



## Full wwPDB EM Validation Report ⓘ

Aug 7, 2025 – 10:53 AM JST

PDB ID : 8ZTV / pdb\_00008ztv  
EMDB ID : EMD-60474  
Title : 70S ribosome arrested by PepNL with RF2  
Authors : Ando, Y.; Kobo, A.; Nureki, O.; Taguchi, H.; Itoh, Y.; Chadani, Y.  
Deposited on : 2024-06-07  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev126  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

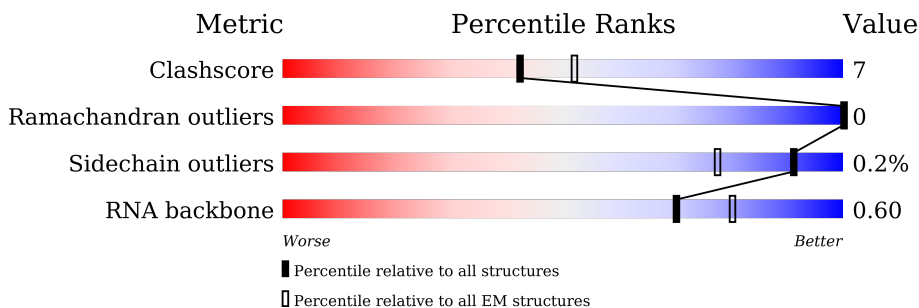
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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.














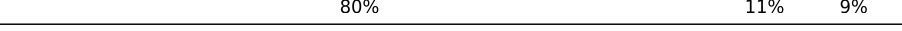



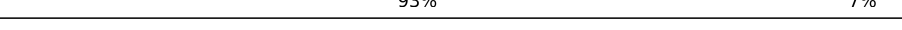



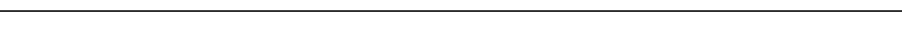

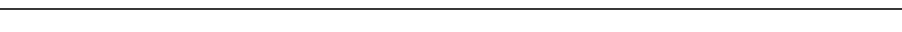
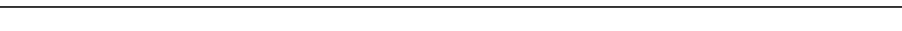


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	1542	
2	B	241	
3	C	233	
4	D	206	
5	E	167	
6	F	135	
7	G	179	


























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Mol	Chain	Length	Quality of chain
8	H	130	 92% 8%
9	I	130	 76% 22%
10	J	103	 76% 20%
11	K	129	 79% 12% 9%
12	L	124	 85% 14%
13	M	118	 82% 15%
14	N	101	 85% 14%
15	O	89	 88% 11%
16	P	82	 90% 9%
17	Q	84	 79% 17% 5%
18	R	75	 76% 12% 12%
19	S	92	 80% 11% 9%
20	T	87	 87% 11%
21	U	71	 83% 15%
22	V	365	 43% 80% 18%
23	W	14	 93% 7%
24	X	9	 89% 11%
25	Y	77	 51% 35% 6% 8%
26	Z	3	 67% 33%
27	a	2904	 57% 35% 5%
28	b	120	 62% 35%
29	c	273	 86% 13%
30	d	209	 88% 12%
31	e	201	 93% 7%
32	f	179	 78% 21%

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Mol	Chain	Length	Quality of chain
33	g	177	
34	h	149	
35	i	142	
36	j	123	
37	k	144	
38	l	136	
39	m	127	
40	n	117	
41	o	115	
42	p	118	
43	q	103	
44	r	110	
45	s	100	
46	t	104	
47	u	94	
48	v	85	
49	w	78	
50	x	63	
51	y	59	
52	z	57	
53	0	55	
54	1	46	
55	2	65	
56	3	38	
57	4	70	

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 143031 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0
			32360	14439	5944	10470	1507		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	225	Total	C	N	O	S	0	0
			1758	1112	316	322	8		

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

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

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

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

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

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

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

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

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

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

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

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

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

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

- Molecule 22 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	357	Total	C	N	O	S	0	0
			2834	1743	498	583	10		

- Molecule 23 is a protein called PepNL.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	14	Total	C	N	O	S	0	0
			108	70	17	20	1		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	9	Total	C	N	O	P	0	0
			194	87	37	61	9		

- Molecule 25 is a RNA chain called RNA (73-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	71	Total	C	N	O	P	0	0
			1517	675	271	500	71		

- Molecule 26 is a RNA chain called RNA (5'-R(P\*CP\*A)-3').

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

- Molecule 27 is a RNA chain called 23S rRNA.



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

- Molecule 28 is a RNA chain called 5S rRNA.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

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

- Molecule 31 is a protein called 50S ribosomal protein L4.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	67	Total	C	N	O	S	0	0
			505	322	90	92	1		

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 39 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 49 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 52 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 53 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

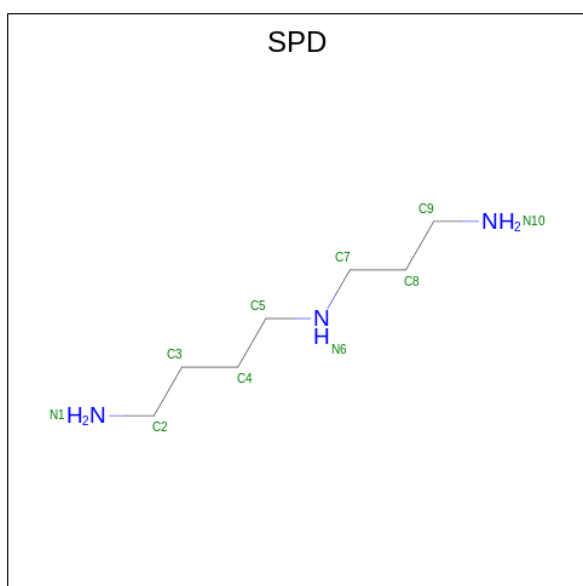
- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	A	83	Total	Mg	0
			83	83	
58	J	1	Total	Mg	0
			1	1	
58	a	209	Total	Mg	0
			209	209	
58	b	5	Total	Mg	0
			5	5	
58	d	1	Total	Mg	0
			1	1	
58	p	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	

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

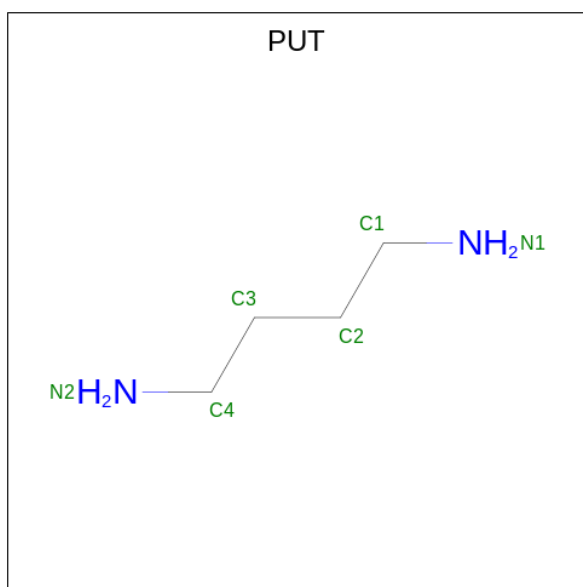
Mol	Chain	Residues	Atoms		AltConf
59	A	4	Total 4	K 4	0
59	D	1	Total 1	K 1	0
59	a	40	Total 40	K 40	0
59	c	2	Total 2	K 2	0

- Molecule 60 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ).



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

- Molecule 61 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula:  $C_4H_{12}N_2$ ).



Mol	Chain	Residues	Atoms			AltConf
61	a	1	Total	C	N	0
			6	4	2	

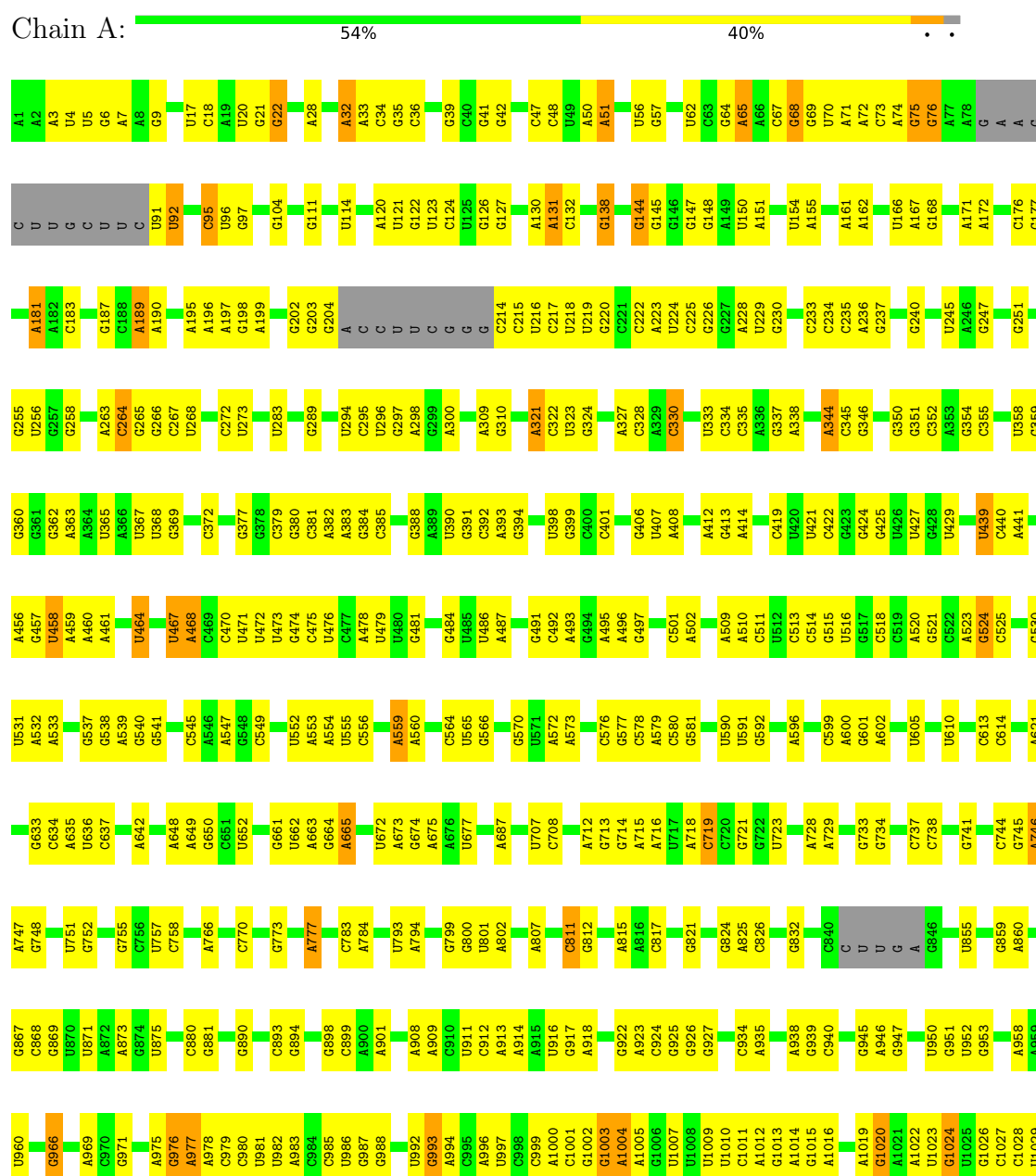
- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	3	1	Total	Zn	0
			1	1	
62	4	1	Total	Zn	0
			1	1	

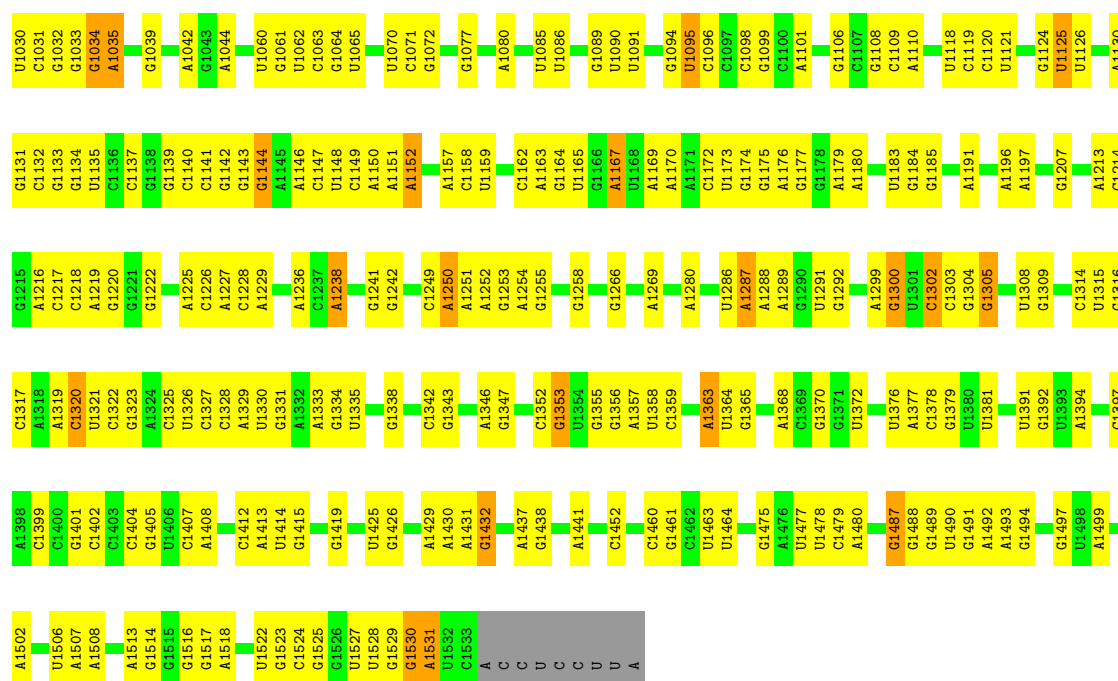
### 3 Residue-property plots

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.

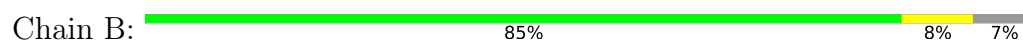
#### • Molecule 1: 16S rRNA



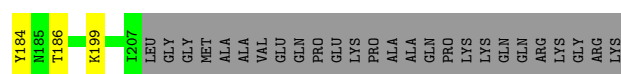




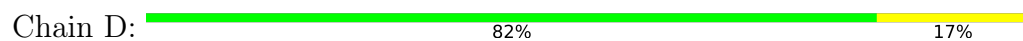
• Molecule 2: 30S ribosomal protein S2




• Molecule 3: 30S ribosomal protein S3

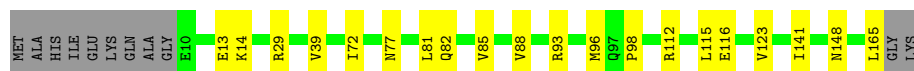


• Molecule 4: 30S ribosomal protein S4



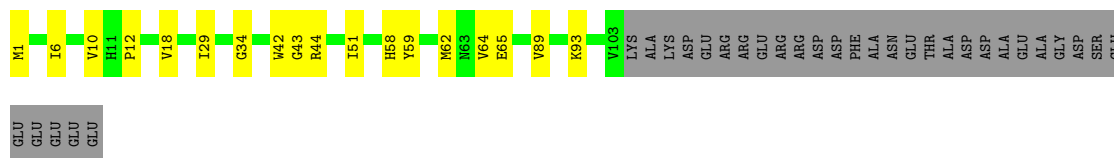
• Molecule 5: 30S ribosomal protein S5

Chain E:  81% 12% 7%




- Molecule 6: 30S ribosomal protein S6, fully modified isoform

Chain F:  63% 13% 24%



- Molecule 7: 30S ribosomal protein S7

Chain G:  79% 6% 15%



- Molecule 8: 30S ribosomal protein S8

Chain H:  92% 8% .




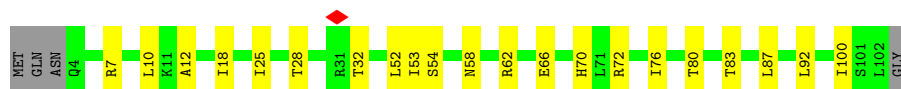
- Molecule 9: 30S ribosomal protein S9

Chain I:  76% 22% .




- Molecule 10: 30S ribosomal protein S10

Chain J:  76% 20% .

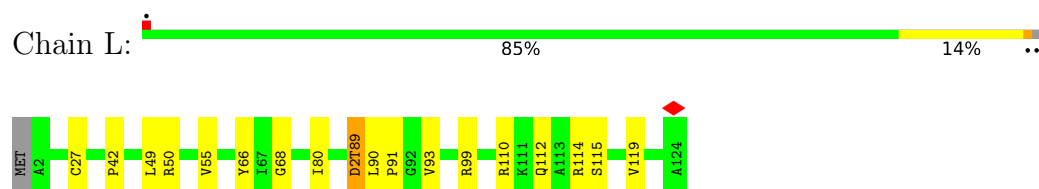


- Molecule 11: 30S ribosomal protein S11

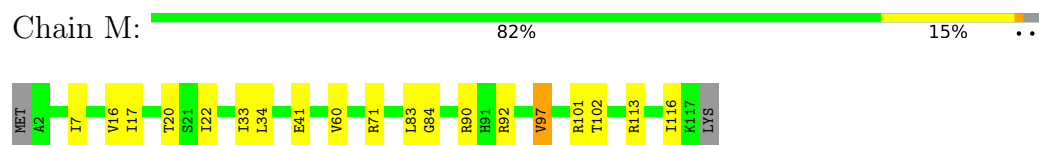
Chain K:  79% 12% 9%



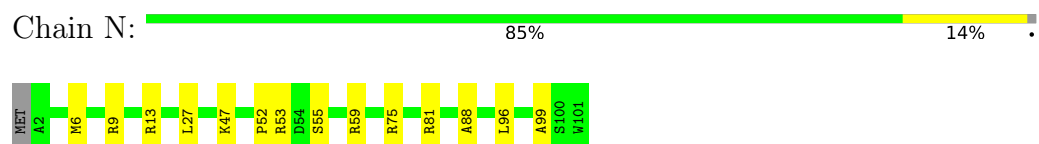
## • Molecule 12: 30S ribosomal protein S12



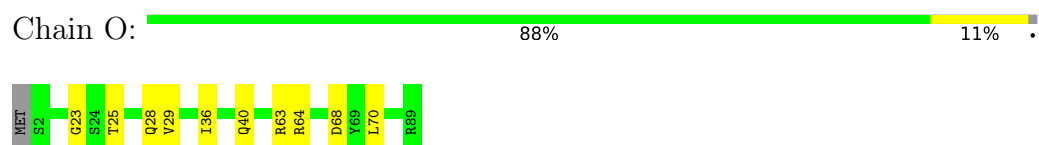
## • Molecule 13: 30S ribosomal protein S13



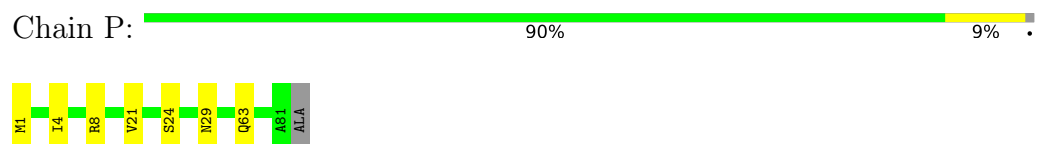
## • Molecule 14: 30S ribosomal protein S14



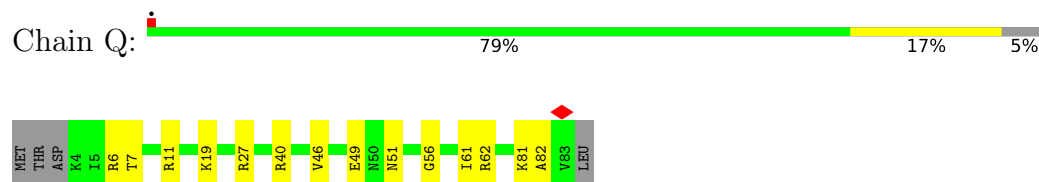
## • Molecule 15: 30S ribosomal protein S15



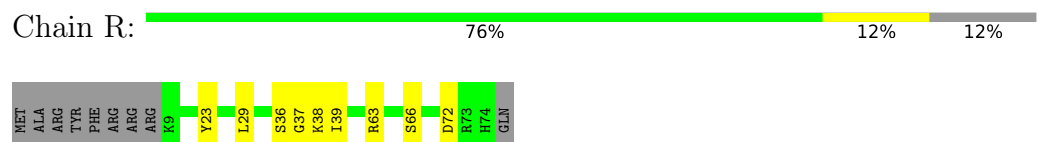
## • Molecule 16: 30S ribosomal protein S16




## • Molecule 17: 30S ribosomal protein S17



## • Molecule 18: 30S ribosomal protein S18




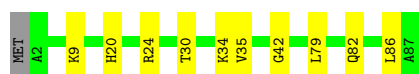
- Molecule 19: 30S ribosomal protein S19

Chain S:  80% 11% 9%




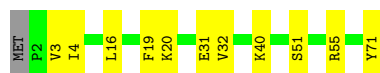
- Molecule 20: 30S ribosomal protein S20

Chain T:  87% 11% .




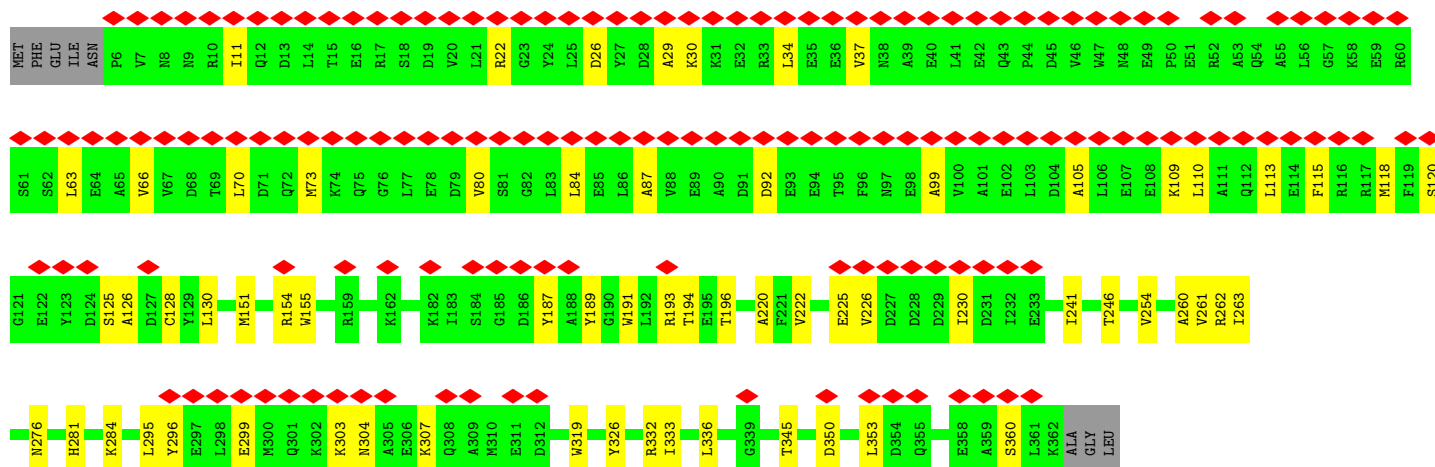
- Molecule 21: 30S ribosomal protein S21

Chain U:  83% 15% .



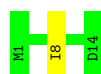
- Molecule 22: Peptide chain release factor 2

Chain V:  43% 80% 18% .



- Molecule 23: PepNL

Chain W:  93% 7%



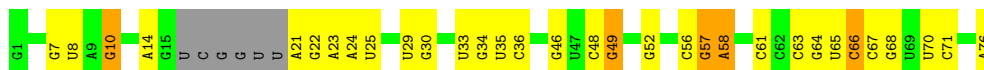
- Molecule 24: mRNA

Chain X:  89% 11%



• Molecule 25: RNA (73-MER)

Chain Y: 51% 35% 6% 8%



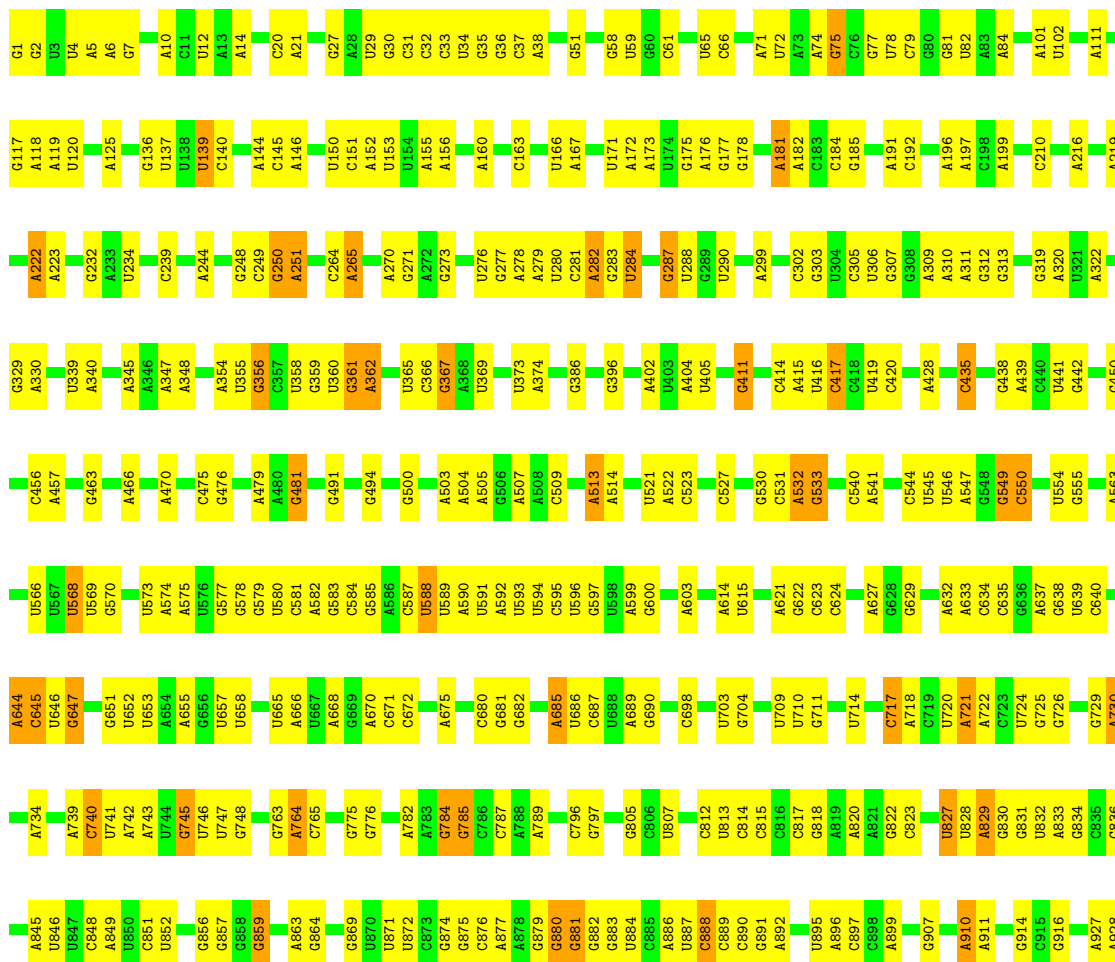
• Molecule 26: RNA (5'-R(P\*CP\*A)-3')

Chain Z: 67% 33%

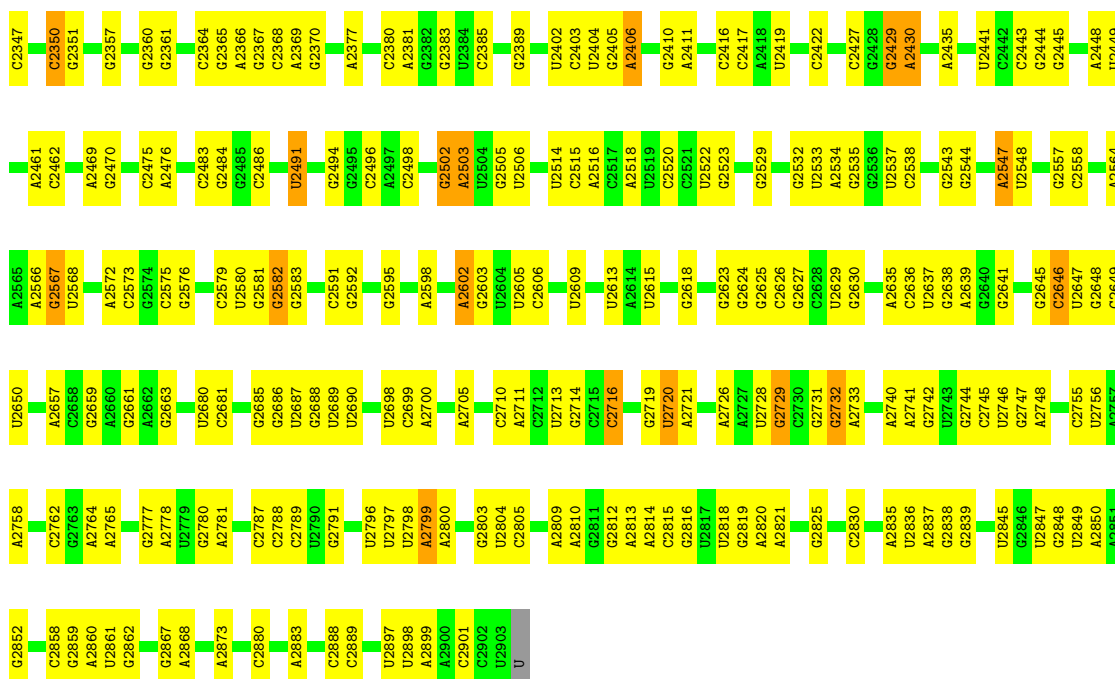


• Molecule 27: 23S rRNA

Chain a: 57% 35% 5%

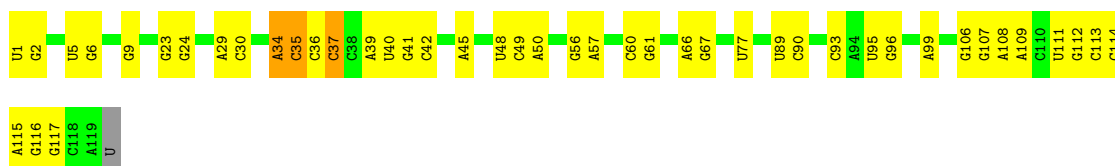


U2244	G2035	A1901	C1790	G1478	A1385	C1278	C1172	A	G1026	U928
U2245	C2036	A1918	A1791	G1482	C1386	G1279	U	A	A1027	G930
G2246	A2037	A1919	A1566	G1490	G1388	G1280	U	G	A1028	U931
A2247	G2038	C1920	A1705	A1493	A1392	G1281	A	C	A1029	U934
G2250	U2039	G1923	A1795	A1494	A1569	U1282	U	U	A1032	C935
G2251	G2040	C1924	A1571	A1495	A1572	U1286	G1177	A	U1033	A936
C2256	C2043	G1927	A1579	A1496	A1572	A1287	U	A	G1036	C937
C2257	G2047	A1928	A1579	U1497	A1572	U1288	G1182	U	G1037	C946
A2266	G2048	G1929	A1583	C1498	U1579	G1289	U1184	G	U1038	A947
A2267	A2051	A1930	U1584	A1505	A1583	G1296	G1187	C	A1039	C948
G2271	C2055	A1936	U1587	U1506	U1584	G1297	U1188	U	A1040	G949
U2272	G2056	A1937	G1587	U1507	U1584	A1287	U1189	C	G1041	A959
A2273	A2057	A1952	A1592	A1508	G1587	A1287	A1189	A	G1042	A960
A2274	G2058	A1953	A1593	A1509	G1587	G1288	G1191	C	C1045	C961
G2278	A2059	U1955	G1593	G1510	G1418	G1289	G1196	G	A1046	G962
G2282	A2060	U1956	A1597	G1511	G1421	A1301	C1197	U	G1047	U963
C2283	G2061	G1964	A1598	C1512	G1425	G1306	G1197	U	A1048	C964
G2285	C2062	U1965	A1608	A1515	G1426	A1307	U1198	C	A1049	C965
C2286	C2063	A1966	G1609	G1516	G1427	A1308	U1199	G	A1050	G966
A2287	G2065	C1967	A1610	G1517	C1428	G1310	G1212	U	G1051	U967
A2288	C2066	G1967	A1618	G1518	G1429	G1311	A1214	C	C1052	C968
G2289	G2067	A1970	A1618	U1519	G1431	G1315	G1215	A	A	G971
C2289	U2068	U1971	G1733	U1520	G1432	A1307	G1216	G	G	A972
C2290	C2069	U1971	G1734	G1521	G1433	A1308	U1219	A	A	G974
U2291	G2070	G1972	A1634	A1522	G1433	G1317	G1220	U	U	A975
U2292	A2071	G1972	A1635	U1523	G1433	U1325	G1220	G	U	G976
U2305	C2072	A1987	U1636	G1524	A1434	U1326	G1223	U	U	A979
U2306	G2073	G1988	A1637	A1525	G1435	U1327	G1224	G	G	A980
G2308	U2074	A1947	C1638	G1526	G1436	A1328	U1225	A	A	A981
A2311	U2075	U1991	G1645	C1526	G1437	U1329	A1226	C	C	C982
A2314	G2076	G1992	U1646	A1528	G1438	U1340	G1227	U	U	A983
G2315	A2077	U1993	U1647	G1529	U1439	G1341	U1231	A	A	G989
A2317	C1996	C1997	U1648	A1535	U1441	U1344	G1232	G	G	G993
G2317	C1997	C1997	U1649	C1536	U1442	U1352	G1236	A	A	A996
A2322	U2011	U2012	A1654	G1537	U1443	U1352	A1237	C	C	A1000
G2325	A2013	A2014	G1659	G1538	U1444	A1353	A1247	A	A	A1001
C2326	G2087	A2015	U1667	U1539	G1447	A1354	G1248	G	G	G1002
A2327	A2088	A2015	A1668	U1542	G1448	G1360	G1250	C	C	G1003
A2328	G2093	A2015	U1669	G1543	G1449	G1361	G1251	A	A	C1007
U2329	C2096	C2021	A1672	A1544	G1451	C1362	G1252	C	C	A1008
U2330	A2097	U2022	G1673	U1548	G1452	G1363	A1253	A	A	A1009
G2333	U2098	C2023	G1674	A1549	C1462	A1365	U1254	U	U	A1010
G2334	U	C2023	A1678	U1554	G1463	G1370	G1256	U	U	G1011
U2334	C	G2025	U1679	U1554	G1465	G1371	A1264	U	U	U1012
G2338	C	U2026	U1779	C1557	C1469	A1378	U1271	A	A	C1013
A2340	C	A2030	G1682	U1558	A1470	U1379	G1273	A	A	A1014
G2341	C	A2031	U1683	U1559	A1470	U1379	A1383	G	G	G1022
A2241	C	G2032	G1684	G1560	U1476	A1383	U1273	A	A	
G2345	U	A2033	U1785	U1561	U1476	A1383	U1273	A	A	
A2346	G	U2034	A1786	U1562	A1477	A1384	U1273	A	A	



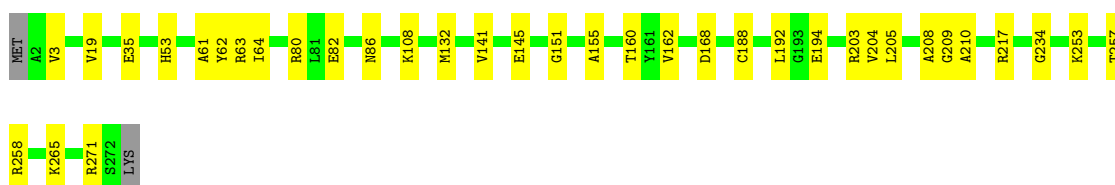
- Molecule 28: 5S rRNA

Chain b: 62% 35%



- Molecule 29: Large ribosomal subunit protein uL2

Chain c: 86% 13%



- Molecule 30: 50S ribosomal protein L3

Chain d: 88% 12%

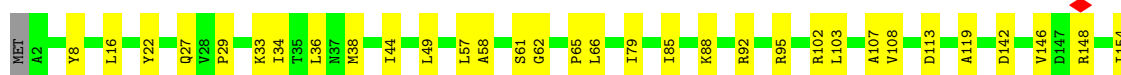
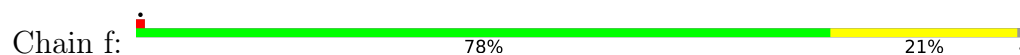


- Molecule 31: 50S ribosomal protein L4

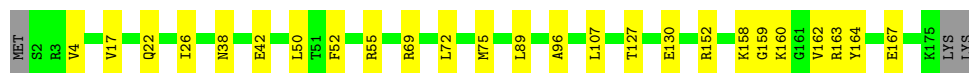
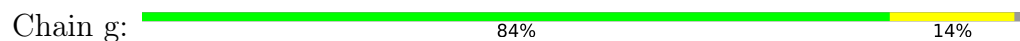
Chain e: 93% 7%



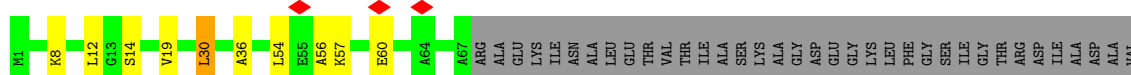
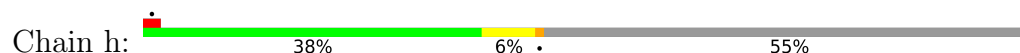
- Molecule 32: Large ribosomal subunit protein uL5



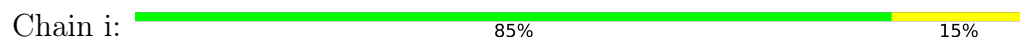
- Molecule 33: Large ribosomal subunit protein uL6



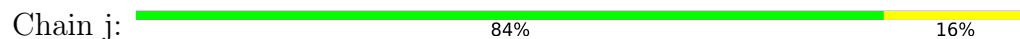
- Molecule 34: 50S ribosomal protein L9



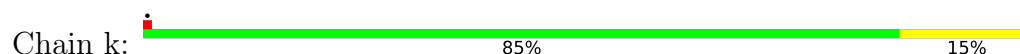
- Molecule 35: 50S ribosomal protein L13



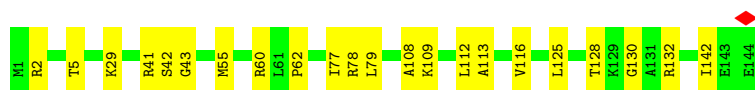
- Molecule 36: 50S ribosomal protein L14



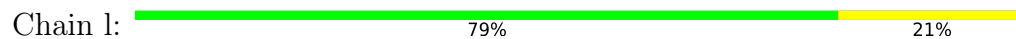
- Molecule 37: 50S ribosomal protein L15



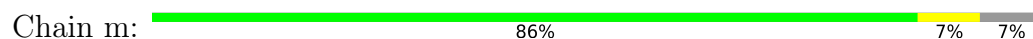




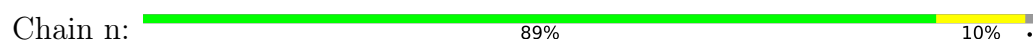
- Molecule 38: 50S ribosomal protein L16



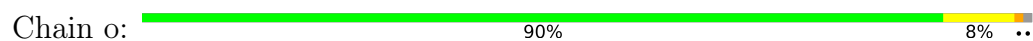
- Molecule 39: Large ribosomal subunit protein bL17



- Molecule 40: Large ribosomal subunit protein uL18



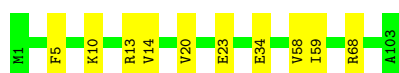
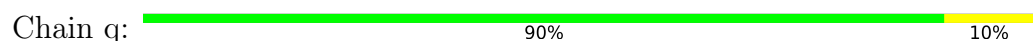
- Molecule 41: Large ribosomal subunit protein bL19



- Molecule 42: Large ribosomal subunit protein bL20



- Molecule 43: 50S ribosomal protein L21



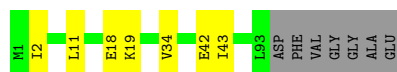
- Molecule 44: 50S ribosomal protein L22





- Molecule 45: Large ribosomal subunit protein uL23

Chain s: 86% 7% 7%



- Molecule 46: 50S ribosomal protein L24

Chain t: 89% 9% .



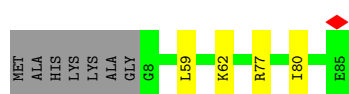
- Molecule 47: 50S ribosomal protein L25

Chain u: 77% 23%



- Molecule 48: Large ribosomal subunit protein bL27

Chain v: 87% 5% 8%



- Molecule 49: Large ribosomal subunit protein bL28

Chain w: 88% 10% .



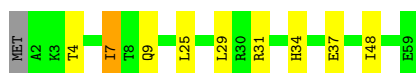
- Molecule 50: Large ribosomal subunit protein uL29

Chain x: 90% 8% .



- Molecule 51: Large ribosomal subunit protein uL30

Chain y: 83% 14% . .



- Molecule 52: Large ribosomal subunit protein bL32

Chain z: 84% 14% .



- Molecule 53: Large ribosomal subunit protein bL33

Chain 0: 75% 18% 7%



- Molecule 54: 50S ribosomal protein L34

Chain 1: 93% 7%



- Molecule 55: Large ribosomal subunit protein bL35

Chain 2: 78% 20% .



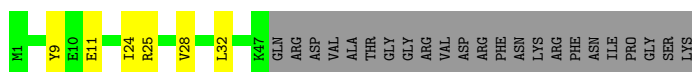
- Molecule 56: 50S ribosomal protein L36

Chain 3: 87% 13%



- Molecule 57: 50S ribosomal protein L31

Chain 4: 59% 9% 33%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71980	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.916	Depositor
Minimum map value	-0.507	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	358.56, 358.56, 358.56	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.10	0/35954	0.23	0/56077
2	B	0.08	0/1789	0.22	0/2410
3	C	0.08	0/1651	0.21	0/2225
4	D	0.08	0/1665	0.20	0/2227
5	E	0.09	0/1165	0.22	0/1568
6	F	0.08	0/858	0.20	0/1160
7	G	0.08	0/1219	0.20	0/1635
8	H	0.08	0/989	0.22	0/1326
9	I	0.08	0/1034	0.22	0/1375
10	J	0.10	0/805	0.27	0/1089
11	K	0.10	0/884	0.20	0/1191
12	L	0.08	0/960	0.22	0/1286
13	M	0.08	0/909	0.23	0/1215
14	N	0.07	0/817	0.18	0/1088
15	O	0.08	0/722	0.20	0/964
16	P	0.08	0/653	0.24	0/877
17	Q	0.08	0/657	0.22	0/881
18	R	0.08	0/553	0.20	0/742
19	S	0.07	0/685	0.19	0/922
20	T	0.08	0/676	0.19	0/895
21	U	0.07	0/597	0.19	0/792
22	V	0.08	0/2863	0.24	0/3855
23	W	0.32	0/99	0.42	0/133
24	X	0.08	0/217	0.25	0/336
25	Y	0.12	0/1693	0.30	0/2636
26	Z	0.05	0/46	0.11	0/69
27	a	0.10	0/65651	0.23	0/102413
28	b	0.08	0/2850	0.21	0/4444
29	c	0.09	0/2121	0.24	0/2852
30	d	0.09	0/1576	0.22	0/2119
31	e	0.08	0/1571	0.21	0/2113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	f	0.09	0/1434	0.23	0/1926
33	g	0.08	0/1324	0.20	0/1794
34	h	0.09	0/510	0.25	0/687
35	i	0.08	0/1152	0.20	0/1551
36	j	0.08	0/955	0.22	0/1279
37	k	0.08	0/1062	0.23	0/1413
38	l	0.08	0/1073	0.22	0/1433
39	m	0.09	0/958	0.26	0/1281
40	n	0.08	0/902	0.21	0/1209
41	o	0.09	0/929	0.20	0/1242
42	p	0.09	0/960	0.20	0/1278
43	q	0.08	0/829	0.20	0/1107
44	r	0.08	0/864	0.20	0/1156
45	s	0.08	0/744	0.21	0/994
46	t	0.07	0/787	0.21	0/1051
47	u	0.08	0/766	0.24	0/1025
48	v	0.08	0/599	0.22	0/792
49	w	0.09	0/635	0.22	0/848
50	x	0.06	0/502	0.15	0/667
51	y	0.08	0/453	0.19	0/605
52	z	0.09	0/450	0.22	0/599
53	0	0.08	0/424	0.21	0/565
54	1	0.08	0/380	0.23	0/498
55	2	0.08	0/513	0.24	0/676
56	3	0.08	0/303	0.22	0/397
57	4	0.07	0/371	0.20	0/496
All	All	0.09	0/153808	0.23	0/229484

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32360	0	16305	417	0
2	B	1758	0	1782	11	0
3	C	1624	0	1696	20	0
4	D	1643	0	1707	23	0
5	E	1152	0	1196	12	0
6	F	839	0	833	11	0
7	G	1203	0	1254	6	0
8	H	979	0	1031	8	0
9	I	1022	0	1070	20	0
10	J	795	0	836	17	0
11	K	877	0	884	10	0
12	L	957	0	1017	16	0
13	M	900	0	965	14	0
14	N	805	0	844	13	0
15	O	714	0	734	5	0
16	P	643	0	661	5	0
17	Q	648	0	691	8	0
18	R	544	0	565	6	0
19	S	668	0	693	6	0
20	T	670	0	719	6	0
21	U	589	0	629	7	0
22	V	2834	0	2731	39	0
23	W	108	0	112	1	0
24	X	194	0	98	0	0
25	Y	1517	0	768	17	0
26	Z	42	0	23	0	0
27	a	59130	0	29761	669	0
28	b	2549	0	1291	34	0
29	c	2082	0	2154	26	0
30	d	1566	0	1617	17	0
31	e	1552	0	1619	9	0
32	f	1410	0	1444	25	0
33	g	1304	0	1345	14	0
34	h	505	0	532	5	0
35	i	1129	0	1162	14	0
36	j	946	0	1023	12	0
37	k	1053	0	1129	14	0
38	l	1075	0	1145	17	0
39	m	945	0	989	4	0
40	n	892	0	923	8	0
41	o	917	0	962	9	0
42	p	947	0	1019	6	0
43	q	816	0	839	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	r	857	0	922	7	0
45	s	738	0	807	5	0
46	t	779	0	831	5	0
47	u	753	0	780	13	0
48	v	592	0	607	3	0
49	w	625	0	652	5	0
50	x	501	0	531	3	0
51	y	449	0	488	5	0
52	z	444	0	458	5	0
53	0	417	0	451	7	0
54	1	377	0	418	3	0
55	2	504	0	572	9	0
56	3	302	0	340	4	0
57	4	364	0	362	4	0
58	A	83	0	0	0	0
58	J	1	0	0	0	0
58	a	209	0	0	0	0
58	b	5	0	0	0	0
58	d	1	0	0	0	0
58	p	1	0	0	0	0
58	z	1	0	0	0	0
59	A	4	0	0	0	0
59	D	1	0	0	0	0
59	a	40	0	0	0	0
59	c	2	0	0	0	0
60	a	70	0	133	3	0
61	a	6	0	12	0	0
62	3	1	0	0	0	0
62	4	1	0	0	0	0
All	All	143031	0	97162	1517	0

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

All (1517) 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)
27:a:881:G:H1	27:a:895:U:H3	1.28	0.82
1:A:111:G:H1	1:A:330:C:H41	1.27	0.80
1:A:1124:G:N2	1:A:1125:U:O4	2.16	0.76
1:A:1149:C:H2'	1:A:1150:A:H8	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:284:U:H3	27:a:356:G:H1	1.35	0.74
1:A:673:A:H2'	1:A:674:G:C8	2.23	0.73
29:c:53:HIS:HA	29:c:217:ARG:HB2	1.71	0.72
22:V:151:MET:HE3	22:V:353:LEU:HD21	1.72	0.72
32:f:102:ARG:HG2	57:4:24:ILE:HD12	1.73	0.71
37:k:108:ALA:HB3	37:k:125:LEU:HD22	1.74	0.70
1:A:1071:C:H2'	1:A:1072:G:H8	1.56	0.70
27:a:1779:U:OP2	27:a:1784:A:N6	2.22	0.69
28:b:30:C:H1'	28:b:57:A:H61	1.57	0.69
27:a:1724:G:O6	27:a:1737:G:N2	2.26	0.69
27:a:2595:G:N2	27:a:2598:A:OP2	2.26	0.69
27:a:2848:G:O2'	27:a:2867:G:N2	2.26	0.69
1:A:1175:G:H2'	1:A:1176:A:H8	1.58	0.68
27:a:197:A:N6	27:a:2430:A:O2'	2.26	0.68
27:a:651:G:H5'	55:2:19:LYS:HB2	1.74	0.68
57:4:11:GLU:HA	57:4:25:ARG:HA	1.75	0.68
1:A:826:C:O2	8:H:16:ASN:ND2	2.27	0.68
1:A:713:G:H2'	1:A:714:G:C8	2.29	0.68
27:a:270:A:N1	27:a:369:U:O2'	2.25	0.67
27:a:820:A:H4'	27:a:836:G:H22	1.60	0.67
5:E:115:LEU:HD13	5:E:123:VAL:HG11	1.76	0.67
1:A:531:U:H2'	22:V:332:ARG:HH22	1.60	0.66
27:a:475:C:O2	27:a:479:A:N6	2.27	0.66
27:a:2728:U:HO2'	27:a:2729:G:H8	1.44	0.66
27:a:1386:C:H2'	27:a:1387:A:H8	1.61	0.65
1:A:1003:G:H21	1:A:1005:A:H5'	1.61	0.65
1:A:492:C:H2'	1:A:493:A:C8	2.32	0.65
27:a:160:A:N3	27:a:2208:C:O2'	2.30	0.65
22:V:22:ARG:HG2	22:V:70:LEU:HD13	1.79	0.65
1:A:1218:C:H2'	1:A:1219:A:H8	1.61	0.64
47:u:51:GLN:HG2	47:u:86:LEU:HD11	1.78	0.64
1:A:219:U:H2'	1:A:220:G:H8	1.63	0.64
1:A:744:C:H2'	1:A:745:G:H8	1.61	0.64
27:a:500:G:N1	27:a:503:A:OP2	2.29	0.64
28:b:77:U:OP1	47:u:21:ARG:NH1	2.32	0.64
27:a:1432:G:H2'	27:a:1433:A:C8	2.34	0.63
27:a:1799:G:OP1	29:c:258:ARG:NH1	2.29	0.63
40:n:83:LEU:HD11	40:n:114:GLY:HA3	1.81	0.63
1:A:309:A:H2'	1:A:310:G:H8	1.64	0.63
22:V:80:VAL:HG13	22:V:99:ALA:HB1	1.81	0.63
27:a:1417:C:HO2'	27:a:1587:G:HO2'	1.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:64:VAL:HG22	47:u:69:GLU:HG2	1.79	0.63
1:A:1218:C:H2'	1:A:1219:A:C8	2.34	0.63
1:A:1266:G:N2	1:A:1269:A:OP2	2.29	0.63
2:B:115:LYS:NZ	2:B:152:LYS:O	2.32	0.63
9:I:130:ARG:NH1	25:Y:33:U:OP2	2.32	0.63
22:V:230:ILE:HG12	22:V:299:GLU:HB2	1.80	0.63
1:A:501:C:OP1	12:L:114:ARG:NH2	2.27	0.63
1:A:1250:A:H2'	1:A:1251:A:C8	2.34	0.62
27:a:1311:G:OP2	27:a:1311:G:N2	2.27	0.62
1:A:552:U:H2'	1:A:553:A:H8	1.62	0.62
27:a:2657:A:O2'	33:g:160:LYS:NZ	2.32	0.62
1:A:75:G:H3'	1:A:76:G:H8	1.64	0.62
1:A:337:G:H2'	1:A:338:A:H8	1.64	0.62
1:A:674:G:H2'	1:A:675:A:H8	1.65	0.62
1:A:1034:G:H2'	1:A:1035:A:H8	1.64	0.62
27:a:832:U:H2'	27:a:833:A:H8	1.65	0.62
1:A:1077:G:N2	1:A:1080:A:OP2	2.31	0.62
27:a:239:C:O2'	27:a:622:G:O2'	2.14	0.62
27:a:1129:A:N6	27:a:2491:U:OP1	2.32	0.62
27:a:2047:C:H2'	27:a:2048:G:H8	1.65	0.62
1:A:714:G:H2'	1:A:715:A:C8	2.35	0.62
1:A:946:A:H2'	1:A:947:G:C8	2.34	0.62
12:L:68:GLY:O	12:L:99:ARG:NH1	2.33	0.62
27:a:1013:C:H2'	27:a:1014:A:H8	1.64	0.62
27:a:2618:G:H21	30:d:155:VAL:HG21	1.63	0.62
27:a:581:C:H2'	27:a:582:A:H8	1.64	0.62
27:a:698:C:O2'	27:a:734:A:N6	2.33	0.62
1:A:346:G:OP1	41:o:39:ARG:NH1	2.31	0.61
1:A:946:A:H2'	1:A:947:G:H8	1.64	0.61
1:A:458:U:H3	1:A:474:G:H1	1.46	0.61
1:A:981:U:OP1	14:N:9:ARG:NH1	2.31	0.61
1:A:1004:A:H2'	1:A:1005:A:O4'	2.00	0.61
1:A:1397:C:OP2	5:E:29:ARG:NH2	2.33	0.61
27:a:1248:G:OP1	31:e:44:ARG:NH1	2.30	0.61
41:o:75:GLN:HB2	41:o:78:SER:HB2	1.83	0.61
28:b:36:C:O2'	28:b:37:C:OP1	2.18	0.61
1:A:358:U:H2'	1:A:359:G:H8	1.64	0.61
27:a:589:U:H2'	27:a:590:A:H8	1.66	0.60
27:a:1386:C:H2'	27:a:1387:A:C8	2.35	0.60
1:A:203:G:N2	1:A:204:G:O6	2.31	0.60
19:S:28:LYS:NZ	19:S:46:GLY:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:463:G:N2	27:a:466:A:OP2	2.26	0.60
27:a:419:U:H2'	27:a:420:C:C6	2.37	0.60
1:A:147:G:H2'	1:A:148:G:C8	2.37	0.60
27:a:1447:C:O2'	27:a:1544:A:N3	2.30	0.60
27:a:1450:G:N2	27:a:1452:G:O6	2.27	0.60
1:A:652:U:O4	1:A:752:G:O2'	2.19	0.60
1:A:999:C:H2'	1:A:1000:A:C8	2.36	0.60
1:A:715:A:H2'	1:A:716:A:C8	2.37	0.60
1:A:938:A:N3	1:A:1376:U:O2'	2.31	0.60
27:a:1252:G:H1	42:p:37:GLN:HE21	1.49	0.60
27:a:993:G:OP2	42:p:51:ARG:NH2	2.33	0.60
1:A:673:A:H2'	1:A:674:G:H8	1.67	0.60
10:J:76:ILE:HG21	10:J:83:THR:HG21	1.83	0.60
27:a:1722:A:N6	27:a:1738:G:O2'	2.35	0.60
27:a:2246:G:H2'	27:a:2247:A:H8	1.67	0.60
4:D:100:ASN:HD22	4:D:111:ARG:HE	1.49	0.59
47:u:72:VAL:HG12	47:u:93:ARG:HA	1.84	0.59
1:A:980:C:O2'	14:N:13:ARG:NH1	2.35	0.59
27:a:219:A:N3	27:a:234:U:O2'	2.29	0.59
27:a:527:C:N4	27:a:2777:G:O2'	2.28	0.59
27:a:1597:A:H5''	27:a:1598:A:H5'	1.85	0.59
39:m:12:ARG:O	39:m:17:ARG:NH1	2.34	0.59
27:a:652:U:H5''	27:a:653:U:H2'	1.84	0.59
27:a:1802:A:H2'	27:a:1803:A:C8	2.37	0.59
27:a:2575:C:H5'	30:d:149:ASN:HB2	1.85	0.59
28:b:60:C:H2'	28:b:61:G:H8	1.67	0.59
53:0:8:LYS:HB3	53:0:54:ILE:HD12	1.83	0.59
27:a:742:A:H2'	27:a:743:A:H8	1.68	0.59
27:a:2258:C:O2'	27:a:2427:C:OP2	2.21	0.59
33:g:164:TYR:HB2	33:g:167:GLU:HB2	1.83	0.59
38:l:77:PRO:HG2	38:l:80:VAL:HG21	1.84	0.59
1:A:401:C:O2'	1:A:621:A:N3	2.34	0.59
27:a:591:U:H2'	27:a:592:A:C8	2.38	0.59
27:a:1506:U:H2'	27:a:1507:C:C6	2.37	0.59
36:j:9:ASN:OD1	36:j:18:ARG:NH1	2.34	0.59
4:D:104:ARG:HB3	4:D:168:PRO:HG2	1.83	0.58
27:a:1153:C:OP1	42:p:92:ARG:NH2	2.36	0.58
7:G:70:ARG:HG2	7:G:96:ARG:HB3	1.85	0.58
22:V:73:MET:HE1	22:V:109:LYS:HB2	1.85	0.58
27:a:568:U:H1'	27:a:2030:6MZ:H9C1	1.84	0.58
27:a:177:G:OP2	27:a:177:G:N2	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:128:CYS:HB3	22:V:189:TYR:HA	1.84	0.58
27:a:2646:C:OP2	27:a:2732:G:O2'	2.22	0.58
1:A:664:G:H22	1:A:741:G:H1	1.51	0.58
27:a:672:C:OP2	37:k:42:SER:OG	2.22	0.58
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.86	0.58
20:T:42:GLY:HA2	20:T:86:LEU:HD11	1.85	0.58
31:e:149:ILE:HB	31:e:188:MET:HG2	1.86	0.58
35:i:96:ARG:HD2	35:i:99:ARG:HG3	1.86	0.58
43:q:10:LYS:NZ	43:q:23:GLU:OE2	2.36	0.58
10:J:10:LEU:HD11	10:J:25:ILE:HD12	1.86	0.58
18:R:36:SER:HA	18:R:72:ASP:HB3	1.86	0.58
22:V:126:ALA:HB1	22:V:225:GLU:HB3	1.84	0.58
27:a:2502:G:H5''	27:a:2503:2MA:H5''	1.84	0.58
1:A:235:C:H2'	1:A:236:A:H8	1.69	0.58
10:J:87:LEU:HD22	10:J:100:ILE:HD13	1.86	0.58
1:A:746:A:H2'	1:A:747:A:C8	2.38	0.58
1:A:1034:G:H2'	1:A:1035:A:C8	2.39	0.58
12:L:50:ARG:HE	12:L:89:D2T:H6	1.69	0.58
27:a:1754:A:N1	27:a:2716:C:O2'	2.35	0.58
53:0:10:LYS:HE3	53:0:54:ILE:HA	1.84	0.58
1:A:34:C:H2'	1:A:35:G:H8	1.69	0.57
10:J:52:LEU:HA	10:J:62:ARG:HB3	1.86	0.57
1:A:297:G:N2	1:A:300:A:OP2	2.26	0.57
3:C:35:SER:OG	3:C:59:ARG:NH2	2.36	0.57
1:A:1147:C:H2'	1:A:1148:U:C6	2.40	0.57
1:A:1255:G:O2'	1:A:1258:G:N3	2.33	0.57
1:A:1327:C:H2'	1:A:1328:C:H6	1.68	0.57
11:K:111:THR:HG23	21:U:3:VAL:HG22	1.86	0.57
1:A:202:G:O2'	1:A:468:A:N3	2.36	0.57
1:A:712:A:H2'	1:A:713:G:C8	2.39	0.57
27:a:590:A:H2'	27:a:591:U:C6	2.39	0.57
27:a:675:A:OP1	31:e:58:LYS:NZ	2.34	0.57
27:a:1231:U:H2'	27:a:1232:G:H8	1.70	0.57
1:A:555:U:H2'	1:A:556:C:C6	2.39	0.57
1:A:811:C:O2'	1:A:901:A:N1	2.37	0.57
27:a:2515:C:H2'	27:a:2516:A:H8	1.69	0.57
27:a:2859:G:H2'	27:a:2860:A:C8	2.40	0.57
1:A:999:C:H2'	1:A:1000:A:H8	1.70	0.57
1:A:1147:C:H1'	9:I:18:ARG:HH21	1.69	0.57
12:L:42:PRO:HB3	12:L:89:D2T:SB	2.45	0.57
27:a:1038:G:H2'	27:a:1039:A:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:G:N2	1:A:1005:A:H5'	2.20	0.57
28:b:30:C:O2'	28:b:57:A:N1	2.35	0.57
1:A:64:G:H4'	1:A:65:A:H3'	1.87	0.56
1:A:745:G:H2'	1:A:746:A:C8	2.40	0.56
22:V:333:ILE:HG13	22:V:345:THR:HG22	1.87	0.56
27:a:1578:U:H2'	27:a:1579:A:H8	1.70	0.56
1:A:1071:C:H2'	1:A:1072:G:C8	2.40	0.56
22:V:276:ASN:O	27:a:2602:A:N6	2.38	0.56
1:A:1308:U:H2'	1:A:1309:G:H8	1.71	0.56
12:L:55:VAL:HG21	12:L:80:ILE:HD11	1.86	0.56
27:a:5:A:H2'	27:a:6:A:C8	2.41	0.56
27:a:5:A:H2'	27:a:6:A:H8	1.70	0.56
1:A:150:U:H2'	1:A:151:A:H8	1.70	0.56
1:A:501:C:H2'	1:A:502:A:H8	1.69	0.56
1:A:718:A:O2'	21:U:31:GLU:OE2	2.21	0.56
27:a:1385:A:O2'	27:a:1396:U:O2	2.23	0.56
5:E:148:ASN:ND2	8:H:73:GLU:OE2	2.38	0.56
29:c:155:ALA:HB2	29:c:162:VAL:HG23	1.87	0.56
38:l:50:ARG:HA	38:l:53:MET:HE2	1.87	0.56
25:Y:22:G:H2'	25:Y:23:A:H8	1.71	0.56
27:a:1901:A:OP2	29:c:253:LYS:NZ	2.34	0.56
27:a:373:U:H2'	27:a:374:A:H8	1.71	0.56
27:a:1028:A:H2'	27:a:1029:A:C8	2.40	0.56
27:a:2705:A:O2'	27:a:2852:G:OP1	2.24	0.56
3:C:19:ASN:O	3:C:40:ARG:NH2	2.39	0.56
35:i:1:MET:SD	35:i:1:MET:N	2.79	0.56
27:a:590:A:H2'	27:a:591:U:H6	1.71	0.56
27:a:591:U:H1'	55:2:2:PRO:HD2	1.88	0.56
27:a:976:G:HO2'	27:a:1155:A:HO2'	1.48	0.56
27:a:1223:G:OP1	43:q:68:ARG:NH1	2.39	0.56
27:a:2537:U:H2'	27:a:2538:C:C6	2.41	0.56
1:A:875:U:O2'	8:H:15:ARG:NH1	2.38	0.56
13:M:90:ARG:HB2	13:M:97:VAL:HG13	1.87	0.56
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.87	0.56
1:A:501:C:H2'	1:A:502:A:C8	2.41	0.55
1:A:1477:U:H2'	1:A:1478:U:C6	2.41	0.55
27:a:591:U:H2'	27:a:592:A:H8	1.69	0.55
29:c:61:ALA:O	29:c:63:ARG:NH1	2.38	0.55
27:a:1808:A:H3'	27:a:1809:A:C8	2.41	0.55
27:a:1638:C:O2	27:a:2698:U:O2'	2.24	0.55
32:f:58:ALA:HB2	32:f:65:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:807:U:OP2	37:k:41:ARG:NH2	2.37	0.55
27:a:1278:C:H2'	27:a:1279:G:H8	1.72	0.55
2:B:214:LEU:HA	2:B:217:VAL:HG22	1.88	0.55
22:V:130:LEU:HG	22:V:222:VAL:HG22	1.88	0.55
27:a:2246:G:H2'	27:a:2247:A:C8	2.41	0.55
27:a:2898:U:H2'	27:a:2899:A:H8	1.72	0.55
27:a:729:G:H5'	27:a:730:A:H5''	1.88	0.55
1:A:1167:A:O2'	1:A:1169:A:N7	2.39	0.55
27:a:581:C:H2'	27:a:582:A:C8	2.39	0.55
27:a:1469:A:H2'	27:a:1470:A:C8	2.42	0.55
32:f:102:ARG:NH1	57:4:9:TYR:OH	2.40	0.55
27:a:589:U:H2'	27:a:590:A:C8	2.42	0.55
27:a:963:U:C2	27:a:964:C:C5	2.95	0.55
32:f:29:PRO:HB3	32:f:160:ALA:HB2	1.87	0.55
1:A:181:A:N6	1:A:195:A:OP2	2.40	0.55
1:A:1412:C:H2'	1:A:1413:A:C8	2.42	0.55
27:a:623:C:H2'	27:a:624:C:H6	1.72	0.55
25:Y:63:C:H2'	25:Y:64:G:H8	1.72	0.55
1:A:1148:U:H2'	1:A:1149:C:O4'	2.06	0.54
43:q:34:GLU:HG3	43:q:58:VAL:HG13	1.89	0.54
27:a:1469:A:H2'	27:a:1470:A:H8	1.72	0.54
27:a:1264:A:OP1	52:z:16:ARG:NH2	2.39	0.54
1:A:56:U:H2'	1:A:57:G:H8	1.72	0.54
1:A:662:U:H2'	1:A:663:A:C8	2.43	0.54
1:A:1012:A:H2'	1:A:1013:G:C8	2.42	0.54
1:A:1013:G:N2	1:A:1016:A:OP2	2.38	0.54
1:A:1086:U:H3	1:A:1099:G:H22	1.55	0.54
27:a:668:A:H2'	27:a:670:A:H62	1.72	0.54
27:a:2836:U:H2'	27:a:2837:A:C8	2.43	0.54
37:k:79:LEU:HB3	37:k:116:VAL:HG23	1.89	0.54
1:A:4:U:H2'	1:A:5:U:H2'	1.88	0.54
1:A:294:U:OP1	1:A:610:U:O2'	2.23	0.54
27:a:2071:A:H2'	27:a:2072:C:C6	2.42	0.54
5:E:165:LEU:O	8:H:114:ARG:NH1	2.41	0.54
27:a:856:G:H2'	27:a:857:G:C8	2.42	0.54
42:p:97:ASP:OD2	43:q:13:ARG:NH2	2.36	0.54
27:a:307:G:N1	27:a:310:A:OP2	2.31	0.54
27:a:1046:A:H3'	27:a:1047:G:H5'	1.90	0.54
27:a:1819:A:H5''	29:c:160:THR:HG21	1.89	0.54
27:a:833:A:H2'	27:a:834:G:C8	2.42	0.54
1:A:144:G:H2'	1:A:145:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:U:H2'	1:A:399:G:H8	1.73	0.54
1:A:427:U:O2'	1:A:541:G:OP1	2.26	0.54
17:Q:11:ARG:HE	17:Q:56:GLY:HA2	1.72	0.54
27:a:503:A:H4'	27:a:504:A:H3'	1.89	0.54
27:a:582:A:H2'	27:a:583:G:H8	1.73	0.54
27:a:1737:G:H2'	27:a:1738:G:H1'	1.90	0.54
44:r:4:ILE:HG22	44:r:106:VAL:HG22	1.90	0.54
51:y:9:GLN:HB2	51:y:29:LEU:HD13	1.90	0.54
27:a:438:G:H2'	27:a:439:A:C8	2.44	0.53
27:a:2847:U:OP1	41:o:96:LYS:NZ	2.37	0.53
1:A:766:A:OP2	1:A:812:G:N2	2.42	0.53
17:Q:27:ARG:HG3	17:Q:40:ARG:HB2	1.88	0.53
25:Y:23:A:H2'	25:Y:24:A:C8	2.42	0.53
27:a:177:G:H3'	27:a:178:G:H8	1.72	0.53
27:a:355:U:H2'	27:a:356:G:C8	2.42	0.53
27:a:1353:A:H2'	27:a:1354:A:H8	1.72	0.53
27:a:2366:A:H4'	48:v:62:LYS:HE3	1.90	0.53
27:a:2514:U:H2'	27:a:2515:C:C6	2.43	0.53
27:a:2581:G:OP2	27:a:2581:G:N2	2.28	0.53
1:A:555:U:H2'	1:A:556:C:H6	1.73	0.53
1:A:1314:C:H2'	1:A:1315:U:C6	2.43	0.53
6:F:12:PRO:O	6:F:44:ARG:NH2	2.42	0.53
27:a:30:G:O2'	27:a:1214:A:N3	2.37	0.53
27:a:1667:G:O2'	27:a:1991:U:O4	2.22	0.53
27:a:1992:G:N2	27:a:1996:C:O2'	2.41	0.53
1:A:1126:U:OP1	10:J:7:ARG:NH2	2.40	0.53
27:a:577:G:O2'	27:a:1254:A:OP1	2.27	0.53
27:a:807:U:O2'	27:a:2060:A:N1	2.39	0.53
38:l:42:THR:HG22	38:l:93:VAL:HG12	1.90	0.53
22:V:261:VAL:HG11	22:V:284:LYS:HG3	1.91	0.53
27:a:742:A:H2'	27:a:743:A:C8	2.43	0.53
27:a:963:U:H2'	27:a:964:C:H6	1.71	0.53
27:a:848:C:H2'	27:a:849:A:H8	1.73	0.53
27:a:2223:G:O2'	29:c:265:LYS:NZ	2.30	0.53
1:A:665:A:H1'	1:A:733:G:H5'	1.90	0.53
1:A:1347:G:O6	9:I:12:ARG:NH2	2.41	0.53
34:h:8:LYS:HA	34:h:14:SER:HA	1.90	0.53
1:A:1356:G:H2'	1:A:1357:A:C8	2.43	0.53
27:a:151:C:H2'	27:a:152:A:H8	1.73	0.53
27:a:832:U:H2'	27:a:833:A:C8	2.43	0.53
27:a:1709:U:H2'	27:a:1710:G:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:125:SER:HA	22:V:187:TYR:HA	1.90	0.53
27:a:1353:A:H2'	27:a:1354:A:C8	2.44	0.53
27:a:1429:G:H2'	27:a:1430:G:H8	1.73	0.53
27:a:2081:U:H2'	27:a:2082:A:H8	1.73	0.53
30:d:136:ASN:ND2	30:d:139:SER:O	2.39	0.53
35:i:58:ASN:HB3	35:i:61:LYS:HD2	1.91	0.53
25:Y:57:G:O2'	25:Y:58:A:OP1	2.25	0.53
27:a:210:C:OP1	54:l:29:GLN:NE2	2.42	0.53
27:a:358:U:H2'	27:a:359:G:C8	2.44	0.53
27:a:1704:C:H2'	27:a:1705:A:H8	1.74	0.53
27:a:1847:A:O2'	27:a:1848:A:H8	1.92	0.53
32:f:49:LEU:HD22	32:f:148:ARG:HH12	1.74	0.53
33:g:89:LEU:HD22	33:g:162:VAL:HG22	1.90	0.53
47:u:1:MET:HE1	47:u:53:LYS:HD3	1.90	0.53
1:A:41:G:H2'	1:A:42:G:H8	1.74	0.52
1:A:514:C:H2'	1:A:515:G:H8	1.74	0.52
1:A:1226:C:OP2	13:M:102:THR:OG1	2.20	0.52
1:A:1314:C:H2'	1:A:1315:U:H6	1.74	0.52
1:A:1513:A:H2'	1:A:1514:G:C8	2.44	0.52
27:a:302:C:H2'	27:a:303:G:H8	1.73	0.52
27:a:1361:G:H2'	27:a:1362:C:C6	2.44	0.52
27:a:1443:U:H2'	27:a:1444:G:H8	1.73	0.52
27:a:1716:U:H2'	27:a:1717:A:H8	1.74	0.52
27:a:2285:C:OP2	53:0:6:ARG:NH1	2.36	0.52
1:A:228:A:O2'	16:P:63:GLN:NE2	2.43	0.52
17:Q:46:VAL:HG21	17:Q:61:ILE:HG21	1.91	0.52
27:a:1744:A:H3'	27:a:1745:A:H8	1.74	0.52
27:a:1796:U:H2'	27:a:1797:G:C8	2.45	0.52
44:r:2:GLU:HG2	44:r:108:SER:HB3	1.90	0.52
52:z:43:ILE:HG22	52:z:49:TYR:HB2	1.89	0.52
1:A:600:A:H2'	1:A:601:G:H8	1.75	0.52
27:a:438:G:H2'	27:a:439:A:H8	1.73	0.52
27:a:1141:U:H4'	27:a:1142:A:O4'	2.09	0.52
27:a:2328:A:H2'	27:a:2329:U:C6	2.44	0.52
28:b:48:U:H2'	28:b:49:C:C6	2.45	0.52
36:j:26:GLY:HA3	36:j:30:ARG:HH11	1.73	0.52
1:A:1359:C:OP2	14:N:75:ARG:NH1	2.41	0.52
27:a:155:A:H2'	27:a:156:A:C8	2.45	0.52
27:a:717:C:H3'	27:a:718:A:H8	1.74	0.52
22:V:326:TYR:HA	22:V:333:ILE:HG12	1.90	0.52
27:a:927:A:H2'	27:a:928:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:2804:U:H2'	27:a:2805:C:H6	1.75	0.52
28:b:115:A:H2'	28:b:116:G:H8	1.74	0.52
55:2:16:LYS:HE3	55:2:20:GLY:HA2	1.92	0.52
1:A:824:G:H2'	1:A:825:A:H8	1.75	0.52
11:K:116:ILE:HD11	21:U:32:VAL:HG22	1.92	0.52
27:a:1361:G:H2'	27:a:1362:C:H6	1.75	0.52
27:a:2291:U:H2'	27:a:2292:U:C6	2.45	0.52
1:A:258:G:H1	1:A:268:U:H3	1.58	0.52
1:A:993:G:O2'	1:A:994:A:N7	2.41	0.52
4:D:15:GLU:OE2	4:D:63:ARG:NH1	2.43	0.52
27:a:360:U:H3'	27:a:361:G:C8	2.44	0.52
27:a:720:U:H2'	27:a:721:A:C8	2.45	0.52
37:k:55:MET:O	37:k:60:ARG:NH1	2.43	0.52
1:A:393:A:C2	1:A:394:G:C8	2.97	0.52
1:A:745:G:H2'	1:A:746:A:H8	1.75	0.52
18:R:37:GLY:O	18:R:63:ARG:NH2	2.43	0.52
27:a:250:G:O2'	27:a:251:A:OP1	2.25	0.52
27:a:796:C:H2'	27:a:797:G:C8	2.45	0.52
27:a:2233:U:H2'	27:a:2234:G:C8	2.45	0.52
52:z:53:LYS:HE2	52:z:56:ALA:HA	1.91	0.52
1:A:909:A:N3	1:A:1413:A:O2'	2.42	0.52
27:a:580:U:H2'	27:a:581:C:C6	2.45	0.52
27:a:633:A:O2'	27:a:2404:U:OP1	2.28	0.52
1:A:460:A:H2'	1:A:461:A:C8	2.45	0.51
27:a:671:C:OP1	37:k:43:GLY:N	2.34	0.51
27:a:675:A:N3	27:a:2443:C:O2'	2.43	0.51
27:a:830:G:OP1	60:a:6193:SPD:N1	2.43	0.51
27:a:1825:U:H2'	27:a:1826:G:C8	2.45	0.51
39:m:44:LEU:HD23	39:m:113:ILE:HD13	1.91	0.51
1:A:579:A:H2'	1:A:580:C:C6	2.45	0.51
1:A:976:G:OP2	1:A:1358:U:O2'	2.28	0.51
1:A:1391:U:H2'	1:A:1392:G:C8	2.45	0.51
4:D:150:LYS:HA	4:D:178:MET:HE1	1.92	0.51
22:V:304:ASN:HA	22:V:307:LYS:HG2	1.91	0.51
27:a:339:U:H2'	27:a:340:A:H8	1.75	0.51
27:a:1746:A:H2'	27:a:1747:U:C6	2.45	0.51
27:a:1997:C:OP2	30:d:129:THR:OG1	2.22	0.51
27:a:2014:A:H2'	27:a:2015:A:C8	2.45	0.51
27:a:411:G:OP2	27:a:2406:A:O2'	2.21	0.51
27:a:827:U:OP1	27:a:2429:G:OP2	2.29	0.51
27:a:1281:G:H2'	27:a:1282:U:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:1306:C:H2'	27:a:1307:A:H8	1.75	0.51
27:a:1528:A:H2'	27:a:1529:G:O4'	2.10	0.51
27:a:1987:A:H2'	27:a:1988:G:H8	1.74	0.51
1:A:56:U:H2'	1:A:57:G:C8	2.45	0.51
6:F:29:ILE:HG21	6:F:64:VAL:HG11	1.93	0.51
22:V:66:VAL:HA	22:V:113:LEU:HD21	1.92	0.51
5:E:88:VAL:HG22	5:E:93:ARG:HG2	1.91	0.51
9:I:54:LEU:HD23	9:I:98:LEU:HD23	1.90	0.51
27:a:75:G:H22	27:a:111:A:H2	1.57	0.51
27:a:2547:A:H2'	27:a:2548:U:C6	2.45	0.51
27:a:2598:A:H5''	29:c:234:GLY:HA3	1.93	0.51
1:A:1183:U:O2'	1:A:1185:G:OP2	2.29	0.51
3:C:64:ILE:HG22	3:C:97:VAL:HG23	1.93	0.51
27:a:665:U:H2'	27:a:666:A:H8	1.76	0.51
27:a:1527:G:N1	27:a:1544:A:OP2	2.40	0.51
27:a:2812:G:H2'	27:a:2813:A:H8	1.76	0.51
47:u:68:LYS:HE2	47:u:70:ILE:HG12	1.92	0.51
25:Y:8:U:O2'	25:Y:21:A:N1	2.36	0.51
27:a:2233:U:H2'	27:a:2234:G:H8	1.74	0.51
1:A:104:G:N7	20:T:9:LYS:NZ	2.44	0.51
1:A:1287:A:H2'	1:A:1288:A:C8	2.45	0.51
27:a:521:U:H2'	27:a:522:A:H8	1.76	0.51
27:a:582:A:H2'	27:a:583:G:C8	2.46	0.51
27:a:880:G:H3'	27:a:881:G:H5''	1.93	0.51
27:a:1709:U:H2'	27:a:1710:G:C8	2.46	0.51
27:a:2836:U:H2'	27:a:2837:A:H8	1.76	0.51
27:a:2861:U:H2'	27:a:2862:G:H8	1.76	0.51
1:A:337:G:H2'	1:A:338:A:C8	2.44	0.51
1:A:662:U:OP2	6:F:93:LYS:NZ	2.39	0.51
1:A:1291:U:H2'	1:A:1292:G:H8	1.75	0.51
22:V:120:SER:O	22:V:193:ARG:NH1	2.43	0.51
27:a:2537:U:H2'	27:a:2538:C:H6	1.74	0.51
27:a:2605:PSU:C4	27:a:2606:C:C5	2.99	0.51
27:a:2837:A:H2'	27:a:2838:G:H8	1.76	0.51
1:A:235:C:H2'	1:A:236:A:C8	2.46	0.51
1:A:358:U:H2'	1:A:359:G:C8	2.45	0.51
1:A:1175:G:H2'	1:A:1176:A:C8	2.43	0.51
27:a:741:U:H2'	27:a:742:A:H8	1.76	0.51
1:A:707:U:H2'	1:A:708:C:H6	1.75	0.50
1:A:1328:C:C2	1:A:1329:A:C8	2.99	0.50
1:A:1414:U:H2'	1:A:1415:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:299:A:N3	27:a:319:G:O2'	2.40	0.50
27:a:1219:U:H2'	27:a:1220:G:C8	2.46	0.50
27:a:1720:U:H2'	27:a:1721:G:O4'	2.11	0.50
27:a:2241:A:H2'	27:a:2242:G:C8	2.46	0.50
28:b:60:C:H2'	28:b:61:G:C8	2.46	0.50
35:i:57:LEU:HD11	35:i:130:HIS:HD2	1.75	0.50
1:A:524:G:H2'	1:A:525:C:C6	2.46	0.50
6:F:1:MET:HE3	6:F:65:GLU:HG2	1.93	0.50
16:P:1:MET:SD	16:P:1:MET:N	2.81	0.50
27:a:554:U:H2'	27:a:555:G:O4'	2.11	0.50
27:a:910:A:H2'	27:a:911:A:C8	2.47	0.50
27:a:1509:A:H2'	27:a:1510:G:C8	2.46	0.50
27:a:2070:A:H2'	27:a:2071:A:H8	1.76	0.50
27:a:2804:U:H2'	27:a:2805:C:C6	2.46	0.50
55:2:28:ASN:O	55:2:36:LYS:NZ	2.39	0.50
1:A:460:A:H2'	1:A:461:A:H8	1.76	0.50
1:A:1142:G:C2	1:A:1143:G:H1'	2.46	0.50
4:D:102:VAL:HG21	4:D:123:ILE:HD13	1.92	0.50
27:a:4:U:H2'	27:a:5:A:H8	1.75	0.50
27:a:1752:C:H2'	27:a:1753:G:C8	2.46	0.50
27:a:1798:U:OP2	29:c:271:ARG:NH1	2.28	0.50
27:a:2645:G:OP2	27:a:2645:G:N2	2.23	0.50
27:a:139:U:H5''	27:a:140:C:H5	1.76	0.50
27:a:1438:U:H2'	27:a:1439:A:H8	1.77	0.50
27:a:1796:U:H2'	27:a:1797:G:H8	1.76	0.50
33:g:127:THR:OG1	33:g:130:GLU:OE1	2.30	0.50
37:k:132:ARG:HG3	37:k:142:ILE:HD12	1.94	0.50
1:A:3:A:H5''	1:A:4:U:O4'	2.10	0.50
1:A:908:A:H2'	1:A:909:A:H8	1.76	0.50
1:A:1143:G:H2'	1:A:1144:G:H8	1.76	0.50
18:R:23:TYR:HA	18:R:29:LEU:HD11	1.92	0.50
27:a:494:G:H4'	44:r:6:LYS:HB2	1.93	0.50
27:a:549:G:H2'	27:a:550:C:C6	2.47	0.50
27:a:1288:G:OP2	27:a:1288:G:N2	2.28	0.50
1:A:1228:C:H1'	13:M:116:ILE:HD11	1.94	0.50
1:A:1251:A:H2'	1:A:1252:A:C8	2.47	0.50
1:A:1404:C:H2'	1:A:1405:G:C8	2.47	0.50
3:C:24:ALA:HB1	3:C:28:GLU:HG2	1.93	0.50
25:Y:63:C:H2'	25:Y:64:G:C8	2.46	0.50
27:a:152:A:H2'	27:a:153:U:C6	2.45	0.50
27:a:2070:A:H2'	27:a:2071:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:49:C:H2'	28:b:50:A:C8	2.46	0.50
43:q:14:VAL:HG12	43:q:20:VAL:HG11	1.93	0.50
20:T:20:HIS:O	20:T:24:ARG:HG2	2.12	0.50
27:a:365:U:H2'	27:a:366:C:C6	2.47	0.50
27:a:593:U:H2'	27:a:594:U:C6	2.47	0.50
27:a:2025:C:H2'	27:a:2026:U:C6	2.46	0.50
27:a:2731:G:H2'	27:a:2732:G:C8	2.47	0.50
36:j:43:ILE:HD12	36:j:56:ASP:HB2	1.93	0.50
1:A:67:C:H2'	1:A:68:G:C8	2.47	0.50
1:A:539:A:H2'	1:A:540:G:C8	2.47	0.50
5:E:72:ILE:HD13	5:E:141:ILE:HG23	1.93	0.50
28:b:111:U:H2'	28:b:112:G:H8	1.76	0.50
1:A:746:A:H2'	1:A:747:A:H8	1.75	0.50
11:K:87:LYS:HB2	11:K:113:VAL:HG23	1.94	0.50
27:a:155:A:H2'	27:a:156:A:H8	1.76	0.50
27:a:1441:G:H2'	27:a:1442:U:C6	2.46	0.50
27:a:1682:G:H2'	27:a:1683:U:C6	2.47	0.50
27:a:2079:U:O2'	49:w:23:ASN:OD1	2.29	0.50
27:a:2522:U:O2'	27:a:2647:U:OP1	2.26	0.50
27:a:2897:U:H2'	27:a:2898:U:C6	2.47	0.50
32:f:103:LEU:HD12	32:f:107:ALA:HB3	1.93	0.50
33:g:17:VAL:HG11	33:g:50:LEU:HD21	1.92	0.50
1:A:950:U:H2'	1:A:951:G:C8	2.47	0.49
4:D:61:VAL:HG21	4:D:200:ILE:HD11	1.94	0.49
27:a:1223:G:N2	27:a:1226:A:OP2	2.37	0.49
27:a:1406:U:H2'	27:a:1407:G:H8	1.77	0.49
27:a:1927:A:H2'	27:a:1928:A:C8	2.47	0.49
27:a:2329:U:H2'	27:a:2330:G:C8	2.47	0.49
27:a:2625:G:H2'	27:a:2626:C:C6	2.46	0.49
27:a:2897:U:H2'	27:a:2898:U:H6	1.77	0.49
28:b:48:U:H2'	28:b:49:C:H6	1.77	0.49
38:l:17:ASN:O	38:l:38:ARG:NH1	2.45	0.49
1:A:28:A:O2'	1:A:296:U:OP1	2.25	0.49
1:A:1522:U:H2'	1:A:1523:G:H8	1.76	0.49
1:A:1524:C:H2'	1:A:1525:G:C8	2.46	0.49
1:A:1524:C:H2'	1:A:1525:G:H8	1.77	0.49
3:C:50:ALA:HB1	3:C:76:VAL:HG22	1.93	0.49
5:E:81:LEU:HB2	5:E:98:PRO:HG3	1.94	0.49
27:a:1563:U:H2'	27:a:1564:C:C6	2.46	0.49
27:a:1704:C:H2'	27:a:1705:A:C8	2.47	0.49
27:a:2787:C:H1'	30:d:63:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:k:77:ILE:HD13	37:k:108:ALA:HB1	1.93	0.49
1:A:728:A:H2'	1:A:729:A:C8	2.47	0.49
1:A:1172:C:H2'	1:A:1173:U:H6	1.77	0.49
27:a:639:U:H2'	27:a:640:C:C6	2.48	0.49
27:a:1164:C:H2'	27:a:1165:A:H8	1.77	0.49
27:a:1476:U:H2'	27:a:1477:A:H8	1.78	0.49
27:a:1570:A:H2'	27:a:1571:A:C8	2.47	0.49
27:a:1672:A:C2	27:a:2582:G:H5'	2.47	0.49
27:a:2523:G:HO2'	27:a:2764:A:HO2'	1.60	0.49
1:A:1376:U:H2'	1:A:1377:A:C8	2.47	0.49
9:I:19:VAL:HG13	9:I:65:ILE:HG12	1.94	0.49
10:J:66:GLU:HB3	14:N:99:ALA:HB3	1.93	0.49
27:a:1387:A:H2'	27:a:1388:G:H8	1.76	0.49
27:a:2796:U:H3	27:a:2799:A:H61	1.60	0.49
1:A:1238:A:OP1	1:A:1335:U:O2'	2.20	0.49
27:a:645:C:H2'	27:a:647:G:C8	2.47	0.49
27:a:1387:A:H2'	27:a:1388:G:C8	2.48	0.49
30:d:152:PRO:HB2	30:d:154:LYS:HG2	1.94	0.49
38:l:10:ARG:HE	38:l:11:LYS:HE3	1.77	0.49
49:w:39:TRP:NE1	49:w:41:GLU:OE1	2.42	0.49
1:A:945:G:C2	1:A:946:A:C8	3.00	0.49
9:I:28:ILE:HD12	9:I:35:LEU:HD22	1.94	0.49
12:L:114:ARG:HB3	12:L:119:VAL:HB	1.94	0.49
27:a:574:A:N6	27:a:2034:U:OP1	2.46	0.49
27:a:624:C:O2'	27:a:657:U:OP1	2.30	0.49
27:a:2020:A:H5'	52:z:9:THR:HG21	1.94	0.49
1:A:801:U:H2'	1:A:802:A:H8	1.76	0.49
1:A:1000:A:H2'	1:A:1001:C:C6	2.48	0.49
1:A:1151:A:O2'	1:A:1152:A:H8	1.96	0.49
1:A:1513:A:H2'	1:A:1514:G:H8	1.77	0.49
4:D:202:GLU:OE1	5:E:112:ARG:NH1	2.42	0.49
27:a:358:U:H2'	27:a:359:G:H8	1.77	0.49
27:a:851:C:H2'	27:a:852:U:C6	2.47	0.49
27:a:1032:A:H1'	56:3:23:ILE:HD13	1.95	0.49
27:a:1548:A:H2'	27:a:1549:A:C8	2.48	0.49
27:a:1571:A:H2'	27:a:1572:A:H8	1.77	0.49
35:i:13:ARG:NH2	35:i:49:ASP:O	2.41	0.49
1:A:154:U:H2'	1:A:155:A:H8	1.78	0.49
27:a:888:C:H2'	27:a:889:C:O4'	2.13	0.49
27:a:2419:U:H4'	53:0:22:THR:HG21	1.95	0.49
1:A:217:C:H2'	1:A:218:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:C:H2'	1:A:1029:U:O4'	2.12	0.49
2:B:115:LYS:O	2:B:118:GLU:HG2	2.13	0.49
4:D:44:ARG:HG3	4:D:46:PRO:HD3	1.95	0.49
27:a:741:U:H2'	27:a:742:A:C8	2.48	0.49
27:a:1049:C:C2	27:a:1050:A:C8	3.01	0.49
27:a:1864:U:OP1	27:a:2410:G:O2'	2.26	0.49
27:a:2799:A:O2'	27:a:2800:A:H5''	2.13	0.49
27:a:2845:U:H5''	41:o:52:ASN:O	2.12	0.49
46:t:26:LYS:HE3	46:t:37:GLU:HB2	1.93	0.49
1:A:458:U:O4	1:A:474:G:O6	2.31	0.49
27:a:1433:A:H2'	27:a:1434:A:C8	2.48	0.49
27:a:1870:C:H3'	27:a:1871:A:H8	1.78	0.49
27:a:2788:C:H2'	27:a:2789:C:C6	2.47	0.49
32:f:108:VAL:HG11	32:f:176:PRO:HG3	1.95	0.49
33:g:107:LEU:O	33:g:152:ARG:NH2	2.41	0.49
1:A:333:U:H2'	1:A:334:C:H6	1.79	0.48
27:a:828:U:H2'	27:a:829:A:C8	2.47	0.48
27:a:1406:U:H2'	27:a:1407:G:C8	2.48	0.48
1:A:380:G:N2	1:A:383:A:OP2	2.34	0.48
1:A:591:U:H2'	1:A:592:G:H8	1.77	0.48
1:A:912:C:H2'	1:A:913:A:C8	2.48	0.48
1:A:923:A:O2'	1:A:1399:C:OP2	2.29	0.48
1:A:1143:G:H2'	1:A:1144:G:C8	2.48	0.48
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.95	0.48
46:t:8:ASP:HA	46:t:24:LYS:HE3	1.95	0.48
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.95	0.48
50:x:9:LYS:HB3	50:x:13:GLU:HB2	1.94	0.48
13:M:34:LEU:HD13	13:M:41:GLU:HA	1.96	0.48
27:a:172:A:H2'	27:a:173:A:C8	2.48	0.48
27:a:2898:U:H2'	27:a:2899:A:C8	2.47	0.48
29:c:35:GLU:HG3	29:c:64:ILE:HD11	1.96	0.48
43:q:5:PHE:HB3	43:q:59:ILE:HD12	1.95	0.48
1:A:384:G:H2'	1:A:385:C:H6	1.79	0.48
1:A:674:G:H2'	1:A:675:A:C8	2.46	0.48
1:A:923:A:H2'	1:A:924:C:C6	2.48	0.48
1:A:1507:A:H2'	1:A:1508:A:C8	2.48	0.48
27:a:569:U:O2'	27:a:983:A:N1	2.45	0.48
13:M:33:ILE:HD13	13:M:60:VAL:HG22	1.95	0.48
27:a:1190:G:H2'	27:a:1191:G:H8	1.78	0.48
27:a:1198:U:H2'	27:a:1199:U:C6	2.49	0.48
27:a:1853:A:H2'	27:a:1854:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:2243:U:H2'	27:a:2244:U:C6	2.48	0.48
1:A:601:G:H2'	1:A:602:A:H8	1.79	0.48
27:a:279:A:C2	27:a:362:A:H5'	2.48	0.48
27:a:1771:C:H2'	27:a:1772:A:H8	1.77	0.48
27:a:2076:U:OP2	27:a:2238:G:N2	2.36	0.48
31:e:5:LEU:HD23	31:e:122:GLU:HB3	1.95	0.48
1:A:41:G:H2'	1:A:42:G:C8	2.49	0.48
1:A:1060:U:H2'	1:A:1061:G:H8	1.79	0.48
1:A:1162:C:H2'	1:A:1163:A:H8	1.78	0.48
1:A:1305:G:N2	1:A:1331:G:O2'	2.45	0.48
3:C:70:THR:HG21	3:C:76:VAL:HG21	1.95	0.48
27:a:75:G:H2'	27:a:75:G:N3	2.27	0.48
27:a:264:C:O2'	27:a:265:A:O5'	2.28	0.48
27:a:354:A:H2'	27:a:355:U:O4'	2.12	0.48
27:a:2250:G:O2'	27:a:2496:C:OP1	2.31	0.48
27:a:2405:G:O2'	27:a:2411:A:N6	2.46	0.48
30:d:8:LYS:NZ	30:d:195:GLY:O	2.40	0.48
32:f:44:ILE:HG21	32:f:79:ILE:HG22	1.96	0.48
47:u:30:ILE:HG12	47:u:91:PHE:HB2	1.95	0.48
1:A:1191:A:OP2	3:C:2:GLY:N	2.47	0.48
25:Y:65:U:H2'	25:Y:66:C:C6	2.48	0.48
27:a:1825:U:H2'	27:a:1826:G:H8	1.78	0.48
38:l:11:LYS:HD3	38:l:86:LYS:HD3	1.95	0.48
55:2:26:HIS:NE2	55:2:48:ALA:HB2	2.29	0.48
1:A:1149:C:H2'	1:A:1150:A:C8	2.41	0.48
27:a:967:U:H2'	27:a:968:C:C6	2.49	0.48
27:a:1432:G:H2'	27:a:1433:A:H8	1.77	0.48
28:b:1:U:H2'	28:b:2:G:H8	1.79	0.48
37:k:62:PRO:HB2	55:2:30:ARG:HH21	1.77	0.48
1:A:464:U:N3	1:A:467:U:OP2	2.44	0.47
1:A:539:A:H2'	1:A:540:G:H8	1.79	0.47
1:A:634:C:H2'	1:A:635:A:H8	1.78	0.47
1:A:867:G:O2'	1:A:873:A:N1	2.45	0.47
1:A:868:C:H2'	1:A:869:G:O4'	2.14	0.47
1:A:966:2MG:N2	25:Y:34:G:H5'	2.28	0.47
1:A:1222:G:OP2	1:A:1322:C:N4	2.45	0.47
1:A:1479:C:H2'	1:A:1480:A:C8	2.48	0.47
10:J:54:SER:OG	10:J:58:ASN:HB2	2.14	0.47
27:a:4:U:H2'	27:a:5:A:C8	2.48	0.47
27:a:20:C:H2'	27:a:21:A:H8	1.79	0.47
27:a:1028:A:H2'	27:a:1029:A:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:1538:G:H2'	27:a:1539:U:H6	1.78	0.47
1:A:439:U:H4'	4:D:121:LYS:HD3	1.96	0.47
1:A:459:A:H2'	1:A:460:A:C8	2.50	0.47
4:D:177:LYS:HG3	4:D:179:GLU:HG2	1.95	0.47
25:Y:29:U:H2'	25:Y:30:G:H8	1.78	0.47
27:a:145:C:H2'	27:a:146:A:H8	1.79	0.47
27:a:729:G:O2'	27:a:763:G:H4'	2.14	0.47
27:a:827:U:O2'	27:a:2068:U:N3	2.47	0.47
27:a:1463:C:H2'	27:a:1464:G:H8	1.79	0.47
1:A:161:A:H2'	1:A:162:A:C8	2.49	0.47
1:A:1401:G:H2'	1:A:1402:4OC:O4'	2.13	0.47
6:F:6:ILE:HB	6:F:62:MET:HG3	1.95	0.47
27:a:629:G:H1'	27:a:639:U:H1'	1.95	0.47
27:a:849:A:H61	27:a:928:A:N6	2.12	0.47
27:a:1405:U:H2'	27:a:1406:U:C6	2.49	0.47
27:a:1463:C:H2'	27:a:1464:G:C8	2.50	0.47
27:a:1727:C:H2'	27:a:1728:C:O4'	2.13	0.47
35:i:18:VAL:HG21	35:i:142:ILE:HD12	1.97	0.47
47:u:4:ILE:HG12	47:u:50:MET:HE1	1.97	0.47
10:J:52:LEU:HD23	10:J:62:ARG:HB3	1.97	0.47
12:L:50:ARG:HG3	12:L:90:LEU:HD21	1.96	0.47
27:a:250:G:HO2'	27:a:251:A:P	2.36	0.47
27:a:302:C:H2'	27:a:303:G:C8	2.48	0.47
27:a:2311:A:H1'	32:f:85:ILE:HD12	1.95	0.47
27:a:2557:G:H2'	27:a:2558:C:C6	2.49	0.47
27:a:2591:C:N4	27:a:2592:G:O6	2.47	0.47
30:d:25:THR:HG21	30:d:193:VAL:HG22	1.96	0.47
40:n:51:ALA:HB3	40:n:78:VAL:HB	1.96	0.47
1:A:229:U:H2'	1:A:230:G:C8	2.49	0.47
13:M:17:ILE:O	13:M:20:THR:OG1	2.24	0.47
13:M:83:LEU:HD21	19:S:65:GLU:HB2	1.95	0.47
27:a:685:A:N1	27:a:787:C:H1'	2.30	0.47
27:a:851:C:H2'	27:a:852:U:H6	1.80	0.47
27:a:1797:G:O2'	29:c:257:THR:OG1	2.31	0.47
27:a:2623:G:H2'	27:a:2624:G:H8	1.80	0.47
28:b:66:A:N6	28:b:107:G:H2'	2.30	0.47
48:v:59:LEU:HD12	48:v:80:ILE:HD12	1.97	0.47
1:A:950:U:H2'	1:A:951:G:H8	1.79	0.47
1:A:1011:C:H2'	1:A:1012:A:C8	2.49	0.47
1:A:1118:U:H1'	1:A:1179:A:C5	2.50	0.47
1:A:1140:C:H2'	1:A:1141:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:59:LEU:O	7:G:63:GLU:HG2	2.14	0.47
7:G:111:ARG:NH1	7:G:123:GLU:OE1	2.47	0.47
27:a:1007:C:OP1	35:i:37:ARG:NH1	2.45	0.47
27:a:1771:C:H2'	27:a:1772:A:C8	2.50	0.47
28:b:115:A:H2'	28:b:116:G:C8	2.48	0.47
1:A:17:U:H2'	1:A:18:C:C6	2.49	0.47
1:A:1217:C:OP2	14:N:9:ARG:NH2	2.40	0.47
19:S:11:ILE:HG13	19:S:38:SER:HB3	1.97	0.47
25:Y:23:A:H2'	25:Y:24:A:H8	1.78	0.47
27:a:145:C:H2'	27:a:146:A:C8	2.50	0.47
27:a:184:C:H2'	27:a:185:G:H8	1.79	0.47
27:a:419:U:H2'	27:a:420:C:H6	1.80	0.47
27:a:1564:C:H2'	27:a:1565:C:C6	2.50	0.47
27:a:2847:U:H2'	27:a:2848:G:O4'	2.14	0.47
37:k:78:ARG:HG2	37:k:113:ALA:HB3	1.97	0.47
1:A:1308:U:H2'	1:A:1309:G:C8	2.50	0.47
1:A:1363:A:O2'	1:A:1365:G:N7	2.40	0.47
3:C:138:VAL:HA	3:C:149:ILE:HD13	1.97	0.47
4:D:105:MET:HE1	4:D:143:VAL:HB	1.97	0.47
13:M:84:GLY:HA2	13:M:92:ARG:HH22	1.80	0.47
17:Q:19:LYS:H	17:Q:51:ASN:HD21	1.63	0.47
27:a:181:A:H1'	27:a:435:C:H5'	1.96	0.47
27:a:373:U:H2'	27:a:374:A:C8	2.50	0.47
27:a:414:C:H2'	27:a:415:A:C8	2.50	0.47
27:a:1000:A:H2'	27:a:1001:A:C8	2.50	0.47
27:a:1703:G:H2'	27:a:1704:C:H6	1.80	0.47
1:A:407:U:H2'	1:A:408:A:H8	1.80	0.47
1:A:994:A:C4	1:A:1216:A:H4'	2.50	0.47
1:A:1001:C:H2'	1:A:1002:G:H8	1.79	0.47
1:A:1399:C:O2	1:A:1502:A:N6	2.48	0.47
4:D:58:LYS:HD3	4:D:203:LEU:HD23	1.96	0.47
11:K:87:LYS:HG3	11:K:115:PRO:HD3	1.96	0.47
27:a:629:G:N3	27:a:639:U:O2'	2.47	0.47
27:a:814:C:H2'	27:a:815:C:H6	1.79	0.47
27:a:1442:U:H2'	27:a:1443:U:C6	2.50	0.47
27:a:2229:U:H2'	27:a:2230:G:H8	1.79	0.47
27:a:2812:G:H2'	27:a:2813:A:C8	2.49	0.47
28:b:49:C:H2'	28:b:50:A:H8	1.79	0.47
1:A:1034:G:O2'	1:A:1035:A:H5'	2.15	0.47
3:C:14:ILE:HG22	3:C:15:VAL:HG13	1.97	0.47
27:a:191:A:H2'	27:a:192:C:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:796:C:H2'	27:a:797:G:H8	1.79	0.47
27:a:1636:U:H2'	27:a:1637:A:C8	2.50	0.47
27:a:1737:G:O5'	27:a:1737:G:H8	1.97	0.47
27:a:1847:A:H4'	27:a:1848:A:OP1	2.15	0.47
44:r:95:ARG:HH11	44:r:97:LEU:HD21	1.80	0.47
53:0:11:LEU:HB3	53:0:49:TYR:HB3	1.97	0.47
56:3:16:ILE:HG12	56:3:25:VAL:HG22	1.97	0.47
1:A:35:G:N3	12:L:115:SER:OG	2.43	0.46
1:A:195:A:N3	1:A:222:C:O2'	2.41	0.46
1:A:321:A:H2'	1:A:322:C:H6	1.78	0.46
1:A:672:U:H2'	1:A:673:A:H8	1.80	0.46
4:D:62:ARG:NH1	4:D:69:GLU:OE1	2.48	0.46
22:V:154:ARG:HH11	22:V:350:ASP:HB3	1.81	0.46
27:a:249:C:H4'	27:a:250:G:O5'	2.15	0.46
27:a:645:C:H2'	27:a:647:G:N7	2.30	0.46
27:a:874:G:H2'	27:a:875:G:H8	1.80	0.46
1:A:131:A:H2'	1:A:132:C:C6	2.50	0.46
1:A:472:U:H2'	1:A:473:U:C6	2.51	0.46
1:A:648:A:H2'	1:A:649:A:C8	2.49	0.46
6:F:29:ILE:HG22	6:F:34:GLY:HA3	1.96	0.46
6:F:42:TRP:HB2	6:F:59:TYR:HB2	1.97	0.46
27:a:1645:G:H5''	27:a:1646:C:H5'	1.97	0.46
27:a:1721:G:N2	27:a:1738:G:H2'	2.30	0.46
27:a:2483:C:N3	38:l:123:LYS:NZ	2.60	0.46
44:r:82:MET:HE3	44:r:98:LYS:HD3	1.96	0.46
1:A:559:A:H4'	1:A:560:A:H3'	1.97	0.46
4:D:170:TRP:HA	4:D:183:LYS:HE2	1.97	0.46
27:a:415:A:H2'	27:a:416:U:C6	2.50	0.46
27:a:1168:G:H2'	27:a:1169:A:H8	1.79	0.46
27:a:1529:G:H1	27:a:1542:U:H3	1.63	0.46
27:a:1710:G:H2'	27:a:1711:A:C8	2.50	0.46
27:a:2193:G:H2'	27:a:2194:U:C6	2.50	0.46
27:a:2728:U:O2'	27:a:2729:G:H8	1.97	0.46
29:c:62:TYR:HA	29:c:86:ASN:HD21	1.81	0.46
1:A:773:G:O6	1:A:807:A:N6	2.48	0.46
1:A:1063:C:OP2	1:A:1064:G:O2'	2.32	0.46
27:a:859:G:O2'	27:a:916:G:O6	2.32	0.46
27:a:1418:G:N2	27:a:1579:A:N7	2.64	0.46
27:a:1495:A:N3	27:a:1578:U:O2'	2.45	0.46
27:a:2081:U:H2'	27:a:2082:A:C8	2.51	0.46
1:A:127:G:H4'	17:Q:6:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:G:N1	1:A:327:A:OP2	2.48	0.46
1:A:634:C:H2'	1:A:635:A:C8	2.51	0.46
9:I:21:ILE:HG12	9:I:63:LEU:HG	1.98	0.46
27:a:570:G:H2'	27:a:2030:6MZ:N7	2.31	0.46
27:a:1278:C:H2'	27:a:1279:G:C8	2.50	0.46
27:a:1434:A:H2'	27:a:1435:G:C8	2.50	0.46
27:a:1443:U:H2'	27:a:1444:G:C8	2.51	0.46
27:a:1790:C:O2'	29:c:208:ALA:HB2	2.16	0.46
27:a:2626:C:H2'	27:a:2627:G:H8	1.81	0.46
28:b:95:U:H2'	28:b:96:G:H8	1.81	0.46
28:b:116:G:H2'	28:b:117:G:H8	1.80	0.46
38:l:75:GLU:HB2	38:l:90:GLU:HG3	1.96	0.46
47:u:6:ALA:HB3	47:u:65:VAL:HG22	1.97	0.46
1:A:916:U:H2'	1:A:917:G:H8	1.79	0.46
1:A:1217:C:P	14:N:9:ARG:HH21	2.37	0.46
5:E:13:GLU:HG2	5:E:39:VAL:HG12	1.96	0.46
5:E:77:ASN:HB2	5:E:82:GLN:CD	2.40	0.46
12:L:66:TYR:HB2	12:L:93:VAL:HG11	1.98	0.46
17:Q:19:LYS:H	17:Q:51:ASN:ND2	2.14	0.46
20:T:30:THR:HG22	20:T:34:LYS:HE3	1.98	0.46
27:a:813:U:H2'	27:a:814:C:C6	2.51	0.46
27:a:1954:G:O2'	27:a:1956:U:O4	2.29	0.46
27:a:2039:U:H2'	27:a:2040:G:C8	2.49	0.46
1:A:34:C:H2'	1:A:35:G:C8	2.49	0.46
1:A:384:G:H2'	1:A:385:C:C6	2.51	0.46
1:A:1152:A:P	10:J:72:ARG:HH22	2.39	0.46
27:a:709:U:H2'	27:a:710:U:C6	2.50	0.46
27:a:871:U:H2'	27:a:872:U:C6	2.51	0.46
27:a:1668:A:O2'	27:a:1674:G:N7	2.44	0.46
28:b:5:U:OP1	28:b:61:G:O2'	2.29	0.46
33:g:26:ILE:HD11	33:g:75:MET:HB3	1.96	0.46
1:A:1229:A:OP2	13:M:113:ARG:NH2	2.49	0.46
27:a:1:G:H2'	27:a:2:G:H8	1.80	0.46
27:a:2830:C:H5''	30:d:59:ARG:HE	1.81	0.46
32:f:22:TYR:HD1	32:f:27:GLN:HE21	1.64	0.46
32:f:62:GLY:O	32:f:95:ARG:NH2	2.49	0.46
57:4:28:VAL:HG11	57:4:32:LEU:HD21	1.98	0.46
1:A:672:U:H2'	1:A:673:A:C8	2.50	0.46
2:B:68:LEU:HD11	2:B:92:VAL:HG23	1.97	0.46
9:I:116:VAL:HG11	10:J:62:ARG:HG3	1.97	0.46
27:a:745:1MG:O2'	27:a:748:G:HI'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:1654:A:O2'	30:d:118:PHE:O	2.33	0.46
27:a:1856:U:H2'	27:a:1857:G:O4'	2.16	0.46
28:b:34:A:H5'	28:b:35:C:OP1	2.15	0.46
38:l:47:GLU:OE2	38:l:51:ARG:NE	2.47	0.46
38:l:102:LEU:HD11	38:l:126:ILE:HD11	1.97	0.46
1:A:1463:U:H2'	1:A:1464:U:C6	2.51	0.46
4:D:105:MET:HA	4:D:173:VAL:HG11	1.98	0.46
25:Y:35:U:H2'	25:Y:36:C:H6	1.81	0.46
27:a:764:A:H5'	29:c:209:GLY:HA2	1.98	0.46
27:a:1149:G:H2'	27:a:1150:C:C6	2.51	0.46
27:a:1447:C:H2'	27:a:1448:G:H8	1.80	0.46
27:a:1464:G:H2'	27:a:1465:G:C8	2.51	0.46
27:a:1880:U:H2'	27:a:1881:C:C6	2.51	0.46
27:a:2087:G:H2'	27:a:2088:A:H8	1.81	0.46
1:A:321:A:H2'	1:A:322:C:C6	2.50	0.45
1:A:1219:A:H2'	1:A:1220:G:C8	2.51	0.45
2:B:157:LEU:HD13	2:B:179:LEU:HD13	1.96	0.45
4:D:101:VAL:HG13	4:D:171:LEU:HD21	1.97	0.45
27:a:414:C:H2'	27:a:415:A:H8	1.80	0.45
27:a:2074:U:H2'	27:a:2075:U:C6	2.52	0.45
27:a:2687:U:H2'	27:a:2688:G:O4'	2.16	0.45
1:A:501:C:H1'	1:A:549:C:H1'	1.99	0.45
1:A:1005:A:O5'	1:A:1005:A:H8	1.99	0.45
15:O:64:ARG:NH1	15:O:68:ASP:OD1	2.49	0.45
27:a:151:C:H2'	27:a:152:A:C8	2.50	0.45
27:a:710:U:H2'	27:a:711:G:H8	1.81	0.45
27:a:739:A:H1'	27:a:740:C:H5	1.80	0.45
27:a:930:G:H1'	51:y:25:LEU:HD11	1.98	0.45
27:a:1028:A:N3	27:a:2486:C:O2'	2.39	0.45
1:A:440:C:C2	1:A:441:A:C8	3.05	0.45
1:A:783:C:H2'	1:A:784:A:H8	1.81	0.45
1:A:1014:A:C2	1:A:1219:A:H1'	2.52	0.45
7:G:5:ARG:HD2	7:G:5:ARG:HA	1.85	0.45
27:a:2266:A:H4'	27:a:2267:A:N3	2.31	0.45
51:y:31:ARG:HG2	51:y:34:HIS:HB2	1.98	0.45
1:A:195:A:H2'	1:A:196:A:C8	2.52	0.45
1:A:470:C:H2'	1:A:471:U:H6	1.81	0.45
1:A:537:G:H2'	1:A:538:G:H8	1.82	0.45
1:A:859:G:H2'	1:A:860:A:C8	2.52	0.45
1:A:1327:C:H2'	1:A:1328:C:C6	2.50	0.45
2:B:187:VAL:HG13	2:B:191:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:196:THR:HA	22:V:220:ALA:O	2.16	0.45
27:a:644:A:C2	27:a:2369:A:H1'	2.51	0.45
27:a:714:U:H1'	27:a:717:C:H5	1.81	0.45
27:a:1425:G:H2'	27:a:1426:G:C8	2.51	0.45
33:g:42:GLU:HA	33:g:55:ARG:HH21	1.80	0.45
36:j:7:MET:HE1	36:j:44:LYS:HG3	1.99	0.45
49:w:3:ARG:O	49:w:12:PRO:HD3	2.17	0.45
1:A:96:U:H2'	1:A:97:G:H8	1.81	0.45
1:A:1032:G:H3'	1:A:1032:G:N3	2.32	0.45
1:A:1488:G:H2'	1:A:1489:G:H8	1.81	0.45
14:N:27:LEU:HD21	14:N:47:LYS:HD3	1.98	0.45
27:a:584:C:N4	27:a:585:G:O6	2.48	0.45
27:a:587:C:H4'	27:a:588:U:H6	1.80	0.45
27:a:639:U:H2'	27:a:640:C:H6	1.81	0.45
27:a:689:A:H2'	27:a:690:G:C8	2.51	0.45
27:a:721:A:H2'	27:a:722:A:C8	2.51	0.45
27:a:876:C:H2'	27:a:877:A:O4'	2.16	0.45
27:a:2377:A:O2'	40:n:117:PHE:O	2.30	0.45
27:a:2430:A:N3	27:a:2430:A:H2'	2.31	0.45
38:l:25:ASP:O	38:l:66:ARG:NH1	2.50	0.45
1:A:154:U:H2'	1:A:155:A:C8	2.52	0.45
1:A:600:A:H2'	1:A:601:G:C8	2.51	0.45
1:A:801:U:H2'	1:A:802:A:C8	2.51	0.45
1:A:925:G:C2	1:A:927:G:C8	3.05	0.45
9:I:85:ARG:HA	9:I:88:MET:HE2	1.98	0.45
27:a:144:A:H2'	27:a:145:C:H6	1.82	0.45
27:a:549:G:H2'	27:a:550:C:H6	1.81	0.45
27:a:1009:A:N3	27:a:1153:C:O2'	2.47	0.45
27:a:1327:A:H2'	27:a:1328:A:O4'	2.17	0.45
27:a:1438:U:H2'	27:a:1439:A:C8	2.51	0.45
27:a:1726:C:H2'	27:a:1727:C:C6	2.52	0.45
27:a:2316:G:H2'	27:a:2317:A:H8	1.82	0.45
27:a:2327:A:H2'	27:a:2328:A:C8	2.52	0.45
27:a:2780:G:OP2	35:i:120:ARG:HD3	2.17	0.45
33:g:4:VAL:HG12	33:g:69:ARG:HG2	1.99	0.45
1:A:377:G:H5''	16:P:24:SER:HB2	1.98	0.45
11:K:35:THR:HG22	11:K:41:ALA:HA	1.99	0.45
27:a:312:G:H2'	27:a:313:G:H8	1.81	0.45
27:a:320:A:H4'	27:a:322:A:N7	2.31	0.45
27:a:441:U:H2'	27:a:442:G:C8	2.52	0.45
27:a:623:C:H2'	27:a:624:C:C6	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:748:G:OP2	60:a:6197:SPD:N10	2.40	0.45
27:a:1198:U:H2'	27:a:1199:U:H6	1.81	0.45
27:a:1734:G:H2'	27:a:1735:A:H8	1.81	0.45
27:a:2314:A:OP1	32:f:88:LYS:NZ	2.50	0.45
27:a:2747:G:O6	27:a:2755:C:H5''	2.15	0.45
1:A:35:G:H2'	1:A:36:C:C6	2.51	0.45
1:A:255:G:H2'	1:A:256:U:C6	2.52	0.45
1:A:344:A:H5''	1:A:345:C:H5	1.82	0.45
14:N:53:ARG:HB3	14:N:59:ARG:NH1	2.32	0.45
27:a:682:G:H5'	54:l:26:ASN:CG	2.42	0.45
27:a:817:C:H2'	27:a:818:G:O4'	2.17	0.45
27:a:947:A:H2'	27:a:948:C:C6	2.52	0.45
35:i:125:TYR:OH	35:i:132:HIS:NE2	2.42	0.45
1:A:1437:A:H2'	1:A:1438:G:H8	1.81	0.45
27:a:703:U:H2'	27:a:704:G:O4'	2.16	0.45
27:a:784:G:H5'	27:a:785:G:OP1	2.16	0.45
27:a:1161:C:H2'	27:a:1162:G:H8	1.81	0.45
27:a:1315:C:O2'	27:a:1392:A:N3	2.49	0.45
27:a:1830:C:H2'	27:a:1831:G:H8	1.82	0.45
27:a:2037:A:H2'	27:a:2038:G:C8	2.51	0.45
32:f:119:ALA:HB1	32:f:167:ARG:HH11	1.81	0.45
32:f:158:THR:HG22	32:f:160:ALA:H	1.82	0.45
38:l:10:ARG:HG3	38:l:11:LYS:HG3	1.99	0.45
1:A:187:G:N2	1:A:190:A:OP2	2.46	0.45
1:A:537:G:H5''	12:L:110:ARG:NH1	2.32	0.45
1:A:1000:A:H2'	1:A:1001:C:H6	1.82	0.45
1:A:1090:U:H2'	1:A:1091:U:C6	2.52	0.45
1:A:1460:C:C2	1:A:1461:G:C8	3.04	0.45
13:M:71:ARG:NH2	32:f:113:ASP:OD2	2.50	0.45
27:a:2815:C:H2'	27:a:2816:G:H8	1.82	0.45
1:A:1425:U:H2'	1:A:1426:G:H8	1.81	0.44
20:T:35:VAL:HG11	20:T:79:LEU:HD13	2.00	0.44
27:a:347:A:H2'	27:a:348:A:C8	2.52	0.44
27:a:594:U:H2'	27:a:595:C:C6	2.52	0.44
27:a:981:A:OP2	27:a:982:C:N4	2.44	0.44
27:a:1523:U:H3'	27:a:1524:G:H8	1.81	0.44
27:a:2720:U:C2	27:a:2721:A:C8	3.05	0.44
28:b:93:C:OP2	47:u:18:ARG:NH1	2.50	0.44
45:s:11:LEU:O	50:x:29:ARG:NH2	2.45	0.44
1:A:1119:C:H2'	1:A:1120:C:H6	1.82	0.44
1:A:1319:A:O2'	1:A:1323:G:N7	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1407:5MC:H2'	1:A:1408:A:H8	1.81	0.44
27:a:264:C:H4'	27:a:265:A:OP1	2.17	0.44
27:a:476:G:N1	27:a:479:A:OP2	2.40	0.44
27:a:724:U:H2'	27:a:725:G:C8	2.52	0.44
27:a:1130:U:C2	27:a:2025:C:H5''	2.52	0.44
27:a:2215:C:H2'	27:a:2216:G:C8	2.52	0.44
27:a:2547:A:H4'	36:j:29:HIS:CE1	2.52	0.44
32:f:8:TYR:HB2	32:f:173:PHE:CZ	2.52	0.44
32:f:38:MET:HE3	32:f:57:LEU:HD13	1.98	0.44
36:j:38:ILE:HD11	36:j:112:PHE:HZ	1.83	0.44
42:p:106:PHE:HA	42:p:109:LEU:HD12	1.99	0.44
1:A:69:G:H2'	1:A:70:U:C6	2.52	0.44
1:A:214:C:C2	1:A:215:C:C5	3.05	0.44
1:A:1134:G:H2'	1:A:1135:U:O4'	2.18	0.44
1:A:1241:G:H2'	1:A:1242:G:H8	1.82	0.44
1:A:1355:G:H2'	1:A:1356:G:H8	1.81	0.44
10:J:12:ALA:HB3	10:J:18:ILE:HB	1.99	0.44
27:a:265:A:O2'	27:a:428:A:N6	2.50	0.44
27:a:540:C:H2'	27:a:541:A:H8	1.82	0.44
27:a:979:A:H2'	27:a:982:C:H42	1.82	0.44
27:a:2215:C:H2'	27:a:2216:G:H8	1.82	0.44
27:a:2329:U:H2'	27:a:2330:G:H8	1.82	0.44
32:f:36:LEU:HD22	32:f:154:ILE:HG12	1.98	0.44
36:j:99:ILE:HD13	36:j:118:LEU:HB2	1.99	0.44
53:O:35:GLU:HG2	53:O:50:LYS:HG2	2.00	0.44
1:A:171:A:H2'	1:A:172:A:C8	2.52	0.44
1:A:922:G:H2'	1:A:923:A:C8	2.53	0.44
1:A:1253:G:H2'	1:A:1254:A:H8	1.82	0.44
4:D:170:TRP:CE2	4:D:186:PRO:HB3	2.53	0.44
27:a:513:A:H5''	27:a:1216:G:O2'	2.17	0.44
27:a:1145:C:N3	27:a:1146:C:C5	2.86	0.44
27:a:1196:C:H2'	27:a:1197:G:H8	1.82	0.44
27:a:1883:U:H2'	27:a:1884:G:O4'	2.18	0.44
1:A:470:C:H2'	1:A:471:U:C6	2.52	0.44
1:A:908:A:H2'	1:A:909:A:C8	2.53	0.44
1:A:958:A:C2	19:S:55:ARG:HB3	2.53	0.44
1:A:1095:U:H2'	1:A:1096:C:C6	2.52	0.44
1:A:1333:A:H2'	1:A:1334:G:O4'	2.18	0.44
9:I:7:TYR:HE1	9:I:18:ARG:HB2	1.81	0.44
10:J:52:LEU:HB2	14:N:81:ARG:HD2	1.98	0.44
27:a:577:G:H2'	27:a:578:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:863:A:H2'	27:a:864:G:H8	1.82	0.44
27:a:964:C:N3	27:a:965:C:C5	2.86	0.44
27:a:1716:U:H2'	27:a:1717:A:C8	2.51	0.44
27:a:2078:C:H2'	27:a:2079:U:C6	2.53	0.44
27:a:2532:G:N2	27:a:2663:G:O2'	2.51	0.44
27:a:2850:A:N7	27:a:2868:A:O2'	2.38	0.44
32:f:33:LYS:HD3	32:f:92:ARG:NH2	2.33	0.44
1:A:982:U:H5''	14:N:6:MET:HE3	1.99	0.44
22:V:241:ILE:HG12	22:V:263:ILE:HG12	2.00	0.44
27:a:171:U:H2'	27:a:172:A:H8	1.82	0.44
27:a:310:A:H5''	46:t:15:THR:HG23	1.98	0.44
27:a:638:G:H2'	27:a:639:U:C6	2.52	0.44
27:a:948:C:H2'	27:a:949:G:H8	1.82	0.44
27:a:1144:A:H2'	27:a:1145:C:H6	1.83	0.44
27:a:1447:C:H2'	27:a:1448:G:C8	2.52	0.44
27:a:1506:U:H2'	27:a:1507:C:H6	1.80	0.44
27:a:1518:C:H2'	27:a:1519:G:H8	1.83	0.44
27:a:2193:G:H2'	27:a:2194:U:H6	1.82	0.44
28:b:39:A:H2'	28:b:40:U:C6	2.53	0.44
1:A:20:U:H2'	1:A:21:G:O4'	2.17	0.44
1:A:1530:G:H2'	1:A:1531:A:C8	2.53	0.44
2:B:66:LYS:HE3	2:B:158:PRO:HA	1.99	0.44
10:J:53:ILE:HG23	10:J:62:ARG:HA	1.99	0.44
27:a:687:C:H5''	54:l:2:LYS:HE2	2.00	0.44
27:a:1710:G:H4'	27:a:2858:C:O2	2.18	0.44
27:a:2819:G:H2'	27:a:2821:A:N7	2.33	0.44
33:g:159:GLY:O	33:g:163:ARG:NH2	2.37	0.44
36:j:107:LEU:HB2	36:j:116:ILE:HD11	1.99	0.44
36:j:114:LYS:HE3	36:j:118:LEU:HD11	2.00	0.44
1:A:677:U:O2	1:A:777:A:O2'	2.31	0.44
1:A:1225:A:H2'	1:A:1225:A:N3	2.33	0.44
9:I:11:ARG:HB3	9:I:106:ARG:HH21	1.83	0.44
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.99	0.44
22:V:254:VAL:HG12	27:a:2583:G:N2	2.32	0.44
27:a:191:A:H2'	27:a:192:C:C6	2.53	0.44
27:a:657:U:H2'	27:a:658:U:C6	2.53	0.44
27:a:934:U:H2'	27:a:935:C:H6	1.83	0.44
27:a:1224:U:H2'	27:a:1225:G:C8	2.52	0.44
27:a:1364:G:OP2	49:w:50:ARG:NH1	2.44	0.44
27:a:1802:A:H2'	27:a:1803:A:H8	1.83	0.44
6:F:6:ILE:HG12	6:F:89:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:51:SER:O	21:U:55:ARG:HG3	2.18	0.44
22:V:230:ILE:HB	22:V:296:TYR:CE2	2.53	0.44
27:a:244:A:OP2	55:2:8:ARG:NH2	2.50	0.44
27:a:307:G:N2	27:a:309:A:H3'	2.32	0.44
27:a:521:U:H2'	27:a:522:A:C8	2.52	0.44
27:a:1571:A:H2'	27:a:1572:A:C8	2.53	0.44
27:a:1880:U:H2'	27:a:1881:C:H6	1.83	0.44
27:a:2286:G:H4'	27:a:2287:A:O4'	2.18	0.44
27:a:2367:G:C2	27:a:2368:C:C5	3.06	0.44
27:a:2443:C:H2'	27:a:2444:G:H8	1.83	0.44
27:a:2514:U:H2'	27:a:2515:C:H6	1.82	0.44
27:a:2685:G:H2'	27:a:2686:G:H8	1.83	0.44
38:l:34:LYS:HE3	38:l:131:VAL:HG11	1.98	0.44
45:s:2:ILE:HD13	45:s:42:GLU:HG2	1.99	0.44
47:u:63:ILE:HG22	47:u:65:VAL:HG23	1.99	0.44
1:A:95:C:H2'	1:A:96:U:C6	2.53	0.43
1:A:799:G:H2'	1:A:800:G:O4'	2.18	0.43
3:C:85:GLU:O	3:C:89:LYS:HG2	2.17	0.43
4:D:139:PRO:HA	4:D:182:PHE:HD2	1.82	0.43
25:Y:10:G:H1	25:Y:25:U:H3	1.65	0.43
27:a:1298:C:H2'	27:a:1299:G:O4'	2.18	0.43
1:A:214:C:H2'	1:A:215:C:H6	1.83	0.43
1:A:1004:A:C5	1:A:1026:G:C4	3.07	0.43
1:A:1330:U:H2'	1:A:1331:G:O4'	2.18	0.43
27:a:20:C:H2'	27:a:21:A:C8	2.52	0.43
27:a:305:C:H2'	27:a:306:U:C6	2.53	0.43
27:a:2251:OMG:H1'	27:a:2251:OMG:HM23	1.74	0.43
28:b:113:C:H2'	28:b:114:C:H6	1.82	0.43
33:g:22:GLN:NE2	33:g:38:ASN:O	2.51	0.43
37:k:109:LYS:HE2	37:k:128:THR:HG22	2.00	0.43
49:w:59:ILE:HG12	49:w:67:VAL:HG21	1.99	0.43
51:y:4:THR:HB	51:y:37:GLU:HG2	2.00	0.43
1:A:978:A:C4	1:A:1319:A:C2	3.06	0.43
27:a:513:A:H2'	27:a:514:A:C8	2.53	0.43
27:a:1219:U:H2'	27:a:1220:G:H8	1.80	0.43
27:a:1316:U:H2'	27:a:1317:G:H8	1.83	0.43
27:a:1703:G:H2'	27:a:1704:C:C6	2.53	0.43
27:a:2636:C:H2'	27:a:2637:U:H6	1.84	0.43
27:a:2699:C:H2'	27:a:2700:A:H8	1.83	0.43
28:b:23:G:H2'	28:b:24:G:C5	2.54	0.43
28:b:106:G:H2'	28:b:107:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:U:H4'	1:A:983:A:O4'	2.19	0.43
1:A:985:C:H2'	1:A:986:U:C6	2.54	0.43
1:A:1005:A:H62	1:A:1024:G:H21	1.66	0.43
1:A:1180:A:P	9:I:99:ARG:HH12	2.41	0.43
1:A:1326:U:C2	1:A:1327:C:C5	3.06	0.43
2:B:97:LEU:H	2:B:100:MET:HE3	1.83	0.43
21:U:4:ILE:HD13	21:U:19:PHE:HD1	1.83	0.43
27:a:588:U:H2'	27:a:589:U:C6	2.53	0.43
27:a:2636:C:H2'	27:a:2637:U:C6	2.52	0.43
27:a:2659:G:OP2	33:g:158:LYS:NZ	2.44	0.43
1:A:486:U:H2'	1:A:487:A:H8	1.83	0.43
2:B:186:ILE:HD13	2:B:213:TYR:CD2	2.53	0.43
3:C:77:ILE:HA	3:C:84:VAL:HG13	2.01	0.43
9:I:55:VAL:HG23	9:I:57:MET:H	1.83	0.43
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.99	0.43
27:a:1183:U:H2'	27:a:1184:U:C6	2.53	0.43
27:a:1417:C:H2'	27:a:1418:G:O4'	2.19	0.43
27:a:2340:A:H2'	27:a:2341:G:H8	1.83	0.43
27:a:2533:U:H2'	27:a:2534:A:O4'	2.18	0.43
27:a:2637:U:H2'	27:a:2638:G:O4'	2.18	0.43
28:b:116:G:H2'	28:b:117:G:C8	2.54	0.43
1:A:202:G:H2'	1:A:203:G:C8	2.54	0.43
1:A:565:U:OP2	1:A:566:G:O2'	2.32	0.43
1:A:590:U:OP1	8:H:31:LYS:HG2	2.18	0.43
1:A:1253:G:H2'	1:A:1254:A:C8	2.53	0.43
22:V:73:MET:HG2	22:V:110:LEU:HD13	2.00	0.43
22:V:115:PHE:O	22:V:118:MET:HG3	2.18	0.43
27:a:30:G:H2'	27:a:31:C:C6	2.54	0.43
27:a:593:U:H2'	27:a:594:U:H6	1.82	0.43
27:a:1437:C:O2'	27:a:1516:G:O2'	2.30	0.43
27:a:1464:G:H2'	27:a:1465:G:H8	1.83	0.43
27:a:1747:U:H2'	27:a:1748:C:C6	2.53	0.43
27:a:1928:A:H2'	27:a:1929:G:O4'	2.18	0.43
27:a:2898:U:C2	27:a:2899:A:C8	3.05	0.43
27:a:2898:U:O2	35:i:134:ALA:HB1	2.19	0.43
1:A:1250:A:H2'	1:A:1251:A:H8	1.79	0.43
15:O:36:ILE:O	15:O:40:GLN:HG2	2.19	0.43
17:Q:81:LYS:HG2	17:Q:82:ALA:H	1.83	0.43
22:V:319:TRP:CD1	22:V:319:TRP:H	2.37	0.43
27:a:65:U:H2'	27:a:66:C:H6	1.82	0.43
27:a:2484:G:OP1	38:l:44:ARG:NH1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:g:52:PHE:HE2	33:g:72:LEU:HD22	1.84	0.43
39:m:114:GLU:OE1	39:m:118:ARG:NH2	2.45	0.43
1:A:6:G:H4'	1:A:298:A:H4'	2.00	0.43
1:A:21:G:H2'	1:A:22:G:C8	2.54	0.43
1:A:579:A:H2'	1:A:580:C:H6	1.83	0.43
1:A:1220:G:P	14:N:53:ARG:HH12	2.42	0.43
27:a:171:U:H2'	27:a:172:A:C8	2.53	0.43
27:a:287:G:H2'	27:a:288:U:C6	2.54	0.43
27:a:596:U:H2'	27:a:597:G:H8	1.82	0.43
27:a:1252:G:N2	42:p:33:ARG:HB3	2.33	0.43
27:a:1316:U:H2'	27:a:1317:G:C8	2.54	0.43
27:a:1325:U:C4	60:a:6197:SPD:H52	2.53	0.43
27:a:2699:C:H2'	27:a:2700:A:C8	2.54	0.43
1:A:1019:A:H2'	1:A:1020:G:O4'	2.19	0.43
1:A:1172:C:H2'	1:A:1173:U:C6	2.54	0.43
12:L:50:ARG:HB3	12:L:66:TYR:HE1	1.83	0.43
19:S:70:LYS:HB2	19:S:73:GLU:HG3	2.00	0.43
22:V:295:LEU:O	22:V:299:GLU:HG2	2.19	0.43
27:a:665:U:H2'	27:a:666:A:C8	2.54	0.43
27:a:1026:G:OP1	27:a:1134:A:O2'	2.35	0.43
27:a:1918:A:O2'	27:a:1920:C:N4	2.52	0.43
27:a:1952:A:C6	36:j:22:ILE:HB	2.54	0.43
27:a:2290:G:H2'	27:a:2291:U:C6	2.54	0.43
27:a:2368:C:C2	27:a:2369:A:C8	3.07	0.43
27:a:2626:C:H2'	27:a:2627:G:C8	2.53	0.43
30:d:121:THR:HG21	30:d:143:PRO:HB3	2.01	0.43
1:A:1236:A:H4'	1:A:1304:G:H4'	2.01	0.43
1:A:1441:A:C4	41:o:114:LEU:HD11	2.54	0.43
27:a:566:U:H5''	37:k:29:LYS:HE3	2.01	0.43
27:a:935:C:H2'	27:a:936:A:H8	1.83	0.43
27:a:1721:G:H22	27:a:1738:G:H2'	1.84	0.43
27:a:2641:G:H5''	35:i:78:THR:HB	1.99	0.43
28:b:1:U:H2'	28:b:2:G:C8	2.54	0.43
31:e:158:PHE:O	31:e:162:ARG:HG3	2.19	0.43
37:k:112:LEU:HD22	37:k:130:GLY:HA3	2.00	0.43
38:l:110:GLU:O	38:l:114:ARG:HG3	2.19	0.43
1:A:334:C:H2'	1:A:335:C:H6	1.84	0.42
1:A:707:U:H2'	1:A:708:C:C6	2.54	0.42
1:A:855:U:OP2	1:A:871:U:N3	2.41	0.42
1:A:1320:C:H2'	1:A:1321:U:C6	2.54	0.42
1:A:1431:A:H2'	1:A:1432:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:U:H2'	1:A:1479:C:H6	1.82	0.42
1:A:1527:U:H2'	1:A:1528:U:C6	2.54	0.42
27:a:32:C:H2'	27:a:33:C:C6	2.54	0.42
27:a:37:C:H2'	27:a:38:A:C8	2.53	0.42
27:a:1286:A:H1'	27:a:1288:G:OP2	2.19	0.42
27:a:1360:G:N7	27:a:1361:G:C8	2.87	0.42
27:a:2461:A:H2'	27:a:2462:C:C6	2.54	0.42
27:a:2543:G:H2'	27:a:2544:G:C8	2.54	0.42
40:n:115:LEU:HD23	40:n:115:LEU:HA	1.90	0.42
41:o:52:ASN:OD1	41:o:52:ASN:N	2.52	0.42
46:t:81:ASP:OD1	46:t:82:ARG:N	2.51	0.42
1:A:75:G:C4	1:A:76:G:C8	3.07	0.42
1:A:204:G:O6	1:A:215:C:H1'	2.18	0.42
1:A:1413:A:H2	1:A:1487:G:H22	1.66	0.42
27:a:514:A:N3	27:a:581:C:O2'	2.49	0.42
27:a:1505:A:H2'	27:a:1506:U:C6	2.54	0.42
27:a:2429:G:OP2	27:a:2430:A:OP2	2.37	0.42
27:a:2623:G:H4'	27:a:2825:G:H8	1.84	0.42
29:c:19:VAL:HG23	29:c:203:ARG:HB3	2.00	0.42
34:h:30:LEU:HB3	34:h:36:ALA:HB3	2.01	0.42
39:m:86:ARG:HH21	39:m:117:ASP:CG	2.27	0.42
44:r:72:THR:OG1	44:r:108:SER:OG	2.26	0.42
1:A:62:U:O2'	1:A:379:C:O2	2.38	0.42
1:A:1169:A:H2'	1:A:1170:A:C8	2.54	0.42
1:A:1219:A:H2'	1:A:1220:G:H8	1.84	0.42
1:A:1478:U:H2'	1:A:1479:C:C6	2.54	0.42
27:a:144:A:H2'	27:a:145:C:C6	2.53	0.42
27:a:632:A:H2'	27:a:633:A:C8	2.53	0.42
27:a:935:C:H2'	27:a:936:A:C8	2.54	0.42
27:a:1003:G:O2'	27:a:1010:A:N1	2.48	0.42
27:a:1440:U:H2'	27:a:1441:G:C8	2.54	0.42
27:a:2011:U:H2'	27:a:2012:G:O4'	2.19	0.42
27:a:2065:C:H2'	27:a:2066:C:H6	1.84	0.42
27:a:2564:A:OP1	27:a:2648:G:O2'	2.32	0.42
27:a:2745:C:H2'	27:a:2746:U:C6	2.54	0.42
1:A:126:G:OP1	1:A:605:U:O2'	2.28	0.42
1:A:362:G:N2	1:A:365:U:OP2	2.52	0.42
1:A:578:C:O2'	1:A:728:A:N3	2.46	0.42
1:A:601:G:H2'	1:A:602:A:C8	2.54	0.42
1:A:1288:A:H2'	1:A:1289:A:C8	2.54	0.42
6:F:43:GLY:HA2	6:F:58:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:51:ILE:HD11	18:R:66:SER:HB2	2.01	0.42
8:H:39:VAL:HG21	8:H:110:VAL:HG12	2.02	0.42
22:V:11:ILE:HD11	22:V:84:LEU:HD12	2.01	0.42
27:a:580:U:H2'	27:a:581:C:H6	1.84	0.42
27:a:634:C:H2'	27:a:635:C:C6	2.54	0.42
27:a:880:G:C2	27:a:881:G:C8	3.06	0.42
27:a:1592:C:H2'	27:a:1593:A:C8	2.55	0.42
27:a:1831:G:H2'	27:a:1832:C:C6	2.54	0.42
27:a:2051:A:H8	27:a:2051:A:OP2	2.02	0.42
27:a:2202:U:O2'	27:a:2204:G:OP1	2.33	0.42
27:a:2282:G:H4'	27:a:2389:G:O2'	2.19	0.42
27:a:2576:G:O2'	27:a:2579:C:OP2	2.32	0.42
28:b:95:U:H2'	28:b:96:G:C8	2.54	0.42
51:y:7:ILE:HD12	51:y:48:ILE:HG12	2.01	0.42
1:A:50:A:O2'	1:A:360:G:N2	2.53	0.42
1:A:51:A:N7	1:A:114:U:O2'	2.48	0.42
1:A:222:C:H2'	1:A:223:A:H8	1.84	0.42
1:A:309:A:H2'	1:A:310:G:C8	2.50	0.42
1:A:591:U:H2'	1:A:592:G:C8	2.54	0.42
3:C:6:HIS:CE1	3:C:8:ASN:HB3	2.54	0.42
22:V:87:ALA:HA	22:V:92:ASP:HB3	2.02	0.42
27:a:540:C:H2'	27:a:541:A:C8	2.54	0.42
27:a:822:G:H2'	27:a:823:C:H6	1.85	0.42
27:a:875:G:H2'	27:a:876:C:C6	2.53	0.42
27:a:1370:C:H2'	27:a:1371:G:O4'	2.19	0.42
27:a:2627:G:O2'	27:a:2781:A:N1	2.50	0.42
1:A:1429:A:H2'	1:A:1430:A:H8	1.85	0.42
23:W:8:ILE:HD11	27:a:2058:A:H2'	2.02	0.42
27:a:184:C:H2'	27:a:185:G:C8	2.55	0.42
27:a:959:A:H2'	27:a:960:A:C8	2.54	0.42
27:a:1340:U:OP1	45:s:19:LYS:NZ	2.52	0.42
27:a:1429:G:H2'	27:a:1430:G:C8	2.54	0.42
27:a:1791:A:H5''	29:c:205:LEU:HD12	2.02	0.42
27:a:2097:A:H2'	27:a:2098:U:C6	2.53	0.42
27:a:2680:U:H2'	27:a:2681:C:C6	2.54	0.42
47:u:80:HIS:CG	47:u:81:PRO:HD2	2.54	0.42
1:A:32:A:H2'	1:A:33:A:C8	2.54	0.42
1:A:580:C:H2'	1:A:581:G:O4'	2.19	0.42
1:A:613:C:H2'	1:A:614:C:C6	2.55	0.42
1:A:737:C:H2'	1:A:738:C:H6	1.84	0.42
1:A:917:G:H2'	1:A:918:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1070:U:H2'	1:A:1071:C:C6	2.54	0.42
1:A:1157:A:H4'	1:A:1158:C:O4'	2.19	0.42
1:A:1164:G:H2'	1:A:1165:U:C6	2.54	0.42
10:J:32:THR:HG21	10:J:83:THR:HA	2.02	0.42
22:V:262:ARG:HH12	27:a:2557:G:H4'	1.84	0.42
27:a:587:C:H4'	27:a:588:U:C6	2.54	0.42
27:a:2567:G:H2'	27:a:2568:U:C6	2.55	0.42
29:c:80:ARG:NE	29:c:82:GLU:OE2	2.53	0.42
29:c:145:GLU:HG2	29:c:151:GLY:C	2.45	0.42
32:f:142:ASP:O	32:f:146:VAL:HG23	2.19	0.42
1:A:294:U:H2'	1:A:295:C:C6	2.55	0.42
1:A:745:G:O2'	1:A:746:A:H5'	2.19	0.42
1:A:1302:C:C6	13:M:17:ILE:HG13	2.55	0.42
3:C:22:TRP:HB3	3:C:59:ARG:HB2	2.01	0.42
14:N:52:PRO:HG2	14:N:55:SER:HB3	2.02	0.42
27:a:58:G:H2'	27:a:59:U:C6	2.54	0.42
27:a:222:A:N6	27:a:232:G:H1'	2.34	0.42
27:a:1164:C:H2'	27:a:1165:A:C8	2.54	0.42
27:a:2291:U:OP1	27:a:2380:C:O2'	2.37	0.42
27:a:2861:U:H2'	27:a:2862:G:C8	2.54	0.42
32:f:119:ALA:O	32:f:167:ARG:NH1	2.53	0.42
1:A:224:U:H2'	1:A:225:C:C6	2.55	0.42
1:A:893:C:C2	1:A:894:G:C8	3.08	0.42
1:A:1062:U:H2'	1:A:1063:C:C6	2.54	0.42
1:A:1176:A:H2'	1:A:1177:G:C8	2.55	0.42
1:A:1325:C:H2'	1:A:1326:U:H6	1.84	0.42
13:M:7:ILE:HD11	13:M:22:ILE:HG12	2.02	0.42
13:M:16:VAL:O	13:M:20:THR:HG23	2.20	0.42
22:V:246:THR:HA	22:V:260:ALA:HB2	2.02	0.42
27:a:78:U:H2'	27:a:79:C:C6	2.55	0.42
27:a:175:G:H2'	27:a:176:A:C8	2.55	0.42
27:a:306:U:H2'	27:a:307:G:O4'	2.19	0.42
27:a:416:U:H2'	27:a:417:C:C6	2.54	0.42
27:a:479:A:O2'	27:a:481:G:H5'	2.20	0.42
27:a:1168:G:H2'	27:a:1169:A:C8	2.54	0.42
27:a:1344:U:O2	27:a:1385:A:H5'	2.19	0.42
28:b:114:C:C2	28:b:115:A:C8	3.08	0.42
1:A:390:U:H2'	1:A:391:G:C8	2.55	0.42
1:A:744:C:H2'	1:A:745:G:C8	2.49	0.42
1:A:1475:G:H4'	27:a:1689:A:H4'	2.01	0.42
9:I:85:ARG:O	9:I:89:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:1678:A:C4	27:a:1679:A:C8	3.08	0.42
29:c:108:LYS:N	29:c:194:GLU:O	2.50	0.42
1:A:258:G:H5''	20:T:82:GLN:HE22	1.85	0.41
1:A:350:G:H2'	1:A:351:G:C8	2.55	0.41
1:A:475:C:H2'	1:A:476:U:C6	2.55	0.41
1:A:719:C:O2'	18:R:39:ILE:O	2.27	0.41
1:A:1412:C:H2'	1:A:1413:A:H8	1.84	0.41
3:C:134:MET:HE2	3:C:168:TYR:HD2	1.85	0.41
9:I:65:ILE:HD13	9:I:79:ILE:HG23	2.02	0.41
27:a:522:A:H2'	27:a:523:C:C6	2.55	0.41
27:a:1704:C:C2	27:a:1705:A:N7	2.87	0.41
27:a:1733:G:H2'	27:a:1734:G:H8	1.85	0.41
27:a:2096:C:H2'	27:a:2097:A:C8	2.55	0.41
27:a:2357:G:N2	27:a:2360:G:OP2	2.36	0.41
27:a:2813:A:C4	27:a:2814:A:C8	3.08	0.41
27:a:2888:C:H2'	27:a:2889:C:C6	2.55	0.41
28:b:5:U:H2'	28:b:6:G:H8	1.85	0.41
29:c:3:VAL:HG12	29:c:19:VAL:HG22	2.02	0.41
37:k:2:ARG:H	37:k:5:THR:HG1	1.64	0.41
1:A:272:C:H2'	1:A:273:U:C6	2.55	0.41
1:A:1109:C:C2	1:A:1110:A:C8	3.08	0.41
5:E:85:VAL:HG23	5:E:96:MET:HE3	2.02	0.41
15:O:29:VAL:HG13	15:O:63:ARG:HG3	2.02	0.41
21:U:16:LEU:HG	21:U:20:LYS:HE2	2.02	0.41
27:a:710:U:H2'	27:a:711:G:C8	2.55	0.41
27:a:881:G:H2'	27:a:882:G:C8	2.55	0.41
27:a:881:G:H2'	27:a:882:G:H8	1.85	0.41
27:a:936:A:H2'	27:a:937:C:C6	2.55	0.41
27:a:1144:A:C4	27:a:1145:C:C5	3.08	0.41
27:a:1153:C:H2'	27:a:1154:G:O4'	2.20	0.41
27:a:1734:G:H2'	27:a:1735:A:C8	2.55	0.41
27:a:2719:G:O2'	27:a:2720:U:H5'	2.20	0.41
30:d:114:LYS:HE3	30:d:196:ALA:HB2	2.02	0.41
31:e:129:PRO:HB3	31:e:156:ASN:HA	2.03	0.41
55:2:62:LEU:HB3	55:2:65:ALA:HB2	2.01	0.41
1:A:17:U:H2'	1:A:18:C:H6	1.85	0.41
1:A:642:A:N7	8:H:107:SER:HA	2.35	0.41
1:A:751:U:H2'	1:A:752:G:O4'	2.20	0.41
1:A:898:G:N2	1:A:901:A:OP2	2.43	0.41
1:A:951:G:H2'	1:A:952:U:H6	1.85	0.41
1:A:1144:G:N2	1:A:1146:A:H62	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1355:G:H2'	1:A:1356:G:C8	2.54	0.41
2:B:105:LYS:H	2:B:105:LYS:HG2	1.64	0.41
12:L:110:ARG:NE	12:L:112:GLN:O	2.45	0.41
27:a:77:G:H2'	27:a:78:U:C6	2.55	0.41
27:a:172:A:H2'	27:a:173:A:H8	1.85	0.41
27:a:1036:G:C6	27:a:1120:G:C6	3.08	0.41
27:a:1683:U:H2'	27:a:1684:G:C8	2.55	0.41
27:a:1792:G:H5'	29:c:204:VAL:HG13	2.01	0.41
29:c:205:LEU:HB3	29:c:210:ALA:HB3	2.01	0.41
1:A:167:A:H2'	1:A:168:G:H8	1.85	0.41
1:A:472:U:H2'	1:A:473:U:H6	1.85	0.41
1:A:520:A:OP1	12:L:49:LEU:HB2	2.20	0.41
1:A:1027:C:N3	1:A:1028:C:N4	2.69	0.41
1:A:1287:A:H2	1:A:1353:G:H1'	1.86	0.41
3:C:47:LEU:HD21	3:C:87:LEU:HD11	2.02	0.41
12:L:90:LEU:HA	12:L:91:PRO:HD3	1.95	0.41
22:V:336:LEU:HD12	22:V:336:LEU:H	1.86	0.41
27:a:1462:C:H2'	27:a:1463:C:H6	1.85	0.41
27:a:1874:C:H2'	27:a:1875:G:O4'	2.20	0.41
27:a:2096:C:H2'	27:a:2097:A:H8	1.85	0.41
27:a:2196:C:H2'	27:a:2197:U:C6	2.56	0.41
27:a:2216:G:H2'	27:a:2217:G:C8	2.55	0.41
27:a:2333:A:P	48:v:77:ARG:HH22	2.43	0.41
29:c:141:VAL:HG12	29:c:192:LEU:HD23	2.02	0.41
34:h:12:LEU:HG	34:h:19:VAL:HG11	2.02	0.41
35:i:140:LEU:HG	35:i:142:ILE:HG13	2.02	0.41
36:j:121:GLU:OE1	41:o:65:SER:OG	2.34	0.41
1:A:1098:C:O2'	21:U:71:TYR:O	2.37	0.41
1:A:1120:C:H2'	1:A:1121:U:C6	2.56	0.41
1:A:1134:G:N2	1:A:1141:C:C2	2.88	0.41
1:A:1432:G:H3'	41:o:106:LYS:HE2	2.02	0.41
10:J:28:THR:O	10:J:32:THR:HG23	2.20	0.41
22:V:281:HIS:CE1	38:l:78:LEU:HD23	2.55	0.41
27:a:282:A:N6	27:a:359:G:O6	2.54	0.41
27:a:680:C:H2'	27:a:681:G:C8	2.56	0.41
27:a:971:G:H2'	27:a:972:A:O4'	2.20	0.41
27:a:1726:C:H2'	27:a:1727:C:H6	1.86	0.41
27:a:1923:U:H2'	27:a:1924:C:C6	2.54	0.41
27:a:2087:G:H2'	27:a:2088:A:C8	2.55	0.41
27:a:2273:A:H2'	27:a:2274:A:C8	2.55	0.41
27:a:2837:A:H2'	27:a:2838:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:2838:G:C4	27:a:2839:G:C8	3.08	0.41
40:n:85:LYS:HD3	40:n:87:ILE:HD11	2.03	0.41
46:t:4:LYS:O	46:t:94:ARG:NH1	2.53	0.41
1:A:770:C:O2'	1:A:899:C:N3	2.44	0.41
1:A:1342:C:H2'	1:A:1343:G:C8	2.55	0.41
4:D:19:LEU:HB2	4:D:21:LEU:HG	2.03	0.41
5:E:14:LYS:NZ	5:E:116:GLU:HG2	2.36	0.41
25:Y:66:C:H2'	25:Y:67:C:O4'	2.20	0.41
27:a:6:A:H2'	27:a:7:G:C8	2.56	0.41
27:a:36:G:N3	27:a:450:G:O2'	2.52	0.41
27:a:2350:C:H2'	27:a:2351:G:O4'	2.21	0.41
28:b:36:C:HO2'	28:b:37:C:P	2.43	0.41
28:b:40:U:H1'	28:b:45:A:H61	1.86	0.41
30:d:12:THR:OG1	30:d:13:ARG:N	2.54	0.41
32:f:36:LEU:HD12	32:f:61:SER:HB3	2.01	0.41
41:o:51:ARG:CZ	41:o:53:ARG:HG3	2.50	0.41
44:r:66:ILE:HG12	44:r:67:ASP:H	1.84	0.41
1:A:215:C:H2'	1:A:216:U:C6	2.55	0.41
1:A:950:U:OP2	13:M:101:ARG:HD2	2.20	0.41
9:I:55:VAL:HG11	9:I:87:LEU:HD13	2.03	0.41
22:V:30:LYS:HE3	22:V:63:LEU:HA	2.02	0.41
22:V:34:LEU:HA	22:V:37:VAL:HB	2.02	0.41
27:a:150:U:H2'	27:a:151:C:C6	2.56	0.41
27:a:181:A:H2'	27:a:182:A:H8	1.86	0.41
27:a:599:A:H2'	27:a:600:G:H8	1.84	0.41
27:a:2635:A:O2'	30:d:81:GLU:OE2	2.37	0.41
36:j:40:LYS:NZ	36:j:89:ASN:OD1	2.54	0.41
1:A:216:U:H2'	1:A:217:C:C6	2.56	0.41
1:A:233:C:H2'	1:A:234:C:H6	1.86	0.41
1:A:952:U:H2'	1:A:953:G:H8	1.86	0.41
1:A:1130:A:C4	1:A:1131:G:C8	3.08	0.41
1:A:1300:G:H1'	1:A:1303:C:N4	2.36	0.41
3:C:7:PRO:HD2	3:C:184:TYR:CD2	2.56	0.41
9:I:47:VAL:HG13	9:I:80:ARG:HD3	2.02	0.41
11:K:18:ASP:HB2	11:K:37:ARG:NH2	2.36	0.41
11:K:20:VAL:HG22	11:K:37:ARG:HH11	1.86	0.41
27:a:1022:G:N7	35:i:68:LYS:HD3	2.36	0.41
27:a:1440:U:H2'	27:a:1441:G:H8	1.86	0.41
27:a:1526:C:H2'	27:a:1527:G:O4'	2.21	0.41
27:a:1683:U:H2'	27:a:1684:G:H8	1.86	0.41
27:a:2484:G:O2'	38:l:123:LYS:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:2647:U:H2'	27:a:2648:G:H8	1.85	0.41
27:a:2809:A:H2'	27:a:2810:A:C8	2.56	0.41
30:d:181:ASP:HB3	30:d:186:LEU:HB2	2.03	0.41
31:e:119:ILE:HD11	31:e:185:LYS:HD3	2.02	0.41
34:h:56:ALA:O	34:h:60:GLU:HG2	2.20	0.41
1:A:33:A:H2'	1:A:34:C:C6	2.56	0.41
1:A:189:A:H8	1:A:189:A:OP2	2.04	0.41
1:A:264:C:H2'	1:A:265:G:O4'	2.21	0.41
1:A:322:C:H2'	1:A:323:U:C6	2.56	0.41
1:A:381:C:H2'	1:A:382:A:O4'	2.21	0.41
1:A:523:A:H61	12:L:89:D2T:H8	1.86	0.41
1:A:545:C:OP1	4:D:62:ARG:NH1	2.54	0.41
1:A:718:A:H2	18:R:38:LYS:HE3	1.86	0.41
1:A:745:G:C2	1:A:746:A:C5	3.09	0.41
1:A:977:A:O2'	1:A:979:C:OP2	2.29	0.41
1:A:987:G:H2'	1:A:988:G:H8	1.86	0.41
1:A:1022:A:C5	1:A:1023:U:C5	3.08	0.41
1:A:1152:A:OP1	10:J:70:HIS:ND1	2.54	0.41
3:C:186:THR:HG22	3:C:199:LYS:HG2	2.03	0.41
4:D:170:TRP:O	4:D:183:LYS:HG2	2.21	0.41
10:J:92:LEU:HD23	10:J:92:LEU:HA	1.91	0.41
11:K:19:GLY:O	11:K:37:ARG:NH1	2.54	0.41
11:K:47:ALA:HB1	11:K:62:ALA:HB1	2.03	0.41
14:N:88:ALA:HB2	14:N:96:LEU:HD23	2.03	0.41
16:P:8:ARG:O	16:P:29:ASN:ND2	2.48	0.41
22:V:105:ALA:O	22:V:109:LYS:HG3	2.21	0.41
27:a:30:G:H2'	27:a:31:C:H6	1.86	0.41
27:a:166:U:H2'	27:a:167:A:H8	1.86	0.41
27:a:743:A:O2'	27:a:1659:G:OP1	2.39	0.41
27:a:822:G:H2'	27:a:823:C:C6	2.56	0.41
27:a:828:U:H4'	27:a:831:G:N1	2.36	0.41
27:a:1392:A:N6	45:s:18:GLU:OE1	2.54	0.41
27:a:1562:U:H2'	27:a:1563:U:C6	2.56	0.41
27:a:1707:G:C8	27:a:1756:G:C5	3.09	0.41
27:a:2345:G:N3	27:a:2381:A:H2'	2.36	0.41
27:a:2688:G:N1	27:a:2720:U:OP2	2.38	0.41
28:b:29:A:OP2	40:n:32:PRO:HD2	2.21	0.41
29:c:168:ASP:OD1	29:c:168:ASP:N	2.54	0.41
30:d:152:PRO:HG3	30:d:156:PHE:CZ	2.55	0.41
31:e:149:ILE:HG22	31:e:192:ALA:HB1	2.02	0.41
40:n:8:ILE:O	40:n:12:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:z:38:HIS:ND1	52:z:39:LEU:O	2.54	0.41
53:0:38:LYS:HB2	53:0:49:TYR:CD1	2.56	0.41
1:A:72:A:H2'	1:A:73:C:H6	1.86	0.41
1:A:176:C:H2'	1:A:177:G:N3	2.36	0.41
1:A:214:C:H2'	1:A:215:C:C6	2.56	0.41
1:A:513:C:H2'	1:A:514:C:C6	2.56	0.41
1:A:757:U:H2'	1:A:758:C:O4'	2.20	0.41
1:A:825:A:H2'	1:A:826:C:C6	2.56	0.41
1:A:1238:A:H2	1:A:1241:G:N3	2.19	0.41
4:D:170:TRP:CD2	4:D:186:PRO:HB3	2.56	0.41
17:Q:7:THR:HG22	17:Q:62:ARG:HB3	2.03	0.41
25:Y:29:U:H2'	25:Y:30:G:C8	2.56	0.41
27:a:886:A:H2'	27:a:887:U:O4'	2.21	0.41
27:a:1710:G:H2'	27:a:1711:A:H8	1.84	0.41
27:a:1857:G:N2	27:a:1884:G:N3	2.69	0.41
27:a:2364:C:H2'	27:a:2365:G:O4'	2.21	0.41
27:a:2369:A:H2'	27:a:2370:G:H8	1.86	0.41
27:a:2416:C:C2	27:a:2417:C:C5	3.09	0.41
27:a:2740:A:H2'	27:a:2741:A:C8	2.56	0.41
27:a:2742:G:H5''	56:3:1:MET:HE3	2.02	0.41
31:e:173:THR:HA	31:e:199:MET:HE1	2.03	0.41
45:s:34:VAL:HG21	45:s:43:ILE:HD11	2.02	0.41
47:u:21:ARG:HA	47:u:25:LYS:O	2.20	0.41
1:A:554:A:H2'	1:A:555:U:C6	2.56	0.40
1:A:599:C:H2'	1:A:600:A:H8	1.85	0.40
1:A:714:G:H2'	1:A:715:A:H8	1.83	0.40
1:A:996:A:H2'	1:A:997:U:C6	2.56	0.40
1:A:1249:C:H4'	9:I:75:GLN:HE22	1.86	0.40
1:A:1315:U:H2'	1:A:1316:G:O4'	2.21	0.40
2:B:32:PHE:HB2	2:B:42:ASN:HB2	2.03	0.40
22:V:194:THR:OG1	22:V:360:SER:HB3	2.21	0.40
25:Y:22:G:H2'	25:Y:23:A:C8	2.55	0.40
27:a:271:G:C6	27:a:367:G:C6	3.10	0.40
27:a:532:A:H4'	27:a:533:G:C8	2.57	0.40
27:a:644:A:H2'	27:a:645:C:O4'	2.21	0.40
27:a:1038:G:H2'	27:a:1039:A:H8	1.83	0.40
27:a:1271:G:OP2	27:a:1648:U:OP1	2.39	0.40
27:a:1511:G:H2'	27:a:1512:C:H6	1.86	0.40
27:a:2419:U:OP1	55:2:41:LYS:NZ	2.47	0.40
28:b:23:G:H2'	28:b:24:G:N7	2.36	0.40
32:f:16:LEU:HD13	32:f:29:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:g:89:LEU:HD11	33:g:96:ALA:HB2	2.03	0.40
35:i:7:LYS:O	35:i:11:VAL:HG23	2.22	0.40
1:A:91:U:H2'	1:A:92:U:C6	2.56	0.40
1:A:130:A:H1'	1:A:263:A:O2'	2.21	0.40
1:A:198:G:H2'	1:A:199:A:H8	1.86	0.40
1:A:636:U:H2'	1:A:637:C:C6	2.56	0.40
1:A:825:A:H2'	1:A:826:C:H6	1.86	0.40
1:A:911:U:H2'	1:A:912:C:C6	2.57	0.40
1:A:1287:A:N3	1:A:1353:G:O2'	2.40	0.40
1:A:1327:C:C2	1:A:1328:C:C5	3.09	0.40
1:A:1352:C:H2'	1:A:1353:G:C8	2.55	0.40
1:A:1405:G:O2'	1:A:1518:MA6:O2'	2.34	0.40
3:C:58:GLU:OE1	3:C:65:ARG:NH2	2.54	0.40
6:F:10:VAL:HG21	6:F:18:VAL:HG22	2.04	0.40
7:G:116:MET:HA	7:G:119:ARG:HG2	2.03	0.40
22:V:26:ASP:HB2	22:V:29:ALA:HB3	2.04	0.40
22:V:226:VAL:HG21	22:V:303:LYS:HE3	2.02	0.40
27:a:177:G:H3'	27:a:178:G:C8	2.53	0.40
27:a:814:C:H1'	27:a:1225:G:N2	2.36	0.40
27:a:1146:C:C2	27:a:1147:A:C8	3.09	0.40
27:a:1441:G:H2'	27:a:1442:U:H6	1.86	0.40
27:a:1794:A:H2'	27:a:1795:C:C6	2.56	0.40
27:a:2036:C:H2'	27:a:2037:A:H8	1.86	0.40
27:a:2064:C:H2'	27:a:2065:C:C6	2.56	0.40
27:a:2334:U:O2'	40:n:13:ARG:NH1	2.53	0.40
27:a:2698:U:H2'	27:a:2699:C:C6	2.56	0.40
27:a:2710:C:H2'	27:a:2711:A:C8	2.56	0.40
29:c:62:TYR:HA	29:c:86:ASN:ND2	2.35	0.40
30:d:24:VAL:HG12	30:d:178:VAL:HG21	2.01	0.40
32:f:34:ILE:HG12	32:f:156:ILE:HG12	2.01	0.40
1:A:123:U:H2'	1:A:124:C:H6	1.86	0.40
1:A:1163:A:H2'	1:A:1164:G:C8	2.56	0.40
3:C:42:TYR:O	3:C:46:GLU:HG2	2.21	0.40
4:D:57:GLU:HG2	4:D:199:LEU:HB2	2.04	0.40
7:G:65:ALA:O	7:G:69:VAL:HG23	2.21	0.40
9:I:81:HIS:NE2	9:I:85:ARG:HD2	2.36	0.40
27:a:166:U:H2'	27:a:167:A:C8	2.56	0.40
27:a:277:G:H8	27:a:361:G:C5	2.39	0.40
27:a:457:A:N1	27:a:470:A:H5''	2.37	0.40
27:a:863:A:H2'	27:a:864:G:C8	2.56	0.40
27:a:948:C:H2'	27:a:949:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:1041:G:C2	27:a:1042:G:N7	2.89	0.40
27:a:1295:C:H2'	27:a:1296:G:H8	1.86	0.40
27:a:2038:G:H2'	27:a:2039:U:O4'	2.21	0.40
28:b:42:C:C5	32:f:66:LEU:HD22	2.56	0.40
1:A:939:G:H2'	1:A:940:C:C6	2.56	0.40
1:A:1015:G:H2'	1:A:1016:A:C8	2.56	0.40
1:A:1120:C:H2'	1:A:1121:U:H6	1.86	0.40
15:O:23:GLY:O	15:O:28:GLN:NE2	2.48	0.40
22:V:155:TRP:HH2	22:V:191:TRP:HB3	1.86	0.40
27:a:175:G:H2'	27:a:176:A:H8	1.85	0.40
27:a:1013:C:H2'	27:a:1014:A:C8	2.52	0.40
27:a:1182:G:H2'	27:a:1183:U:O4'	2.21	0.40
27:a:1187:G:N2	27:a:1188:U:O4	2.55	0.40
27:a:2649:C:H2'	27:a:2650:U:H6	1.86	0.40
27:a:2756:U:OP2	56:3:19:ARG:NE	2.52	0.40
27:a:2803:G:H2'	27:a:2804:U:C6	2.57	0.40
27:a:2815:C:C2	27:a:2816:G:C8	3.09	0.40
29:c:132:MET:HE2	29:c:188:CYS:HB2	2.03	0.40
34:h:54:LEU:O	34:h:57:LYS:HG2	2.22	0.40
50:x:39:GLN:HB3	50:x:41:HIS:CE1	2.56	0.40
1:A:138:G:C6	1:A:226:G:C6	3.10	0.40
1:A:236:A:H2'	1:A:237:G:H8	1.87	0.40
1:A:363:A:N6	12:L:27:CYS:SG	2.95	0.40
1:A:419:C:N3	1:A:425:G:N1	2.70	0.40
1:A:880:C:C2	1:A:881:G:C8	3.09	0.40
1:A:1010:U:H2'	1:A:1011:C:O4'	2.22	0.40
1:A:1130:A:C8	1:A:1146:A:C2	3.09	0.40
1:A:1163:A:H2'	1:A:1164:G:H8	1.87	0.40
11:K:36:ASP:OD1	11:K:40:ASN:N	2.53	0.40
25:Y:7:G:O2'	25:Y:49:G:O5'	2.39	0.40
27:a:81:G:H2'	27:a:82:U:O4'	2.21	0.40
27:a:117:G:OP2	27:a:119:A:O2'	2.28	0.40
27:a:222:A:H61	27:a:232:G:H1'	1.87	0.40
27:a:579:G:H2'	27:a:580:U:C6	2.55	0.40
27:a:1196:C:H2'	27:a:1197:G:C8	2.56	0.40
27:a:1496:A:H2'	27:a:1498:C:C5	2.57	0.40
27:a:1521:G:OP2	27:a:1522:A:O2'	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	223/241 (92%)	220 (99%)	3 (1%)	0	100	100
3	C	204/233 (88%)	200 (98%)	4 (2%)	0	100	100
4	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
5	E	154/167 (92%)	153 (99%)	1 (1%)	0	100	100
6	F	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
7	G	151/179 (84%)	148 (98%)	3 (2%)	0	100	100
8	H	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
9	I	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	J	97/103 (94%)	96 (99%)	1 (1%)	0	100	100
11	K	113/129 (88%)	111 (98%)	2 (2%)	0	100	100
12	L	120/124 (97%)	118 (98%)	2 (2%)	0	100	100
13	M	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
14	N	98/101 (97%)	98 (100%)	0	0	100	100
15	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	Q	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	R	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
19	S	82/92 (89%)	82 (100%)	0	0	100	100
20	T	84/87 (97%)	84 (100%)	0	0	100	100
21	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
22	V	354/365 (97%)	350 (99%)	4 (1%)	0	100	100
23	W	12/14 (86%)	12 (100%)	0	0	100	100
29	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
30	d	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
31	e	199/201 (99%)	199 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	f	175/179 (98%)	173 (99%)	2 (1%)	0	100	100
33	g	172/177 (97%)	169 (98%)	3 (2%)	0	100	100
34	h	65/149 (44%)	64 (98%)	1 (2%)	0	100	100
35	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
36	j	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
37	k	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
38	l	132/136 (97%)	132 (100%)	0	0	100	100
39	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
40	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
41	o	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
42	p	115/118 (98%)	115 (100%)	0	0	100	100
43	q	101/103 (98%)	101 (100%)	0	0	100	100
44	r	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
45	s	91/100 (91%)	91 (100%)	0	0	100	100
46	t	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
47	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
48	v	76/85 (89%)	76 (100%)	0	0	100	100
49	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
50	x	60/63 (95%)	60 (100%)	0	0	100	100
51	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
52	z	54/57 (95%)	54 (100%)	0	0	100	100
53	0	49/55 (89%)	49 (100%)	0	0	100	100
54	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
55	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
56	3	36/38 (95%)	36 (100%)	0	0	100	100
57	4	45/70 (64%)	45 (100%)	0	0	100	100
All	All	5864/6292 (93%)	5786 (99%)	78 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	87/90 (97%)	86 (99%)	1 (1%)	70	90
11	K	89/98 (91%)	89 (100%)	0	100	100
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	94/96 (98%)	93 (99%)	1 (1%)	70	90
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	74/78 (95%)	73 (99%)	1 (1%)	62	86
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	59 (98%)	1 (2%)	56	83
22	V	303/310 (98%)	303 (100%)	0	100	100
23	W	10/10 (100%)	10 (100%)	0	100	100
29	c	216/218 (99%)	216 (100%)	0	100	100
30	d	163/163 (100%)	163 (100%)	0	100	100
31	e	165/165 (100%)	165 (100%)	0	100	100
32	f	148/150 (99%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	g	135/138 (98%)	135 (100%)	0	100	100
34	h	50/114 (44%)	49 (98%)	1 (2%)	50	79
35	i	116/116 (100%)	115 (99%)	1 (1%)	75	92
36	j	104/104 (100%)	104 (100%)	0	100	100
37	k	103/103 (100%)	103 (100%)	0	100	100
38	l	107/107 (100%)	106 (99%)	1 (1%)	75	92
39	m	98/103 (95%)	97 (99%)	1 (1%)	73	91
40	n	86/87 (99%)	86 (100%)	0	100	100
41	o	99/100 (99%)	98 (99%)	1 (1%)	73	91
42	p	89/90 (99%)	89 (100%)	0	100	100
43	q	84/84 (100%)	84 (100%)	0	100	100
44	r	93/93 (100%)	93 (100%)	0	100	100
45	s	80/84 (95%)	80 (100%)	0	100	100
46	t	83/85 (98%)	83 (100%)	0	100	100
47	u	78/78 (100%)	78 (100%)	0	100	100
48	v	59/63 (94%)	59 (100%)	0	100	100
49	w	67/68 (98%)	67 (100%)	0	100	100
50	x	54/55 (98%)	54 (100%)	0	100	100
51	y	48/49 (98%)	47 (98%)	1 (2%)	48	78
52	z	47/48 (98%)	47 (100%)	0	100	100
53	0	46/49 (94%)	46 (100%)	0	100	100
54	1	38/38 (100%)	38 (100%)	0	100	100
55	2	51/52 (98%)	51 (100%)	0	100	100
56	3	34/34 (100%)	34 (100%)	0	100	100
57	4	43/62 (69%)	43 (100%)	0	100	100
All	All	4893/5145 (95%)	4883 (100%)	10 (0%)	91	98

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	80	THR
13	M	97	VAL
17	Q	49	GLU

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Mol	Chain	Res	Type
21	U	40	LYS
34	h	30	LEU
35	i	17	VAL
38	l	36	VAL
39	m	98	LEU
41	o	52	ASN
51	y	7	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	39	HIS
2	B	93	ASN
2	B	94	HIS
2	B	177	ASN
3	C	3	GLN
3	C	100	GLN
3	C	139	GLN
4	D	40	GLN
4	D	100	ASN
4	D	131	ASN
5	E	82	GLN
5	E	122	ASN
6	F	3	HIS
6	F	46	GLN
6	F	94	HIS
7	G	52	GLN
7	G	68	ASN
7	G	142	HIS
9	I	75	GLN
11	K	15	GLN
11	K	38	GLN
11	K	40	ASN
11	K	101	ASN
12	L	112	GLN
13	M	8	ASN
14	N	4	GLN
14	N	35	ASN
14	N	60	GLN
15	O	35	GLN
15	O	50	HIS
15	O	80	GLN

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Mol	Chain	Res	Type
16	P	9	HIS
16	P	40	ASN
16	P	63	GLN
17	Q	51	ASN
19	S	14	HIS
19	S	57	HIS
20	T	3	ASN
20	T	13	GLN
20	T	61	GLN
20	T	68	HIS
20	T	82	GLN
20	T	84	ASN
21	U	9	ASN
21	U	64	ASN
22	V	38	ASN
22	V	43	GLN
22	V	214	HIS
22	V	273	GLN
22	V	290	GLN
29	c	86	ASN
29	c	90	ASN
29	c	115	GLN
29	c	163	GLN
29	c	260	ASN
30	d	49	GLN
30	d	173	GLN
31	e	115	GLN
31	e	136	GLN
32	f	27	GLN
32	f	135	GLN
33	g	88	GLN
33	g	115	HIS
34	h	2	GLN
34	h	18	GLN
35	i	80	HIS
35	i	136	GLN
36	j	90	ASN
37	k	104	GLN
38	l	13	HIS
38	l	60	GLN
39	m	31	HIS
41	o	10	GLN

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Mol	Chain	Res	Type
41	o	66	ASN
42	p	37	GLN
42	p	52	GLN
42	p	71	GLN
42	p	81	ASN
43	q	12	HIS
44	r	40	ASN
45	s	72	GLN
45	s	91	GLN
47	u	5	ASN
47	u	49	ASN
49	w	20	HIS
49	w	36	HIS
50	x	27	ASN
50	x	45	GLN
50	x	58	ASN
55	2	26	HIS
56	3	35	GLN
57	4	30	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1542 (97%)	197 (13%)	2 (0%)
24	X	8/9 (88%)	1 (12%)	0
25	Y	69/77 (89%)	14 (20%)	1 (1%)
26	Z	1/3 (33%)	0	0
27	a	2749/2904 (94%)	356 (12%)	0
28	b	118/120 (98%)	12 (10%)	0
All	All	4448/4655 (95%)	580 (13%)	3 (0%)

All (580) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C

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Mol	Chain	Res	Type
1	A	51	A
1	A	65	A
1	A	68	G
1	A	71	A
1	A	74	A
1	A	75	G
1	A	76	G
1	A	92	U
1	A	95	C
1	A	121	U
1	A	122	G
1	A	131	A
1	A	138	G
1	A	144	G
1	A	166	U
1	A	181	A
1	A	183	C
1	A	189	A
1	A	197	A
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	283	U
1	A	289	G
1	A	321	A
1	A	328	C
1	A	330	C
1	A	344	A
1	A	352	C
1	A	354	G
1	A	355	C
1	A	367	U
1	A	368	U
1	A	369	G
1	A	372	C
1	A	388	G
1	A	392	C
1	A	406	G
1	A	412	A

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Mol	Chain	Res	Type
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	439	U
1	A	456	A
1	A	457	G
1	A	458	U
1	A	464	U
1	A	467	U
1	A	468	A
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	491	G
1	A	495	A
1	A	496	A
1	A	497	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	524	G
1	A	530	G
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	564	C
1	A	570	G
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	596	A
1	A	633	G
1	A	650	G
1	A	661	G

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Mol	Chain	Res	Type
1	A	665	A
1	A	687	A
1	A	719	C
1	A	721	G
1	A	723	U
1	A	734	G
1	A	746	A
1	A	748	G
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	811	C
1	A	815	A
1	A	817	C
1	A	821	G
1	A	832	G
1	A	890	G
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	993	G
1	A	1003	G
1	A	1004	A
1	A	1007	U
1	A	1009	U
1	A	1020	G
1	A	1024	G
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1034	G
1	A	1035	A
1	A	1039	G

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Mol	Chain	Res	Type
1	A	1042	A
1	A	1044	A
1	A	1065	U
1	A	1085	U
1	A	1089	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1108	G
1	A	1125	U
1	A	1132	C
1	A	1133	G
1	A	1137	C
1	A	1139	G
1	A	1144	G
1	A	1152	A
1	A	1159	U
1	A	1167	A
1	A	1174	G
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1250	A
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1364	U
1	A	1368	A

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Mol	Chain	Res	Type
1	A	1370	G
1	A	1372	U
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1419	G
1	A	1432	G
1	A	1452	C
1	A	1487	G
1	A	1490	U
1	A	1491	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
24	X	19	U
25	Y	10	G
25	Y	14	A
25	Y	46	G
25	Y	48	C
25	Y	49	G
25	Y	52	G
25	Y	56	C
25	Y	58	A
25	Y	61	C
25	Y	66	C
25	Y	68	G
25	Y	70	U
25	Y	71	C
25	Y	76	A
27	a	10	A
27	a	12	U
27	a	14	A
27	a	27	G
27	a	29	U

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Mol	Chain	Res	Type
27	a	34	U
27	a	35	G
27	a	51	G
27	a	61	C
27	a	71	A
27	a	72	U
27	a	74	A
27	a	75	G
27	a	84	A
27	a	101	A
27	a	102	U
27	a	118	A
27	a	120	U
27	a	125	A
27	a	136	G
27	a	137	U
27	a	139	U
27	a	163	C
27	a	181	A
27	a	196	A
27	a	199	A
27	a	216	A
27	a	222	A
27	a	223	A
27	a	248	G
27	a	250	G
27	a	251	A
27	a	265	A
27	a	273	G
27	a	276	U
27	a	278	A
27	a	280	U
27	a	281	C
27	a	282	A
27	a	283	G
27	a	284	U
27	a	287	G
27	a	290	U
27	a	311	A
27	a	329	G
27	a	330	A
27	a	345	A

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Mol	Chain	Res	Type
27	a	356	G
27	a	361	G
27	a	362	A
27	a	367	G
27	a	386	G
27	a	396	G
27	a	402	A
27	a	404	A
27	a	405	U
27	a	411	G
27	a	417	C
27	a	435	C
27	a	456	C
27	a	481	G
27	a	491	G
27	a	505	A
27	a	507	A
27	a	509	C
27	a	513	A
27	a	530	G
27	a	531	C
27	a	532	A
27	a	533	G
27	a	544	C
27	a	545	U
27	a	546	U
27	a	547	A
27	a	549	G
27	a	550	C
27	a	563	A
27	a	568	U
27	a	573	U
27	a	575	A
27	a	588	U
27	a	603	A
27	a	614	A
27	a	615	U
27	a	621	A
27	a	627	A
27	a	637	A
27	a	644	A
27	a	645	C

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Mol	Chain	Res	Type
27	a	646	U
27	a	647	G
27	a	655	A
27	a	685	A
27	a	686	U
27	a	717	C
27	a	721	A
27	a	726	G
27	a	730	A
27	a	740	C
27	a	747	5MU
27	a	764	A
27	a	765	C
27	a	775	G
27	a	776	G
27	a	782	A
27	a	784	G
27	a	785	G
27	a	789	A
27	a	805	G
27	a	812	C
27	a	827	U
27	a	829	A
27	a	845	A
27	a	846	U
27	a	859	G
27	a	869	G
27	a	879	G
27	a	880	G
27	a	881	G
27	a	883	G
27	a	884	U
27	a	888	C
27	a	890	C
27	a	891	G
27	a	892	A
27	a	896	A
27	a	897	C
27	a	899	A
27	a	907	G
27	a	910	A
27	a	914	G

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Mol	Chain	Res	Type
27	a	931	U
27	a	946	C
27	a	961	C
27	a	974	G
27	a	983	A
27	a	989	G
27	a	996	A
27	a	1009	A
27	a	1012	U
27	a	1013	C
27	a	1026	G
27	a	1033	U
27	a	1045	C
27	a	1047	G
27	a	1110	G
27	a	1111	A
27	a	1112	G
27	a	1115	G
27	a	1116	G
27	a	1132	U
27	a	1133	A
27	a	1135	C
27	a	1142	A
27	a	1169	A
27	a	1172	C
27	a	1212	G
27	a	1213	A
27	a	1227	G
27	a	1236	G
27	a	1237	A
27	a	1247	A
27	a	1250	G
27	a	1253	A
27	a	1256	G
27	a	1271	G
27	a	1272	A
27	a	1273	U
27	a	1279	G
27	a	1300	G
27	a	1301	A
27	a	1309	G
27	a	1325	U

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Mol	Chain	Res	Type
27	a	1329	U
27	a	1341	G
27	a	1352	U
27	a	1365	A
27	a	1378	A
27	a	1379	U
27	a	1383	A
27	a	1395	A
27	a	1398	C
27	a	1416	G
27	a	1417	C
27	a	1421	G
27	a	1428	C
27	a	1434	A
27	a	1437	C
27	a	1452	G
27	a	1478	G
27	a	1482	G
27	a	1490	A
27	a	1493	C
27	a	1508	A
27	a	1509	A
27	a	1515	A
27	a	1524	G
27	a	1535	A
27	a	1536	C
27	a	1554	U
27	a	1557	C
27	a	1558	C
27	a	1560	G
27	a	1566	A
27	a	1569	A
27	a	1571	A
27	a	1583	A
27	a	1584	U
27	a	1608	A
27	a	1610	A
27	a	1634	A
27	a	1647	U
27	a	1648	U
27	a	1649	G
27	a	1674	G

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Mol	Chain	Res	Type
27	a	1715	G
27	a	1729	U
27	a	1730	C
27	a	1733	G
27	a	1738	G
27	a	1756	G
27	a	1758	U
27	a	1764	C
27	a	1773	A
27	a	1784	A
27	a	1786	A
27	a	1800	C
27	a	1801	A
27	a	1808	A
27	a	1816	C
27	a	1827	U
27	a	1829	A
27	a	1847	A
27	a	1848	A
27	a	1858	A
27	a	1868	C
27	a	1869	G
27	a	1870	C
27	a	1871	A
27	a	1872	A
27	a	1927	A
27	a	1929	G
27	a	1930	G
27	a	1936	A
27	a	1955	U
27	a	1964	G
27	a	1966	A
27	a	1967	C
27	a	1970	A
27	a	1971	U
27	a	1972	G
27	a	1991	U
27	a	1993	U
27	a	2021	C
27	a	2023	C
27	a	2030	6MZ
27	a	2031	A

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Mol	Chain	Res	Type
27	a	2033	A
27	a	2043	C
27	a	2055	C
27	a	2056	G
27	a	2060	A
27	a	2061	G
27	a	2062	A
27	a	2069	G7M
27	a	2093	G
27	a	2198	A
27	a	2203	U
27	a	2204	G
27	a	2211	A
27	a	2225	A
27	a	2238	G
27	a	2239	G
27	a	2271	G
27	a	2278	A
27	a	2283	C
27	a	2287	A
27	a	2288	A
27	a	2305	U
27	a	2308	G
27	a	2322	A
27	a	2325	G
27	a	2333	A
27	a	2345	G
27	a	2347	C
27	a	2350	C
27	a	2361	G
27	a	2383	G
27	a	2385	C
27	a	2402	U
27	a	2403	C
27	a	2406	A
27	a	2422	C
27	a	2429	G
27	a	2430	A
27	a	2435	A
27	a	2441	U
27	a	2448	A
27	a	2469	A

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Mol	Chain	Res	Type
27	a	2470	G
27	a	2475	C
27	a	2476	A
27	a	2491	U
27	a	2494	G
27	a	2498	OMC
27	a	2502	G
27	a	2505	G
27	a	2506	U
27	a	2518	A
27	a	2520	C
27	a	2529	G
27	a	2535	G
27	a	2547	A
27	a	2566	A
27	a	2567	G
27	a	2572	A
27	a	2573	C
27	a	2582	G
27	a	2602	A
27	a	2603	G
27	a	2609	U
27	a	2613	U
27	a	2615	U
27	a	2629	U
27	a	2630	G
27	a	2639	A
27	a	2646	C
27	a	2661	G
27	a	2689	U
27	a	2690	U
27	a	2713	U
27	a	2714	G
27	a	2716	C
27	a	2720	U
27	a	2726	A
27	a	2729	G
27	a	2732	G
27	a	2733	A
27	a	2744	G
27	a	2748	A
27	a	2758	A

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Mol	Chain	Res	Type
27	a	2762	C
27	a	2765	A
27	a	2778	A
27	a	2791	G
27	a	2797	U
27	a	2798	U
27	a	2799	A
27	a	2818	U
27	a	2820	A
27	a	2835	A
27	a	2849	U
27	a	2873	A
27	a	2880	C
27	a	2883	A
27	a	2901	C
28	b	9	G
28	b	34	A
28	b	35	C
28	b	37	C
28	b	41	G
28	b	56	G
28	b	67	G
28	b	89	U
28	b	90	C
28	b	99	A
28	b	108	A
28	b	109	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	120	A
1	A	264	C
25	Y	57	G

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

41 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
27	2MG	a	2445	27	18,26,27	0.93	2 (11%)	16,38,41	0.69	0
27	PSU	a	2580	27,58	18,21,22	0.52	0	22,30,33	0.62	1 (4%)
27	PSU	a	1911	27	18,21,22	0.46	0	22,30,33	0.58	0
27	PSU	a	2605	27	18,21,22	0.56	0	22,30,33	0.63	0
1	5MC	A	967	1	18,22,23	0.30	0	26,32,35	0.44	0
27	OMU	a	2552	27	19,22,23	0.28	0	26,31,34	0.42	0
1	UR3	A	1498	1	19,22,23	0.28	0	26,32,35	0.37	0
1	G7M	A	527	1	20,26,27	0.57	0	17,39,42	0.42	0
12	D2T	L	89	12	7,9,10	0.90	0	6,11,13	1.63	2 (33%)
27	OMG	a	2251	25,27,59	18,26,27	0.91	1 (5%)	19,38,41	0.62	0
27	OMC	a	2498	27,58	19,22,23	0.28	0	26,31,34	0.41	0
1	2MG	A	1516	1	18,26,27	0.93	1 (5%)	16,38,41	0.69	0
30	MEQ	d	150	30	8,9,10	0.88	0	5,10,12	0.40	0
27	PSU	a	2604	27	18,21,22	0.45	0	22,30,33	0.58	0
27	G7M	a	2069	27,59	20,26,27	0.58	0	17,39,42	0.48	0
27	PSU	a	955	27,59	18,21,22	0.56	0	22,30,33	0.59	0
27	1MG	a	745	27	18,26,27	0.84	2 (11%)	19,39,42	0.47	0
27	PSU	a	2457	27	18,21,22	0.48	0	22,30,33	0.58	0
38	4D4	l	81	38	9,11,12	0.85	0	8,13,15	1.94	3 (37%)
1	MA6	A	1518	1	18,26,27	0.74	0	19,38,41	0.66	0
27	PSU	a	746	27,58	18,21,22	0.57	1 (5%)	22,30,33	0.67	1 (4%)
22	MEQ	V	252	22	8,9,10	0.90	0	5,10,12	0.44	0
27	PSU	a	1917	27	18,21,22	0.51	0	22,30,33	0.55	0
27	PSU	a	2504	27,59	18,21,22	0.49	0	22,30,33	0.56	0
27	6MZ	a	1618	27	18,25,26	0.74	0	16,36,39	0.79	1 (6%)
27	6MZ	a	2030	27	18,25,26	0.74	0	16,36,39	0.77	1 (6%)
27	5MU	a	1939	27,59	19,22,23	0.28	0	28,32,35	0.38	0
1	2MG	A	966	1	18,26,27	0.92	1 (5%)	16,38,41	0.74	0
11	IAS	K	119	11	6,7,8	0.87	0	6,8,10	0.95	0
1	4OC	A	1402	1	20,23,24	0.32	0	26,32,35	0.46	0
27	3TD	a	1915	27	18,22,23	0.46	0	22,32,35	0.58	0
1	2MG	A	1207	1	18,26,27	0.91	1 (5%)	16,38,41	0.69	0
23	FME	W	1	23	8,9,10	0.51	0	7,9,11	0.44	0
27	5MU	a	747	27	19,22,23	0.29	0	28,32,35	0.33	0
27	2MG	a	1835	27	18,26,27	0.92	1 (5%)	16,38,41	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	A	516	58,1	18,21,22	0.52	0	22,30,33	0.65	1 (4%)
1	5MC	A	1407	1	18,22,23	0.30	0	26,32,35	0.46	0
27	H2U	a	2449	27	18,21,22	0.45	0	21,30,33	1.02	1 (4%)
1	MA6	A	1519	1	18,26,27	0.75	0	19,38,41	0.67	0
27	5MC	a	1962	27,59	18,22,23	0.28	0	26,32,35	0.46	0
27	2MA	a	2503	27,58	19,25,26	1.00	2 (10%)	21,37,40	3.07	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	2MG	a	2445	27	-	0/5/27/28	0/3/3/3
27	PSU	a	2580	27,58	-	0/7/25/26	0/2/2/2
27	PSU	a	1911	27	-	0/7/25/26	0/2/2/2
27	PSU	a	2605	27	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
27	OMU	a	2552	27	-	0/9/27/28	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	2/3/25/26	0/3/3/3
12	D2T	L	89	12	-	2/7/12/14	-
27	OMG	a	2251	25,27,59	-	1/5/27/28	0/3/3/3
27	OMC	a	2498	27,58	-	0/9/27/28	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
30	MEQ	d	150	30	-	3/8/9/11	-
27	PSU	a	2604	27	-	0/7/25/26	0/2/2/2
27	G7M	a	2069	27,59	-	1/3/25/26	0/3/3/3
27	PSU	a	955	27,59	-	0/7/25/26	0/2/2/2
27	1MG	a	745	27	-	0/3/25/26	0/3/3/3
27	PSU	a	2457	27	-	0/7/25/26	0/2/2/2
38	4D4	l	81	38	-	5/11/12/14	-
1	MA6	A	1518	1	-	3/7/29/30	0/3/3/3
27	PSU	a	746	27,58	-	1/7/25/26	0/2/2/2
22	MEQ	V	252	22	-	4/8/9/11	-
27	PSU	a	1917	27	-	0/7/25/26	0/2/2/2
27	PSU	a	2504	27,59	-	2/7/25/26	0/2/2/2
27	6MZ	a	1618	27	-	0/5/27/28	0/3/3/3
27	6MZ	a	2030	27	-	2/5/27/28	0/3/3/3
27	5MU	a	1939	27,59	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	966	1	-	0/5/27/28	0/3/3/3
11	IAS	K	119	11	-	2/7/7/8	-
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
27	3TD	a	1915	27	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
23	FME	W	1	23	-	3/7/9/11	-
27	5MU	a	747	27	-	0/7/25/26	0/2/2/2
27	2MG	a	1835	27	-	0/5/27/28	0/3/3/3
1	PSU	A	516	58,1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
27	H2U	a	2449	27	-	0/7/38/39	0/2/2/2
1	MA6	A	1519	1	-	4/7/29/30	0/3/3/3
27	5MC	a	1962	27,59	-	0/7/25/26	0/2/2/2
27	2MA	a	2503	27,58	-	1/3/25/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	966	2MG	C5-C6	-2.35	1.42	1.47
27	a	1835	2MG	C5-C6	-2.32	1.42	1.47
1	A	1516	2MG	C5-C6	-2.31	1.42	1.47
27	a	2445	2MG	C5-C6	-2.29	1.42	1.47
1	A	1207	2MG	C5-C6	-2.28	1.42	1.47
27	a	745	1MG	C5-C4	-2.24	1.37	1.43
27	a	2251	OMG	C5-C6	-2.19	1.43	1.47
27	a	2503	2MA	C6-N1	2.14	1.37	1.33
27	a	2503	2MA	C6-N6	-2.09	1.26	1.34
27	a	746	PSU	O4'-C1'	-2.08	1.41	1.43
27	a	745	1MG	C8-N7	-2.02	1.31	1.35
27	a	2445	2MG	C8-N7	-2.02	1.31	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	2503	2MA	C5-C6-N1	-12.36	112.90	121.01
38	l	81	4D4	NE-CZ-NH2	3.95	127.65	120.70
27	a	2503	2MA	C2-N1-C6	3.83	124.05	118.08
27	a	2503	2MA	C2-N3-C4	-3.82	112.42	115.52
27	a	2449	H2U	C5-C4-N3	-3.12	113.14	116.65
12	L	89	D2T	O-C-CA	-2.78	117.49	124.78
38	l	81	4D4	NH1-CZ-NE	-2.67	113.02	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	l	81	4D4	O-C-CA	-2.65	117.84	124.78
27	a	2503	2MA	N6-C6-N1	2.33	123.39	117.07
1	A	516	PSU	O4'-C1'-C2'	2.28	108.36	105.14
12	L	89	D2T	OD1-CG-CB	-2.26	117.71	122.44
27	a	746	PSU	O4'-C1'-C2'	2.24	108.31	105.14
27	a	2503	2MA	C5-C6-N6	2.21	123.71	120.35
27	a	2580	PSU	O4'-C1'-C2'	2.13	108.15	105.14
27	a	1618	6MZ	C2-N1-C6	2.09	118.38	116.59
27	a	2030	6MZ	C2-N1-C6	2.00	118.31	116.59

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	C5-C6-N6-C9
1	A	1518	MA6	C5-C6-N6-C10
1	A	1519	MA6	C5-C6-N6-C10
38	l	81	4D4	N-CA-CB-CG
38	l	81	4D4	NH2-CZ-NE-CD
22	V	252	MEQ	C-CA-CB-CG
23	W	1	FME	O1-CN-N-CA
23	W	1	FME	C-CA-CB-CG
27	a	2251	OMG	C1'-C2'-O2'-CM2
27	a	2030	6MZ	O4'-C4'-C5'-O5'
27	a	2504	PSU	O4'-C4'-C5'-O5'
1	A	1518	MA6	N1-C6-N6-C10
30	d	150	MEQ	NE2-CD-CG-CB
27	a	2030	6MZ	C3'-C4'-C5'-O5'
30	d	150	MEQ	OE1-CD-CG-CB
30	d	150	MEQ	CA-CB-CG-CD
27	a	2504	PSU	C3'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	O4'-C4'-C5'-O5'
12	L	89	D2T	CG-CB-SB-CB1
27	a	2503	2MA	O4'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
38	l	81	4D4	NH1-CZ-NE-CD
22	V	252	MEQ	N-CA-CB-CG
11	K	119	IAS	OXT-C-CA-CB
22	V	252	MEQ	OE1-CD-CG-CB
11	K	119	IAS	O-C-CA-CB
22	V	252	MEQ	NE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
27	a	746	PSU	O4'-C1'-C5-C4
23	W	1	FME	N-CA-CB-CG
27	a	2069	G7M	O4'-C4'-C5'-O5'
12	L	89	D2T	CA-CB-SB-CB1
38	l	81	4D4	C-CA-CB-OB
1	A	1519	MA6	C3'-C4'-C5'-O5'
38	l	81	4D4	C-CA-CB-CG
1	A	527	G7M	C4'-C5'-O5'-P

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	2605	PSU	1	0
12	L	89	D2T	3	0
27	a	2251	OMG	1	0
27	a	745	1MG	1	0
1	A	1518	MA6	1	0
27	a	2030	6MZ	2	0
1	A	966	2MG	1	0
1	A	1402	4OC	1	0
1	A	1407	5MC	1	0
27	a	2503	2MA	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 358 ligands modelled in this entry, 350 are monoatomic - leaving 8 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
60	SPD	a	6194	-	9,9,9	0.27	0	8,8,8	0.86	0
60	SPD	a	6193	-	9,9,9	0.27	0	8,8,8	0.86	0
60	SPD	a	6199	-	9,9,9	0.20	0	8,8,8	0.81	0
60	SPD	a	6197	-	9,9,9	0.23	0	8,8,8	0.89	0
60	SPD	a	6195	-	9,9,9	0.29	0	8,8,8	0.83	0
61	PUT	a	6200	-	5,5,5	0.13	0	4,4,4	0.15	0
60	SPD	a	6198	-	9,9,9	0.23	0	8,8,8	0.88	0
60	SPD	a	6196	-	9,9,9	0.24	0	8,8,8	0.83	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
60	SPD	a	6194	-	-	0/7/7/7	-
60	SPD	a	6193	-	-	0/7/7/7	-
60	SPD	a	6199	-	-	0/7/7/7	-
60	SPD	a	6197	-	-	2/7/7/7	-
60	SPD	a	6195	-	-	0/7/7/7	-
61	PUT	a	6200	-	-	0/3/3/3	-
60	SPD	a	6198	-	-	0/7/7/7	-
60	SPD	a	6196	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	a	6196	SPD	N6-C7-C8-C9
60	a	6197	SPD	N6-C7-C8-C9
60	a	6197	SPD	C3-C4-C5-N6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	a	6193	SPD	1	0
60	a	6197	SPD	2	0



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

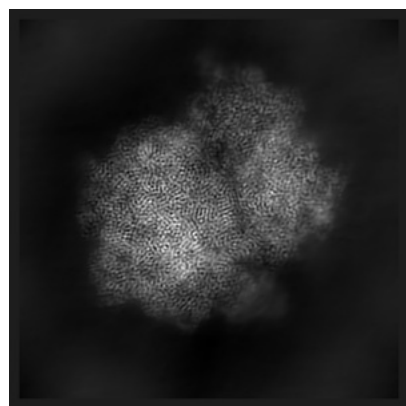
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60474. These allow visual inspection of the internal detail of the map and identification of artifacts.

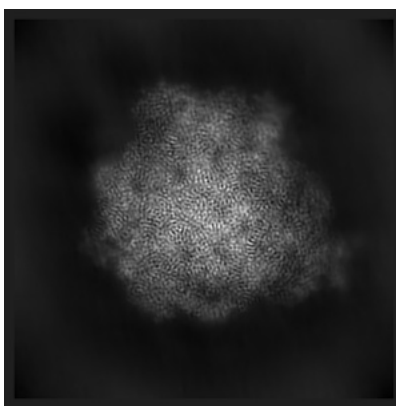
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

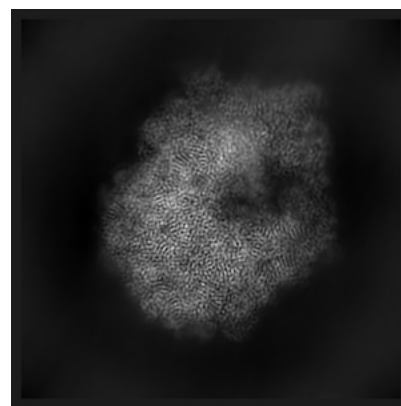
#### 6.1.1 Primary map



X

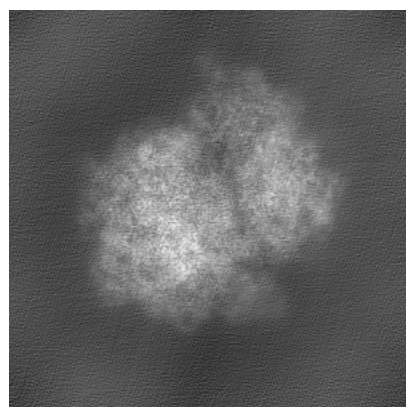


Y

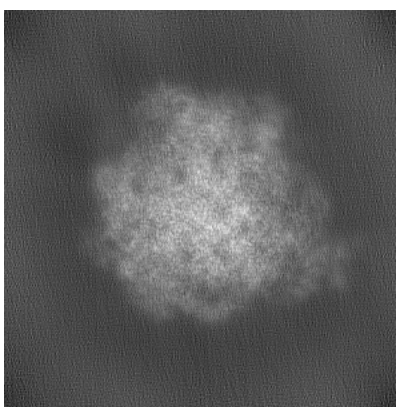


Z

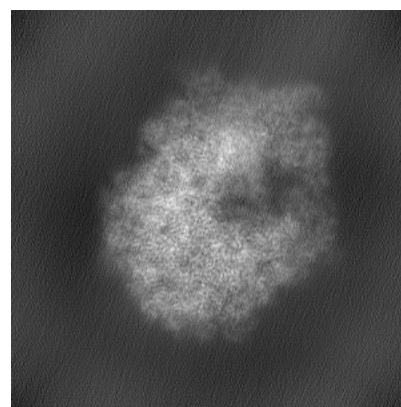
#### 6.1.2 Raw map



X



Y

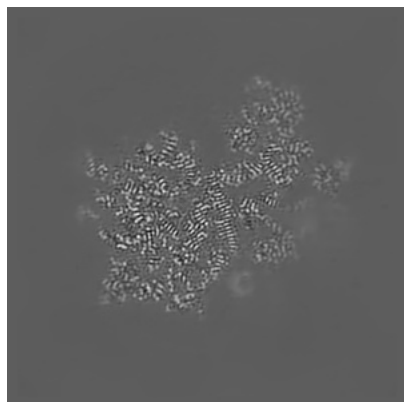


Z

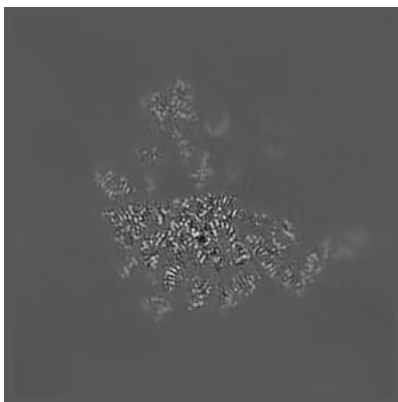
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

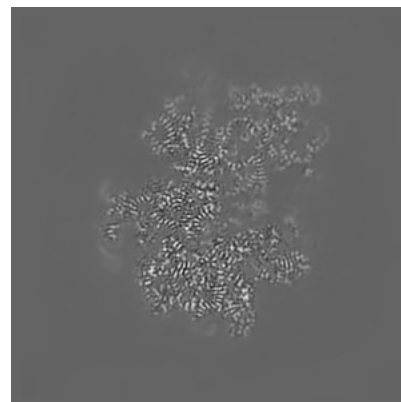
### 6.2.1 Primary map



X Index: 216

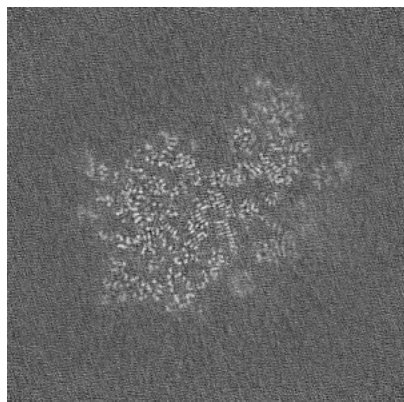


Y Index: 216

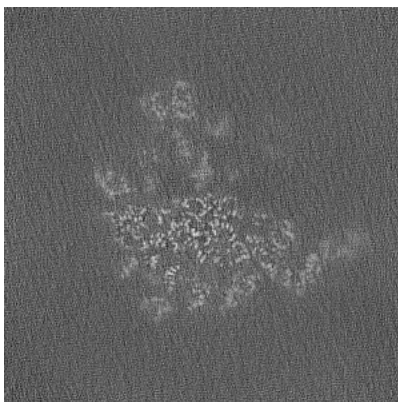


Z Index: 216

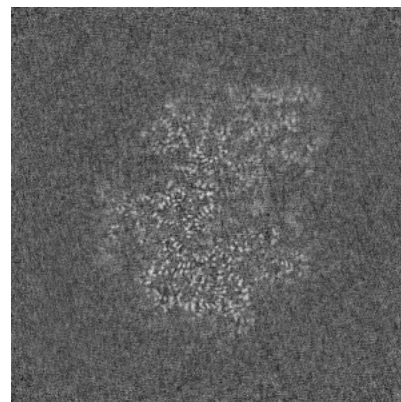
### 6.2.2 Raw map



X Index: 216



Y Index: 216

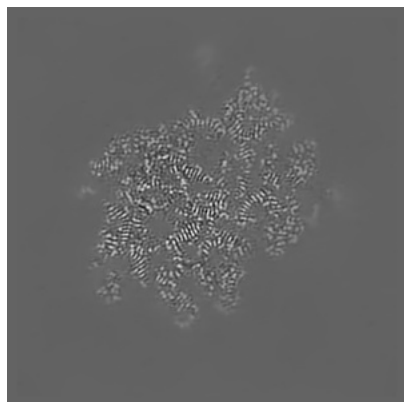


Z Index: 216

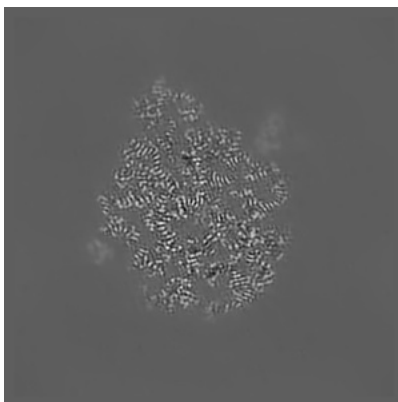
The images above show central slices of the map in three orthogonal directions.

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

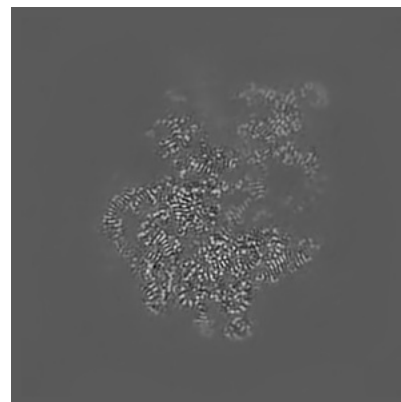
### 6.3.1 Primary map



X Index: 186

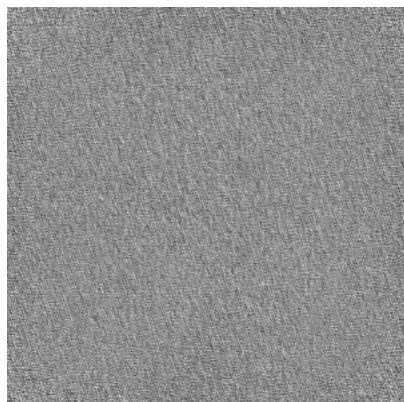


Y Index: 177

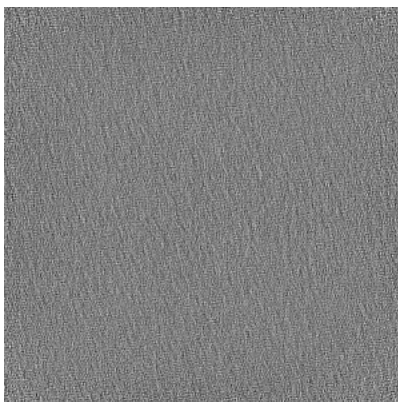


Z Index: 208

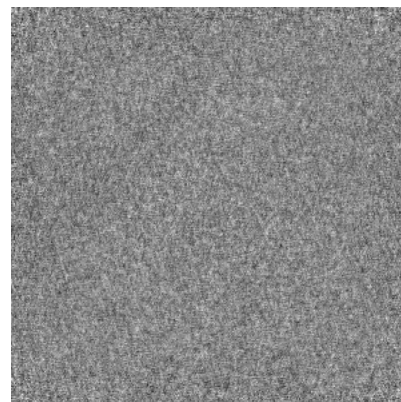
### 6.3.2 Raw map



X Index: 0



Y Index: 0



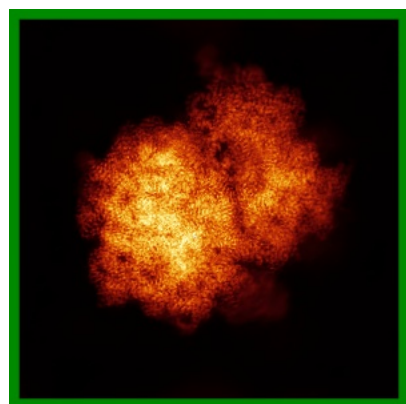
Z Index: 0

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

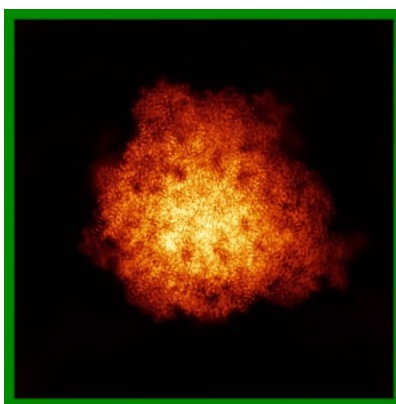


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

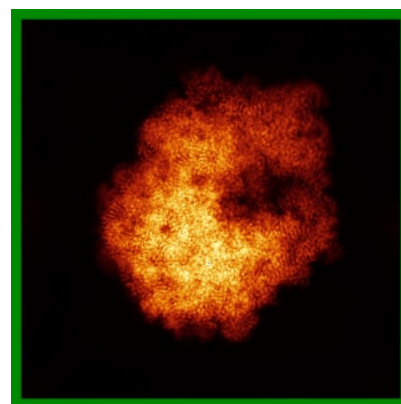
### 6.4.1 Primary map



X

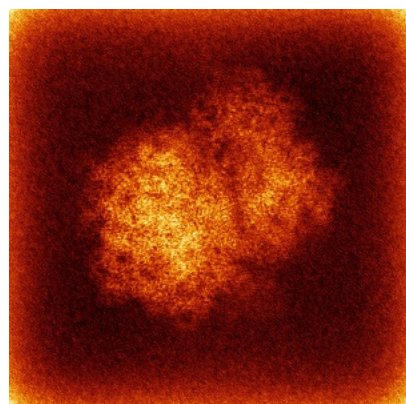


Y

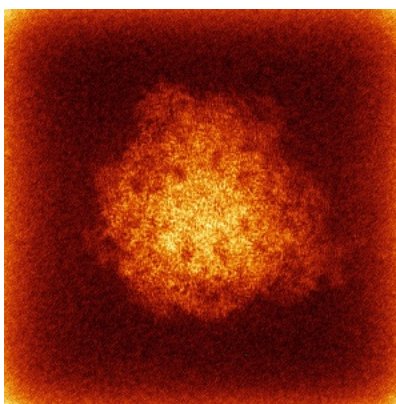


Z

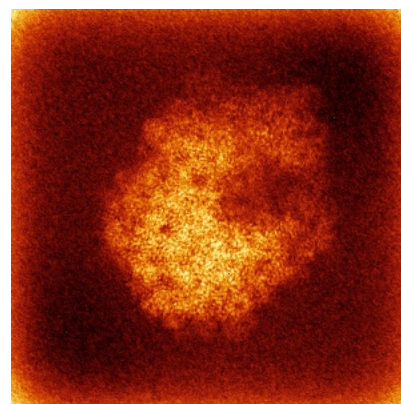
### 6.4.2 Raw map



X



Y

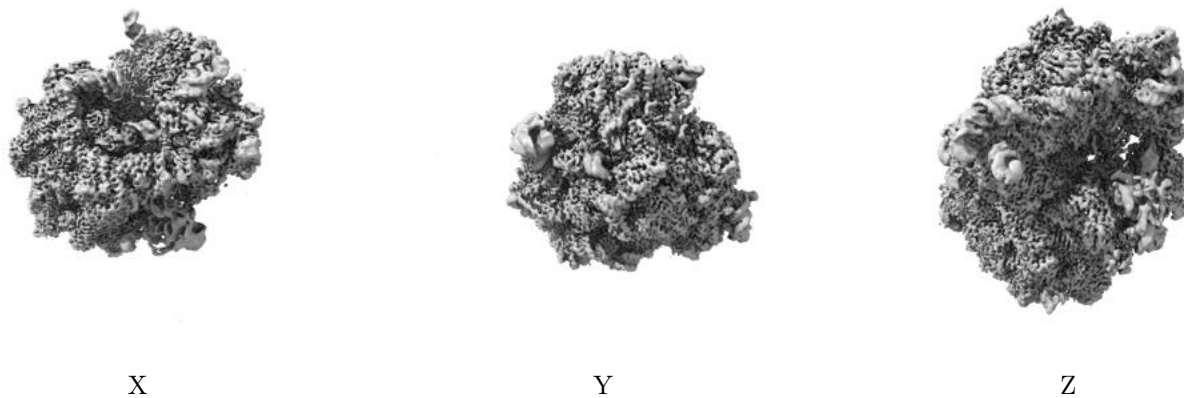


Z

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

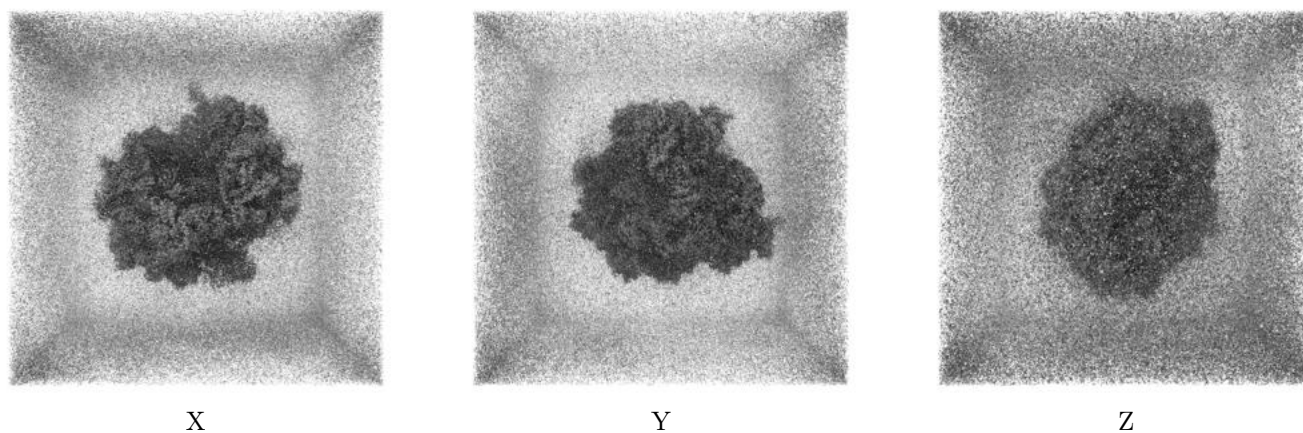
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

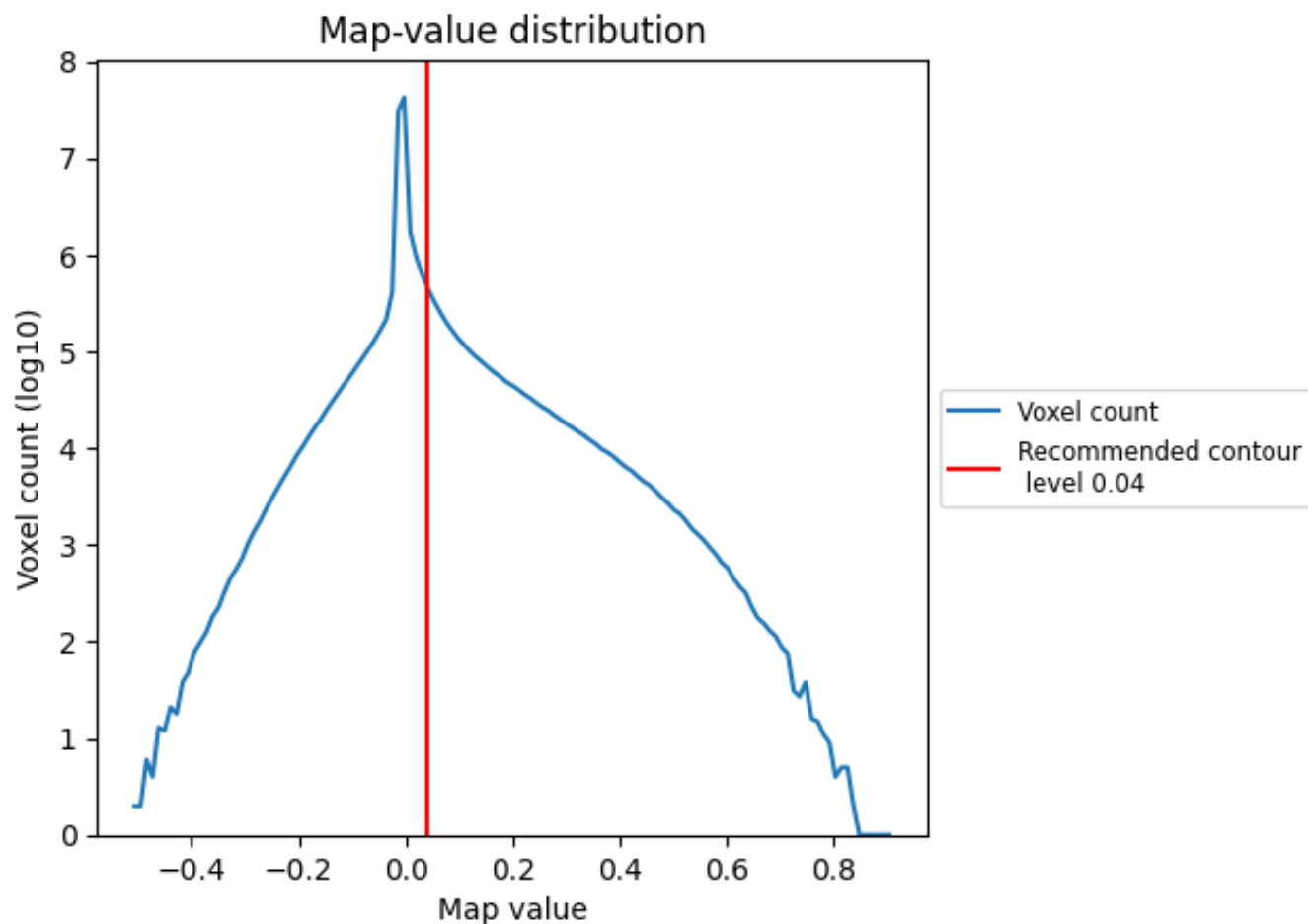
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

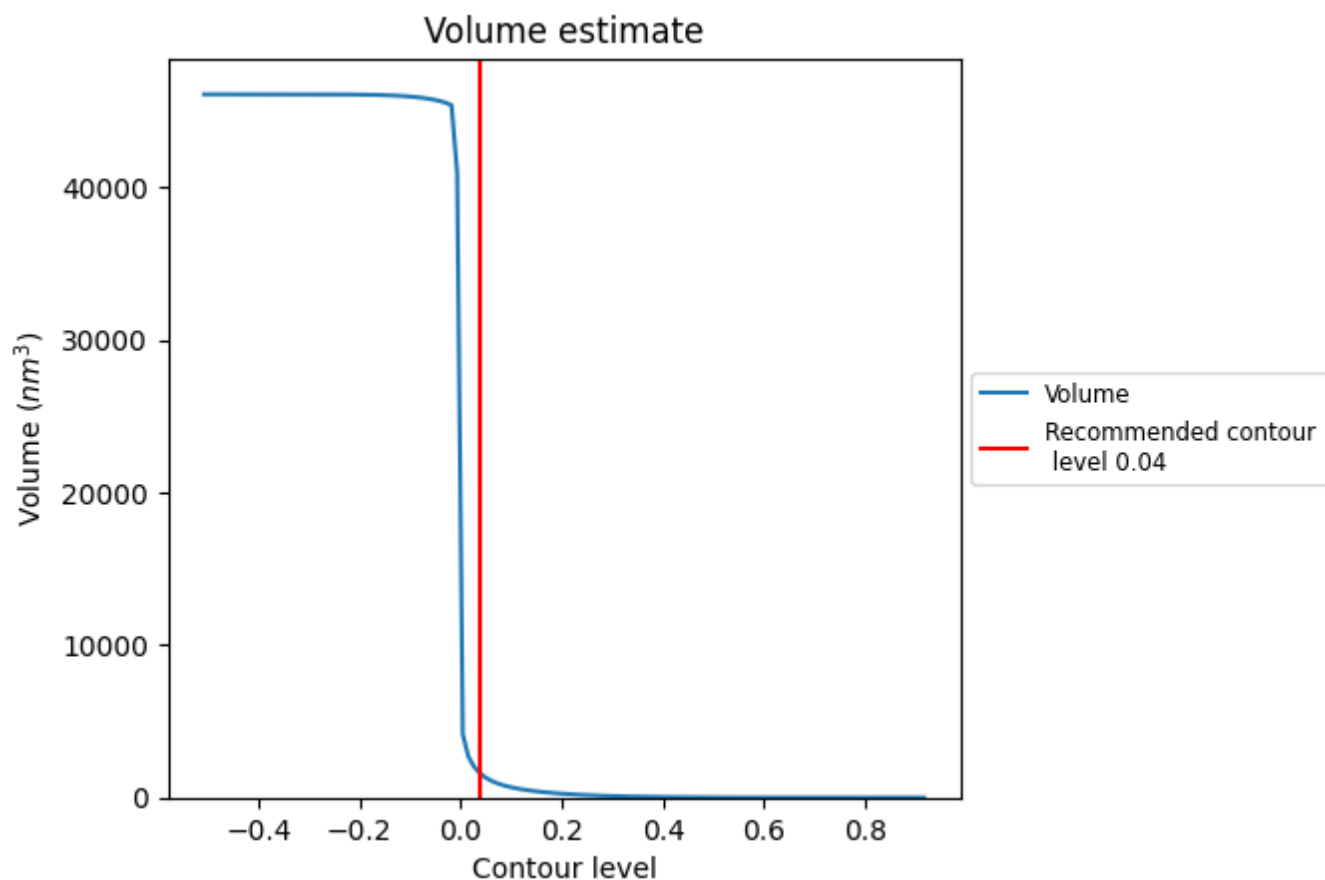
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

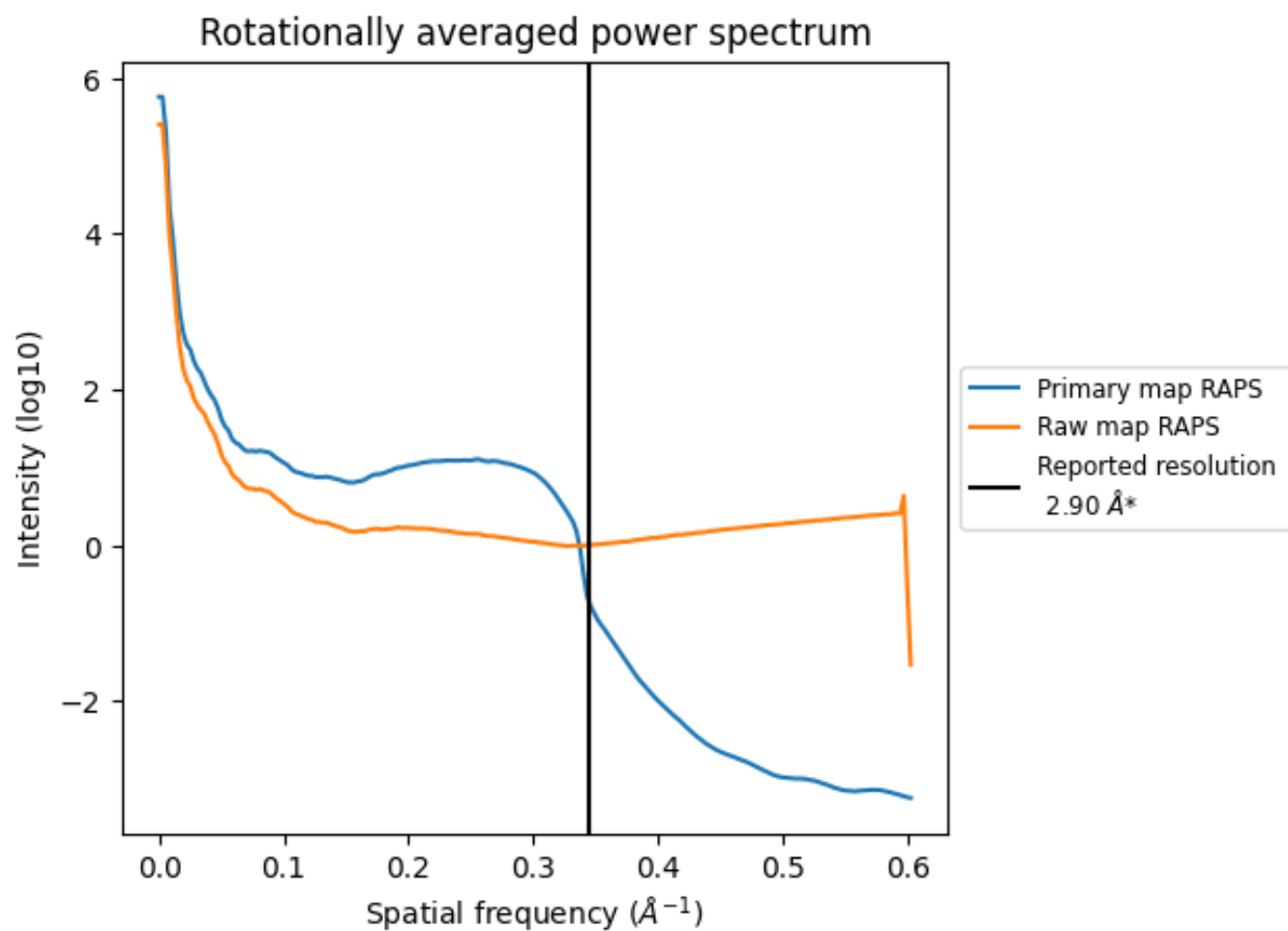


The volume at the recommended contour level is 1554 nm<sup>3</sup>; this corresponds to an approximate mass of 1403 kDa.

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 ⓘ

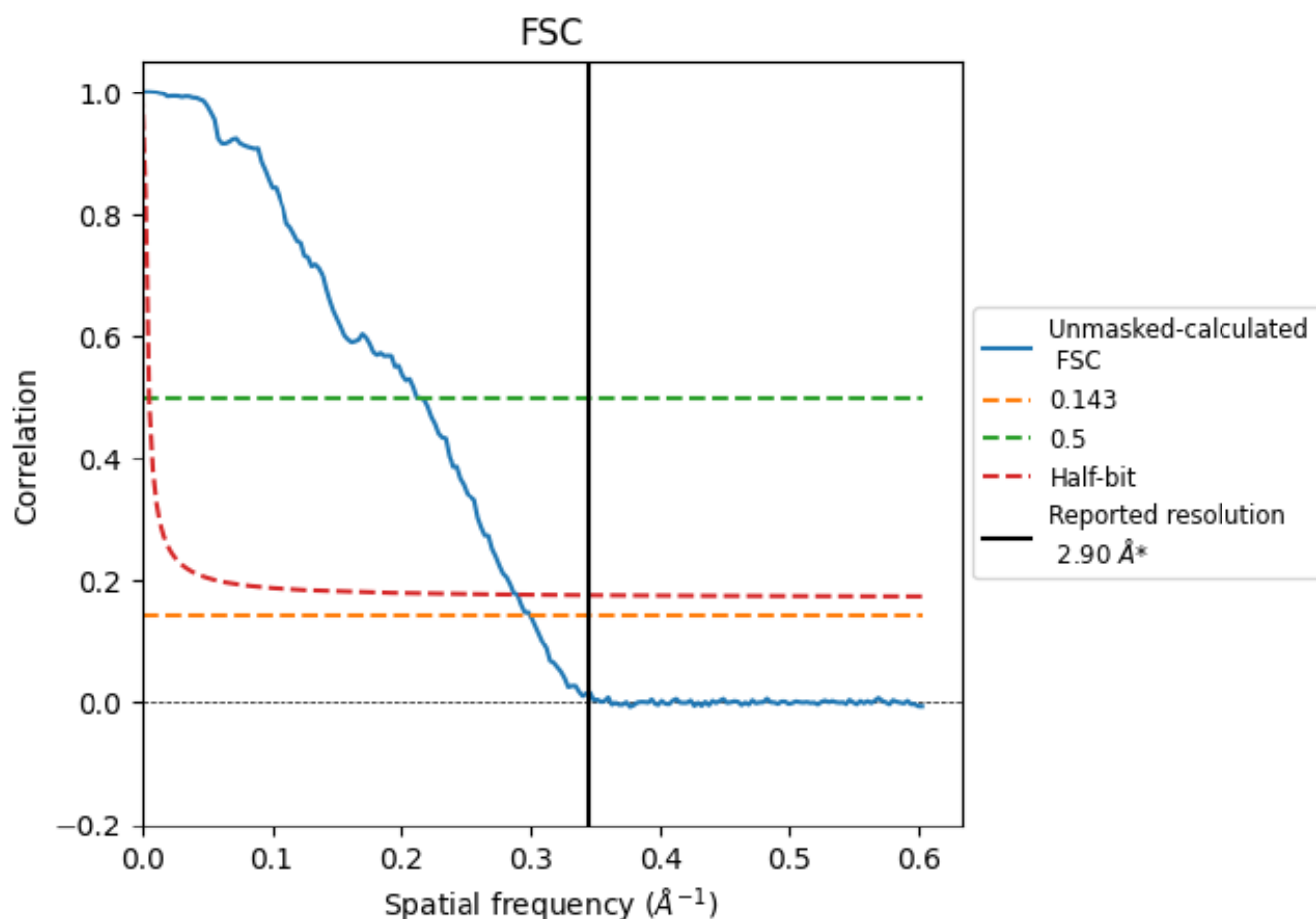


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

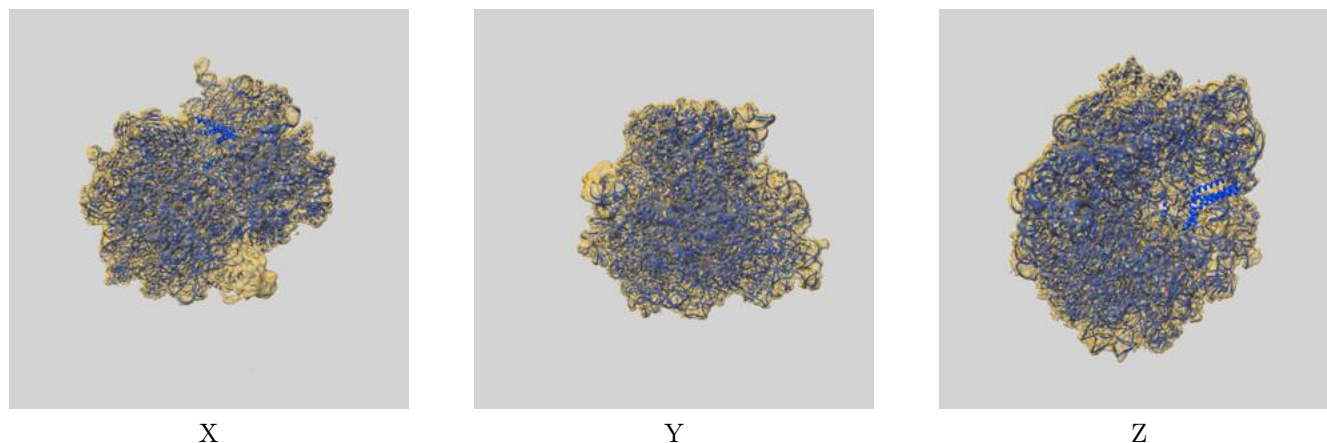
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	4.72	3.45

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.34 differs from the reported value 2.9 by more than 10 %

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

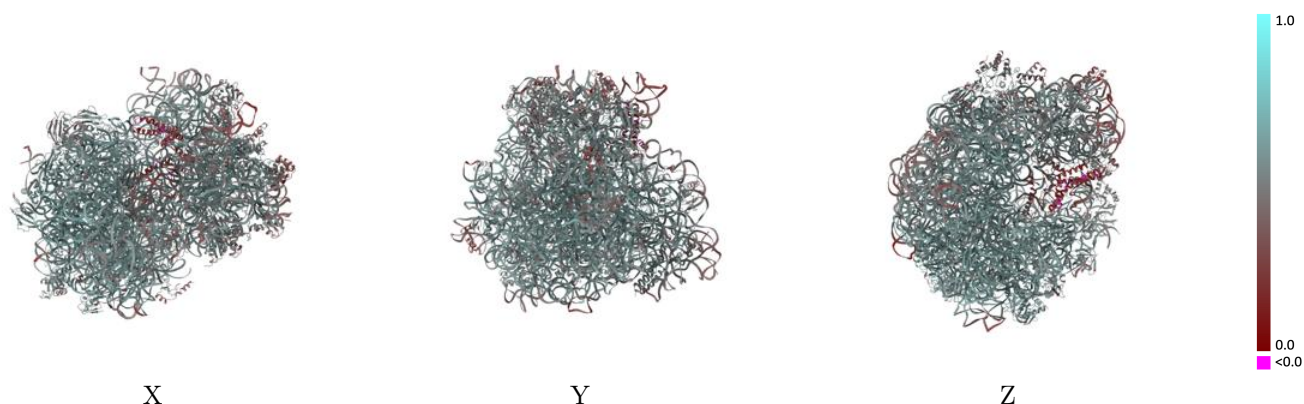
This section contains information regarding the fit between EMDB map EMD-60474 and PDB model 8ZTV. Per-residue inclusion information can be found in section 3 on page 16.

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



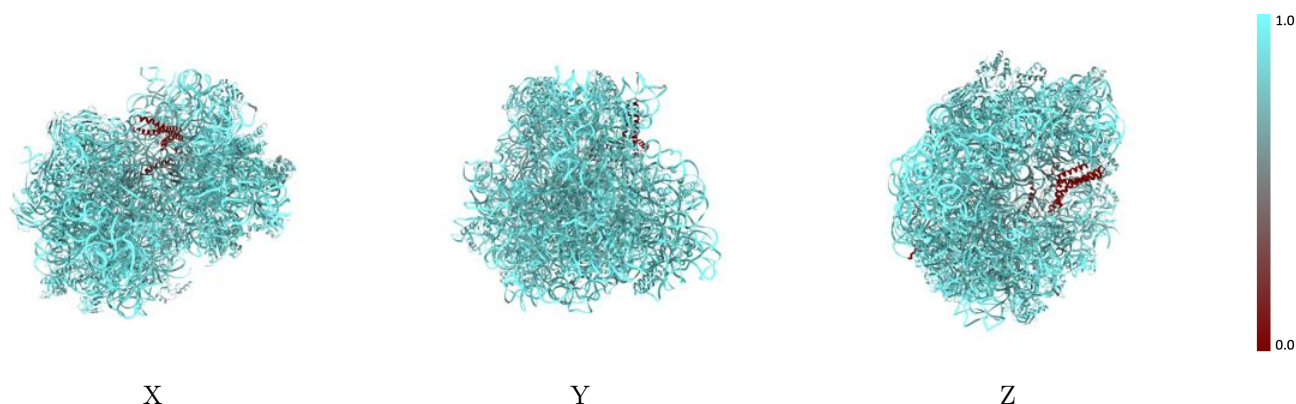
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



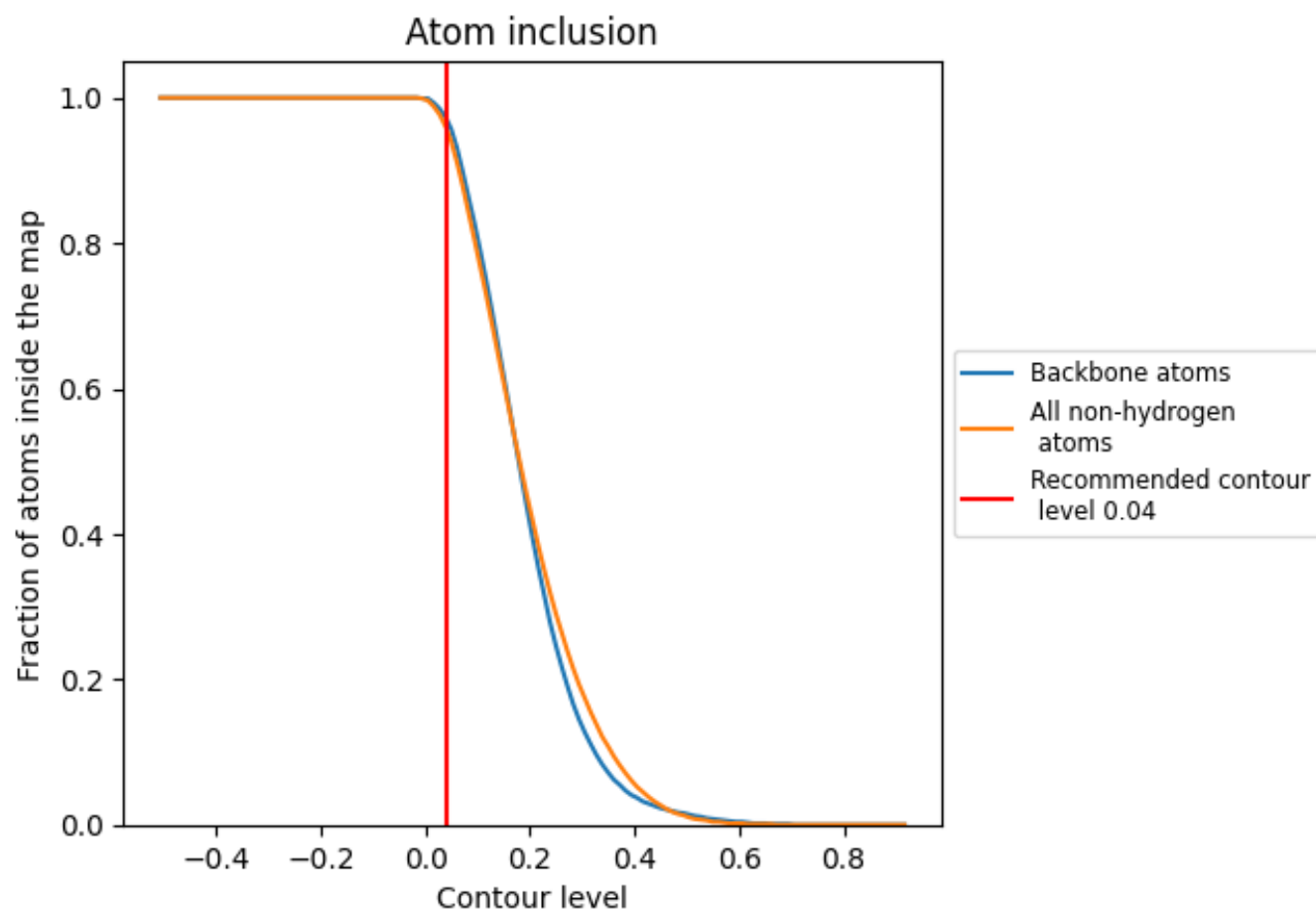
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.5530
0	 0.9220	 0.5410
1	 0.9800	 0.6120
2	 0.9860	 0.6100
3	 0.9830	 0.5900
4	 0.8070	 0.4240
A	 0.9860	 0.5430
B	 0.8410	 0.4520
C	 0.9280	 0.5160
D	 0.9030	 0.4920
E	 0.9410	 0.5580
F	 0.8860	 0.5150
G	 0.8820	 0.4790
H	 0.9280	 0.5410
I	 0.8910	 0.4780
J	 0.8500	 0.4320
K	 0.9400	 0.5440
L	 0.9270	 0.5430
M	 0.8820	 0.4750
N	 0.9150	 0.5000
O	 0.9060	 0.5410
P	 0.9210	 0.5140
Q	 0.9020	 0.5180
R	 0.9180	 0.5340
S	 0.8620	 0.4820
T	 0.9240	 0.5100
U	 0.8590	 0.4600
V	 0.4610	 0.3120
W	 0.9440	 0.5140
X	 0.9900	 0.5580
Y	 0.9570	 0.4930
Z	 0.9760	 0.5740
a	 0.9900	 0.5850
b	 0.9800	 0.5400
c	 0.9680	 0.6030



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Chain	Atom inclusion	Q-score
d	 0.9620	 0.5850
e	 0.9260	 0.5480
f	 0.8500	 0.4720
g	 0.8650	 0.4920
h	 0.7810	 0.4120
i	 0.9680	 0.5920
j	 0.9610	 0.5840
k	 0.9470	 0.5760
l	 0.9630	 0.5870
m	 0.9800	 0.5950
n	 0.9140	 0.5260
o	 0.9410	 0.5730
p	 0.9850	 0.6120
q	 0.9500	 0.5730
r	 0.9560	 0.5820
s	 0.9470	 0.5620
t	 0.9350	 0.5430
u	 0.9170	 0.5350
v	 0.9500	 0.5840
w	 0.9630	 0.5790
x	 0.9160	 0.5300
y	 0.9430	 0.5750
z	 0.9560	 0.5740