	a	2325	G
53	a	2333	A

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Mol	Chain	Res	Type
53	a	2335	A
53	a	2347	C
53	a	2361	G
53	a	2366	A
53	a	2379	G
53	a	2383	G
53	a	2385	C
53	a	2402	U
53	a	2403	C
53	a	2406	A
53	a	2409	G
53	a	2425	A
53	a	2429	G
53	a	2435	A
53	a	2441	U
53	a	2448	A
53	a	2469	A
53	a	2476	A
53	a	2478	A
53	a	2482	A
53	a	2484	G
53	a	2491	U
53	a	2492	U
53	a	2498	OMC
53	a	2502	G
53	a	2505	G
53	a	2518	A
53	a	2529	G
53	a	2535	G
53	a	2547	A
53	a	2554	U
53	a	2566	A
53	a	2567	G
53	a	2573	C
53	a	2592	G
53	a	2602	A
53	a	2609	U
53	a	2613	U
53	a	2629	U
53	a	2630	G
53	a	2663	G
53	a	2689	U

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Mol	Chain	Res	Type
53	a	2690	U
53	a	2714	G
53	a	2716	C
53	a	2726	A
53	a	2733	A
53	a	2744	G
53	a	2748	A
53	a	2765	A
53	a	2778	A
53	a	2790	U
53	a	2792	A
53	a	2798	U
53	a	2799	A
53	a	2800	A
53	a	2820	A
53	a	2821	A
53	a	2849	U
53	a	2873	A
53	a	2879	A
53	a	2883	A
53	a	2884	U
53	a	2902	C
53	a	2903	U
55	Y	2	G
55	Y	4	G
55	Y	5	G
55	Y	10	G
55	Y	11	G
55	Y	12	U
55	Y	18	G
55	Y	20	C
55	Y	22	G
55	Y	24	C
55	Y	25	C
55	Y	25(A)	A
55	Y	28	G
55	Y	29	G
55	Y	30	G
55	Y	32	C
55	Y	34	C
55	Y	39	A
55	Y	40	C

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Mol	Chain	Res	Type
55	Y	41	C
55	Y	42(A)	A
55	Y	44	C
55	Y	45	C
55	Y	48	G
55	Y	49	C
55	Y	50	G
55	Y	51	G
55	Y	53	G
55	Y	55	U
55	Y	60	G
55	Y	61	C
55	Y	63	C
55	Y	65	G
55	Y	68	C
55	Y	69	U
55	Y	72	C
55	Y	74	C

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	X	24	A
26	Z	19	G
52	A	121	U
52	A	411	A
52	A	467	U
52	A	1026	G
52	A	1114	C
55	Y	10	G
55	Y	17	G
55	Y	18	G
55	Y	25	C
55	Y	43	G
55	Y	44	C
55	Y	48	G
55	Y	71	U

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

42 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$
53	2MG	a	1835	53	23,26,27	1.26	4 (17%)	33,38,41	2.20	6 (18%)
53	H2U	a	2449	53	18,21,22	1.07	2 (11%)	19,30,33	1.00	2 (10%)
52	MA6	A	1519	52	23,26,27	1.54	5 (21%)	33,38,41	2.10	10 (30%)
53	3TD	a	1915	53	19,22,23	1.63	5 (26%)	23,32,35	2.07	4 (17%)
53	PSU	a	2580	53	18,21,22	1.43	3 (16%)	21,30,33	2.01	4 (19%)
15	D2T	L	89	15	8,9,10	2.53	3 (37%)	6,11,13	1.54	1 (16%)
53	2MG	a	2445	53	23,26,27	1.26	4 (17%)	33,38,41	2.17	7 (21%)
53	5MU	a	1939	53	19,22,23	1.39	5 (26%)	27,32,35	2.16	6 (22%)
53	OMG	a	2251	53,59,26	23,26,27	1.20	3 (13%)	32,38,41	2.04	6 (18%)
53	G7M	a	2069	53	23,26,27	1.51	3 (13%)	34,39,42	1.74	5 (14%)
52	2MG	A	1516	52	23,26,27	1.22	3 (13%)	33,38,41	2.20	8 (24%)
53	OMC	a	2498	53,57	19,22,23	0.78	0	25,31,34	0.86	1 (4%)
53	PSU	a	1917	53	18,21,22	1.34	2 (11%)	21,30,33	2.15	5 (23%)
53	6MZ	a	1618	53	22,25,26	1.51	5 (22%)	29,36,39	2.16	10 (34%)
53	6MZ	a	2030	53	22,25,26	1.45	5 (22%)	29,36,39	2.37	11 (37%)
52	4OC	A	1402	52	20,23,24	0.75	0	25,32,35	0.91	1 (4%)
52	PSU	A	516	52,57	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
53	PSU	a	2604	53	18,21,22	1.37	3 (16%)	21,30,33	1.99	5 (23%)
53	1MG	a	745	53	23,26,27	1.19	3 (13%)	33,39,42	1.75	5 (15%)
53	OMU	a	2552	53,57	19,22,23	1.23	3 (15%)	25,31,34	1.85	5 (20%)
53	PSU	a	1911	53	18,21,22	1.31	2 (11%)	21,30,33	2.08	3 (14%)
52	G7M	A	527	52	23,26,27	1.55	3 (13%)	34,39,42	1.73	5 (14%)
37	MS6	l	138	37	5,7,8	0.22	0	2,7,9	0.12	0
53	PSU	a	2504	53,59	18,21,22	1.37	2 (11%)	21,30,33	2.02	3 (14%)
29	MEQ	d	150	29	8,9,10	0.50	0	5,10,12	0.27	0
52	5MC	A	967	52	19,22,23	1.54	3 (15%)	26,32,35	1.11	2 (7%)
53	PSU	a	746	53,57	18,21,22	1.37	3 (16%)	21,30,33	1.95	4 (19%)
53	5MU	a	747	53	19,22,23	1.37	5 (26%)	27,32,35	2.10	9 (33%)
53	PSU	a	2605	53	18,21,22	1.39	3 (16%)	21,30,33	2.02	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
52	MA6	A	1518	52	23,26,27	1.52	4 (17%)	33,38,41	2.10	10 (30%)
55	8AN	Y	76	53,55,63	21,24,25	1.61	4 (19%)	26,35,38	2.26	7 (26%)
53	PSU	a	955	53	18,21,22	1.34	2 (11%)	21,30,33	2.09	4 (19%)
52	UR3	A	1498	52	19,22,23	0.99	1 (5%)	26,32,35	1.75	4 (15%)
52	5MC	A	1407	52	19,22,23	1.67	3 (15%)	26,32,35	1.17	3 (11%)
37	4D4	l	137	37	9,11,12	2.04	2 (22%)	7,13,15	0.89	0
53	2MA	a	2503	53,57,59	22,25,26	1.49	4 (18%)	32,37,40	2.33	8 (25%)
14	IAS	K	119	14	6,7,8	1.42	1 (16%)	3,8,10	1.30	1 (33%)
26	8AN	Z	76	57,26,58	21,24,25	0.90	1 (4%)	26,35,38	0.61	0
53	5MC	a	1962	53	19,22,23	1.54	3 (15%)	26,32,35	1.18	2 (7%)
53	PSU	a	2457	53	18,21,22	1.36	3 (16%)	21,30,33	2.09	3 (14%)
52	2MG	A	966	52	23,26,27	1.24	4 (17%)	33,38,41	2.20	7 (21%)
52	2MG	A	1207	52	23,26,27	1.30	4 (17%)	33,38,41	2.27	9 (27%)

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
53	2MG	a	1835	53	-	0/9/27/28	0/3/3/3
53	H2U	a	2449	53	-	0/7/38/39	0/2/2/2
52	MA6	A	1519	52	-	2/11/29/30	0/3/3/3
53	3TD	a	1915	53	-	0/7/25/26	0/2/2/2
53	PSU	a	2580	53	-	0/7/25/26	0/2/2/2
15	D2T	L	89	15	-	4/7/12/14	-
53	2MG	a	2445	53	-	1/9/27/28	0/3/3/3
53	5MU	a	1939	53	-	0/7/25/26	0/2/2/2
53	OMG	a	2251	53,59,26	-	0/9/27/28	0/3/3/3
53	G7M	a	2069	53	-	0/7/25/26	0/3/3/3
52	2MG	A	1516	52	-	0/9/27/28	0/3/3/3
53	OMC	a	2498	53,57	-	1/9/27/28	0/2/2/2
53	PSU	a	1917	53	-	0/7/25/26	0/2/2/2
53	6MZ	a	1618	53	-	0/9/27/28	0/3/3/3
53	6MZ	a	2030	53	-	2/9/27/28	0/3/3/3
52	4OC	A	1402	52	-	0/9/29/30	0/2/2/2
52	PSU	A	516	52,57	-	0/7/25/26	0/2/2/2
53	PSU	a	2604	53	-	0/7/25/26	0/2/2/2
53	1MG	a	745	53	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	OMU	a	2552	53,57	-	0/9/27/28	0/2/2/2
53	PSU	a	1911	53	-	0/7/25/26	0/2/2/2
52	G7M	A	527	52	-	1/7/25/26	0/3/3/3
37	MS6	l	138	37	-	0/4/6/8	-
53	PSU	a	2504	53,59	-	0/7/25/26	0/2/2/2
29	MEQ	d	150	29	-	2/8/9/11	-
52	5MC	A	967	52	-	0/7/25/26	0/2/2/2
53	PSU	a	746	53,57	-	2/7/25/26	0/2/2/2
53	5MU	a	747	53	-	0/7/25/26	0/2/2/2
53	PSU	a	2605	53	-	0/7/25/26	0/2/2/2
52	MA6	A	1518	52	-	0/11/29/30	0/3/3/3
55	8AN	Y	76	53,55,63	-	1/7/25/26	0/3/3/3
53	PSU	a	955	53	-	0/7/25/26	0/2/2/2
52	UR3	A	1498	52	-	0/7/25/26	0/2/2/2
52	5MC	A	1407	52	-	0/7/25/26	0/2/2/2
37	4D4	l	137	37	-	0/11/12/14	-
53	2MA	a	2503	53,57,59	-	1/7/25/26	0/3/3/3
14	IAS	K	119	14	-	2/7/7/8	-
26	8AN	Z	76	57,26,58	-	3/7/25/26	0/3/3/3
53	5MC	a	1962	53	-	1/7/25/26	0/2/2/2
53	PSU	a	2457	53	-	0/7/25/26	0/2/2/2
52	2MG	A	966	52	-	0/9/27/28	0/3/3/3
52	2MG	A	1207	52	-	1/9/27/28	0/3/3/3

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A	1407	5MC	C5-C4	5.96	1.48	1.44
52	A	967	5MC	C5-C4	5.45	1.48	1.44
53	a	1962	5MC	C5-C4	5.42	1.48	1.44
15	L	89	D2T	CB-CA	5.22	1.56	1.54
53	a	2069	G7M	C5-N7	-4.86	1.33	1.39
53	a	1618	6MZ	C5-C4	4.84	1.47	1.39
55	Y	76	8AN	C5-C4	4.82	1.47	1.39
52	A	527	G7M	C5-N7	-4.79	1.33	1.39
52	A	1518	MA6	C5-C4	4.72	1.47	1.39
52	A	1519	MA6	C5-C4	4.64	1.47	1.39
53	a	2503	2MA	C5-C4	4.59	1.47	1.39
53	a	2030	6MZ	C5-C4	4.32	1.46	1.39
37	l	137	4D4	CZ-NE	4.23	1.41	1.33
15	L	89	D2T	CB-CG	3.62	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	a	1915	3TD	C6-C5	3.52	1.39	1.35
53	a	2604	PSU	C6-C5	3.41	1.39	1.35
53	a	2605	PSU	C6-C5	3.36	1.39	1.35
53	a	2457	PSU	C6-C5	3.35	1.39	1.35
53	a	2580	PSU	C6-C5	3.33	1.39	1.35
53	a	1915	3TD	C4-N3	-3.30	1.33	1.40
52	A	527	G7M	C5-C4	3.28	1.46	1.38
26	Z	76	8AN	C3'-N3'	-3.23	1.42	1.47
52	A	1207	2MG	C5-C4	3.22	1.47	1.38
53	a	2504	PSU	C6-C5	3.21	1.38	1.35
53	a	2251	OMG	C5-C4	3.20	1.47	1.38
53	a	745	1MG	C5-C4	3.20	1.47	1.38
53	a	746	PSU	C6-C5	3.20	1.38	1.35
52	A	1519	MA6	C5-C6	3.18	1.49	1.41
53	a	1917	PSU	C6-C5	3.16	1.38	1.35
53	a	2445	2MG	C5-C4	3.09	1.47	1.38
53	a	2069	G7M	C5-C4	3.09	1.46	1.38
53	a	1915	3TD	C10-N3	3.09	1.52	1.47
52	A	516	PSU	C6-C5	3.08	1.38	1.35
53	a	1835	2MG	C5-C4	3.07	1.47	1.38
52	A	966	2MG	C5-C4	3.07	1.47	1.38
53	a	955	PSU	C6-C5	3.07	1.38	1.35
53	a	2605	PSU	C4-N3	-3.05	1.33	1.38
53	a	1911	PSU	C6-C5	3.02	1.38	1.35
52	A	1518	MA6	C5-C6	3.00	1.49	1.41
53	a	1939	5MU	C6-C5	3.00	1.39	1.34
52	A	1516	2MG	C5-C4	2.97	1.46	1.38
53	a	2449	H2U	C2-N3	-2.91	1.32	1.38
53	a	2580	PSU	C4-N3	-2.89	1.33	1.38
55	Y	76	8AN	C5-C6	2.86	1.49	1.41
52	A	1407	5MC	C6-C5	2.84	1.39	1.34
53	a	1962	5MC	C6-C5	2.79	1.39	1.34
37	l	137	4D4	CZ-NH2	2.79	1.42	1.32
53	a	2604	PSU	C4-N3	-2.75	1.33	1.38
53	a	2030	6MZ	C5-C6	2.75	1.48	1.41
53	a	955	PSU	C4-N3	-2.74	1.33	1.38
53	a	746	PSU	C4-N3	-2.70	1.33	1.38
53	a	1618	6MZ	C5-C6	2.68	1.48	1.41
53	a	2504	PSU	C4-N3	-2.67	1.33	1.38
53	a	1917	PSU	C4-N3	-2.67	1.33	1.38
53	a	747	5MU	C4-N3	-2.64	1.33	1.38
53	a	2457	PSU	C4-N3	-2.64	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	a	1939	5MU	C4-N3	-2.64	1.33	1.38
53	a	2552	OMU	C4-N3	-2.63	1.34	1.38
53	a	1835	2MG	C6-N1	-2.62	1.33	1.38
52	A	516	PSU	C4-N3	-2.60	1.34	1.38
53	a	745	1MG	C2-N1	2.58	1.41	1.37
53	a	1911	PSU	C4-N3	-2.57	1.34	1.38
52	A	1207	2MG	C6-N1	-2.56	1.34	1.38
53	a	2251	OMG	C6-N1	-2.55	1.34	1.38
52	A	966	2MG	C6-N1	-2.51	1.34	1.38
52	A	527	G7M	C6-N1	-2.51	1.34	1.38
52	A	967	5MC	C6-C5	2.50	1.38	1.34
15	L	89	D2T	CB-SB	2.49	1.84	1.82
53	a	2503	2MA	C5-C6	2.48	1.47	1.41
53	a	2449	H2U	C4-N3	-2.47	1.33	1.37
53	a	2030	6MZ	C4-N9	-2.46	1.32	1.37
55	Y	76	8AN	C8-N7	2.45	1.36	1.31
52	A	967	5MC	C6-N1	-2.45	1.33	1.38
53	a	747	5MU	C6-N1	-2.44	1.33	1.38
53	a	2445	2MG	C6-N1	-2.44	1.34	1.38
53	a	1939	5MU	C4-C5	2.43	1.48	1.44
53	a	747	5MU	C6-C5	2.41	1.38	1.34
52	A	1516	2MG	C6-N1	-2.41	1.34	1.38
55	Y	76	8AN	C5-N7	-2.41	1.34	1.39
52	A	1407	5MC	C6-N1	-2.40	1.33	1.38
53	a	747	5MU	C4-C5	2.40	1.48	1.44
53	a	1962	5MC	C6-N1	-2.37	1.34	1.38
52	A	1519	MA6	C8-N7	2.36	1.36	1.31
53	a	2503	2MA	C5-N7	-2.36	1.34	1.39
14	K	119	IAS	CB-CG	2.36	1.56	1.50
53	a	2552	OMU	C2-N3	-2.35	1.33	1.38
53	a	2030	6MZ	C5-N7	-2.35	1.34	1.39
53	a	2069	G7M	C6-N1	-2.31	1.34	1.38
53	a	1939	5MU	C2-N3	-2.31	1.33	1.38
53	a	1835	2MG	C5-N7	-2.31	1.34	1.39
52	A	1207	2MG	C5-N7	-2.28	1.34	1.39
53	a	2503	2MA	C8-N7	2.28	1.36	1.31
53	a	2030	6MZ	C8-N7	2.27	1.36	1.31
53	a	1618	6MZ	C8-N7	2.25	1.36	1.31
53	a	2251	OMG	C5-N7	-2.24	1.34	1.39
52	A	1519	MA6	C4-N9	-2.24	1.33	1.37
52	A	1518	MA6	C5-N7	-2.23	1.35	1.39
53	a	1618	6MZ	C5-N7	-2.20	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	a	2552	OMU	C5-C4	-2.20	1.38	1.43
52	A	1518	MA6	C8-N7	2.17	1.35	1.31
53	a	745	1MG	C5-N7	-2.15	1.34	1.39
53	a	2445	2MG	C2-N3	2.15	1.36	1.32
52	A	1516	2MG	C5-N7	-2.13	1.34	1.39
53	a	1618	6MZ	C4-N9	-2.13	1.33	1.37
52	A	1207	2MG	C2-N3	2.12	1.36	1.32
53	a	2604	PSU	C2-N3	-2.12	1.34	1.37
53	a	1915	3TD	C2-N3	-2.11	1.34	1.38
52	A	1498	UR3	C2-N1	2.10	1.41	1.38
53	a	2580	PSU	C2-N3	-2.10	1.34	1.37
52	A	966	2MG	C2-N3	2.10	1.36	1.32
53	a	1939	5MU	C6-N1	-2.09	1.34	1.38
52	A	966	2MG	C5-N7	-2.09	1.34	1.39
53	a	746	PSU	C2-N3	-2.09	1.34	1.37
53	a	747	5MU	C2-N1	2.09	1.41	1.38
53	a	1915	3TD	C2-N1	-2.08	1.34	1.37
53	a	2445	2MG	C5-N7	-2.08	1.34	1.39
53	a	2457	PSU	C2-N3	-2.07	1.34	1.37
53	a	1835	2MG	C2-N3	2.05	1.35	1.32
53	a	2605	PSU	C2-N3	-2.05	1.34	1.37
52	A	1519	MA6	C5-N7	-2.04	1.35	1.39

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	a	2503	2MA	C5-C4-N3	-7.97	118.78	127.18
53	a	1915	3TD	N1-C2-N3	7.92	121.89	116.13
52	A	1207	2MG	C2-N3-C4	7.35	121.19	112.00
53	a	2445	2MG	C2-N3-C4	7.32	121.16	112.00
52	A	966	2MG	C2-N3-C4	7.32	121.16	112.00
53	a	1835	2MG	C2-N3-C4	7.26	121.08	112.00
52	A	1516	2MG	C2-N3-C4	6.92	120.66	112.00
52	A	1498	UR3	C4-N3-C2	-6.82	119.09	124.58
53	a	2251	OMG	C5-C4-N3	-6.59	117.91	128.39
53	a	2605	PSU	N1-C2-N3	6.52	122.04	115.17
53	a	955	PSU	N1-C2-N3	6.49	122.01	115.17
53	a	2457	PSU	N1-C2-N3	6.48	122.01	115.17
53	a	1917	PSU	N1-C2-N3	6.45	121.97	115.17
53	a	2503	2MA	N3-C4-N9	6.42	135.13	126.99
52	A	1207	2MG	C5-C4-N3	-6.40	118.20	128.39
53	a	1911	PSU	N1-C2-N3	6.38	121.89	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	a	2604	PSU	N1-C2-N3	6.29	121.81	115.17
55	Y	76	8AN	C5-C4-N3	-6.27	118.08	126.72
52	A	516	PSU	N1-C2-N3	6.25	121.76	115.17
53	a	2504	PSU	N1-C2-N3	6.25	121.76	115.17
53	a	2580	PSU	N1-C2-N3	6.22	121.73	115.17
53	a	746	PSU	N1-C2-N3	6.21	121.72	115.17
53	a	1835	2MG	C5-C4-N3	-6.14	118.62	128.39
52	A	966	2MG	C5-C4-N3	-6.03	118.80	128.39
53	a	2445	2MG	C5-C4-N3	-5.99	118.86	128.39
53	a	1618	6MZ	C5-C4-N3	-5.62	118.98	126.72
52	A	1516	2MG	C5-C4-N3	-5.58	119.51	128.39
52	A	1518	MA6	C5-C4-N3	-5.44	119.22	126.72
52	A	527	G7M	C5-C4-N3	-5.34	118.05	128.15
52	A	527	G7M	N9-C4-N3	5.32	136.59	125.95
53	a	745	1MG	C5-C4-N3	-5.28	119.98	128.39
53	a	2069	G7M	N9-C4-N3	5.26	136.47	125.95
53	a	1939	5MU	C4-N3-C2	-5.22	120.50	127.34
53	a	2251	OMG	C2-N3-C4	5.18	121.23	112.30
53	a	2069	G7M	C5-C4-N3	-5.12	118.47	128.15
52	A	1519	MA6	C5-C4-N3	-5.10	119.69	126.72
53	a	2030	6MZ	C9-N6-C6	-5.10	118.12	122.85
53	a	1939	5MU	N3-C2-N1	5.04	121.45	114.89
53	a	747	5MU	C4-N3-C2	-4.98	120.81	127.34
53	a	2552	OMU	C4-N3-C2	-4.95	120.46	126.61
53	a	2030	6MZ	C5-C4-N3	-4.86	120.02	126.72
53	a	2251	OMG	N9-C4-N3	4.84	135.62	125.95
53	a	1939	5MU	C5-C4-N3	4.81	119.51	115.32
53	a	747	5MU	N3-C2-N1	4.81	121.15	114.89
53	a	2069	G7M	C2-N3-C4	4.77	120.52	112.30
52	A	1207	2MG	N9-C4-N3	4.64	135.23	125.95
53	a	1835	2MG	N9-C4-N3	4.64	135.22	125.95
55	Y	76	8AN	N3-C4-N9	4.58	134.95	127.17
53	a	745	1MG	C2-N3-C4	4.56	122.24	111.98
52	A	1519	MA6	C4-C5-N7	-4.56	105.36	110.58
53	a	1917	PSU	C4-N3-C2	-4.54	120.12	126.37
52	A	527	G7M	C2-N3-C4	4.53	120.10	112.30
53	a	1618	6MZ	N3-C4-N9	4.44	134.72	127.17
53	a	2445	2MG	N9-C4-N3	4.44	134.82	125.95
52	A	1518	MA6	C2-N1-C6	4.43	122.65	111.83
52	A	966	2MG	N9-C4-N3	4.40	134.75	125.95
52	A	1519	MA6	C2-N1-C6	4.39	122.54	111.83
53	a	2552	OMU	N3-C2-N1	4.34	120.54	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	a	2030	6MZ	C6-C5-N7	4.32	137.14	132.43
53	a	2457	PSU	C4-N3-C2	-4.26	120.50	126.37
53	a	1911	PSU	C4-N3-C2	-4.26	120.51	126.37
53	a	955	PSU	C4-N3-C2	-4.21	120.57	126.37
52	A	1518	MA6	N3-C4-N9	4.19	134.30	127.17
53	a	747	5MU	C5-C4-N3	4.18	118.96	115.32
53	a	746	PSU	C4-N3-C2	-4.15	120.66	126.37
52	A	516	PSU	C4-N3-C2	-4.12	120.69	126.37
53	a	2604	PSU	C4-N3-C2	-4.11	120.70	126.37
53	a	2030	6MZ	N3-C4-N9	4.04	134.03	127.17
52	A	1518	MA6	C4-C5-N7	-4.00	106.01	110.58
53	a	2504	PSU	C4-N3-C2	-3.99	120.88	126.37
53	a	2605	PSU	C4-N3-C2	-3.98	120.89	126.37
53	a	1939	5MU	O4-C4-C5	-3.96	120.39	124.92
53	a	955	PSU	O2-C2-N1	-3.96	118.71	122.79
53	a	1911	PSU	O2-C2-N1	-3.94	118.73	122.79
53	a	2580	PSU	C4-N3-C2	-3.94	120.95	126.37
53	a	745	1MG	N9-C4-N3	3.93	133.82	125.95
52	A	1516	2MG	N9-C4-N3	3.93	133.81	125.95
55	Y	76	8AN	C4-C5-N7	-3.93	106.09	110.58
53	a	2552	OMU	C5-C4-N3	3.91	120.28	114.80
53	a	1962	5MC	C5-C6-N1	-3.87	119.11	123.31
53	a	747	5MU	O4-C4-C5	-3.85	120.51	124.92
53	a	1939	5MU	C5-C6-N1	-3.84	119.15	123.31
53	a	2030	6MZ	C4-N9-C8	3.82	109.75	105.74
55	Y	76	8AN	C2-N3-C4	3.80	121.11	111.83
52	A	516	PSU	O2-C2-N1	-3.77	118.90	122.79
53	a	1917	PSU	O2-C2-N1	-3.74	118.93	122.79
53	a	1618	6MZ	C6-C5-N7	3.72	136.49	132.43
53	a	1618	6MZ	C2-N3-C4	3.69	120.83	111.83
52	A	1518	MA6	C2-N3-C4	3.67	120.80	111.83
52	A	1516	2MG	C6-C5-N7	3.64	136.91	130.29
53	a	2504	PSU	O2-C2-N1	-3.59	119.08	122.79
52	A	1519	MA6	C2-N3-C4	3.56	120.54	111.83
52	A	1519	MA6	N3-C4-N9	3.51	133.14	127.17
52	A	1518	MA6	N1-C2-N3	-3.50	123.28	128.58
53	a	2503	2MA	N6-C6-N1	3.50	121.75	117.03
53	a	1618	6MZ	C4-C5-N7	-3.49	106.59	110.58
53	a	2457	PSU	O2-C2-N1	-3.49	119.19	122.79
53	a	2030	6MZ	C2-N3-C4	3.45	120.25	111.83
53	a	2030	6MZ	C4-C5-N7	-3.45	106.64	110.58
53	a	1915	3TD	C4-N3-C2	-3.45	120.97	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	a	1618	6MZ	N1-C2-N3	-3.44	123.38	128.58
53	a	2030	6MZ	N1-C2-N3	-3.40	123.43	128.58
53	a	2445	2MG	C6-C5-N7	3.36	136.40	130.29
53	a	2503	2MA	C4-C5-N7	-3.32	106.78	110.58
52	A	966	2MG	C6-C5-N7	3.32	136.33	130.29
53	a	1939	5MU	O2-C2-N1	-3.31	118.49	122.80
52	A	1519	MA6	N1-C2-N3	-3.27	123.63	128.58
53	a	747	5MU	C5-C6-N1	-3.23	119.80	123.31
53	a	1835	2MG	C6-C5-N7	3.19	136.10	130.29
52	A	1498	UR3	C5-C4-N3	3.19	119.24	115.04
52	A	1407	5MC	C5-C6-N1	-3.13	119.92	123.31
53	a	746	PSU	O2-C2-N1	-3.11	119.58	122.79
52	A	1207	2MG	C6-C5-N7	3.11	135.96	130.29
52	A	1519	MA6	C5-N7-C8	3.08	108.29	103.45
53	a	2580	PSU	O2-C2-N1	-3.02	119.67	122.79
53	a	2552	OMU	O4-C4-C5	-3.01	119.98	125.16
52	A	1519	MA6	C6-C5-N7	2.98	138.19	133.43
53	a	2251	OMG	C6-C5-N7	2.97	135.70	130.29
53	a	2030	6MZ	N9-C8-N7	-2.96	109.73	113.94
52	A	1518	MA6	C5-N7-C8	2.93	108.06	103.45
53	a	745	1MG	C6-C5-N7	2.92	135.85	129.36
55	Y	76	8AN	N1-C2-N3	-2.91	124.18	128.58
53	a	2030	6MZ	C5-N7-C8	2.85	107.93	103.45
52	A	967	5MC	C5-C4-N3	-2.84	118.84	121.75
52	A	1407	5MC	C5-C4-N3	-2.83	118.85	121.75
52	A	967	5MC	C5-C6-N1	-2.83	120.24	123.31
52	A	1518	MA6	C4-N9-C8	2.82	108.70	105.74
52	A	1519	MA6	C4-N9-C8	2.81	108.69	105.74
53	a	2503	2MA	C2-N1-C6	2.80	122.40	118.10
53	a	2503	2MA	C4-N9-C8	2.79	108.67	105.74
55	Y	76	8AN	C5-N7-C8	2.77	107.81	103.45
53	a	1618	6MZ	C4-N9-C8	2.72	108.59	105.74
53	a	745	1MG	C4-C5-N7	-2.68	106.42	110.67
52	A	1516	2MG	N1-C2-N2	2.68	119.30	116.56
52	A	1516	2MG	C4-C5-N7	-2.68	106.43	110.67
53	a	2251	OMG	C4-C5-N7	-2.68	106.43	110.67
53	a	1618	6MZ	C9-N6-C6	-2.68	120.37	122.85
53	a	2069	G7M	O6-C6-C5	-2.66	122.08	128.01
53	a	1962	5MC	C5-C4-N3	-2.63	119.06	121.75
53	a	2604	PSU	O2-C2-N1	-2.61	120.09	122.79
52	A	1207	2MG	C4-C5-N7	-2.58	106.58	110.67
53	a	2445	2MG	C4-C5-N7	-2.58	106.59	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A	1207	2MG	N1-C2-N2	2.57	119.18	116.56
52	A	966	2MG	C4-C5-N7	-2.55	106.64	110.67
52	A	1407	5MC	O2-C2-N3	-2.54	118.33	122.33
53	a	2605	PSU	O2-C2-N1	-2.54	120.17	122.79
53	a	1835	2MG	C4-C5-N7	-2.51	106.70	110.67
53	a	747	5MU	C5M-C5-C4	2.48	121.43	118.78
52	A	527	G7M	O6-C6-C5	-2.48	122.48	128.01
53	a	2580	PSU	O4'-C1'-C2'	2.47	108.57	105.15
53	a	2503	2MA	C5-N7-C8	2.47	107.33	103.45
15	L	89	D2T	OD1-CG-CB	-2.44	117.32	122.44
52	A	1519	MA6	N9-C8-N7	-2.44	110.47	113.94
52	A	516	PSU	O4'-C1'-C2'	2.44	108.52	105.15
53	a	2552	OMU	O2-C2-N1	-2.42	119.64	122.80
53	a	747	5MU	O2-C2-N1	-2.41	119.66	122.80
53	a	1618	6MZ	C5-N7-C8	2.40	107.22	103.45
52	A	1402	4OC	C6-C5-C4	2.39	119.88	117.00
52	A	1518	MA6	C6-C5-N7	2.32	137.14	133.43
53	a	1915	3TD	O2-C2-N3	-2.32	118.55	121.82
53	a	2605	PSU	O2-C2-N3	-2.29	117.79	121.86
52	A	1498	UR3	C1'-N1-C2	2.29	120.79	117.04
53	a	1917	PSU	C5-C6-N1	-2.29	118.96	122.14
53	a	1915	3TD	C1'-C5-C4	2.27	121.06	117.61
52	A	966	2MG	N1-C2-N2	2.25	118.85	116.56
52	A	1518	MA6	N9-C8-N7	-2.24	110.75	113.94
52	A	527	G7M	C5-C6-N1	2.20	116.40	111.84
53	a	2449	H2U	N3-C2-N1	2.20	118.86	116.65
53	a	2069	G7M	C5-C6-N1	2.19	116.37	111.84
52	A	1207	2MG	CM2-N2-C2	-2.19	118.94	123.65
53	a	2251	OMG	O6-C6-C5	-2.18	120.77	126.53
53	a	1917	PSU	O4'-C1'-C2'	2.18	108.17	105.15
53	a	746	PSU	C5-C6-N1	-2.18	119.12	122.14
53	a	2503	2MA	C6-C5-N7	2.17	136.28	132.09
53	a	2030	6MZ	C2-N1-C6	2.15	122.38	115.24
52	A	1207	2MG	N2-C2-N3	-2.14	117.79	120.51
52	A	1498	UR3	C3U-N3-C2	2.13	121.04	117.33
53	a	2604	PSU	O2-C2-N3	-2.12	118.10	121.86
55	Y	76	8AN	C6-C5-N7	2.11	136.15	132.09
52	A	1516	2MG	O6-C6-C5	-2.11	120.97	126.53
52	A	1207	2MG	O6-C6-C5	-2.10	120.99	126.53
53	a	2498	OMC	O2-C2-N3	-2.10	119.02	122.33
53	a	1618	6MZ	C2-N1-C6	2.09	122.17	115.24
53	a	2604	PSU	C5-C6-N1	-2.08	119.25	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A	1516	2MG	N2-C2-N3	-2.07	117.87	120.51
53	a	2449	H2U	O2-C2-N1	-2.07	120.62	123.10
14	K	119	IAS	OD1-CG-CB	-2.06	119.37	125.38
53	a	747	5MU	C5M-C5-C6	-2.06	120.06	122.85
53	a	1835	2MG	O6-C6-C5	-2.05	121.11	126.53
53	a	2445	2MG	O6-C6-C5	-2.04	121.14	126.53
53	a	747	5MU	C1'-N1-C2	2.02	121.23	117.59
53	a	2605	PSU	C5-C6-N1	-2.02	119.33	122.14
53	a	955	PSU	C5-C6-N1	-2.02	119.34	122.14
52	A	966	2MG	O6-C6-C5	-2.00	121.24	126.53
53	a	2445	2MG	N1-C2-N2	2.00	118.61	116.56

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	L	89	D2T	CA-CB-CG-OD1
15	L	89	D2T	CA-CB-CG-OD2
26	Z	76	8AN	O4'-C4'-C5'-O5'
52	A	1207	2MG	N3-C2-N2-CM2
26	Z	76	8AN	C3'-C4'-C5'-O5'
52	A	1519	MA6	O4'-C4'-C5'-O5'
29	d	150	MEQ	NE2-CD-CG-CB
26	Z	76	8AN	C4'-C5'-O5'-P
29	d	150	MEQ	OE1-CD-CG-CB
53	a	2030	6MZ	O4'-C4'-C5'-O5'
53	a	2030	6MZ	C3'-C4'-C5'-O5'
52	A	1519	MA6	C3'-C4'-C5'-O5'
14	K	119	IAS	CA-CB-CG-OD1
53	a	2503	2MA	C4'-C5'-O5'-P
52	A	527	G7M	C4'-C5'-O5'-P
55	Y	76	8AN	O4'-C4'-C5'-O5'
15	L	89	D2T	SB-CB-CG-OD2
53	a	746	PSU	O4'-C1'-C5-C6
53	a	2445	2MG	C3'-C4'-C5'-O5'
15	L	89	D2T	CG-CB-SB-CB1
53	a	746	PSU	C2'-C1'-C5-C6
14	K	119	IAS	N-CA-CB-CG
53	a	2498	OMC	C4'-C5'-O5'-P
53	a	1962	5MC	O4'-C1'-N1-C6

There are no ring outliers.

16 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A	1519	MA6	1	0
53	a	1915	3TD	1	0
53	a	1939	5MU	1	0
52	A	1516	2MG	1	0
53	a	1917	PSU	2	0
53	a	2030	6MZ	2	0
52	A	1402	4OC	2	0
52	A	516	PSU	1	0
53	a	745	1MG	1	0
29	d	150	MEQ	1	0
52	A	967	5MC	1	0
52	A	1518	MA6	1	0
52	A	1498	UR3	1	0
14	K	119	IAS	1	0
26	Z	76	8AN	5	0
52	A	1207	2MG	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 350 ligands modelled in this entry, 332 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
61	SPD	a	3216	-	9,9,9	0.34	0	8,8,8	0.72	0
61	SPD	a	3210	-	9,9,9	0.34	0	8,8,8	0.64	0
61	SPD	a	3219	-	9,9,9	0.35	0	8,8,8	0.66	0
63	A1B71	Y	101	55	16,16,17	0.90	0	16,20,22	2.14	3 (18%)
61	SPD	a	3208	-	9,9,9	0.34	0	8,8,8	0.63	0
61	SPD	a	3212	-	9,9,9	0.35	0	8,8,8	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
61	SPD	a	3209	-	9,9,9	0.33	0	8,8,8	0.77	0
61	SPD	a	3211	-	9,9,9	0.34	0	8,8,8	0.90	0
61	SPD	a	3213	-	9,9,9	0.33	0	8,8,8	0.69	0
61	SPD	a	3214	-	9,9,9	0.33	0	8,8,8	0.78	0
61	SPD	a	3217	-	9,9,9	0.34	0	8,8,8	0.55	0
61	SPD	a	3218	-	9,9,9	0.34	0	8,8,8	0.73	0
58	FME	Z	101	26	8,9,10	0.99	0	8,9,11	1.10	1 (12%)
61	SPD	a	3221	-	9,9,9	0.34	0	8,8,8	0.85	0
62	SPM	a	3220	-	13,13,13	0.35	0	12,12,12	0.74	0
61	SPD	a	3215	-	9,9,9	0.29	0	8,8,8	0.81	0
60	PAR	A	1601	-	44,45,45	0.53	0	63,67,67	0.93	3 (4%)
61	SPD	A	1691	-	9,9,9	0.33	0	8,8,8	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SPD	a	3216	-	-	4/7/7/7	-
61	SPD	a	3210	-	-	2/7/7/7	-
61	SPD	a	3219	-	-	3/7/7/7	-
63	A1B71	Y	101	55	-	1/17/17/19	-
61	SPD	a	3208	-	-	5/7/7/7	-
61	SPD	a	3212	-	-	1/7/7/7	-
61	SPD	a	3209	-	-	3/7/7/7	-
61	SPD	a	3211	-	-	4/7/7/7	-
61	SPD	a	3213	-	-	4/7/7/7	-
61	SPD	a	3214	-	-	3/7/7/7	-
61	SPD	a	3217	-	-	4/7/7/7	-
61	SPD	a	3218	-	-	2/7/7/7	-
58	FME	Z	101	26	-	3/7/9/11	-
61	SPD	a	3221	-	-	3/7/7/7	-
62	SPM	a	3220	-	-	4/11/11/11	-
61	SPD	a	3215	-	-	4/7/7/7	-
60	PAR	A	1601	-	-	3/18/94/94	0/4/4/4
61	SPD	A	1691	-	-	5/7/7/7	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	Y	101	A1B71	O10-C09-N08	5.71	118.11	110.00
63	Y	101	A1B71	O15-C09-N08	-3.98	118.94	124.93
63	Y	101	A1B71	O01-C02-C03	-3.51	117.21	125.24
60	A	1601	PAR	C22-C12-C62	-2.37	106.54	110.08
60	A	1601	PAR	C13-O52-C52	-2.25	112.64	117.98
58	Z	101	FME	C-CA-N	2.24	113.82	109.50
60	A	1601	PAR	C34-C44-C54	2.06	113.96	110.23

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	Z	101	FME	N-CA-CB-CG
58	Z	101	FME	C-CA-CB-CG
60	A	1601	PAR	C44-C54-C64-N64
60	A	1601	PAR	O54-C54-C64-N64
61	a	3212	SPD	C2-C3-C4-C5
61	A	1691	SPD	N6-C7-C8-C9
61	a	3210	SPD	C3-C4-C5-N6
61	a	3211	SPD	N6-C7-C8-C9
61	a	3219	SPD	N6-C7-C8-C9
61	a	3217	SPD	N6-C7-C8-C9
61	A	1691	SPD	C4-C5-N6-C7
61	a	3209	SPD	C8-C7-N6-C5
61	a	3214	SPD	C4-C5-N6-C7
61	a	3217	SPD	C4-C5-N6-C7
61	a	3217	SPD	C8-C7-N6-C5
61	a	3208	SPD	C2-C3-C4-C5
61	a	3211	SPD	C3-C4-C5-N6
61	a	3208	SPD	C4-C5-N6-C7
61	a	3211	SPD	C4-C5-N6-C7
61	a	3214	SPD	C8-C7-N6-C5
61	a	3216	SPD	C2-C3-C4-C5
61	A	1691	SPD	C3-C4-C5-N6
61	a	3208	SPD	C3-C4-C5-N6
61	a	3219	SPD	C2-C3-C4-C5
61	a	3208	SPD	C8-C7-N6-C5
61	a	3213	SPD	C8-C7-N6-C5
61	a	3209	SPD	C2-C3-C4-C5
61	a	3215	SPD	N6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
58	Z	101	FME	CB-CG-SD-CE
62	a	3220	SPM	N5-C6-C7-C8
61	a	3213	SPD	N1-C2-C3-C4
61	a	3215	SPD	C2-C3-C4-C5
61	a	3221	SPD	C2-C3-C4-C5
61	a	3208	SPD	C7-C8-C9-N10
61	a	3219	SPD	C7-C8-C9-N10
61	A	1691	SPD	C2-C3-C4-C5
60	A	1601	PAR	C52-C42-O11-C11
61	a	3221	SPD	C3-C4-C5-N6
61	a	3215	SPD	N1-C2-C3-C4
61	a	3209	SPD	C7-C8-C9-N10
61	a	3210	SPD	C7-C8-C9-N10
61	a	3211	SPD	C7-C8-C9-N10
61	a	3217	SPD	C7-C8-C9-N10
61	a	3218	SPD	C4-C5-N6-C7
61	a	3218	SPD	C7-C8-C9-N10
62	a	3220	SPM	N1-C2-C3-C4
61	A	1691	SPD	N1-C2-C3-C4
63	Y	101	A1B71	C02-C03-C04-C05
61	a	3213	SPD	C3-C4-C5-N6
61	a	3214	SPD	N1-C2-C3-C4
61	a	3216	SPD	C4-C5-N6-C7
61	a	3216	SPD	N6-C7-C8-C9
61	a	3216	SPD	C8-C7-N6-C5
61	a	3215	SPD	C3-C4-C5-N6
61	a	3221	SPD	C8-C7-N6-C5
62	a	3220	SPM	C11-C12-C13-N14
62	a	3220	SPM	C7-C8-C9-N10
61	a	3213	SPD	C2-C3-C4-C5

There are no ring outliers.

12 monomers are involved in 20 short contacts:

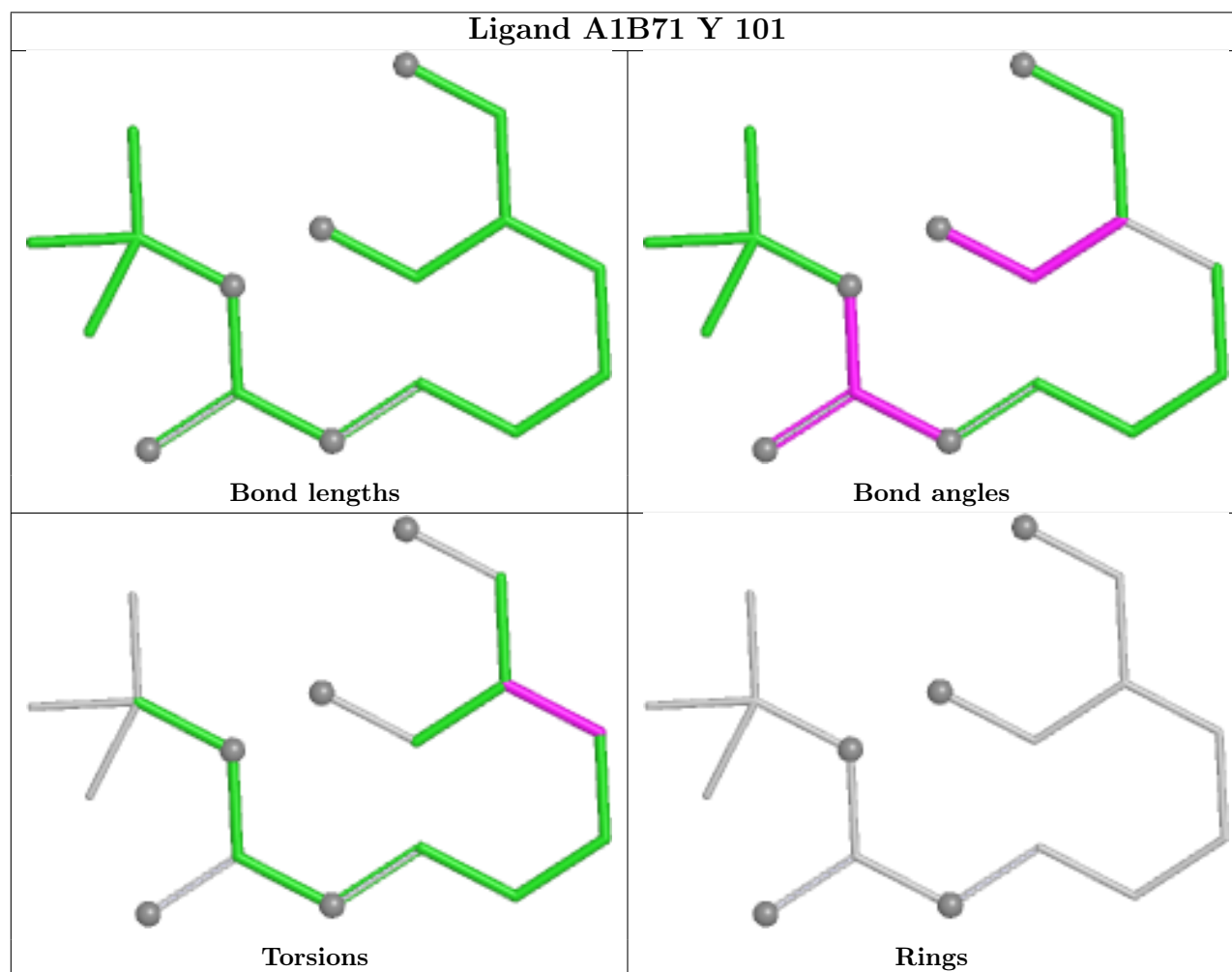
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	a	3216	SPD	2	0
61	a	3208	SPD	2	0
61	a	3212	SPD	1	0
61	a	3209	SPD	1	0
61	a	3213	SPD	1	0
61	a	3214	SPD	2	0
61	a	3217	SPD	3	0

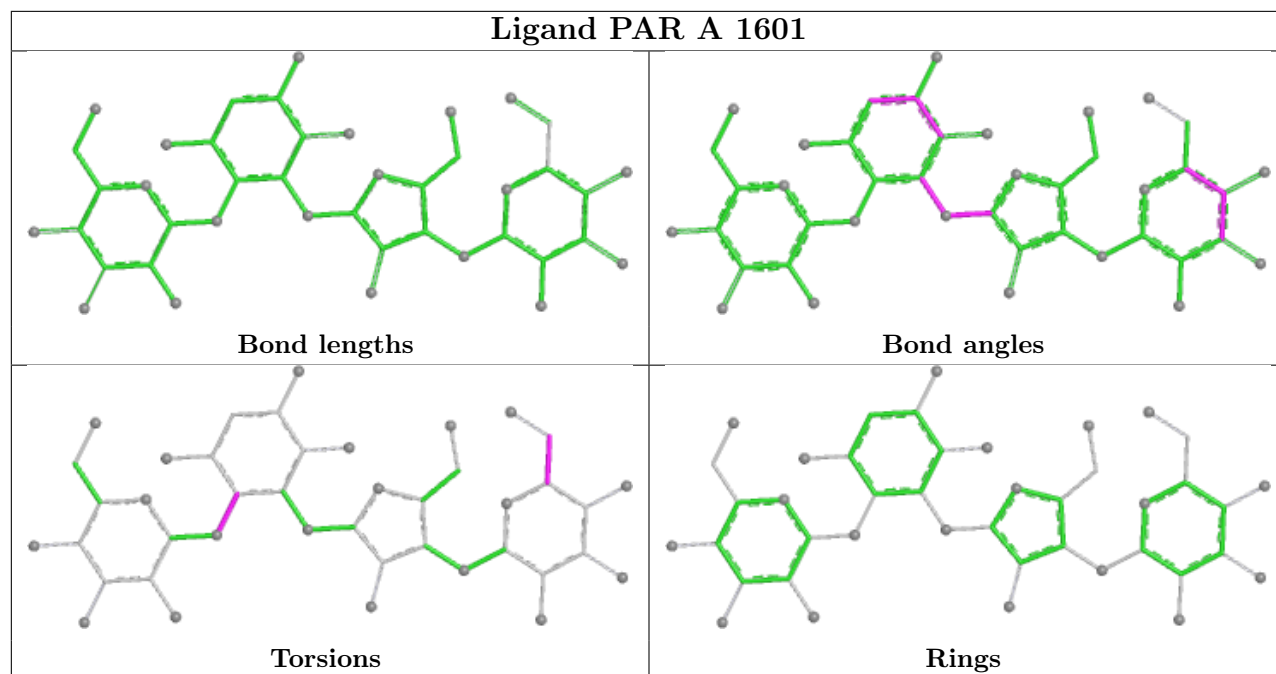
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	a	3218	SPD	2	0
61	a	3221	SPD	1	0
62	a	3220	SPM	3	0
61	a	3215	SPD	1	0
60	A	1601	PAR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	Y	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	15:C	O3'	17:G	P	5.81
1	Y	45:C	O3'	47:A	P	5.36
1	Y	13:C	O3'	15:C	P	5.22
1	Y	66:G	O3'	67:U	P	4.34
1	Y	7:C	O3'	10:G	P	3.06

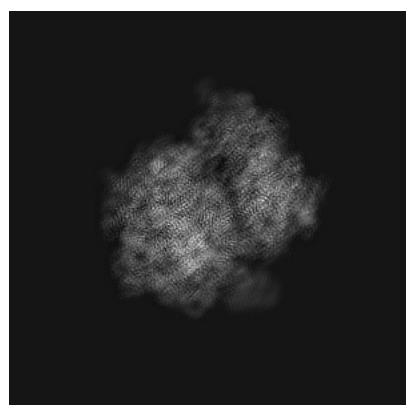
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70050. These allow visual inspection of the internal detail of the map and identification of artifacts.

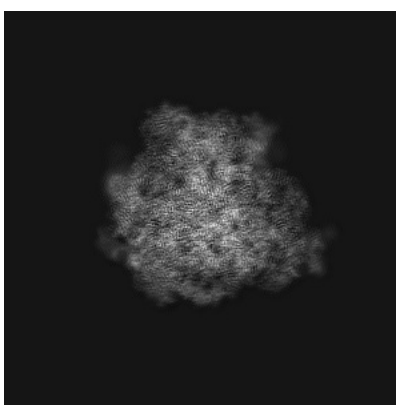
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

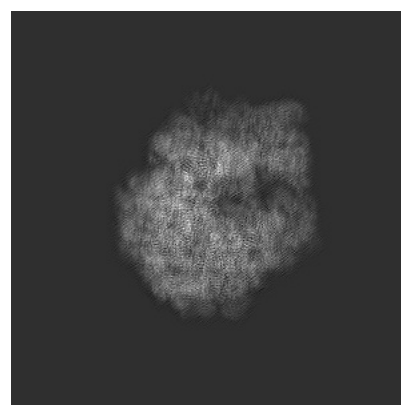
#### 6.1.1 Primary map



X



Y

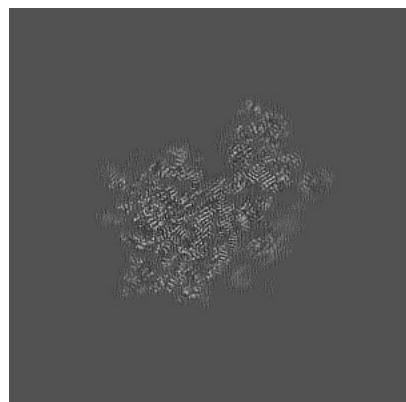


Z

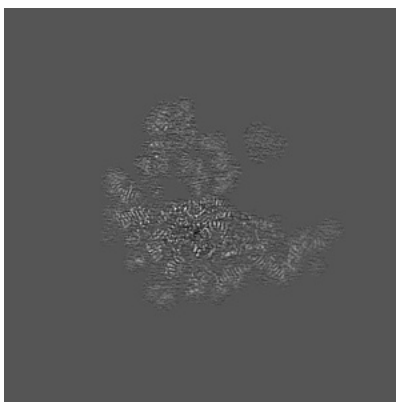
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

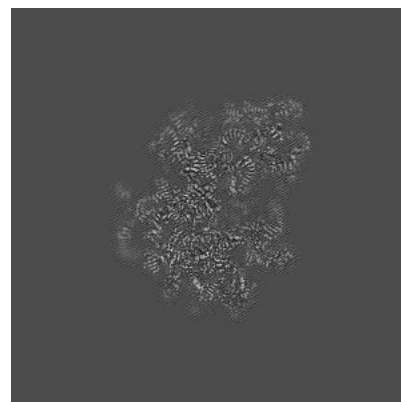
#### 6.2.1 Primary map



X Index: 256



Y Index: 256



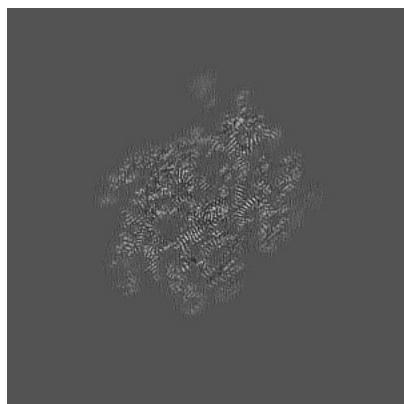
Z Index: 256



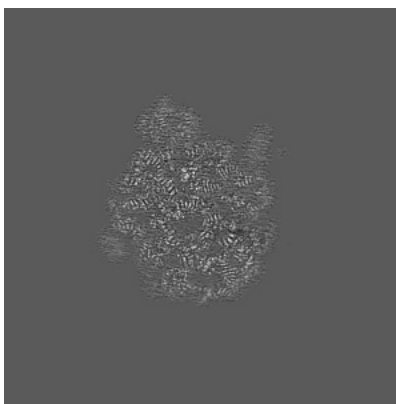
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

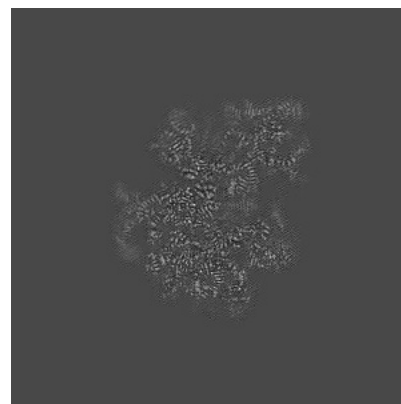
### 6.3.1 Primary map



X Index: 226



Y Index: 219

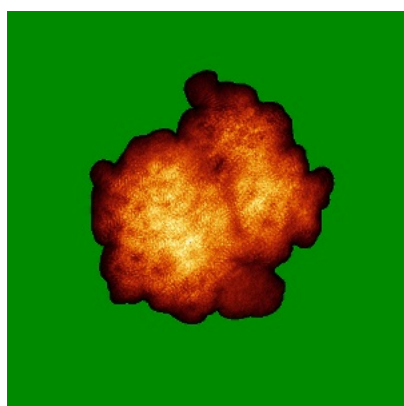


Z Index: 252

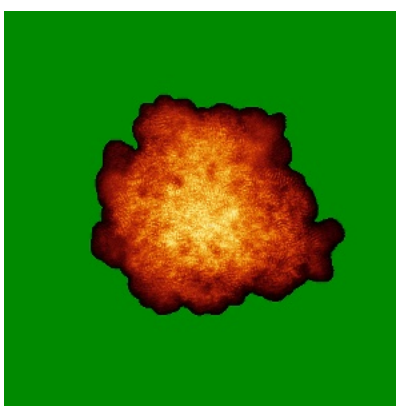
The images above show the largest variance slices of the map in three orthogonal directions.

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

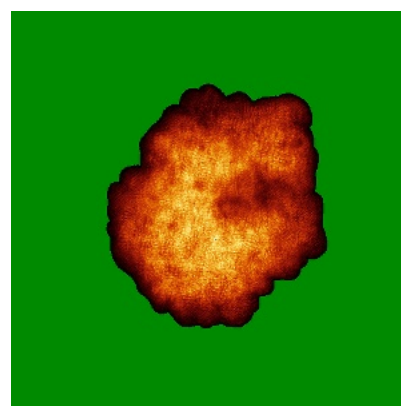
### 6.4.1 Primary map



X



Y

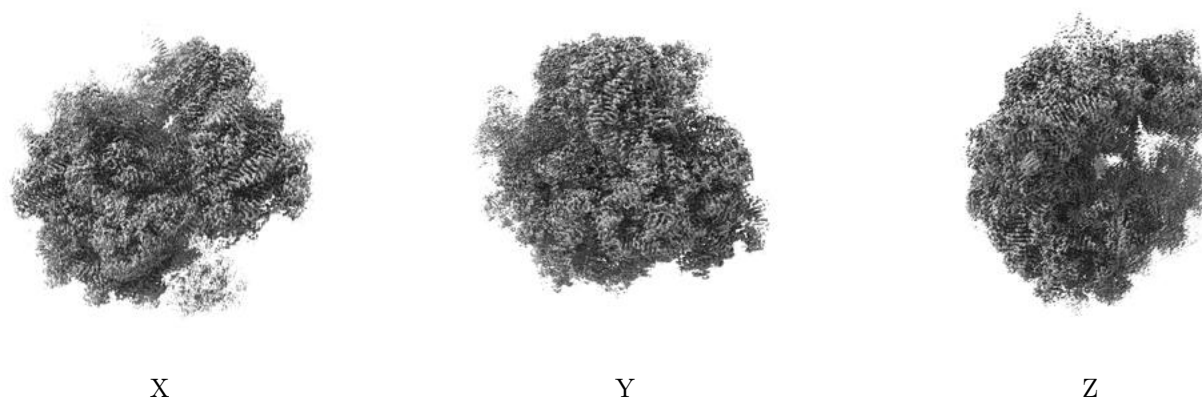


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0267. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

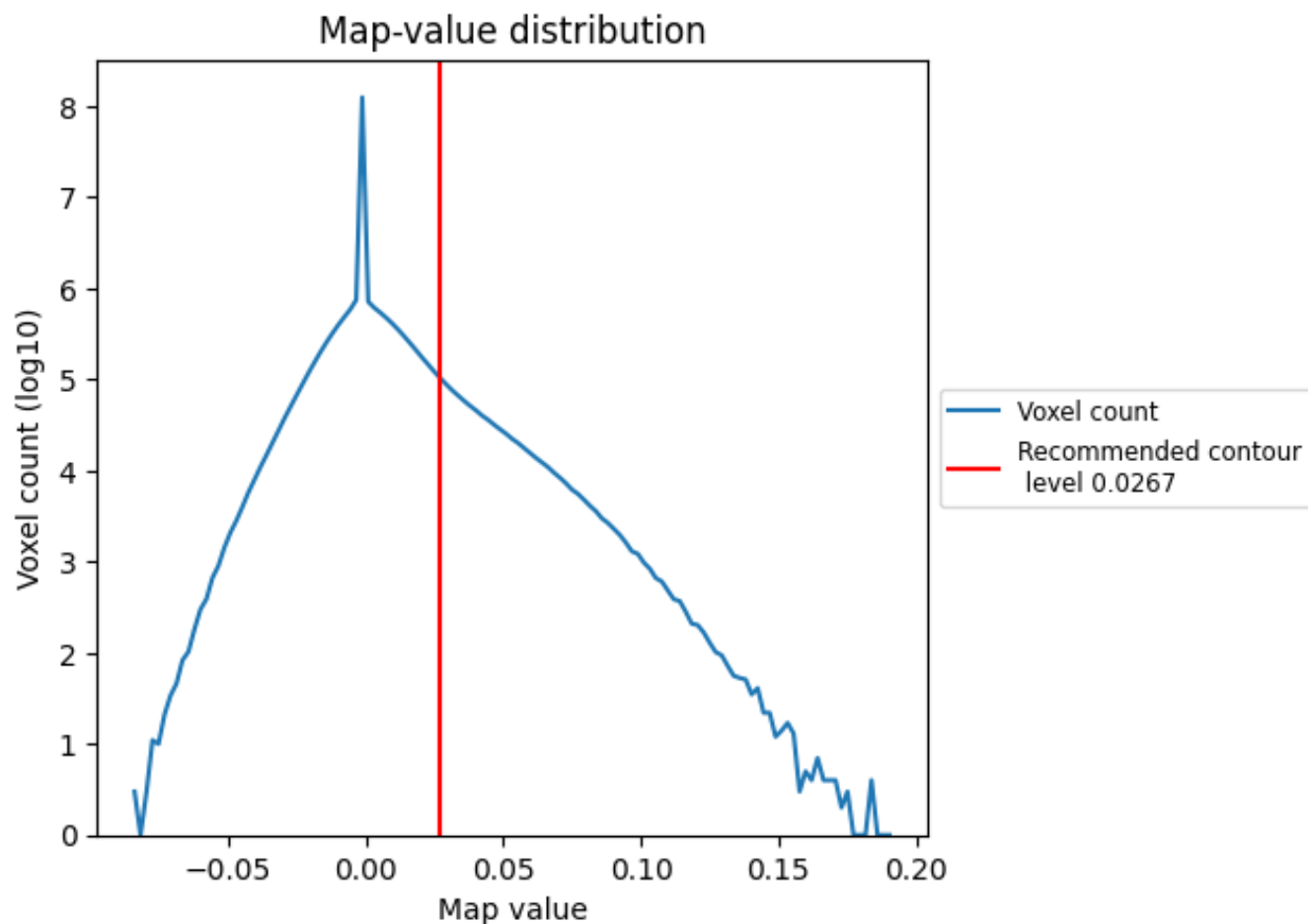
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

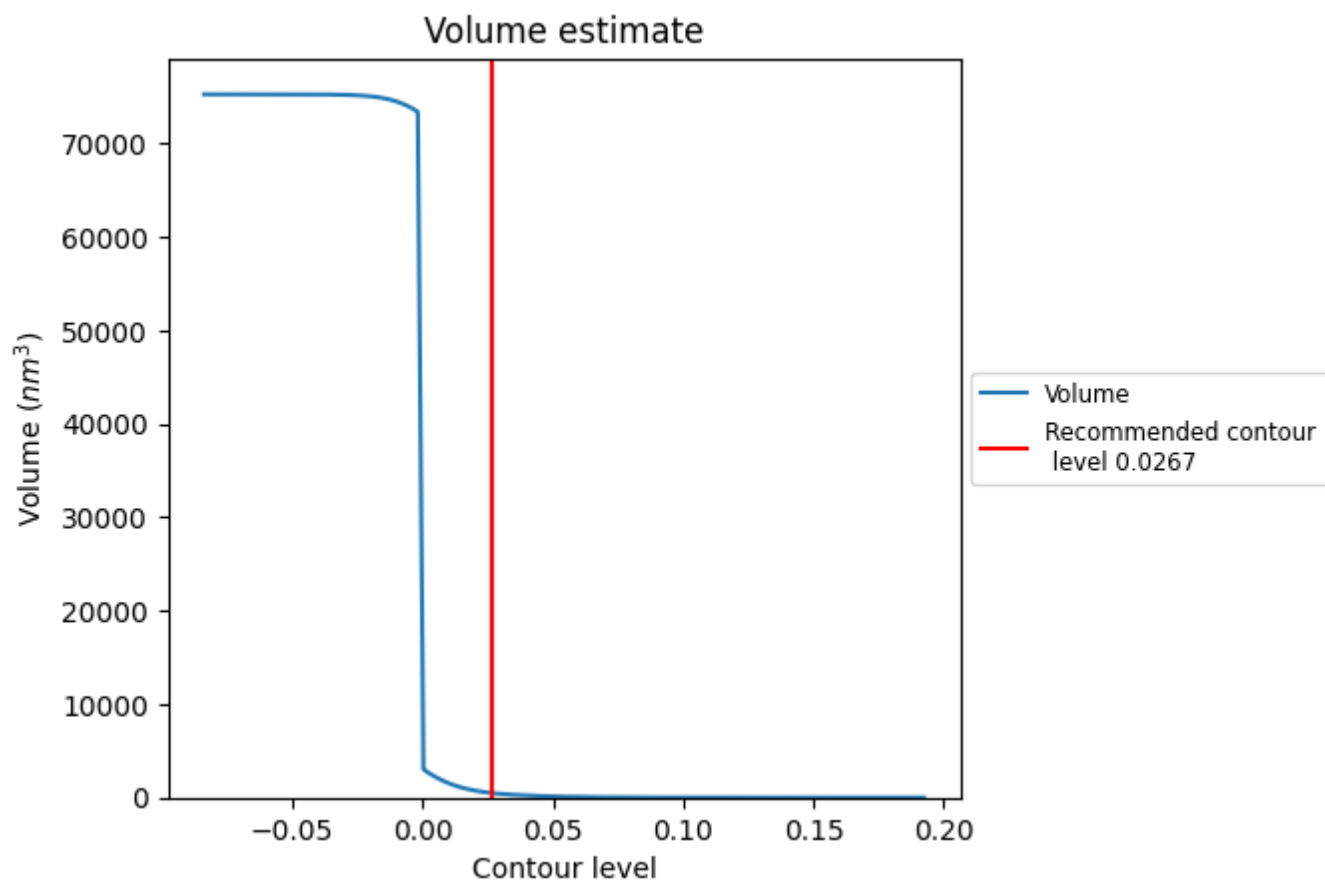
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

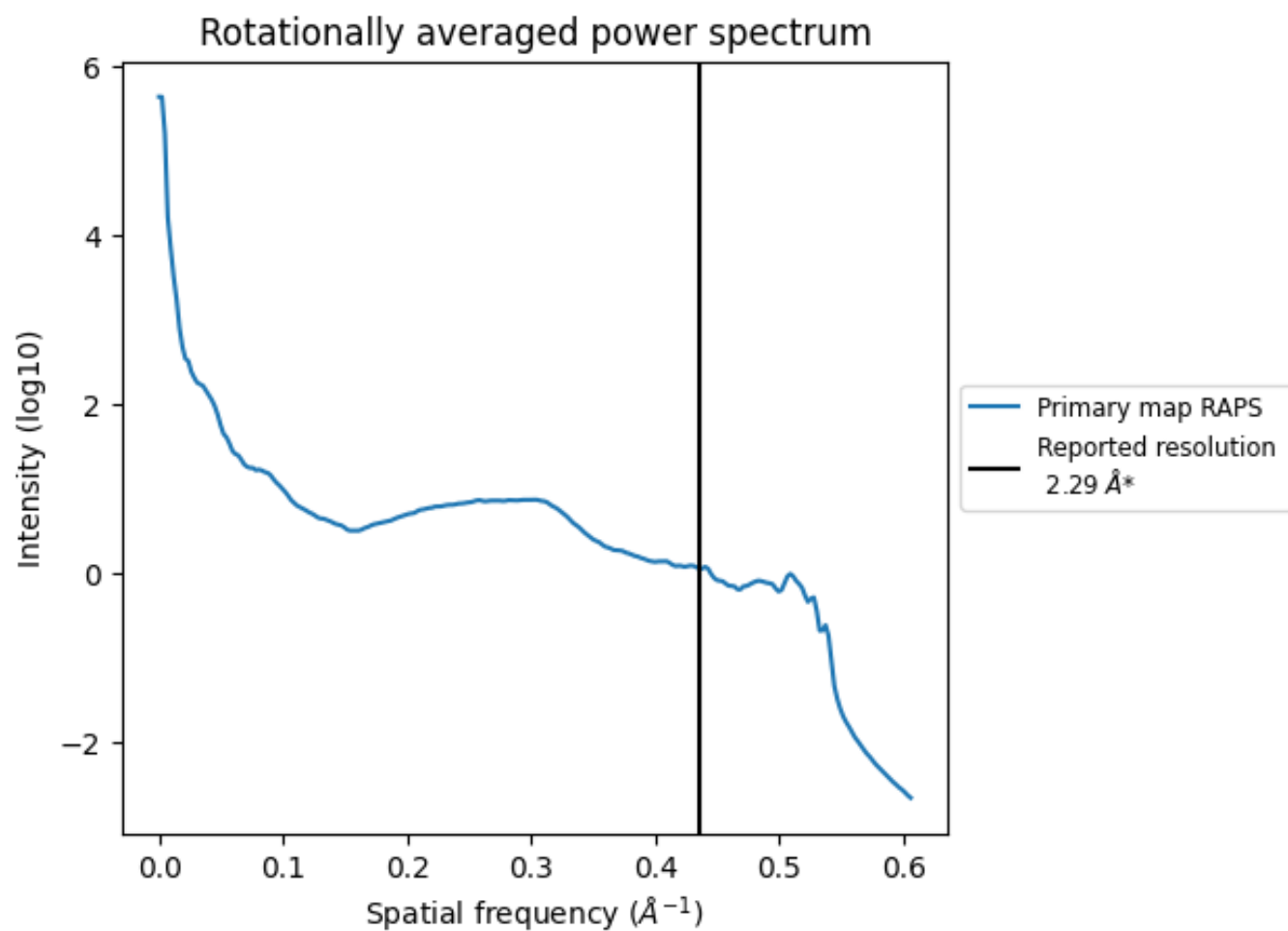
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 480 nm<sup>3</sup>; this corresponds to an approximate mass of 434 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 ⓘ

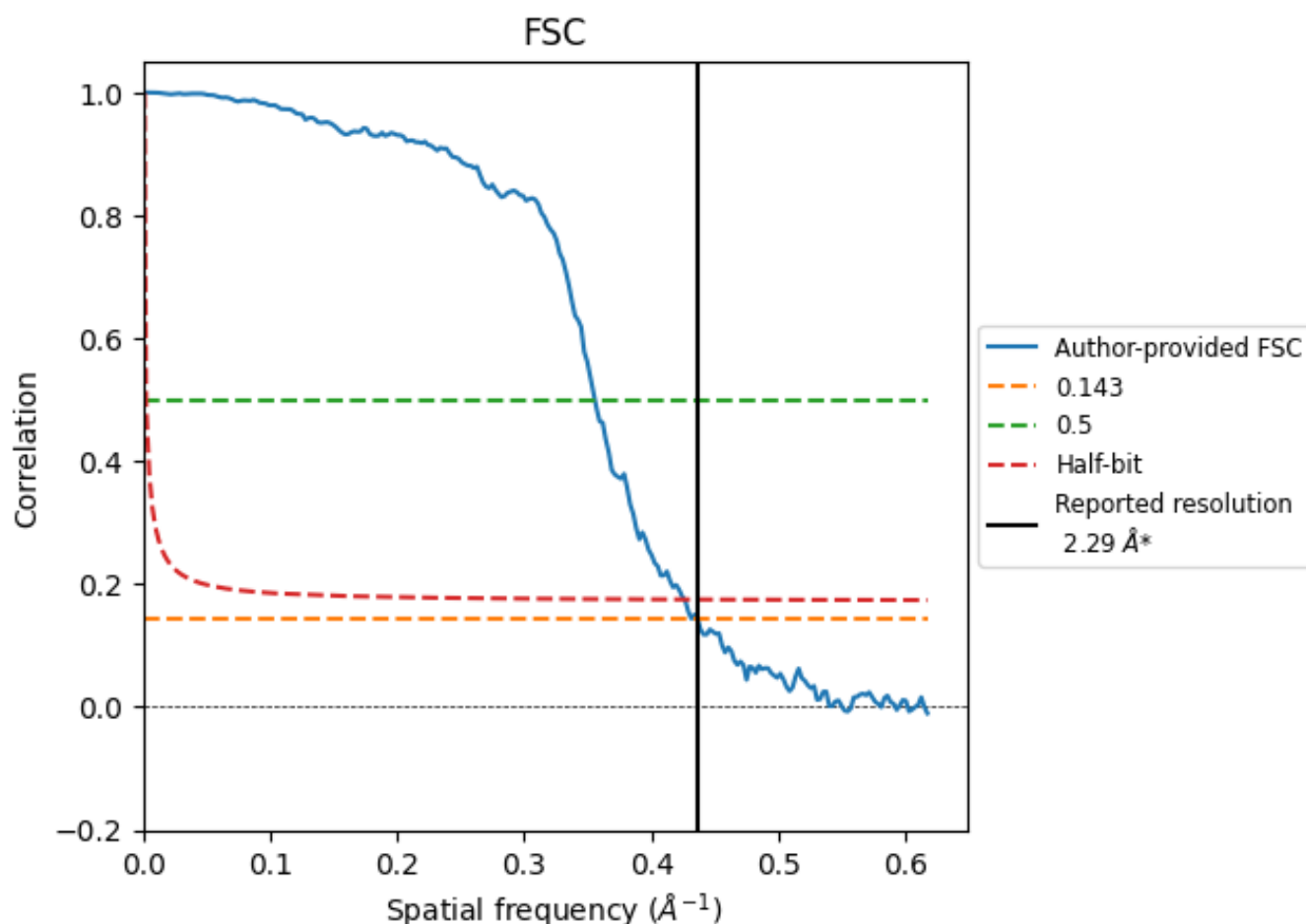


\*Reported resolution corresponds to spatial frequency of 0.437 Å<sup>-1</sup>

## 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 0.437 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

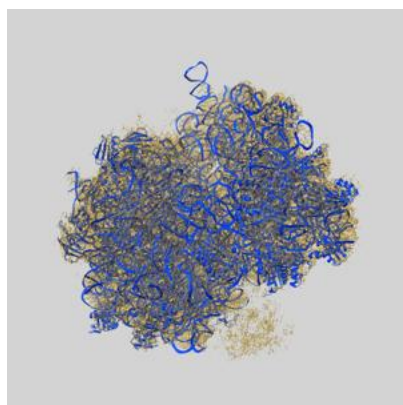
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	2.29	2.81	2.35
Unmasked-calculated*	-	-	-

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

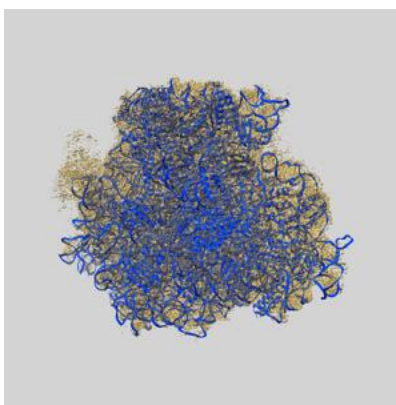
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70050 and PDB model 9O2X. Per-residue inclusion information can be found in section 3 on page 20.

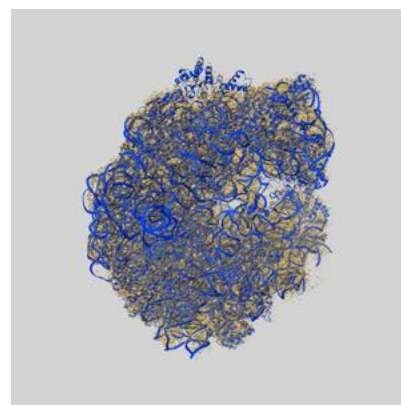
### 9.1 Map-model overlay [i](#)



X



Y

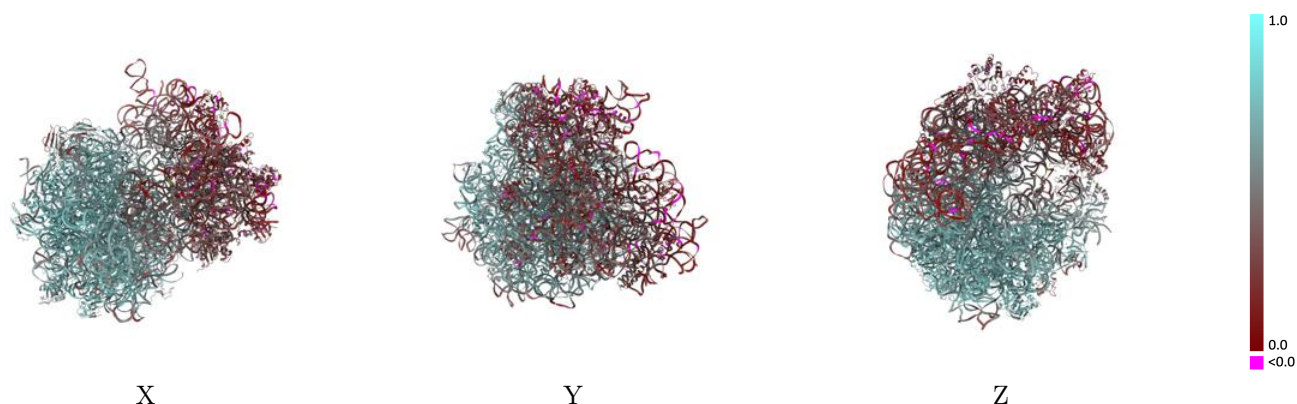


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0267 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.

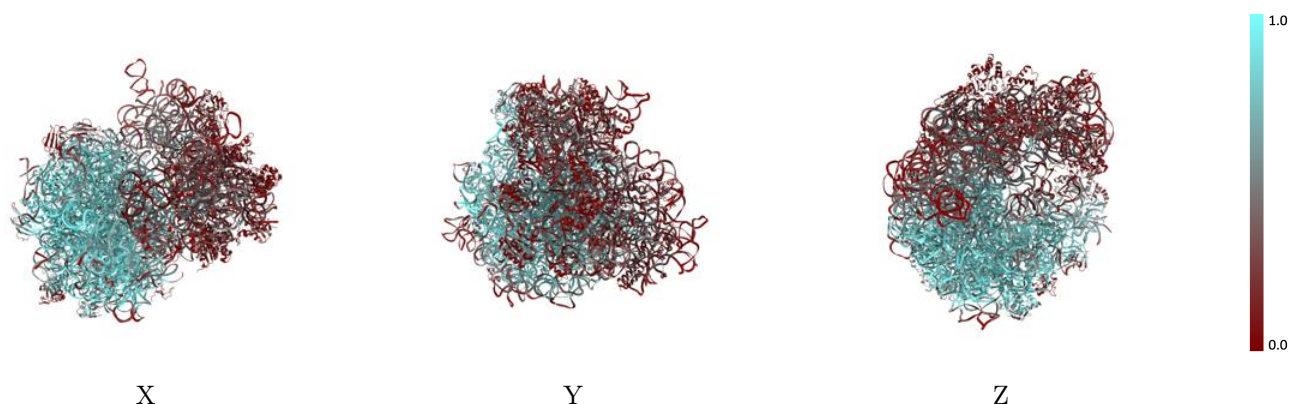


## 9.2 Q-score mapped to coordinate model [i](#)



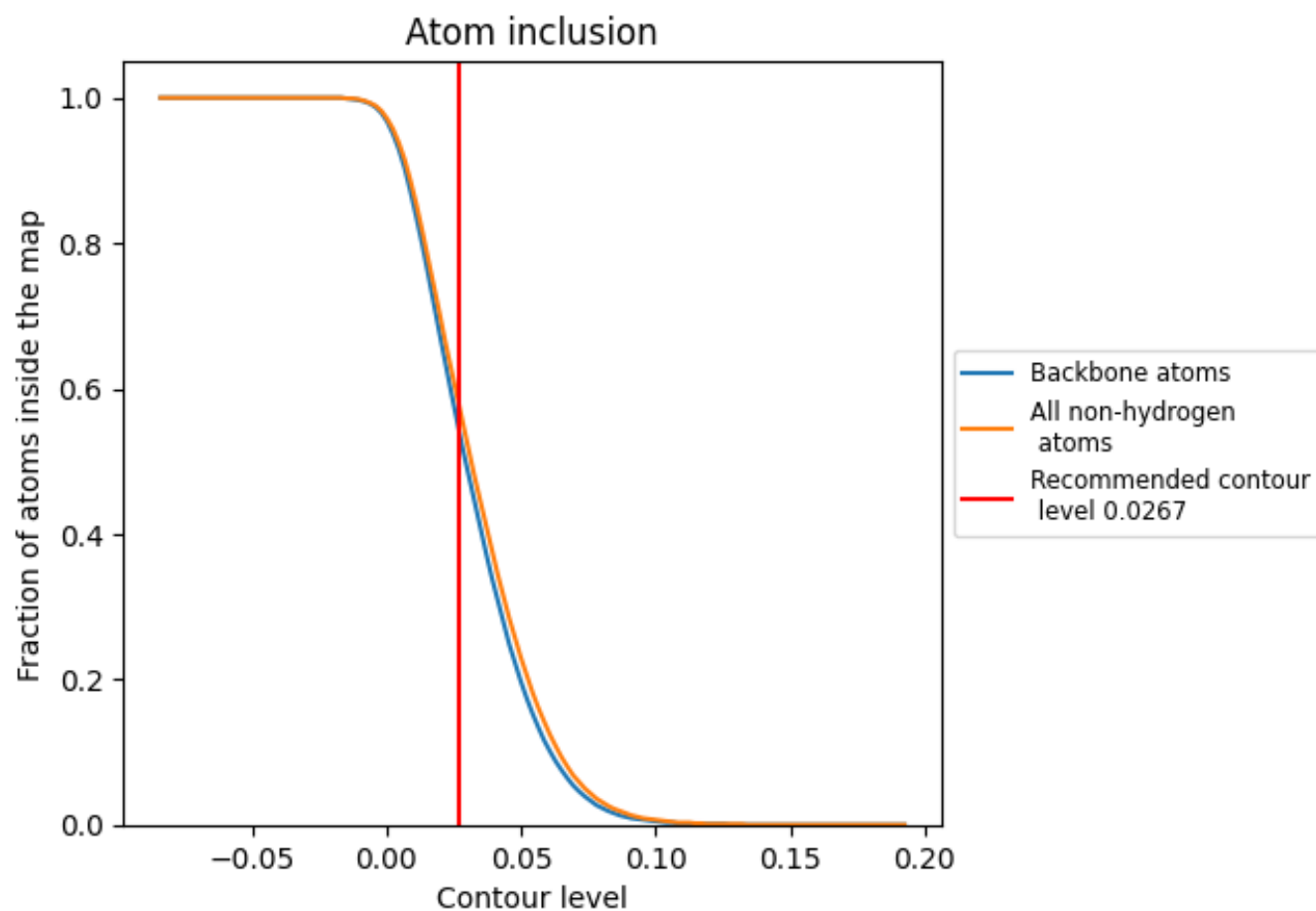
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0267).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 58% 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 (0.0267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5800	 0.5260
0	 0.6500	 0.6560
1	 0.8700	 0.7330
2	 0.8840	 0.7360
3	 0.7440	 0.6770
4	 0.0980	 0.3010
A	 0.3590	 0.3330
B	 0.0670	 0.2580
C	 0.2120	 0.2870
D	 0.1570	 0.2580
E	 0.2570	 0.3380
F	 0.1300	 0.3690
G	 0.1550	 0.3020
H	 0.2460	 0.3240
I	 0.2040	 0.2660
J	 0.1510	 0.1960
K	 0.2170	 0.3620
L	 0.2870	 0.4270
M	 0.1770	 0.3160
N	 0.2050	 0.2140
O	 0.2170	 0.3790
P	 0.2500	 0.2640
Q	 0.2010	 0.3360
R	 0.2030	 0.3350
S	 0.1400	 0.2350
T	 0.2370	 0.3800
U	 0.0450	 0.2690
X	 0.2670	 0.3190
Y	 0.3110	 0.3820
Z	 0.3840	 0.4460
a	 0.8040	 0.6590
b	 0.7260	 0.6020
c	 0.7330	 0.6710
d	 0.7710	 0.7010
e	 0.5800	 0.6610



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Chain	Atom inclusion	Q-score
f	 0.3090	 0.4540
g	 0.3030	 0.4810
h	 0.2100	 0.5190
i	 0.8140	 0.7100
j	 0.6660	 0.6520
k	 0.7290	 0.6890
l	 0.8120	 0.7050
m	 0.8510	 0.7210
n	 0.6790	 0.6250
o	 0.6330	 0.6520
p	 0.8790	 0.7390
q	 0.7060	 0.6810
r	 0.7490	 0.6940
s	 0.5720	 0.6480
t	 0.4620	 0.6110
u	 0.6560	 0.6320
v	 0.8570	 0.7240
w	 0.7140	 0.6800
x	 0.4170	 0.5750
y	 0.7800	 0.6910
z	 0.7110	 0.7030