Full wwPDB EM Validation Report

Oct 20, 2026 – 06:02 pm BST

PDB ID	:	9SVJ / pdb_00009svj
EMDB ID	:	EMD-55260
Title	:	Structural characterization of hibernating ribosomes in the Gram-negative pathogen Acinetobacter baumannii
Authors	:	Vasanthakrishnan, R.K.B.S.; Olivier, D.; Sophie, C.; Yann, L.C.; Sylvie, G.D.; Sassi, M.; Emmanuel, G.; Reynald, G.
Deposited on	:	2025-10-03
Resolution	:	2.50 Å(reported)
Based on initial model	:	8B0X

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

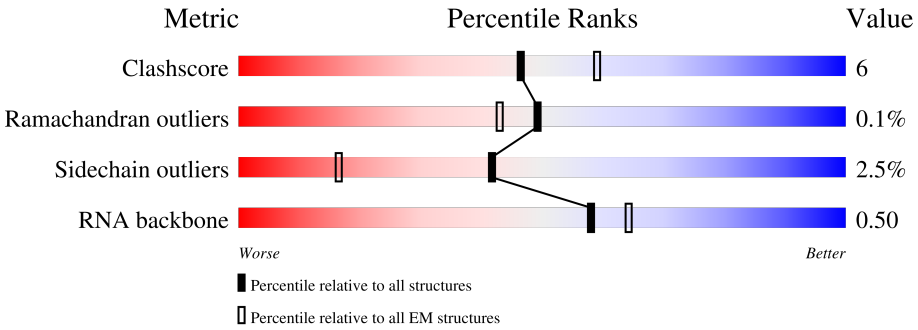
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

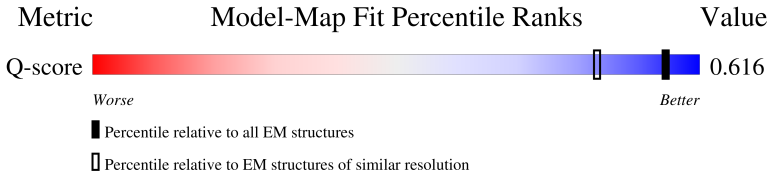
1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

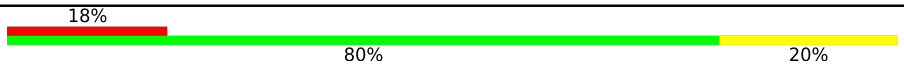
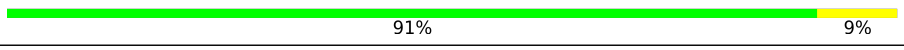
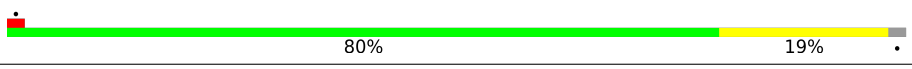
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	0	51	
2	1	44	
3	2	64	

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Mol	Chain	Length	Quality of chain
4	3	38	5% 71% 29%
5	4	74	96% 80% 16%
6	A	1537	21% 57% 37% 6%
7	B	250	90% 68% 22% 8%
8	C	215	61% 79% 20%
9	D	208	74% 78% 21%
10	E	165	22% 80% 13% 6%
11	F	127	74% 67% 16% 17%
12	G	156	85% 81% 16%
13	H	131	31% 80% 19%
14	I	128	66% 85% 14%
15	J	103	66% 68% 29%
16	K	128	47% 72% 18% 9%
17	L	124	35% 81% 17%
18	M	118	84% 81% 18%
19	N	101	59% 71% 27%
20	O	89	39% 87% 12%
21	P	83	45% 90% 8%
22	Q	85	53% 75% 18% 7%
23	R	75	67% 69% 19% 12%
24	S	91	79% 68% 23% 8%
25	T	88	36% 82% 16%
26	V	77	99% 23% 47% 27%
27	W	15	67% 47% 20% 33%
28	X	116	44% 72% 17% 10%

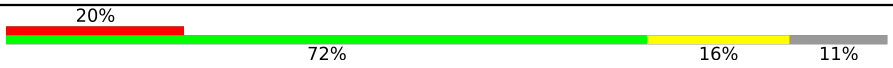
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Mol	Chain	Length	Quality of chain
29	a	2893	14% 60% 35% 5%
30	b	115	13% 75% 20% 5%
31	c	274	5% 86% 13%
32	d	212	10% 87% 12%
33	e	200	23% 89% 10%
34	f	178	90% 74% 25%
35	g	177	69% 77% 20%
36	h	148	41% 30% 10% 59%
37	i	142	84% 16%
38	j	122	16% 83% 17%
39	k	146	11% 88% 11%
40	l	137	19% 82% 18%
41	m	125	86% 10% 5%
42	n	116	35% 87% 11%
43	o	122	15% 82% 13%
44	p	119	89% 9%
45	q	103	16% 79% 21%
46	r	109	8% 81% 19%
47	s	106	18% 80% 7% 13%
48	t	105	40% 90% 9%
49	u	98	38% 93% 5%
50	v	85	6% 79% 12% 8%
51	w	78	21% 88% 9%
52	x	64	52% 80% 17%
53	y	58	10% 76% 24%

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Mol	Chain	Length	Quality of chain
54	z	61	

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 144017 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	71	Total	C	N	O	S	0	0
			552	343	101	102	6		

- Molecule 6 is a RNA chain called 16S rRNA (1537-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1536	Total	C	N	O	P	0	0
			32947	14705	6016	10690	1536		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	229	Total	C	N	O	S	0	0
			1801	1130	333	332	6		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	106	Total	C	N	O	S	0	0
			878	552	160	162	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1210	758	229	216	7		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	127	Total	C	N	O	S	0	0
			995	621	198	175	1		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			861	535	166	159	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	118	IAS	ASN	conflict	UNP D0CD20

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	122	Total	C	N	O	S	0	0
			947	581	193	167	6		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	116	Total	C	N	O	S	0	0
			912	564	186	159	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	82	Total	C	N	O	S	0	0
			644	403	128	112	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	66	Total	C	N	O	S	0	0
			545	349	96	99	1		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			657	419	127	109	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	86	Total	C	N	O	S	0	0
			663	409	139	113	2		

- Molecule 26 is a RNA chain called tRNA (77-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
26	V	77	Total	C	N	O	P	S	0	0
			1644	734	297	535	77	1		

- Molecule 27 is a RNA chain called non-Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	10	Total	C	N	O	P	0	0
			219	97	41	71	10		

- Molecule 28 is a protein called Putative ribosomal subunit interface protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	104	Total	C	N	O	S	0	0
			841	519	161	158	3		

- Molecule 29 is a RNA chain called 23S rRNA (2890-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	2890	Total	C	N	O	P	0	0
			61984	27671	11335	20088	2890		

- Molecule 30 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	272	Total	C	N	O	S	0	0
			2111	1302	436	365	8		

- Molecule 32 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	211	Total	C	N	O	S	0	0
			1573	973	297	300	3		

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	199	Total	C	N	O	S	0	0
			1511	950	280	276	5		

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	177	Total	C	N	O	S	0	0
			1395	886	250	251	8		

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	175	Total	C	N	O	S	0	0
			1327	838	238	250	1		

- Molecule 36 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 37 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 38 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

- Molecule 39 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	146	Total	C	N	O	S	0	0
			1089	673	215	200	1		

- Molecule 40 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	137	Total	C	N	O	S	0	0
			1088	687	210	185	6		

- Molecule 41 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	119	Total 942	C 590	N 186	O 163	S 3	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	115	Total 865	C 532	N 175	O 157	S 1	0	0

- Molecule 43 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	o	117	Total 919	C 578	N 177	O 164	0	0

- Molecule 44 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	117	Total 934	C 589	N 197	O 146	S 2	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	103	Total 807	C 506	N 155	O 143	S 3	0	0

- Molecule 46 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	109	Total 826	C 514	N 158	O 150	S 4	0	0

- Molecule 47 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	92	Total 717	C 457	N 129	O 130	S 1	0	0

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	t	103	Total	C	N	O	0	0
			766	476	142	148		

- Molecule 49 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	97	Total	C	N	O	S	0	0
			760	477	143	139	1		

- Molecule 50 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	78	Total	C	N	O	S	0	0
			589	365	113	109	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	77	Total	C	N	O	S	0	0
			632	395	130	105	2		

- Molecule 52 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	62	Total	C	N	O	S	0	0
			498	308	96	93	1		

- Molecule 53 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	58	Total	C	N	O	S	0	0
			463	286	88	85	4		

- Molecule 54 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	54	Total	C	N	O	S	0	0
			447	265	100	81	1		

- Molecule 55 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
55	1	1	Total K 1 1	0
55	3	1	Total K 1 1	0
55	A	47	Total K 47 47	0
55	L	1	Total K 1 1	0
55	a	111	Total K 111 111	0
55	b	1	Total K 1 1	0
55	c	4	Total K 4 4	0
55	d	2	Total K 2 2	0
55	t	1	Total K 1 1	0

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

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

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

Mol	Chain	Residues	Atoms	AltConf
57	A	95	Total Mg 95 95	0
57	J	1	Total Mg 1 1	0
57	M	1	Total Mg 1 1	0
57	X	1	Total Mg 1 1	0
57	a	251	Total Mg 251 251	0
57	b	5	Total Mg 5 5	0
57	c	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
57	d	1	Total Mg 1 1	0
57	k	1	Total Mg 1 1	0
57	p	1	Total Mg 1 1	0
57	v	1	Total Mg 1 1	0
57	z	1	Total Mg 1 1	0

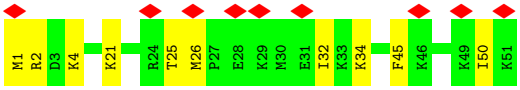
3 Residue-property plots (i)

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

• Molecule 1: Large ribosomal subunit protein bL33

Chain 0:





• Molecule 2: Large ribosomal subunit protein bL34

Chain 1:

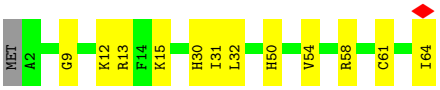




• Molecule 3: Large ribosomal subunit protein bL35

Chain 2:

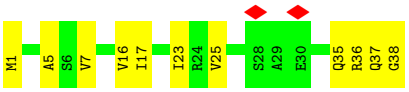




• Molecule 4: Large ribosomal subunit protein bL36

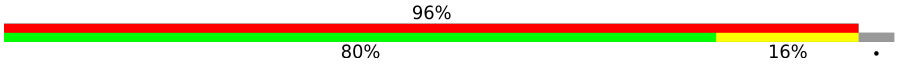
Chain 3:

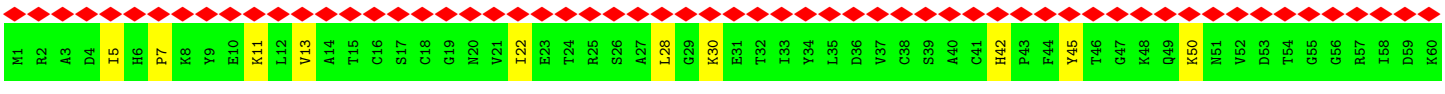


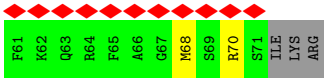


• Molecule 5: Large ribosomal subunit protein bL31

Chain 4:



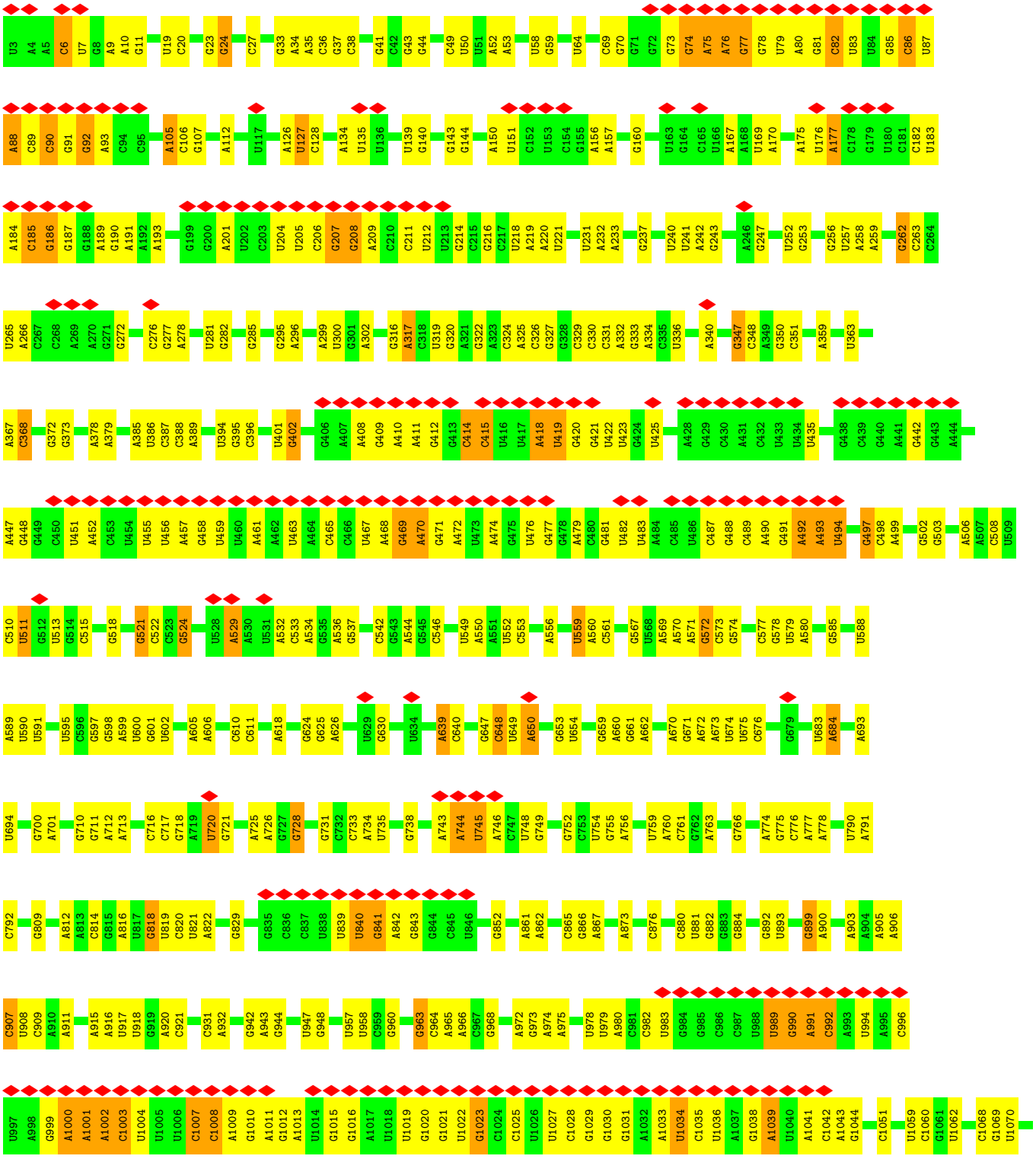


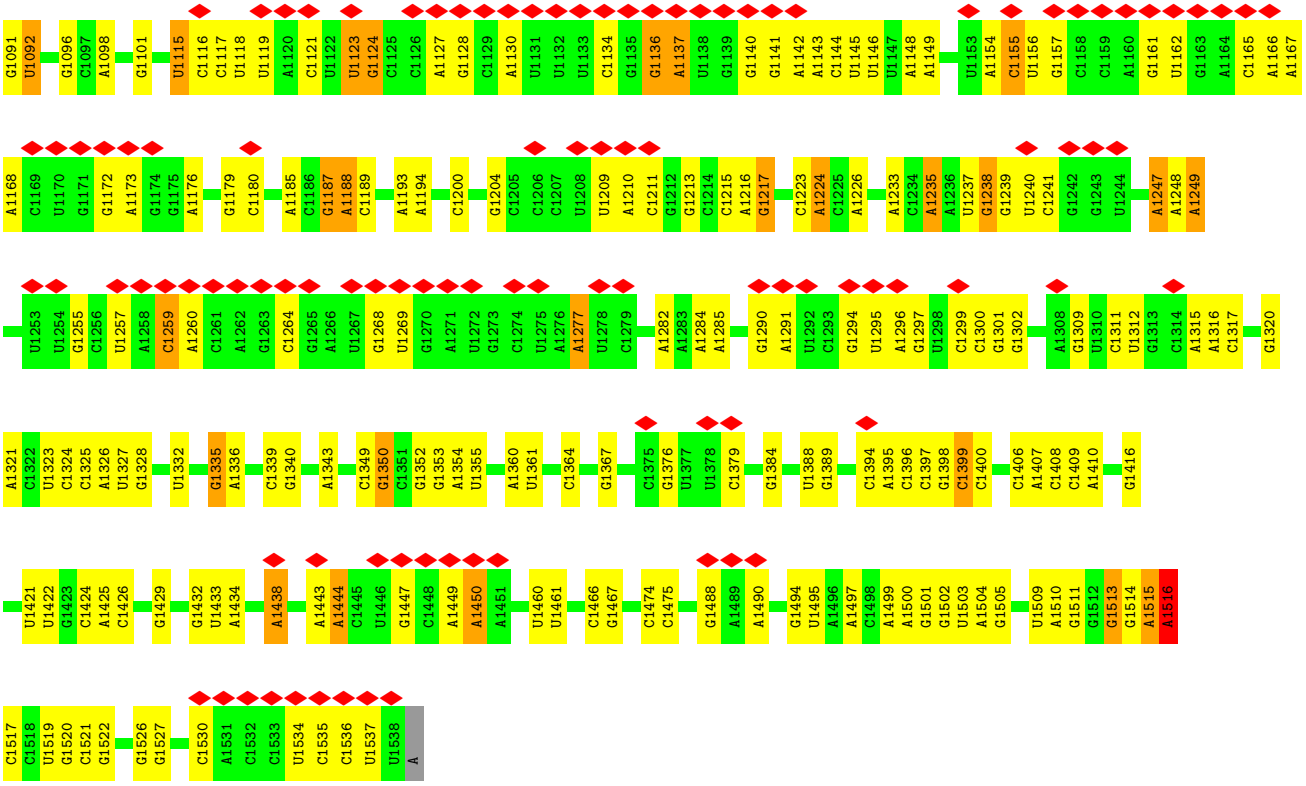


• Molecule 6: 16S rRNA (1537-MER)

Chain A:

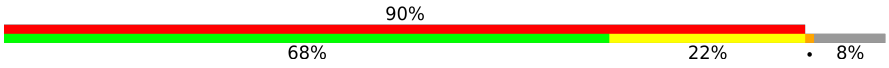






• Molecule 7: Small ribosomal subunit protein uS2

Chain B:

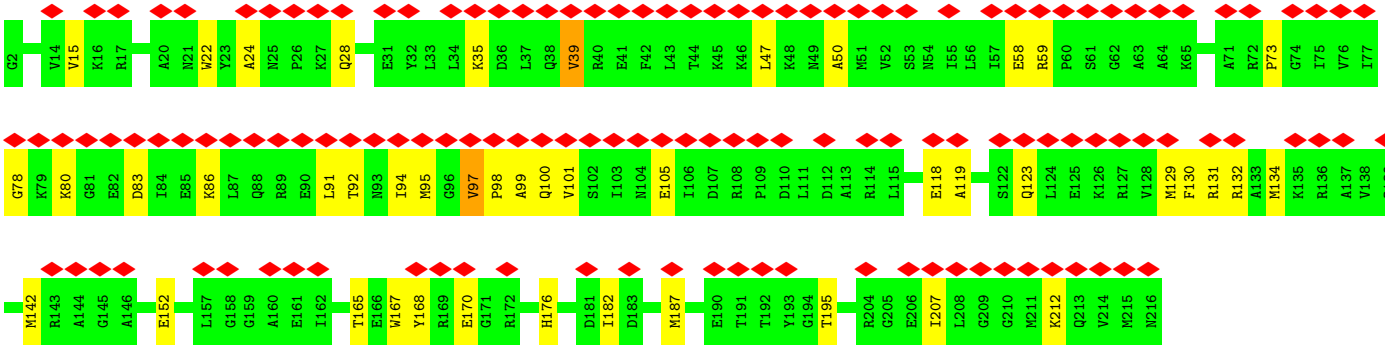




• Molecule 8: Small ribosomal subunit protein uS3

Chain C:





• Molecule 9: Small ribosomal subunit protein uS4

Chain D:

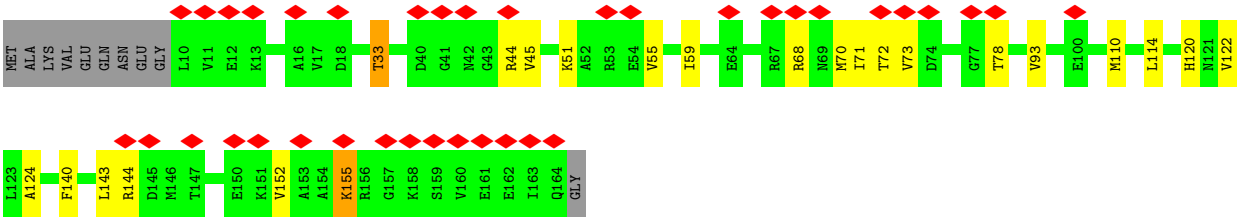




• Molecule 10: Small ribosomal subunit protein uS5

Chain E:

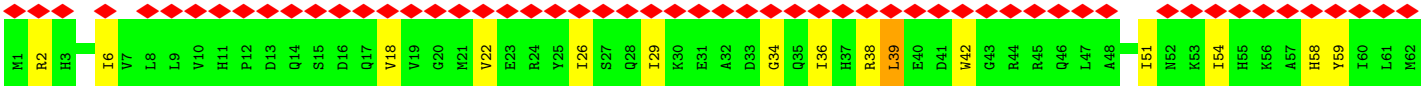


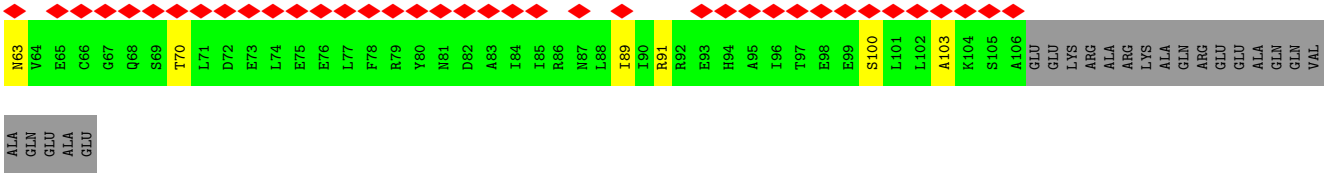


• Molecule 11: Small ribosomal subunit protein bS6

Chain F:

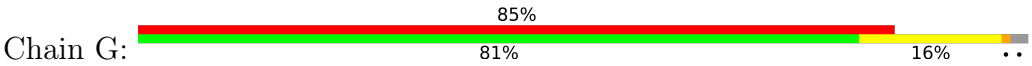


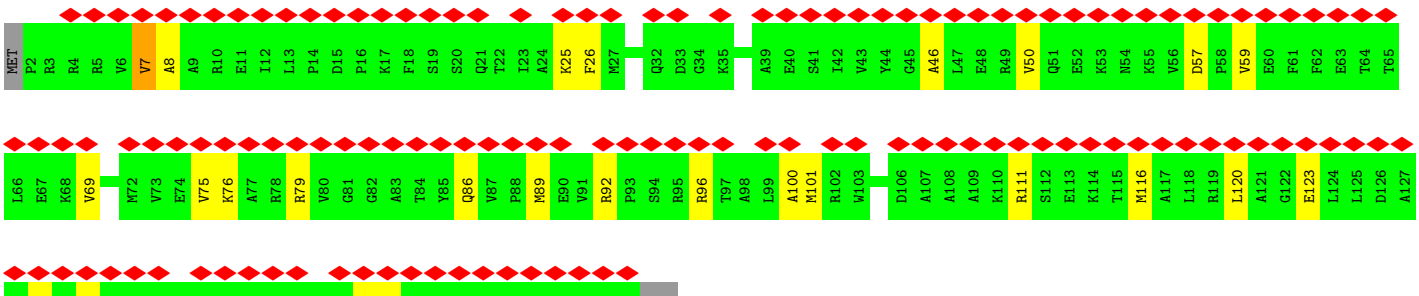




• Molecule 12: Small ribosomal subunit protein uS7

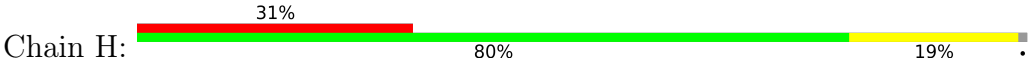
Chain G:

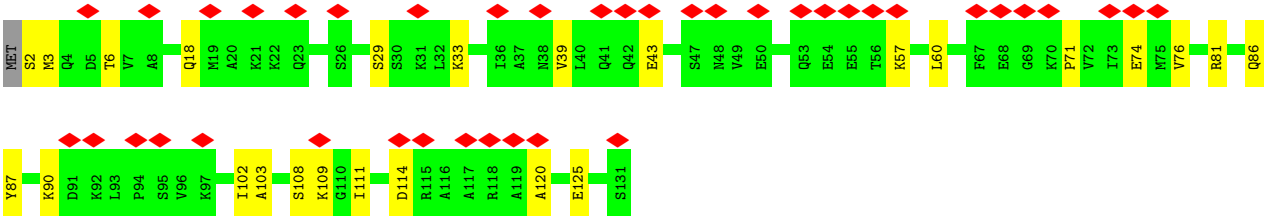




• Molecule 13: Small ribosomal subunit protein uS8

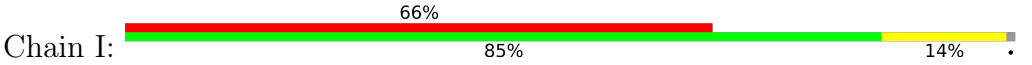
Chain H:

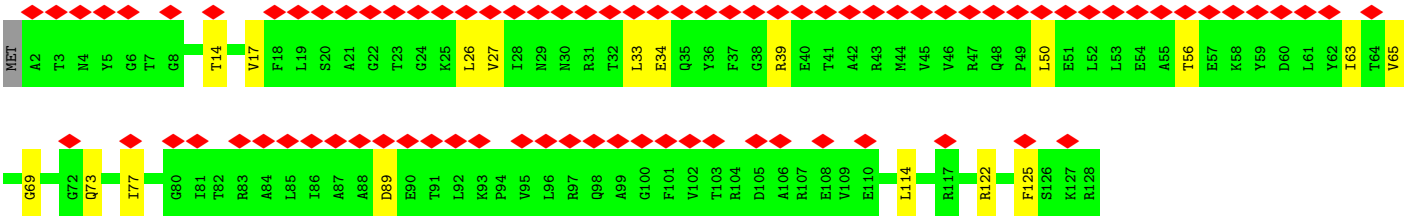




• Molecule 14: Small ribosomal subunit protein uS9

Chain I:

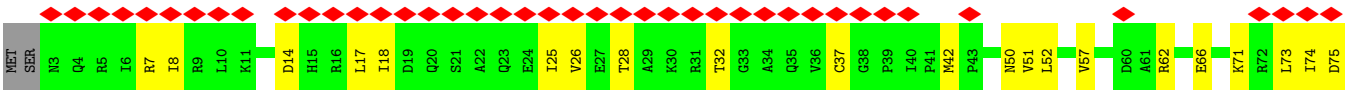


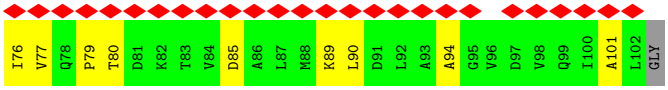


• Molecule 15: Small ribosomal subunit protein uS10

Chain J:



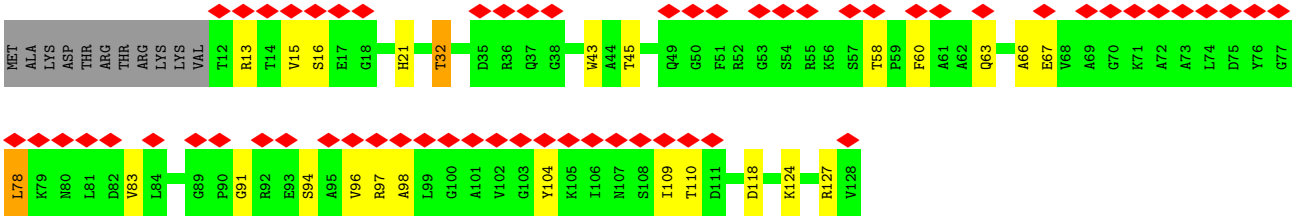




• Molecule 16: Small ribosomal subunit protein uS11

Chain K:

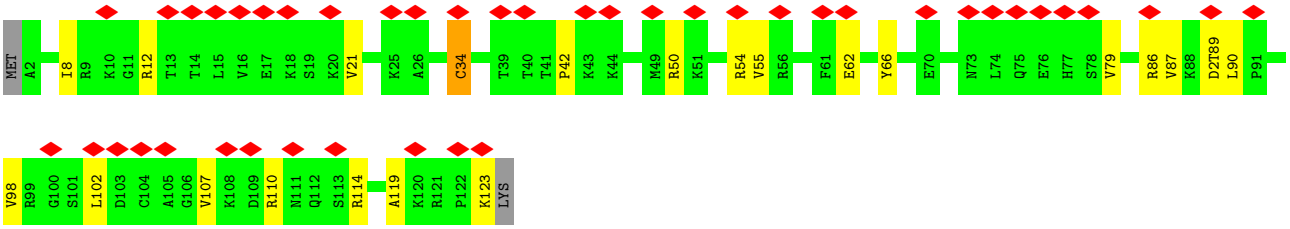




• Molecule 17: Small ribosomal subunit protein uS12

Chain L:

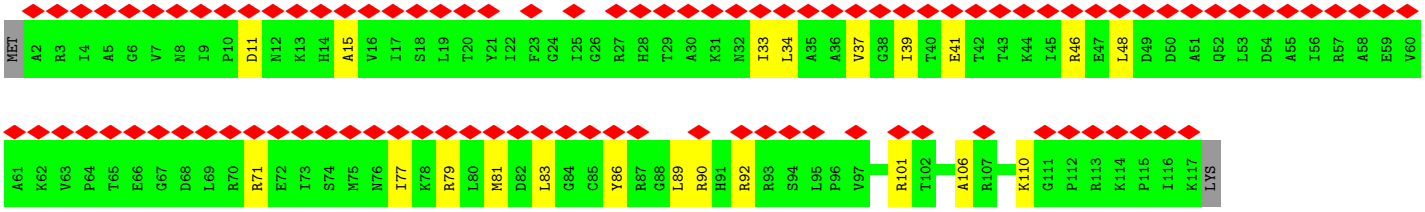




• Molecule 18: Small ribosomal subunit protein uS13

Chain M:

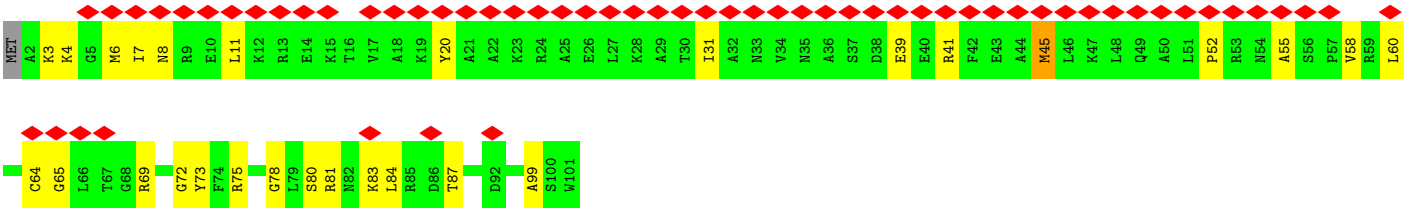




• Molecule 19: Small ribosomal subunit protein uS14

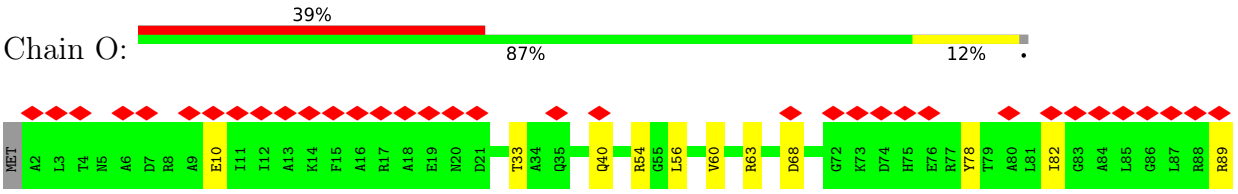
Chain N:





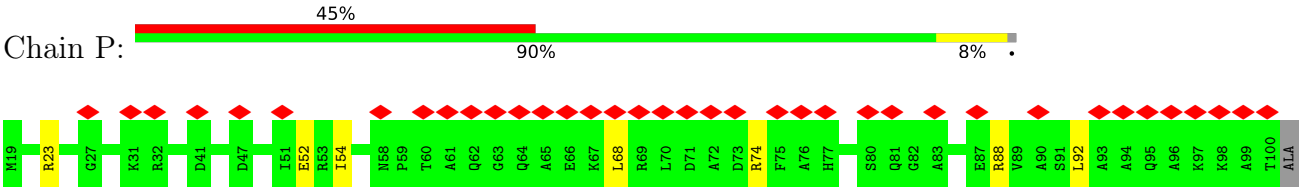
• Molecule 20: Small ribosomal subunit protein uS15

Chain O:



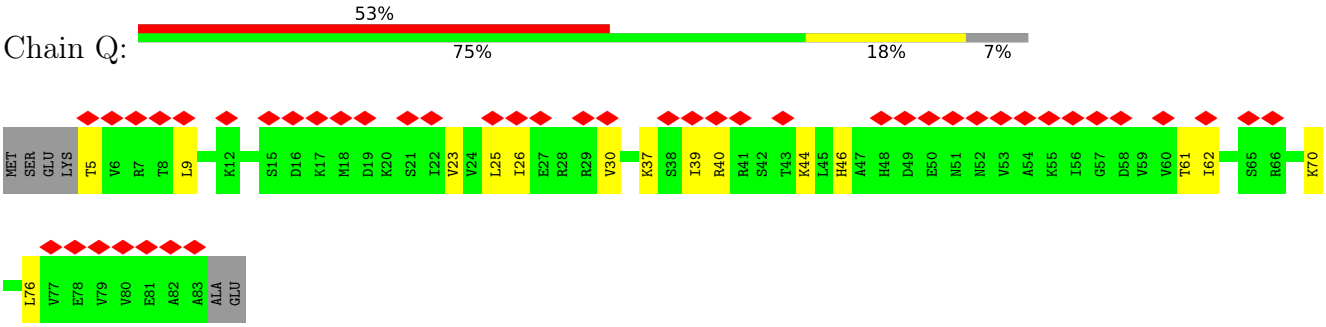
• Molecule 21: Small ribosomal subunit protein bS16

Chain P:



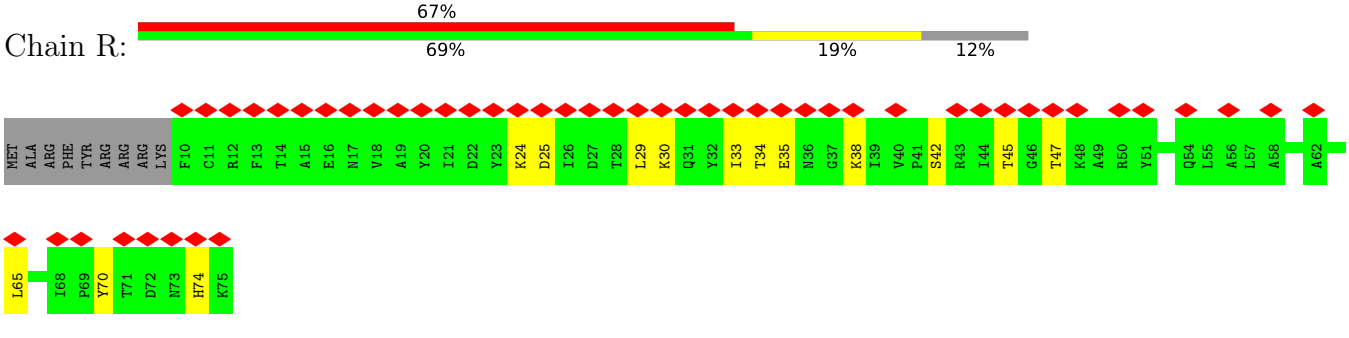
• Molecule 22: Small ribosomal subunit protein uS17

Chain Q:



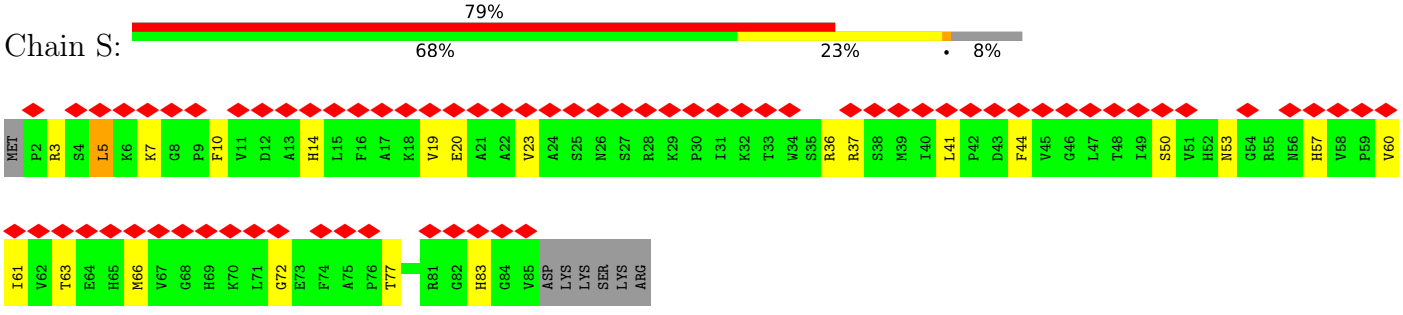
• Molecule 23: Small ribosomal subunit protein bS18

Chain R:



• Molecule 24: Small ribosomal subunit protein uS19

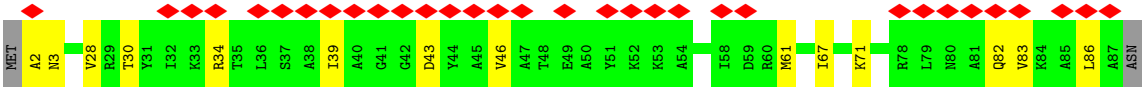
Chain S:



• Molecule 25: Small ribosomal subunit protein bS20

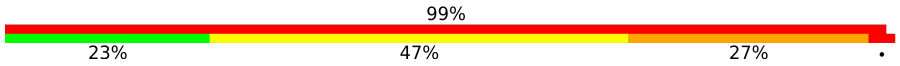
Chain T:

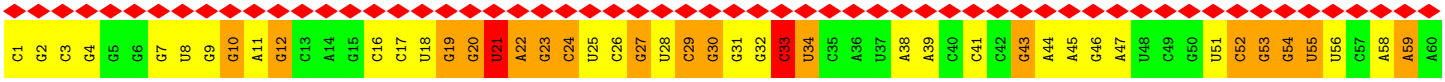


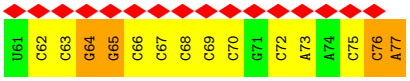


• Molecule 26: tRNA (77-MER)

Chain V:



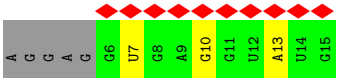




• Molecule 27: non-Stop mRNA

Chain W:



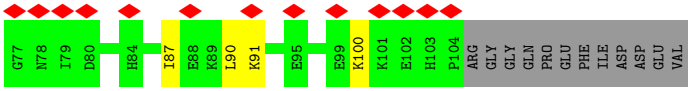


• Molecule 28: Putative ribosomal subunit interface protein

Chain X:



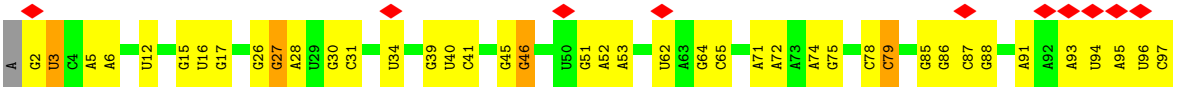


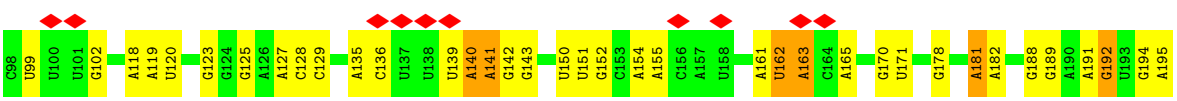


• Molecule 29: 23S rRNA (2890-MER)

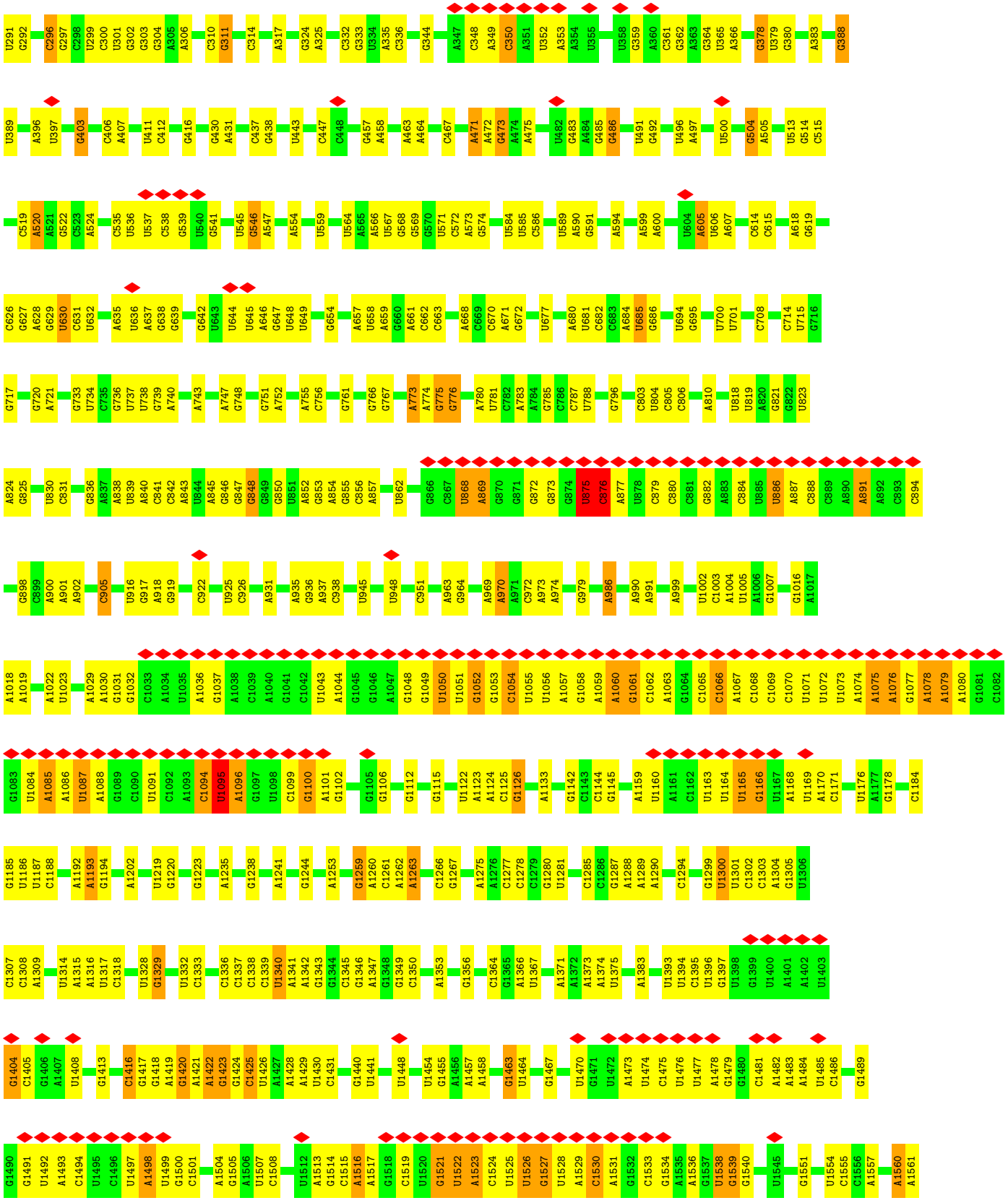
Chain a:

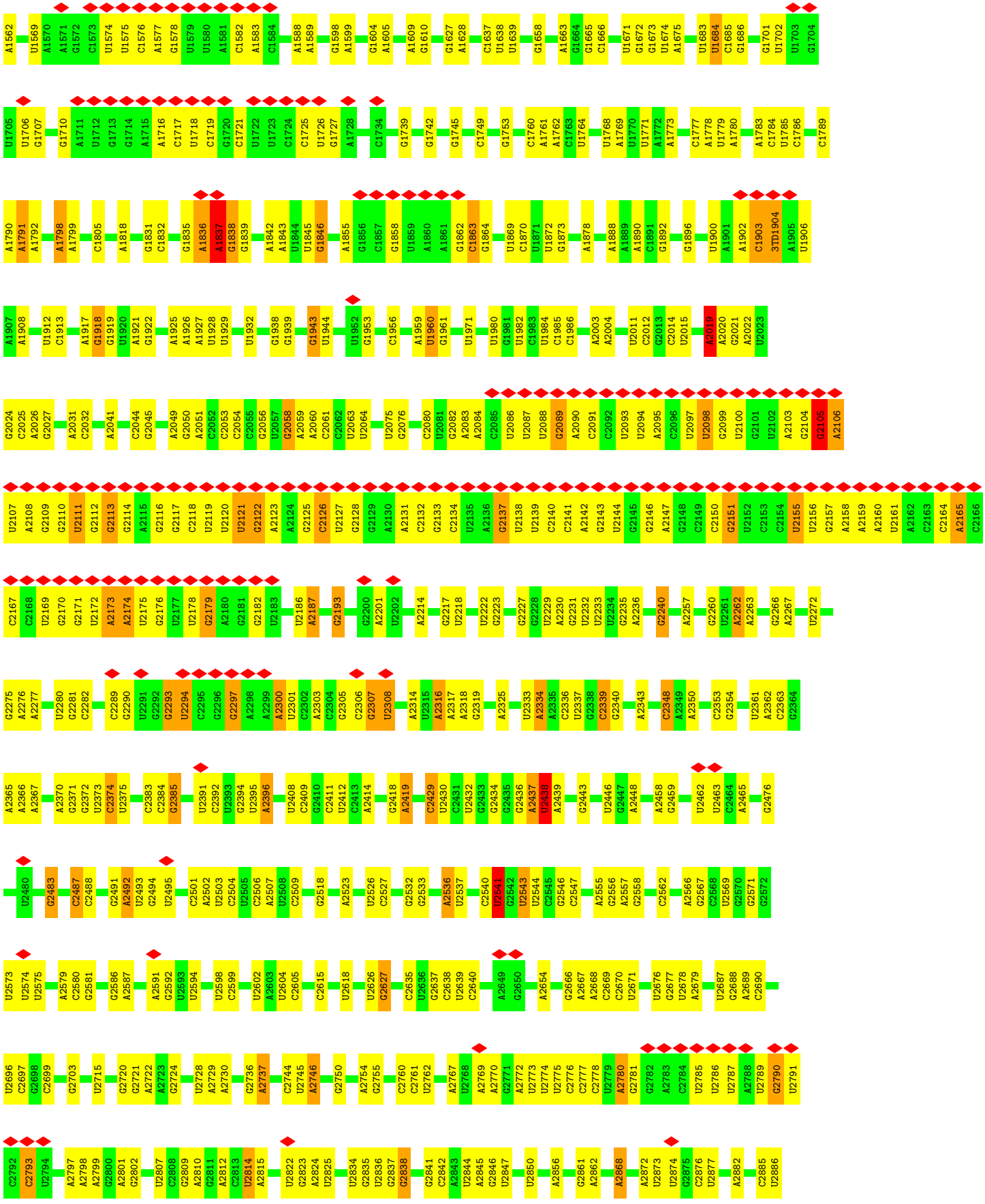


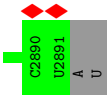








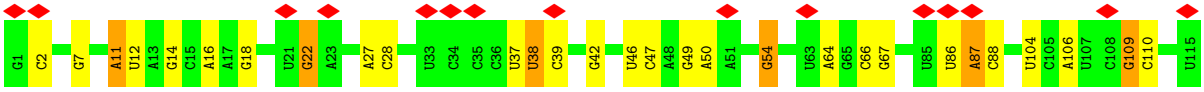




• Molecule 30: 5S rRNA

Chain b:

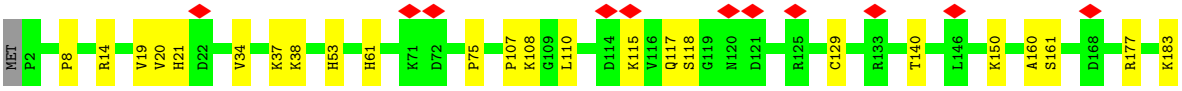


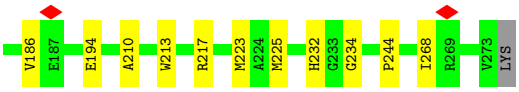


• Molecule 31: Large ribosomal subunit protein uL2

Chain c:



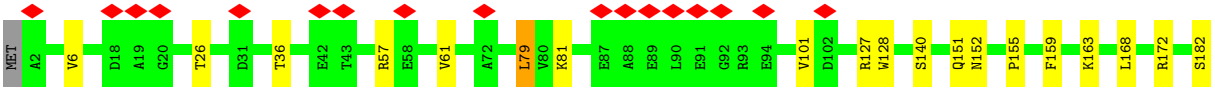


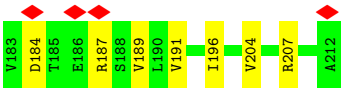


• Molecule 32: Large ribosomal subunit protein uL3

Chain d:

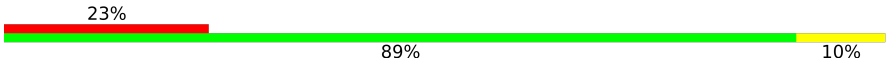


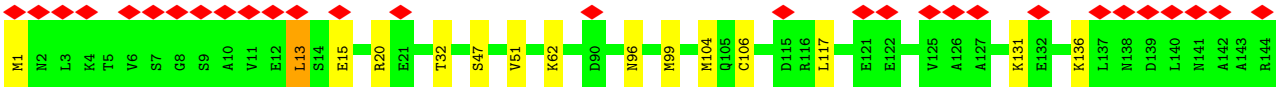


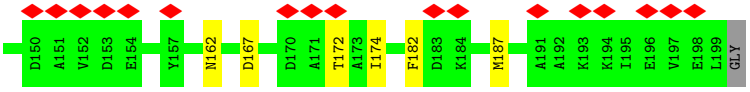


• Molecule 33: Large ribosomal subunit protein uL4

Chain e:



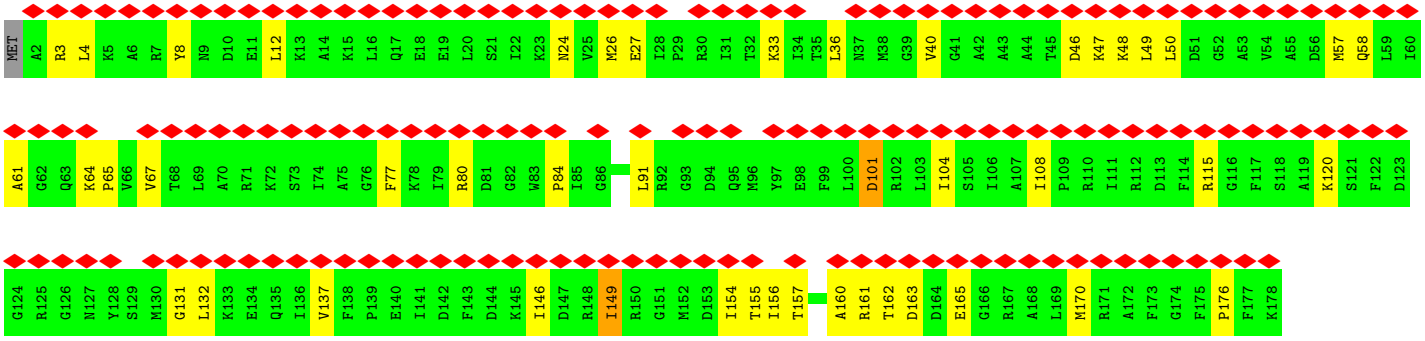




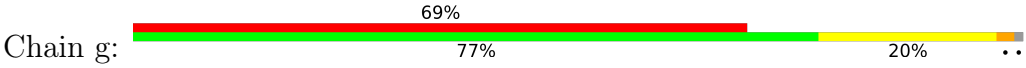
• Molecule 34: Large ribosomal subunit protein uL5

Chain f:





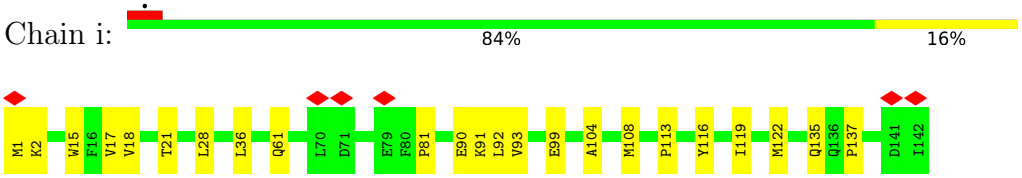
• Molecule 35: Large ribosomal subunit protein uL6



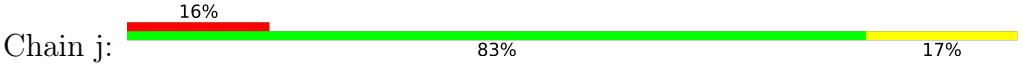
• Molecule 36: Large ribosomal subunit protein bL9

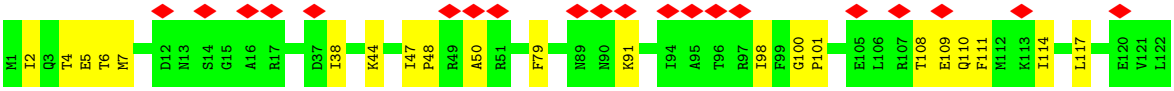


• Molecule 37: Large ribosomal subunit protein uL13

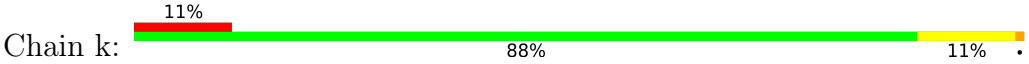


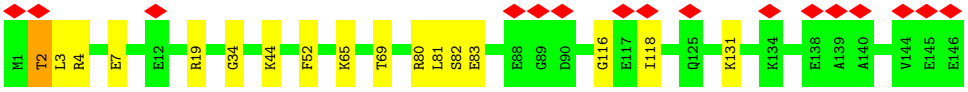
• Molecule 38: Large ribosomal subunit protein uL14



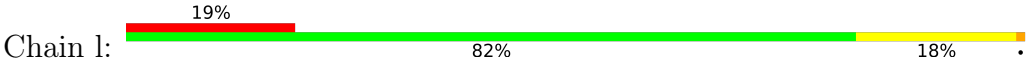


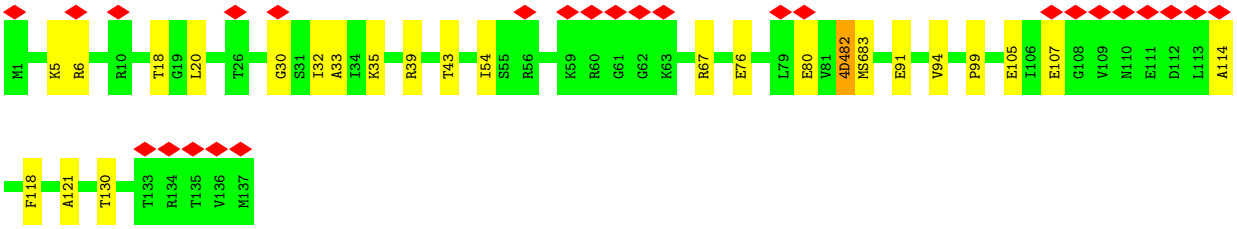
• Molecule 39: Large ribosomal subunit protein uL15



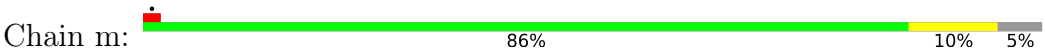


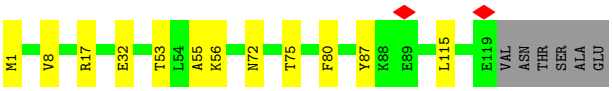
• Molecule 40: Large ribosomal subunit protein uL16



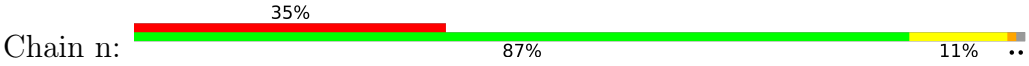


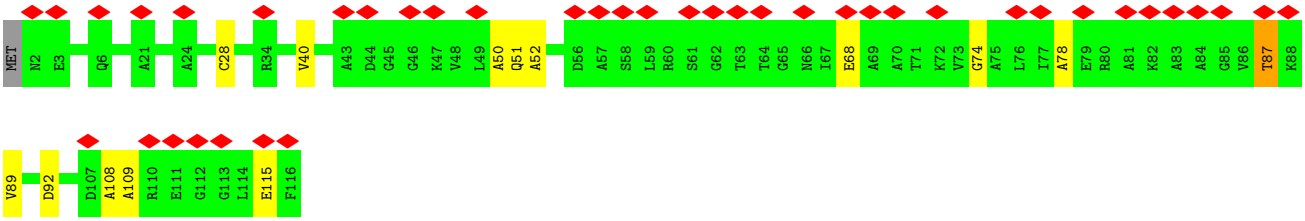
• Molecule 41: Large ribosomal subunit protein bL17



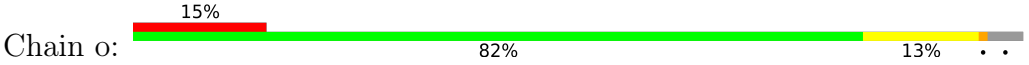


• Molecule 42: Large ribosomal subunit protein uL18





• Molecule 43: Large ribosomal subunit protein bL19





• Molecule 44: Large ribosomal subunit protein bL20

Chain p:

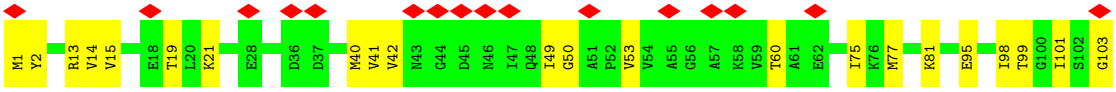




• Molecule 45: Large ribosomal subunit protein bL21

Chain q:

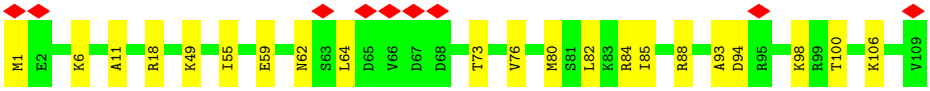




• Molecule 46: Large ribosomal subunit protein uL22

Chain r:

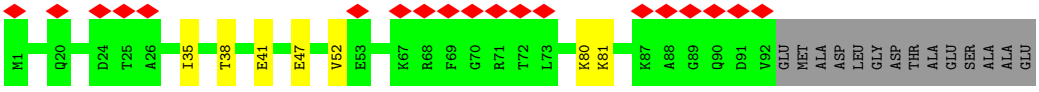




• Molecule 47: Large ribosomal subunit protein uL23

Chain s:

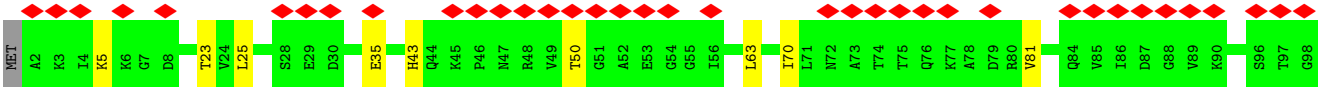


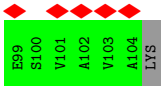


• Molecule 48: Large ribosomal subunit protein uL24

Chain t:

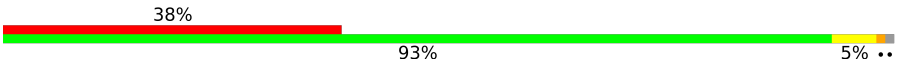


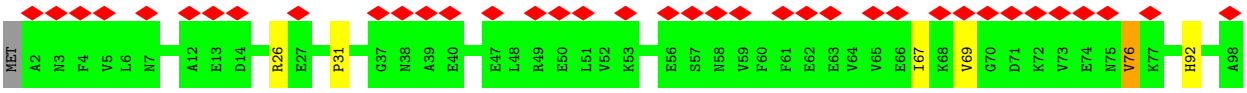




• Molecule 49: Large ribosomal subunit protein bL25

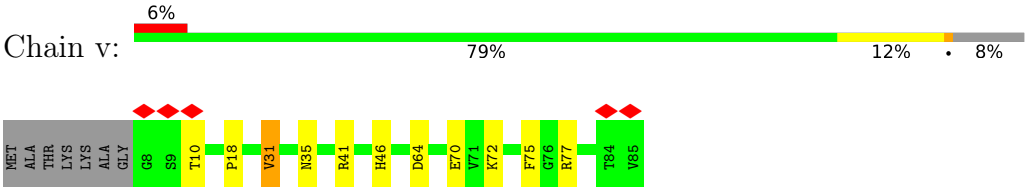
Chain u:





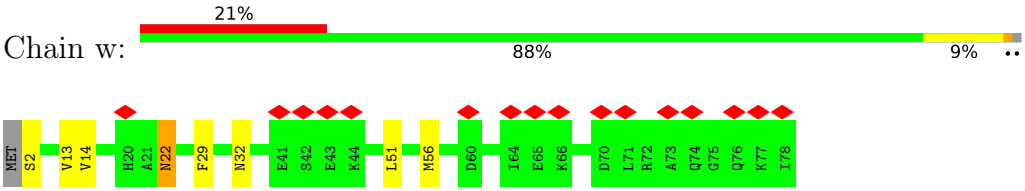
• Molecule 50: Large ribosomal subunit protein bL27

Chain v:



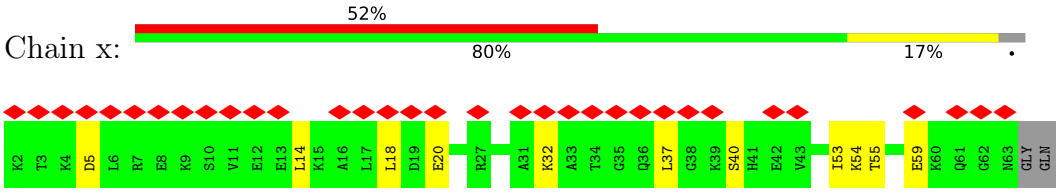
• Molecule 51: Large ribosomal subunit protein bL28

Chain w:



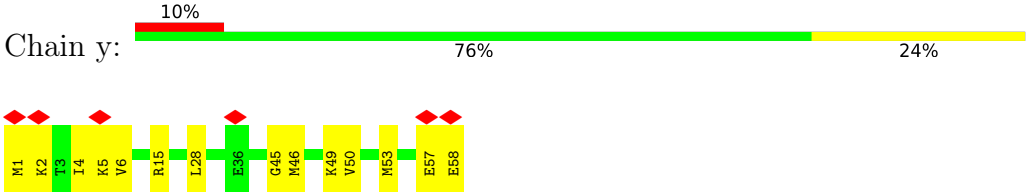
• Molecule 52: Large ribosomal subunit protein uL29

Chain x:



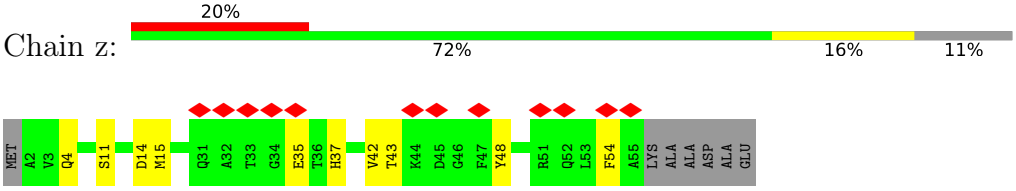
• Molecule 53: Large ribosomal subunit protein uL30

Chain y:



• Molecule 54: Large ribosomal subunit protein bL32

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	225259	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 ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.429	Depositor
Minimum map value	-1.526	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.21	0/434	0.38	0/573
2	1	0.24	0/367	0.30	0/481
3	2	0.22	0/515	0.34	0/678
4	3	0.22	0/296	0.27	0/389
5	4	0.13	0/561	0.37	0/750
6	A	0.46	0/36630	0.75	5/57129 (0.0%)
7	B	0.13	0/1832	0.30	0/2474
8	C	0.16	0/1714	0.30	0/2304
9	D	0.15	0/1653	0.29	0/2213
10	E	0.20	0/1141	0.31	0/1537
11	F	0.15	0/893	0.28	0/1204
12	G	0.13	0/1229	0.27	0/1647
13	H	0.17	0/993	0.28	0/1331
14	I	0.16	0/1006	0.28	0/1346
15	J	0.17	0/811	0.30	0/1096
16	K	0.17	0/869	0.33	0/1175
17	L	0.18	0/949	0.38	0/1270
18	M	0.14	0/922	0.29	0/1237
19	N	0.16	0/803	0.29	0/1071
20	O	0.18	0/715	0.30	0/958
21	P	0.16	0/655	0.29	0/879
22	Q	0.16	0/628	0.32	0/847
23	R	0.16	0/555	0.32	0/749
24	S	0.15	0/675	0.32	0/912
25	T	0.19	0/669	0.24	0/892
26	V	0.29	0/1724	0.81	1/2687 (0.0%)
27	W	0.29	0/245	0.77	0/381
28	X	0.16	0/858	0.26	0/1150
29	a	0.59	0/68962	0.79	32/107563 (0.0%)
30	b	0.46	0/2739	0.76	0/4266
31	c	0.23	0/2152	0.33	0/2891

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	d	0.23	0/1580	0.33	0/2127
33	e	0.22	0/1532	0.31	0/2068
34	f	0.20	0/1415	0.44	0/1895
35	g	0.15	0/1346	0.29	0/1818
36	h	0.12	0/461	0.35	0/616
37	i	0.23	0/1151	0.35	0/1551
38	j	0.22	0/956	0.30	0/1286
39	k	0.21	0/1097	0.31	0/1461
40	l	0.20	0/1084	0.30	0/1448
41	m	0.23	0/956	0.35	0/1282
42	n	0.19	0/873	0.32	0/1167
43	o	0.20	0/931	0.31	0/1249
44	p	0.24	0/947	0.32	0/1262
45	q	0.22	0/818	0.35	0/1094
46	r	0.22	0/831	0.36	0/1113
47	s	0.19	0/723	0.26	0/967
48	t	0.16	0/770	0.26	0/1034
49	u	0.19	0/770	0.34	0/1036
50	v	0.22	0/597	0.29	0/798
51	w	0.22	0/642	0.29	0/856
52	x	0.17	0/499	0.26	0/662
53	y	0.23	0/468	0.39	0/624
54	z	0.23	0/453	0.32	0/604
All	All	0.47	0/155095	0.69	38/232098 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
40	l	0	1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	1301	U	C2-N1-C1'	7.27	126.43	117.70
6	A	415	C	N3-C2-O2	-6.72	117.20	121.90
29	a	875	U	N3-C2-O2	-6.44	117.69	122.20
29	a	781	U	C2-N1-C1'	6.26	125.21	117.70
29	a	520	A	C2-N3-C4	-6.07	107.57	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	1837	A	O4'-C1'-N9	6.05	113.04	108.20
29	a	739	G	O4'-C1'-N9	5.93	112.65	108.50
6	A	653	G	O4'-C1'-N9	5.90	112.92	108.20
29	a	1301	U	N1-C2-O2	5.80	126.86	122.80
29	a	1301	U	N3-C2-O2	-5.76	118.17	122.20
29	a	2443	G	O4'-C1'-N9	5.75	112.53	108.50
29	a	2462	U	C2-N1-C1'	5.68	124.51	117.70
29	a	876	C	O4'-C1'-N1	5.67	112.74	108.20
29	a	504	G	O4'-C1'-N9	5.66	112.46	108.50
29	a	880	C	C2-N1-C1'	5.49	124.84	118.80
29	a	781	U	N1-C2-O2	5.49	126.64	122.80
29	a	2793	C	C2-N1-C1'	5.45	124.79	118.80
29	a	471	A	O5'-C5'-C4'	5.37	113.70	109.40
29	a	880	C	N1-C2-O2	5.35	122.11	118.90
29	a	1095	U	C2-N1-C1'	5.33	124.09	117.70
29	a	2443	G	O5'-C5'-C4'	5.32	113.66	109.40
26	V	41	C	C2-N1-C1'	5.31	124.64	118.80
29	a	192	G	C8-N9-C1'	-5.26	120.16	127.00
29	a	1094	C	C2-N1-C1'	5.21	124.53	118.80
29	a	905	C	C2-N1-C1'	5.20	124.52	118.80
29	a	249	C	N3-C2-O2	-5.17	118.28	121.90
6	A	1200	C	C2-N1-C1'	5.16	124.47	118.80
29	a	2105	G	O5'-C5'-C4'	5.13	113.51	109.40
29	a	1521	G	P-O3'-C3'	5.13	125.85	119.70
29	a	2429	C	C2-N1-C1'	5.11	124.42	118.80
29	a	192	G	O4'-C1'-N9	5.10	112.07	108.50
29	a	970	A	N9-C1'-C2'	5.09	117.60	112.00
29	a	2814	U	C2-N1-C1'	5.09	123.81	117.70
29	a	361	C	P-O3'-C3'	5.05	125.77	119.70
29	a	720	G	O4'-C1'-N9	5.05	112.03	108.50
29	a	708	C	N1-C2-O2	5.05	121.93	118.90
6	A	1092	U	N3-C2-O2	-5.02	118.68	122.20
6	A	1155	C	C2-N1-C1'	5.02	124.32	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	l	82	4D4	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	427	0	462	7	0
2	1	363	0	401	5	0
3	2	509	0	566	8	0
4	3	295	0	325	8	0
5	4	552	0	552	10	0
6	A	32947	0	16585	343	0
7	B	1801	0	1814	33	0
8	C	1690	0	1774	24	0
9	D	1631	0	1691	29	0
10	E	1129	0	1174	12	0
11	F	878	0	878	14	0
12	G	1210	0	1255	19	0
13	H	985	0	1047	14	0
14	I	995	0	1053	14	0
15	J	801	0	832	18	0
16	K	861	0	873	16	0
17	L	947	0	997	14	0
18	M	912	0	975	16	0
19	N	792	0	833	23	0
20	O	705	0	712	6	0
21	P	644	0	655	5	0
22	Q	621	0	665	8	0
23	R	545	0	556	11	0
24	S	657	0	675	20	0
25	T	663	0	715	9	0
26	V	1644	0	842	42	0
27	W	219	0	108	2	0
28	X	841	0	824	11	0
29	a	61984	0	31148	551	0
30	b	2450	0	1241	14	0
31	c	2111	0	2176	23	0
32	d	1573	0	1611	14	0
33	e	1511	0	1566	12	0
34	f	1395	0	1450	33	0
35	g	1327	0	1386	21	0
36	h	458	0	480	7	0
37	i	1125	0	1148	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	j	946	0	1007	14	0
39	k	1089	0	1158	12	0
40	l	1088	0	1150	16	0
41	m	942	0	987	7	0
42	n	865	0	905	6	0
43	o	919	0	973	12	0
44	p	934	0	997	7	0
45	q	807	0	842	12	0
46	r	826	0	894	13	0
47	s	717	0	777	4	0
48	t	766	0	816	4	0
49	u	760	0	783	4	0
50	v	589	0	592	6	0
51	w	632	0	667	8	0
52	x	498	0	537	6	0
53	y	463	0	488	7	0
54	z	447	0	435	5	0
55	1	1	0	0	0	0
55	3	1	0	0	0	0
55	A	47	0	0	0	0
55	L	1	0	0	0	0
55	a	111	0	0	2	0
55	b	1	0	0	0	0
55	c	4	0	0	0	0
55	d	2	0	0	0	0
55	t	1	0	0	1	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	95	0	0	0	0
57	J	1	0	0	0	0
57	M	1	0	0	0	0
57	X	1	0	0	0	0
57	a	251	0	0	2	0
57	b	5	0	0	0	0
57	c	1	0	0	0	0
57	d	1	0	0	0	0
57	k	1	0	0	0	0
57	p	1	0	0	0	0
57	v	1	0	0	0	0
57	z	1	0	0	0	0
All	All	144017	0	96053	1458	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1458) 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)
29:a:1059:A:H1'	29:a:1086:A:H4'	1.54	0.89
26:V:51:U:H3	26:V:65:G:H1	0.92	0.88
29:a:1925:A:H2	29:a:1932:U:H3	1.20	0.86
6:A:74:G:H8	6:A:93:A:H62	1.22	0.85
43:o:30:VAL:HG22	43:o:47:GLU:HG3	1.59	0.84
29:a:536:U:O2	29:a:539:G:O6	1.96	0.83
29:a:467:C:O2	29:a:471:A:N6	2.14	0.80
33:e:96:ASN:HB2	33:e:99:MET:HG3	1.63	0.80
53:y:1:MET:HE3	53:y:2:LYS:H	1.46	0.80
6:A:1309:G:H5'	24:S:5:LEU:HD21	1.64	0.79
34:f:8:TYR:HA	34:f:12:LEU:HB2	1.62	0.79
6:A:201:A:H61	6:A:209:A:H61	1.28	0.79
29:a:1837:A:HO2'	29:a:1838:G:H8	1.29	0.77
19:N:4:LYS:HA	19:N:7:ILE:HD12	1.66	0.77
39:k:4:ARG:HB2	39:k:7:GLU:HG3	1.67	0.77
14:I:17:VAL:HG22	14:I:63:ILE:HG12	1.66	0.77
29:a:868:U:O2	29:a:891:A:N7	2.18	0.76
6:A:471:G:H2'	6:A:472:A:C8	2.21	0.76
6:A:670:A:H2'	6:A:671:G:C8	2.20	0.76
29:a:520:A:H5'	37:i:113:PRO:HG3	1.67	0.76
6:A:991:A:H8	19:N:8:ASN:HD22	1.33	0.75
29:a:2141:C:H2'	29:a:2142:A:H8	1.52	0.74
29:a:1588:A:H5"	29:a:1589:A:H5'	1.70	0.73
44:p:43:GLY:HA3	45:q:75:ILE:HD12	1.71	0.73
33:e:1:MET:HB3	33:e:13:LEU:O	1.90	0.72
26:V:29:C:H2'	26:V:30:G:H8	1.55	0.72
29:a:2317:A:H2'	29:a:2318:A:C8	2.25	0.72
16:K:78:LEU:HB3	16:K:104:TYR:HE1	1.54	0.72
29:a:2125:G:H1	29:a:2144:U:H3	1.34	0.71
29:a:45:G:H5"	29:a:46:G:H5'	1.72	0.71
29:a:2294:U:H5"	34:f:131:GLY:HA3	1.72	0.71
6:A:661:G:H22	6:A:738:G:H1	1.39	0.71
13:H:39:VAL:HG21	13:H:111:ILE:HG22	1.72	0.71
38:j:98:ILE:HD12	38:j:117:LEU:HB2	1.73	0.70
29:a:559:U:H1'	29:a:2019:6MZ:H9C1	1.74	0.70
12:G:129:GLU:HB3	12:G:131:LYS:HE3	1.73	0.69
26:V:29:C:H2'	26:V:30:G:C8	2.28	0.69
24:S:3:ARG:HE	24:S:7:LYS:HB2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:140:A:HO2'	29:a:141:A:H8	1.40	0.69
6:A:1002:A:H8	6:A:1020:G:H21	1.41	0.69
29:a:78:C:HO2'	29:a:79:C:H6	1.41	0.68
29:a:1018:A:H2'	29:a:1019:A:C8	2.27	0.68
6:A:943:A:H2'	6:A:944:G:C8	2.29	0.68
34:f:61:ALA:HB1	34:f:91:LEU:HD21	1.74	0.68
49:u:67:ILE:HD12	49:u:76:VAL:HG21	1.76	0.68
29:a:902:A:H8	29:a:2266:G:H21	1.42	0.68
29:a:2280:U:H2'	29:a:2281:G:C8	2.29	0.68
29:a:28:A:N6	29:a:504:G:H1'	2.09	0.68
10:E:93:VAL:HB	10:E:110:MET:HE3	1.75	0.67
29:a:2120:U:H5'	29:a:2121:U:H2'	1.75	0.67
6:A:1320:G:H2'	6:A:1321:A:C8	2.30	0.66
6:A:1364:C:H5"	14:I:114:LEU:HD12	1.77	0.66
28:X:11:ILE:HD12	28:X:43:PHE:HB3	1.77	0.66
49:u:26:ARG:HG2	49:u:26:ARG:HH11	1.60	0.66
16:K:21:HIS:HB2	16:K:32:THR:HG22	1.76	0.66
29:a:349:A:HO2'	29:a:350:C:H6	1.41	0.66
29:a:1457:A:H2'	29:a:1458:A:C8	2.29	0.66
32:d:159:PHE:HB3	37:i:81:PRO:HG3	1.77	0.66
6:A:994:U:H3	6:A:1041:A:H62	1.43	0.66
45:q:40:MET:HE3	45:q:49:ILE:HG12	1.78	0.66
29:a:1837:A:O2'	29:a:1838:G:H8	1.79	0.66
6:A:489:C:H2'	6:A:490:A:C8	2.30	0.66
6:A:456:U:H2'	6:A:457:A:H8	1.61	0.66
29:a:2109:G:H2'	29:a:2110:G:H8	1.61	0.66
6:A:536:A:H2'	6:A:537:G:C8	2.32	0.65
14:I:26:LEU:HD22	14:I:33:LEU:HB2	1.78	0.65
35:g:9:VAL:HG13	35:g:50:LEU:HB2	1.78	0.65
1:0:4:LYS:HB3	1:0:50:ILE:HD13	1.79	0.65
29:a:28:A:H61	29:a:504:G:H1'	1.61	0.65
8:C:73:PRO:HG3	8:C:105:GLU:HG3	1.79	0.65
29:a:1627:G:H2'	29:a:1628:A:C8	2.32	0.65
6:A:1068:C:H2'	6:A:1069:G:H8	1.61	0.64
9:D:56:GLN:HB3	9:D:205:LEU:HB2	1.79	0.64
3:2:32:LEU:HB2	29:a:2408:U:H5"	1.79	0.64
6:A:1020:G:H2'	6:A:1021:G:C8	2.33	0.64
6:A:725:A:H2'	6:A:726:A:C8	2.32	0.64
35:g:43:LEU:HD11	35:g:50:LEU:HD22	1.79	0.64
29:a:1791:A:H2'	29:a:1792:A:C8	2.32	0.64
2:1:1:MET:H2	29:a:1610:G:H21	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1215:C:H2'	6:A:1216:A:C8	2.33	0.64
29:a:2056:G:H1	29:a:2432:U:H3	1.45	0.64
6:A:27:C:H5'	6:A:521:G:H1'	1.80	0.63
26:V:51:U:O4	26:V:65:G:O6	2.15	0.63
37:i:21:THR:HA	37:i:61:GLN:HB3	1.78	0.63
6:A:766:G:H4'	6:A:1510:A:H4'	1.80	0.63
40:l:39:ARG:HB3	40:l:99:PRO:HD3	1.80	0.63
6:A:733:C:H2'	6:A:734:A:C8	2.33	0.63
33:e:117:LEU:HD11	33:e:187:MET:HE3	1.80	0.63
6:A:1353:G:H2'	6:A:1354:A:C8	2.34	0.63
5:4:22:ILE:HG23	34:f:3:ARG:HH12	1.64	0.62
24:S:10:PHE:HE2	24:S:37:ARG:HG3	1.63	0.62
15:J:85:ASP:O	15:J:89:LYS:HG3	1.99	0.62
29:a:1785:U:H2'	29:a:1786:C:C6	2.35	0.62
9:D:38:ALA:HB3	9:D:43:GLY:HA2	1.81	0.62
29:a:2232:U:H2'	29:a:2233:U:C6	2.34	0.62
6:A:77:G:H3'	6:A:78:G:H8	1.65	0.62
6:A:610:C:H2'	6:A:611:C:C6	2.34	0.62
29:a:161:A:H3'	29:a:162:U:H5"	1.82	0.62
29:a:1342:A:H4'	31:c:38:LYS:HE3	1.81	0.62
6:A:989:U:H5	6:A:1041:A:H2	1.46	0.62
6:A:1388:U:H2'	6:A:1389:G:C8	2.34	0.62
36:h:9:ILE:HB	36:h:12:LEU:HB3	1.82	0.62
6:A:19:U:H2'	6:A:20:C:C6	2.35	0.62
10:E:33:THR:HG23	10:E:51:LYS:HG2	1.82	0.61
26:V:10:G:N2	26:V:27:G:H1'	2.15	0.61
29:a:2836:U:H2'	29:a:2837:G:O4'	2.00	0.61
7:B:116:LEU:HB2	7:B:146:LEU:HB3	1.82	0.61
29:a:2075:U:H2'	29:a:2076:G:C8	2.36	0.61
23:R:30:LYS:HA	23:R:33:ILE:HG12	1.81	0.61
29:a:584:U:H2'	29:a:585:U:C6	2.35	0.61
29:a:2088:U:H3	29:a:2179:G:H1	1.48	0.61
35:g:52:LEU:HD21	35:g:72:LEU:HD12	1.82	0.61
6:A:711:G:H2'	6:A:712:A:C8	2.36	0.61
29:a:572:C:H2'	29:a:573:A:C8	2.36	0.61
6:A:451:U:H2'	6:A:452:A:H8	1.66	0.61
29:a:2790:G:H2'	29:a:2791:U:C6	2.36	0.61
29:a:140:A:O2'	29:a:141:A:H8	1.83	0.60
29:a:1192:A:H4'	29:a:1193:A:H5"	1.82	0.60
37:i:92:LEU:HD21	37:i:99:GLU:HG2	1.82	0.60
6:A:710:G:H2'	6:A:711:G:C8	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1003:C:N3	6:A:1019:U:O4	2.35	0.60
6:A:1247:A:H2'	6:A:1248:A:C8	2.37	0.60
6:A:455:U:H3	6:A:469:G:H1	1.49	0.60
6:A:1044:G:H5"	19:N:4:LYS:HD3	1.82	0.60
6:A:143:G:H2'	6:A:144:G:C8	2.36	0.60
40:l:6:ARG:NH1	40:l:6:ARG:HB3	2.16	0.60
14:I:122:ARG:HD3	14:I:125:PHE:HE2	1.66	0.60
26:V:51:U:H2'	26:V:52:C:C6	2.36	0.60
6:A:820:C:HO2'	13:H:2:SER:N	2.00	0.60
17:L:107:VAL:HG23	17:L:110:ARG:HG3	1.84	0.60
29:a:2141:C:H2'	29:a:2142:A:C8	2.36	0.60
6:A:419:U:H2'	6:A:420:G:O4'	2.01	0.60
15:J:52:LEU:HD23	15:J:62:ARG:HG3	1.83	0.60
7:B:45:LEU:HA	7:B:48:THR:HG23	1.83	0.59
4:3:36:ARG:HG2	4:3:37:GLN:H	1.66	0.59
6:A:1409:C:H2'	6:A:1410:A:C8	2.38	0.59
6:A:457:A:H2'	6:A:458:G:H8	1.66	0.59
29:a:840:A:H2'	29:a:841:C:C6	2.36	0.59
15:J:37:CYS:HB2	15:J:75:ASP:HB2	1.84	0.59
26:V:19:G:H21	26:V:59:A:H5'	1.67	0.59
29:a:1785:U:H2'	29:a:1786:C:H6	1.67	0.59
29:a:1050:U:H4'	29:a:1052:G:O4'	2.02	0.59
6:A:572:G:O2'	6:A:818:G:H5'	2.03	0.59
29:a:16:U:H5"	54:z:14:ASP:HB2	1.85	0.59
29:a:2222:U:H2'	29:a:2223:G:C8	2.38	0.59
34:f:67:VAL:HG11	34:f:84:PRO:HB3	1.83	0.59
6:A:252:U:H2'	6:A:253:G:H8	1.68	0.59
6:A:1320:G:H2'	6:A:1321:A:H8	1.68	0.59
29:a:1474:U:H2'	29:a:1475:C:C6	2.38	0.59
8:C:152:GLU:HG3	8:C:167:TRP:HB3	1.84	0.58
29:a:273:A:H2'	29:a:274:A:C8	2.37	0.58
29:a:1421:A:H2'	29:a:1422:A:C8	2.37	0.58
29:a:2164:C:H2'	29:a:2165:A:C8	2.38	0.58
40:l:76:GLU:HB2	40:l:91:GLU:HG3	1.84	0.58
16:K:67:GLU:HG2	16:K:98:ALA:HB1	1.83	0.58
29:a:839:U:H2'	29:a:840:A:H8	1.69	0.58
6:A:6:C:H2'	6:A:7:U:H2'	1.84	0.58
19:N:83:LYS:O	19:N:87:THR:HG23	2.03	0.58
29:a:733:G:H2'	29:a:734:U:C6	2.38	0.58
31:c:107:PRO:HD2	31:c:110:LEU:HD22	1.84	0.58
6:A:588:U:H2'	6:A:589:A:C8	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2230:A:H2'	29:a:2231:G:C8	2.39	0.58
6:A:647:G:H2'	6:A:648:C:H5'	1.85	0.58
6:A:1008:C:H4'	6:A:1009:A:H5'	1.85	0.58
6:A:1323:U:H2'	6:A:1324:C:H6	1.68	0.58
14:I:69:GLY:O	14:I:73:GLN:HB2	2.03	0.58
20:O:89:ARG:HB2	20:O:89:ARG:HH11	1.69	0.58
29:a:840:A:H2'	29:a:841:C:H6	1.69	0.58
6:A:77:G:H3'	6:A:78:G:C8	2.39	0.58
6:A:650:A:C6	13:H:57:LYS:HB3	2.39	0.58
29:a:1374:A:H2'	29:a:1375:U:C6	2.39	0.58
6:A:23:G:H2'	6:A:24:G:C8	2.39	0.57
12:G:143:ARG:NH2	26:V:43:G:H5'	2.19	0.57
29:a:2579:A:H2'	29:a:2580:C:C6	2.38	0.57
2:1:1:MET:HE1	29:a:743:A:H3'	1.85	0.57
29:a:536:U:O2	29:a:539:G:C6	2.57	0.57
6:A:498:C:H2'	6:A:499:A:C8	2.39	0.57
29:a:823:U:H2'	29:a:824:A:C8	2.39	0.57
29:a:1530:C:H2'	29:a:1531:A:C8	2.39	0.57
29:a:2262:A:H2'	29:a:2263:A:C8	2.39	0.57
45:q:2:TYR:CD1	45:q:13:ARG:HD2	2.40	0.57
6:A:1438:A:C4	43:o:117:LEU:HD11	2.40	0.57
29:a:648:U:H2'	29:a:649:U:C6	2.39	0.57
5:4:7:PRO:HG3	34:f:58:GLN:HG2	1.86	0.57
29:a:2316:A:H2'	29:a:2317:A:C8	2.40	0.57
6:A:231:U:H2'	6:A:232:A:C8	2.39	0.57
6:A:1038:G:H2'	6:A:1039:A:C8	2.39	0.57
6:A:73:G:C2	6:A:74:G:H1'	2.39	0.57
6:A:960:G:H5'	28:X:9:LYS:HD3	1.87	0.57
29:a:1018:A:N6	29:a:1115:G:H2'	2.19	0.57
29:a:277:U:H3	29:a:353:A:N6	2.02	0.57
3:2:12:LYS:HB3	39:k:65:LYS:HG2	1.87	0.57
6:A:1530:C:H42	27:W:13:A:H61	1.52	0.57
29:a:2834:U:H2'	29:a:2835:G:C8	2.40	0.57
18:M:83:LEU:HD11	24:S:66:MET:HG2	1.87	0.56
29:a:467:C:N3	29:a:471:A:N7	2.53	0.56
29:a:1526:U:H3'	29:a:1527:G:O4'	2.05	0.56
6:A:85:G:H21	6:A:87:U:H3	1.50	0.56
6:A:777:A:H5"	16:K:124:LYS:HD3	1.87	0.56
14:I:65:VAL:HG22	14:I:73:GLN:HG2	1.87	0.56
15:J:42:MET:HB2	15:J:71:LYS:HB3	1.87	0.56
22:Q:25:LEU:HD12	22:Q:44:LYS:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:27:G:O6	26:V:45:A:N1	2.38	0.56
29:a:1474:U:H3	29:a:1491:G:H1	1.54	0.56
29:a:2175:U:H2'	29:a:2176:G:C8	2.39	0.56
31:c:183:LYS:HG3	31:c:268:ILE:HD11	1.87	0.56
46:r:82:LEU:HB2	46:r:98:LYS:HB2	1.86	0.56
5:4:11:LYS:HE2	5:4:13:VAL:HG22	1.88	0.56
6:A:43:G:H2'	6:A:44:G:H8	1.70	0.56
6:A:1068:C:H2'	6:A:1069:G:C8	2.41	0.56
6:A:1315:A:H5"	24:S:3:ARG:NH1	2.21	0.56
15:J:52:LEU:HB2	19:N:81:ARG:HD2	1.86	0.56
6:A:252:U:H2'	6:A:253:G:C8	2.41	0.56
23:R:42:SER:HA	23:R:45:THR:HG22	1.87	0.56
6:A:144:G:HO2'	6:A:1443:A:H8	1.54	0.56
6:A:550:A:H5"	17:L:21:VAL:HG21	1.88	0.56
30:b:46:U:H2'	30:b:47:C:C6	2.40	0.56
6:A:733:C:H2'	6:A:734:A:H8	1.69	0.56
6:A:906:A:H3'	6:A:907:C:H6	1.71	0.56
7:B:168:VAL:HG23	7:B:193:SER:OG	2.06	0.56
20:O:78:TYR:O	20:O:82:ILE:HG23	2.06	0.56
29:a:2823:G:H2'	29:a:2868:A:H61	1.71	0.56
29:a:2536:A:H2'	29:a:2537:U:C6	2.42	0.55
6:A:201:A:N6	6:A:209:A:H61	2.01	0.55
8:C:24:ALA:HB1	8:C:28:GLN:HG3	1.86	0.55
29:a:411:U:H2'	29:a:412:C:C6	2.40	0.55
13:H:43:GLU:HG3	13:H:102:ILE:HG21	1.87	0.55
17:L:34:CYS:HA	17:L:55:VAL:HA	1.87	0.55
29:a:188:G:H5'	51:w:14:VAL:HG21	1.88	0.55
29:a:630:U:H2'	29:a:631:C:C6	2.41	0.55
6:A:420:G:H2'	6:A:421:G:C8	2.42	0.55
6:A:1447:G:H21	6:A:1450:A:H2	1.54	0.55
14:I:34:GLU:CD	14:I:34:GLU:H	2.14	0.55
46:r:11:ALA:HA	46:r:100:THR:HG22	1.89	0.55
6:A:58:U:H2'	6:A:59:G:C8	2.42	0.55
6:A:674:U:H3	6:A:710:G:H22	1.54	0.55
29:a:62:U:H5	29:a:93:A:H61	1.54	0.55
29:a:1071:U:H2'	29:a:1072:U:C6	2.42	0.55
29:a:2235:G:H2'	29:a:2236:A:C8	2.42	0.55
29:a:773:A:C2	31:c:225:MET:HG2	2.42	0.55
29:a:1836:A:HO2'	29:a:1837:A:H8	1.53	0.55
36:h:25:TYR:HE1	36:h:29:PHE:HD2	1.54	0.55
6:A:1215:C:H2'	6:A:1216:A:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:156:MET:HE3	7:B:160:PRO:HD3	1.89	0.55
15:J:51:VAL:HG21	19:N:84:LEU:HD12	1.89	0.55
29:a:599:A:H2'	29:a:600:A:C8	2.42	0.55
29:a:2318:A:H2'	29:a:2319:G:C8	2.42	0.55
47:s:35:ILE:HD12	47:s:80:LYS:HB2	1.87	0.55
8:C:58:GLU:HB3	15:J:94:ALA:HB1	1.88	0.55
13:H:87:TYR:CE1	13:H:125:GLU:HG3	2.41	0.55
31:c:118:SER:HB3	31:c:129:CYS:HB3	1.88	0.55
32:d:6:VAL:HG11	32:d:79:LEU:HD11	1.89	0.55
35:g:164:TYR:HB2	35:g:167:GLU:HB2	1.87	0.55
20:O:33:THR:HA	20:O:63:ARG:HH21	1.72	0.55
29:a:694:U:H2'	29:a:695:G:O4'	2.07	0.55
31:c:161:SER:HB3	31:c:194:GLU:HG2	1.89	0.55
45:q:1:MET:HA	45:q:42:VAL:O	2.07	0.55
6:A:43:G:H2'	6:A:44:G:C8	2.42	0.54
6:A:588:U:H2'	6:A:589:A:H8	1.72	0.54
6:A:639:A:H2'	6:A:640:C:H6	1.72	0.54
12:G:143:ARG:HH21	26:V:43:G:H5'	1.70	0.54
29:a:700:U:H2'	29:a:701:U:C6	2.42	0.54
29:a:1178:G:H5'	39:k:34:GLY:HA2	1.88	0.54
6:A:333:G:H2'	6:A:334:A:C8	2.42	0.54
26:V:1:C:H42	26:V:73:A:H61	1.54	0.54
29:a:181:A:H2'	29:a:182:A:C8	2.42	0.54
41:m:32:GLU:HG2	41:m:115:LEU:HD12	1.88	0.54
6:A:989:U:H4'	6:A:990:G:O5'	2.06	0.54
16:K:63:GLN:O	16:K:67:GLU:HG3	2.07	0.54
16:K:83:VAL:HG21	16:K:96:VAL:HG23	1.88	0.54
24:S:50:SER:HB2	24:S:57:HIS:HB3	1.89	0.54
30:b:109:G:H2'	30:b:110:C:C6	2.43	0.54
1:0:2:ARG:HA	1:0:21:LYS:O	2.08	0.54
35:g:143:GLN:O	35:g:147:GLU:HG3	2.07	0.54
6:A:79:U:H2'	6:A:80:A:H8	1.72	0.54
6:A:372:G:H4'	21:P:23:ARG:HD2	1.89	0.54
26:V:11:A:H2'	26:V:12:G:C8	2.42	0.54
29:a:1528:U:H2'	29:a:1529:A:H8	1.72	0.54
29:a:1783:A:H2'	29:a:1784:C:C6	2.42	0.54
38:j:47:ILE:HG13	38:j:48:PRO:HD2	1.90	0.54
29:a:872:G:H1	29:a:886:U:H3	1.54	0.54
29:a:2041:A:H4'	32:d:151:GLN:O	2.07	0.54
29:a:2174:A:H2'	29:a:2175:U:H6	1.73	0.54
10:E:71:ILE:HD13	10:E:144:ARG:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2060:A:H2'	29:a:2061:C:C6	2.42	0.54
6:A:265:U:H2'	6:A:266:A:C8	2.43	0.54
6:A:456:U:H2'	6:A:457:A:C8	2.41	0.54
29:a:5:A:H2'	29:a:6:A:C8	2.43	0.54
29:a:1516:A:HO2'	29:a:1517:A:H8	1.56	0.54
7:B:48:THR:HG22	7:B:203:PRO:HG2	1.89	0.54
19:N:31:ILE:HG12	19:N:45:MET:HG2	1.90	0.54
29:a:2103:A:H3'	29:a:2104:G:H8	1.73	0.54
40:l:20:LEU:HD23	40:l:99:PRO:HG2	1.90	0.54
6:A:943:A:H2'	6:A:944:G:H8	1.73	0.53
6:A:1141:G:N2	6:A:1143:A:H62	2.05	0.53
7:B:168:VAL:HG23	7:B:193:SER:HG	1.72	0.53
10:E:78:THR:HB	10:E:120:HIS:HB2	1.89	0.53
29:a:990:A:H2'	29:a:991:A:C8	2.44	0.53
29:a:1051:U:H4'	29:a:1060:A:C4	2.43	0.53
29:a:2116:G:H2'	29:a:2117:G:C8	2.44	0.53
38:j:47:ILE:HG22	38:j:50:ALA:HB2	1.90	0.53
21:P:68:LEU:HD13	21:P:92:LEU:HD22	1.90	0.53
26:V:30:G:H2'	26:V:31:G:H8	1.72	0.53
29:a:78:C:O2'	29:a:79:C:H6	1.91	0.53
29:a:285:U:H2'	29:a:286:U:C6	2.42	0.53
29:a:1345:C:H2'	29:a:1346:G:O4'	2.08	0.53
6:A:35:A:H2'	6:A:36:C:C6	2.44	0.53
6:A:671:G:H2'	6:A:672:A:H8	1.73	0.53
6:A:759:U:H2'	6:A:760:A:C8	2.44	0.53
29:a:1457:A:H2'	29:a:1458:A:H8	1.71	0.53
6:A:69:C:H2'	6:A:70:G:C8	2.44	0.53
6:A:1311:C:H2'	6:A:1312:U:C6	2.44	0.53
11:F:2:ARG:HG2	11:F:91:ARG:HE	1.74	0.53
29:a:2503:U:H2'	29:a:2504:C:C6	2.44	0.53
4:3:23:ILE:HD13	29:a:1022:A:H1'	1.91	0.53
26:V:52:C:H2'	26:V:53:G:O4'	2.09	0.53
29:a:1516:A:N6	29:a:1534:G:H2'	2.24	0.53
6:A:218:U:H2'	6:A:219:A:C8	2.44	0.53
7:B:138:GLU:O	7:B:142:GLU:HG2	2.09	0.53
23:R:34:THR:HG22	23:R:38:LYS:H	1.72	0.53
29:a:2097:U:H2'	29:a:2098:U:C6	2.43	0.53
31:c:232:HIS:NE2	31:c:244:PRO:HA	2.23	0.53
6:A:79:U:H2'	6:A:80:A:C8	2.44	0.53
6:A:1136:G:H4'	6:A:1137:A:H5'	1.91	0.53
6:A:1172:G:H2'	6:A:1173:A:H8	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2580:C:H2'	29:a:2581:G:C8	2.44	0.53
6:A:991:A:H3'	6:A:992:C:H5"	1.90	0.53
6:A:1035:C:H2'	6:A:1036:U:H6	1.73	0.53
29:a:839:U:H2'	29:a:840:A:C8	2.44	0.53
5:4:28:LEU:HD22	5:4:30:LYS:HB2	1.91	0.53
26:V:30:G:H2'	26:V:31:G:C8	2.44	0.53
29:a:1049:G:H3'	29:a:1050:U:C5'	2.39	0.53
29:a:1492:U:H2'	29:a:1493:A:H8	1.74	0.53
29:a:2235:G:H2'	29:a:2236:A:H8	1.74	0.53
6:A:33:G:C5	6:A:302:A:H1'	2.44	0.52
6:A:295:G:H2'	6:A:296:A:C8	2.44	0.52
29:a:2090:A:H2'	29:a:2091:C:H6	1.75	0.52
29:a:2097:U:H2'	29:a:2098:U:H6	1.73	0.52
29:a:2834:U:H5"	43:o:55:ASN:O	2.08	0.52
29:a:200:U:H4'	51:w:22:ASN:HB3	1.91	0.52
5:4:50:LYS:HE2	34:f:115:ARG:HD2	1.91	0.52
6:A:218:U:H2'	6:A:219:A:H8	1.74	0.52
6:A:712:A:H2'	6:A:713:A:C8	2.44	0.52
7:B:69:VAL:HG22	7:B:162:ALA:HB3	1.92	0.52
9:D:10:LYS:HD2	9:D:39:PRO:HB2	1.90	0.52
29:a:191:A:H2'	29:a:192:G:N3	2.24	0.52
29:a:250:G:H2'	29:a:251:A:C8	2.44	0.52
34:f:40:VAL:HG11	34:f:49:LEU:HB3	1.90	0.52
2:1:10:LEU:HD23	29:a:761:G:H5"	1.91	0.52
6:A:414:C:H2'	6:A:415:C:C6	2.44	0.52
6:A:498:C:H2'	6:A:499:A:H8	1.73	0.52
24:S:3:ARG:NH1	24:S:10:PHE:HB2	2.23	0.52
29:a:27:G:H22	29:a:504:G:H2'	1.75	0.52
29:a:2169:U:H2'	29:a:2170:G:C8	2.44	0.52
29:a:301:U:H2'	29:a:302:G:O4'	2.09	0.52
29:a:1528:U:H2'	29:a:1529:A:C8	2.44	0.52
29:a:2090:A:H2'	29:a:2091:C:C6	2.45	0.52
29:a:2094:U:H2'	29:a:2095:A:C8	2.45	0.52
29:a:2587:A:H5"	31:c:234:GLY:HA3	1.92	0.52
44:p:49:ASP:HA	44:p:52:GLN:HB2	1.92	0.52
6:A:549:U:H2'	6:A:550:A:H8	1.74	0.52
6:A:917:U:H2'	6:A:918:U:C6	2.45	0.52
8:C:78:GLY:HA3	8:C:83:ASP:HB2	1.90	0.52
29:a:486:G:H4'	46:r:6:LYS:HB2	1.91	0.52
29:a:2579:A:H2'	29:a:2580:C:H6	1.74	0.52
30:b:109:G:H2'	30:b:110:C:H6	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:32:ILE:HG21	40:l:114:ALA:HB1	1.92	0.52
6:A:1020:G:H2'	6:A:1021:G:H8	1.74	0.52
9:D:161:ILE:HD12	9:D:177:HIS:ND1	2.23	0.52
25:T:43:ASP:HB3	25:T:46:VAL:HG22	1.92	0.52
29:a:1527:G:H2'	29:a:1528:U:C6	2.45	0.52
29:a:2014:C:H2'	29:a:2015:U:C6	2.44	0.52
29:a:2111:U:H2'	29:a:2112:G:O4'	2.10	0.52
33:e:1:MET:CB	33:e:13:LEU:O	2.57	0.52
36:h:26:GLY:HA2	36:h:30:LEU:HD12	1.92	0.52
13:H:103:ALA:HB3	13:H:114:ASP:HB3	1.91	0.52
26:V:54:G:H3'	26:V:55:5MU:H73	1.92	0.52
29:a:1165:U:H4'	29:a:1166:G:C2	2.44	0.52
29:a:1417:G:H2'	29:a:1418:G:H8	1.74	0.52
29:a:2362:A:H2'	29:a:2363:C:C6	2.45	0.52
40:l:30:GLY:HA2	40:l:107:GLU:HB3	1.91	0.52
6:A:319:U:H2'	6:A:320:G:O4'	2.10	0.52
6:A:982:C:H2'	6:A:983:U:C6	2.45	0.52
6:A:1145:U:H2'	6:A:1146:U:O4'	2.09	0.52
29:a:2172:U:H2'	29:a:2173:A:C8	2.45	0.52
6:A:1059:U:H2'	6:A:1060:C:C6	2.45	0.52
8:C:129:MET:HE2	8:C:131:ARG:HB2	1.92	0.52
15:J:66:GLU:HB3	19:N:99:ALA:HB2	1.90	0.52
29:a:2317:A:H2'	29:a:2318:A:H8	1.73	0.52
29:a:2626:U:H2'	29:a:2627:G:O4'	2.10	0.52
29:a:2720:G:H2'	29:a:2721:G:C8	2.45	0.52
52:x:18:LEU:HB2	52:x:53:ILE:HG21	1.92	0.52
8:C:130:PHE:O	8:C:134:MET:HG3	2.08	0.51
29:a:630:U:H2'	29:a:631:C:H6	1.75	0.51
38:j:100:GLY:HA2	43:o:69:SER:HB2	1.92	0.51
17:L:54:ARG:CZ	17:L:62:GLU:HG2	2.40	0.51
29:a:2125:G:N2	29:a:2144:U:O2	2.32	0.51
29:a:2729:A:H2'	29:a:2730:A:C8	2.45	0.51
45:q:41:VAL:HG11	45:q:103:GLY:HA3	1.90	0.51
4:3:16:VAL:HG22	4:3:25:VAL:HG22	1.91	0.51
6:A:207:G:C2	6:A:208:G:H1'	2.45	0.51
6:A:552:U:H2'	6:A:553:C:C6	2.45	0.51
6:A:748:U:H2'	6:A:749:G:O4'	2.10	0.51
6:A:1248:A:H2'	6:A:1249:A:C8	2.45	0.51
7:B:133:LYS:O	7:B:137:LEU:HD23	2.11	0.51
7:B:135:GLU:O	7:B:139:ARG:HG2	2.11	0.51
15:J:7:ARG:HB2	15:J:101:ALA:HB3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:139:U:H1'	29:a:140:A:H5"	1.92	0.51
29:a:277:U:H3	29:a:353:A:H62	1.57	0.51
32:d:26:THR:HG21	32:d:196:ILE:HG12	1.92	0.51
38:j:108:THR:HG23	38:j:110:GLN:H	1.75	0.51
6:A:231:U:H2'	6:A:232:A:H8	1.74	0.51
10:E:71:ILE:HG12	10:E:140:PHE:CE2	2.44	0.51
29:a:317:A:OP2	33:e:162:ASN:HB2	2.11	0.51
29:a:1043:U:H2'	29:a:1044:A:C8	2.46	0.51
29:a:1921:A:H2'	29:a:1922:G:O4'	2.10	0.51
29:a:2483:G:H4'	40:l:80:GLU:HG2	1.91	0.51
29:a:2638:C:H2'	29:a:2639:U:H6	1.74	0.51
31:c:160:ALA:HA	31:c:177:ARG:HD3	1.93	0.51
37:i:18:VAL:HG11	37:i:28:LEU:HD11	1.93	0.51
52:x:55:THR:O	52:x:59:GLU:HG3	2.09	0.51
6:A:639:A:H2'	6:A:640:C:C6	2.45	0.51
6:A:942:G:C2	6:A:943:A:C8	2.98	0.51
6:A:1311:C:H2'	6:A:1312:U:H6	1.74	0.51
14:I:65:VAL:HG11	14:I:77:ILE:HD11	1.93	0.51
29:a:868:U:H2'	29:a:869:A:H8	1.74	0.51
29:a:1835:G:H5'	29:a:1836:A:OP2	2.10	0.51
29:a:2604:U:C2	54:z:4:GLN:HA	2.44	0.51
37:i:1:MET:N	37:i:1:MET:HE2	2.26	0.51
11:F:2:ARG:HE	11:F:91:ARG:CZ	2.24	0.51
16:K:78:LEU:HB3	16:K:104:TYR:CE1	2.42	0.51
29:a:1628:A:H5'	29:a:1749:C:O2'	2.09	0.51
29:a:2116:G:N2	29:a:2151:G:H1'	2.26	0.51
29:a:2383:C:H5"	39:k:65:LYS:HD3	1.92	0.51
29:a:2671:U:H5"	43:o:2:SER:HB2	1.93	0.51
36:h:13:GLY:HA3	36:h:19:VAL:HG11	1.93	0.51
17:L:87:VAL:HB	17:L:90:LEU:HB2	1.92	0.51
29:a:627:G:OP1	39:k:131:LYS:HE2	2.10	0.51
29:a:1842:A:H2'	29:a:1843:A:C8	2.46	0.51
35:g:15:VAL:HA	35:g:27:LYS:O	2.11	0.51
6:A:1011:A:H2'	6:A:1012:G:C8	2.46	0.51
29:a:30:G:H2'	29:a:31:C:C6	2.46	0.51
29:a:127:A:H5"	29:a:128:C:C6	2.46	0.51
29:a:2777:C:H2'	29:a:2778:C:C6	2.45	0.51
32:d:182:SER:HB2	32:d:191:VAL:HB	1.91	0.51
6:A:176:U:H2'	6:A:177:A:H5'	1.92	0.51
6:A:386:U:H2'	6:A:387:C:C6	2.46	0.51
6:A:457:A:H2'	6:A:458:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:470:A:H2'	6:A:471:G:H8	1.75	0.51
6:A:1001:A:H5'	6:A:1023:G:H22	1.76	0.51
16:K:83:VAL:HB	16:K:109:ILE:HG22	1.90	0.51
18:M:34:LEU:HD23	18:M:41:GLU:HA	1.93	0.51
22:Q:40:ARG:HB3	22:Q:40:ARG:NH1	2.26	0.51
29:a:572:C:H2'	29:a:573:A:H8	1.75	0.51
35:g:30:LYS:HD2	35:g:82:GLY:H	1.76	0.51
54:z:42:VAL:HG12	54:z:48:TYR:HB2	1.93	0.51
4:3:25:VAL:HB	4:3:35:GLN:HB2	1.91	0.51
9:D:50:GLN:HB2	9:D:54:SER:HB3	1.93	0.51
29:a:406:C:H2'	29:a:407:A:C8	2.46	0.51
29:a:1528:U:C2	29:a:1529:A:C8	2.99	0.51
29:a:2667:A:H2'	29:a:2668:A:C8	2.46	0.51
14:I:65:VAL:CG2	14:I:73:GLN:HG2	2.41	0.50
29:a:585:U:H2'	29:a:586:C:C6	2.46	0.50
29:a:1087:U:H2'	29:a:1088:A:O4'	2.11	0.50
6:A:208:G:H2'	6:A:209:A:H8	1.75	0.50
12:G:111:ARG:HD2	12:G:123:GLU:HG2	1.94	0.50
13:H:6:THR:HB	13:H:33:LYS:HE2	1.93	0.50
29:a:855:G:H2'	29:a:856:C:C6	2.47	0.50
29:a:1504:A:H3'	29:a:1505:G:H8	1.76	0.50
29:a:2156:U:H2'	29:a:2157:G:C8	2.46	0.50
29:a:1837:A:C4	29:a:1838:G:C8	2.99	0.50
51:w:13:VAL:HG22	51:w:29:PHE:HB2	1.93	0.50
6:A:989:U:H5	6:A:1041:A:C2	2.28	0.50
10:E:152:VAL:HA	10:E:155:LYS:HD3	1.93	0.50
17:L:34:CYS:HB3	17:L:55:VAL:HG22	1.93	0.50
29:a:875:U:H2'	29:a:876:C:C6	2.45	0.50
29:a:1538:U:HO2'	29:a:1539:G:H8	1.57	0.50
29:a:2573:U:H2'	29:a:2574:U:H2'	1.94	0.50
9:D:106:ARG:HB3	9:D:170:PRO:HG2	1.92	0.50
26:V:69:C:H2'	26:V:70:C:C6	2.47	0.50
29:a:154:A:H2'	29:a:155:A:C8	2.46	0.50
29:a:2174:A:H2'	29:a:2175:U:C6	2.46	0.50
49:u:26:ARG:HG2	49:u:26:ARG:NH1	2.26	0.50
6:A:728:G:H5'	6:A:763:A:H4'	1.94	0.50
6:A:1140:G:H2'	6:A:1141:G:H8	1.77	0.50
9:D:28:PHE:O	9:D:32:THR:HG22	2.12	0.50
29:a:195:A:H61	29:a:198:C:H3'	1.75	0.50
29:a:1420:G:H2'	29:a:1421:A:C8	2.46	0.50
29:a:2798:A:H2'	29:a:2799:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:k:80:ARG:HB2	39:k:83:GLU:HG3	1.93	0.50
26:V:28:U:H2'	26:V:29:C:C6	2.47	0.50
29:a:40:U:H2'	29:a:41:C:C6	2.46	0.50
29:a:1779:U:H2'	29:a:1780:A:C5	2.47	0.50
41:m:53:THR:HA	41:m:56:LYS:HD2	1.94	0.50
6:A:333:G:H2'	6:A:334:A:H8	1.76	0.50
9:D:97:GLU:HG2	9:D:188:PRO:HG3	1.94	0.50
29:a:571:U:H2'	29:a:572:C:C6	2.47	0.50
29:a:2526:U:H2'	29:a:2527:C:C6	2.47	0.50
31:c:8:PRO:HB3	31:c:14:ARG:HG3	1.93	0.50
6:A:281:U:H2'	6:A:282:G:C8	2.46	0.50
7:B:37:ARG:HB2	7:B:42:ILE:HD13	1.93	0.50
8:C:97:VAL:HG22	8:C:98:PRO:HD2	1.94	0.50
17:L:8:ILE:HD11	22:Q:37:LYS:HB3	1.93	0.50
26:V:76:C:H5'	26:V:77:A:O5'	2.12	0.50
29:a:513:U:H2'	29:a:514:G:C8	2.47	0.50
29:a:545:U:C2'	29:a:546:G:H5'	2.42	0.50
29:a:740:A:H4'	29:a:1259:G:N3	2.27	0.50
29:a:2086:U:H2'	29:a:2087:U:C6	2.47	0.50
6:A:759:U:H2'	6:A:760:A:H8	1.76	0.49
6:A:905:A:H2'	6:A:906:A:C8	2.47	0.49
6:A:1504:A:H2'	6:A:1505:G:C8	2.47	0.49
6:A:1510:A:H2'	6:A:1511:G:C8	2.47	0.49
20:O:40:GLN:OE1	20:O:40:GLN:HA	2.12	0.49
29:a:1673:G:H2'	29:a:1674:U:C6	2.46	0.49
29:a:2336:C:H2'	29:a:2337:U:C6	2.47	0.49
46:r:88:ARG:HG3	46:r:94:ASP:OD2	2.11	0.49
6:A:840:U:H3'	6:A:841:G:C8	2.47	0.49
11:F:51:ILE:O	11:F:54:ILE:HG13	2.11	0.49
29:a:196:A:C2	39:k:52:PHE:HZ	2.30	0.49
29:a:389:U:H5"	51:w:32:ASN:HB2	1.94	0.49
29:a:430:G:H2'	29:a:431:A:C8	2.47	0.49
29:a:1529:A:H2'	29:a:1530:C:H6	1.77	0.49
29:a:1783:A:H2'	29:a:1784:C:H6	1.77	0.49
29:a:1903:C:H2'	29:a:1904:3TD:H6	1.94	0.49
29:a:2053:C:H2'	29:a:2054:C:C6	2.47	0.49
19:N:64:CYS:HB2	19:N:69:ARG:H	1.76	0.49
22:Q:23:VAL:HG22	22:Q:46:HIS:CD2	2.46	0.49
29:a:2142:A:H2'	29:a:2143:G:H8	1.77	0.49
37:i:17:VAL:CG2	37:i:137:PRO:HB2	2.43	0.49
44:p:86:ALA:HB2	44:p:116:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:42:TRP:CZ2	23:R:24:LYS:HD3	2.48	0.49
29:a:2:G:H2'	29:a:3:U:C6	2.48	0.49
29:a:847:G:H2'	29:a:848:G:C8	2.48	0.49
29:a:1341:A:H2'	29:a:1342:A:C8	2.47	0.49
29:a:1395:C:H2'	29:a:1396:U:H6	1.76	0.49
34:f:46:ASP:OD1	34:f:49:LEU:HB2	2.13	0.49
3:2:50:HIS:CG	29:a:2348:C:H5'	2.48	0.49
6:A:693:A:H2'	6:A:694:U:H6	1.77	0.49
14:I:50:LEU:HB3	14:I:56:THR:HA	1.95	0.49
29:a:2158:A:H2'	29:a:2159:A:C8	2.48	0.49
29:a:2639:U:H2'	29:a:2640:C:C6	2.48	0.49
29:a:2790:G:H2'	29:a:2791:U:H6	1.76	0.49
29:a:1287:G:H5"	29:a:1288:A:H5"	1.94	0.49
29:a:1463:G:O2'	29:a:1464:U:H6	1.96	0.49
29:a:2762:U:H5"	32:d:172:ARG:HG2	1.95	0.49
34:f:48:LYS:HE2	34:f:48:LYS:N	2.26	0.49
35:g:42:GLU:HG2	35:g:55:ALA:HB2	1.94	0.49
6:A:597:G:H5"	13:H:90:LYS:HD3	1.95	0.49
6:A:905:A:H2'	6:A:906:A:H8	1.78	0.49
9:D:172:TRP:CD2	9:D:188:PRO:HB3	2.47	0.49
29:a:1395:C:H2'	29:a:1396:U:C6	2.48	0.49
29:a:2546:G:H2'	29:a:2547:C:C6	2.48	0.49
22:Q:62:ILE:HG22	22:Q:76:LEU:HA	1.94	0.49
29:a:804:U:H2'	29:a:805:C:C6	2.47	0.49
32:d:196:ILE:HD12	32:d:204:VAL:HG11	1.95	0.49
53:y:4:ILE:HG22	53:y:58:GLU:HA	1.95	0.49
9:D:8:LYS:HD2	9:D:21:LEU:HD13	1.94	0.49
29:a:590:A:H2'	29:a:591:G:H8	1.78	0.49
29:a:824:A:H2'	29:a:825:G:C8	2.47	0.49
29:a:1492:U:H2'	29:a:1493:A:C8	2.47	0.49
29:a:2543:U:H2'	29:a:2544:U:C6	2.48	0.49
34:f:156:ILE:HG21	34:f:170:MET:HE1	1.94	0.49
53:y:6:VAL:HG12	53:y:28:LEU:HD11	1.95	0.49
6:A:1519:U:H2'	6:A:1520:G:H8	1.78	0.49
7:B:101:GLY:HA2	7:B:104:THR:OG1	2.13	0.49
18:M:81:MET:HG2	18:M:92:ARG:HG3	1.95	0.49
29:a:751:G:H2'	29:a:752:A:O4'	2.13	0.49
34:f:80:ARG:HD3	34:f:80:ARG:N	2.28	0.49
36:h:31:ILE:HG12	36:h:32:PRO:HD3	1.95	0.49
6:A:1035:C:H2'	6:A:1036:U:C6	2.46	0.48
9:D:157:ILE:O	9:D:161:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:91:GLY:HA2	16:K:94:SER:HB2	1.95	0.48
26:V:21:H2U:H1'	26:V:22:A:H5'	1.95	0.48
29:a:2086:U:H2'	29:a:2087:U:H6	1.77	0.48
6:A:75:A:H4'	6:A:76:A:C8	2.48	0.48
6:A:725:A:H2'	6:A:726:A:H8	1.78	0.48
29:a:1018:A:H61	29:a:1115:G:H2'	1.78	0.48
29:a:1393:U:H2'	29:a:1394:U:C6	2.48	0.48
6:A:1399:4OC:H2'	6:A:1400:C:O4'	2.12	0.48
42:n:74:GLY:HA3	42:n:108:ALA:HB3	1.95	0.48
6:A:536:A:H2'	6:A:537:G:H8	1.78	0.48
8:C:142:MET:HE2	8:C:170:GLU:HG3	1.96	0.48
29:a:2026:A:H2'	29:a:2027:G:C8	2.48	0.48
29:a:2138:U:H2'	29:a:2139:U:H6	1.78	0.48
7:B:131:LEU:HD23	7:B:135:GLU:HB3	1.94	0.48
8:C:100:GLN:HG2	8:C:101:VAL:N	2.29	0.48
11:F:18:VAL:HG21	11:F:58:HIS:ND1	2.29	0.48
29:a:1493:A:H2'	29:a:1494:C:C6	2.48	0.48
29:a:2885:C:H2'	29:a:2886:U:C6	2.48	0.48
47:s:38:THR:HB	47:s:41:GLU:HG3	1.95	0.48
17:L:50:ARG:HB3	17:L:66:TYR:HE1	1.77	0.48
18:M:106:ALA:HB3	18:M:110:LYS:HD3	1.95	0.48
29:a:657:A:H2'	29:a:658:U:C6	2.49	0.48
29:a:2138:U:H2'	29:a:2139:U:C6	2.48	0.48
35:g:17:VAL:HG11	35:g:50:LEU:HD11	1.95	0.48
43:o:56:ARG:H	43:o:60:SER:HB3	1.78	0.48
53:y:46:MET:O	53:y:50:VAL:HG22	2.14	0.48
6:A:818:G:H2'	6:A:819:U:C6	2.49	0.48
15:J:50:ASN:HB3	15:J:62:ARG:HD2	1.96	0.48
29:a:1031:G:H2'	29:a:1032:G:H8	1.78	0.48
29:a:1187:U:H2'	29:a:1188:C:H6	1.79	0.48
39:k:82:SER:HB3	39:k:116:GLY:HA3	1.95	0.48
42:n:28:CYS:HA	42:n:92:ASP:HB3	1.95	0.48
6:A:521:G:H2'	6:A:522:C:C6	2.49	0.48
6:A:1217:G:O3'	24:S:36:ARG:HD3	2.14	0.48
7:B:71:PHE:HB3	7:B:82:ILE:HG23	1.96	0.48
29:a:12:U:O2	29:a:2615:C:H4'	2.13	0.48
29:a:1798:A:H2'	29:a:1799:A:C8	2.48	0.48
31:c:20:VAL:HG23	31:c:21:HIS:H	1.79	0.48
31:c:140:THR:HG23	31:c:161:SER:HB2	1.95	0.48
33:e:20:ARG:HD3	33:e:106:CYS:SG	2.54	0.48
43:o:95:VAL:HG11	43:o:100:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:899:G:H2'	6:A:900:A:H8	1.78	0.48
6:A:1406:C:H2'	6:A:1407:A:H8	1.79	0.48
7:B:113:ILE:HG13	7:B:150:LEU:HD13	1.95	0.48
11:F:100:SER:H	11:F:103:ALA:HB3	1.79	0.48
29:a:1527:G:H2'	29:a:1528:U:H6	1.79	0.48
29:a:2137:G:H2'	29:a:2138:U:C6	2.49	0.48
29:a:2689:A:H2'	29:a:2690:C:C6	2.49	0.48
7:B:138:GLU:HG3	7:B:139:ARG:HH21	1.79	0.48
29:a:39:G:H2'	29:a:40:U:C6	2.49	0.48
29:a:875:U:H2'	29:a:876:C:H6	1.78	0.48
29:a:1422:A:H2'	29:a:1423:G:O4'	2.14	0.48
29:a:2676:U:H2'	29:a:2677:G:O4'	2.13	0.48
6:A:1069:G:H2'	6:A:1070:U:C6	2.49	0.47
10:E:110:MET:SD	10:E:124:ALA:HB1	2.54	0.47
11:F:29:ILE:HG23	11:F:34:GLY:HA3	1.96	0.47
26:V:20:G:H4'	26:V:21:H2U:OP2	2.14	0.47
29:a:64:G:H2'	29:a:65:C:C6	2.48	0.47
29:a:151:U:H2'	29:a:152:G:C8	2.49	0.47
29:a:1482:A:H2'	29:a:1483:A:C8	2.49	0.47
29:a:1582:C:H2'	29:a:1583:A:C8	2.48	0.47
29:a:2098:U:H2'	29:a:2099:G:C8	2.49	0.47
29:a:2121:U:H5'	29:a:2122:G:C5	2.48	0.47
29:a:2132:C:H2'	29:a:2133:G:O4'	2.14	0.47
29:a:2142:A:H2'	29:a:2143:G:C8	2.49	0.47
29:a:2232:U:H2'	29:a:2233:U:H6	1.78	0.47
30:b:46:U:H2'	30:b:47:C:H6	1.79	0.47
6:A:58:U:H2'	6:A:59:G:H8	1.79	0.47
6:A:89:C:H5"	6:A:90:C:H6	1.78	0.47
6:A:1188:A:OP2	6:A:1188:A:H8	1.96	0.47
6:A:1352:G:H2'	6:A:1353:G:H8	1.78	0.47
6:A:1513:2MG:H2'	6:A:1515:MA6:OP2	2.14	0.47
29:a:411:U:H2'	29:a:412:C:H6	1.78	0.47
29:a:1304:A:H2'	29:a:1305:G:C8	2.49	0.47
57:a:2959:MG:MG	55:a:3239:K:K	1.50	0.47
31:c:210:ALA:HA	31:c:213:TRP:CE3	2.49	0.47
6:A:487:C:H2'	6:A:488:G:H8	1.79	0.47
6:A:1115:U:H2'	6:A:1116:C:H6	1.80	0.47
29:a:2118:C:H2'	29:a:2119:U:O4'	2.14	0.47
6:A:1353:G:H2'	6:A:1354:A:H8	1.79	0.47
29:a:659:A:H2'	29:a:661:A:H62	1.80	0.47
29:a:1554:U:H2'	29:a:1555:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:184:ASP:HB3	32:d:189:VAL:HG22	1.95	0.47
38:j:2:ILE:HD12	38:j:6:THR:HG21	1.96	0.47
38:j:109:GLU:CD	38:j:109:GLU:H	2.22	0.47
44:p:58:ARG:HA	44:p:61:TRP:CE3	2.49	0.47
54:z:37:HIS:HB3	54:z:43:THR:HG22	1.96	0.47
1:0:1:MET:HG2	1:0:1:MET:O	2.14	0.47
6:A:754:U:H2'	6:A:755:G:O4'	2.14	0.47
6:A:1409:C:H2'	6:A:1410:A:H8	1.80	0.47
7:B:109:LEU:HD12	7:B:150:LEU:HD11	1.96	0.47
5:4:22:ILE:HG23	34:f:3:ARG:NH1	2.27	0.47
6:A:915:A:H2'	6:A:916:A:C8	2.49	0.47
6:A:1323:U:H2'	6:A:1324:C:C6	2.47	0.47
29:a:222:A:C2	29:a:233:A:H5"	2.50	0.47
29:a:483:G:O6	46:r:49:LYS:HE3	2.14	0.47
29:a:1186:U:H2'	29:a:1187:U:C6	2.50	0.47
29:a:1314:U:H2'	29:a:1315:A:H8	1.80	0.47
6:A:447:A:H5'	21:P:88:ARG:HH22	1.80	0.47
6:A:502:G:H2'	6:A:503:G:C8	2.50	0.47
6:A:1216:A:H2'	6:A:1217:G:C8	2.50	0.47
6:A:1238:G:H2'	6:A:1239:G:H8	1.78	0.47
8:C:47:LEU:HB3	8:C:50:ALA:HB3	1.96	0.47
18:M:92:ARG:HG2	29:a:879:C:C5	2.49	0.47
26:V:33:OMC:H2'	26:V:34:U:C6	2.49	0.47
29:a:189:G:OP2	51:w:14:VAL:HG11	2.15	0.47
29:a:513:U:H2'	29:a:514:G:H8	1.80	0.47
29:a:1280:G:H2'	29:a:1281:U:C6	2.50	0.47
29:a:1394:U:H2'	29:a:1395:C:H6	1.80	0.47
29:a:1404:G:H2'	29:a:1405:C:H6	1.79	0.47
29:a:1684:U:H5"	29:a:1685:C:H5	1.80	0.47
30:b:87:A:H5'	40:l:18:THR:HG22	1.95	0.47
6:A:502:G:H2'	6:A:503:G:H8	1.79	0.47
29:a:917:G:H2'	29:a:918:A:H8	1.80	0.47
29:a:1514:G:H2'	29:a:1515:C:O4'	2.14	0.47
29:a:2116:G:H2'	29:a:2117:G:H8	1.78	0.47
29:a:2366:A:H2'	29:a:2367:A:C8	2.50	0.47
45:q:21:LYS:HG2	45:q:95:GLU:HG2	1.97	0.47
6:A:577:C:H2'	6:A:578:G:O4'	2.15	0.47
6:A:671:G:H2'	6:A:672:A:C8	2.49	0.47
26:V:24:C:H2'	26:V:25:U:C6	2.49	0.47
29:a:310:C:H2'	29:a:311:G:O4'	2.15	0.47
29:a:2150:C:H2'	29:a:2151:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:z:11:SER:O	54:z:15:MET:HG3	2.15	0.47
10:E:55:VAL:O	10:E:59:ILE:HG13	2.15	0.47
29:a:314:C:OP2	33:e:131:LYS:HE3	2.14	0.47
29:a:2280:U:H2'	29:a:2281:G:H8	1.78	0.47
29:a:2293:G:H5'	29:a:2294:U:OP2	2.15	0.47
31:c:53:HIS:HA	31:c:217:ARG:HB2	1.97	0.47
35:g:145:ALA:HB1	35:g:164:TYR:HE1	1.80	0.47
6:A:467:U:H2'	6:A:468:A:C8	2.50	0.46
6:A:624:G:H2'	6:A:625:G:O4'	2.15	0.46
9:D:13:ARG:NH2	9:D:39:PRO:HA	2.30	0.46
12:G:69:VAL:HG13	12:G:100:ALA:HB1	1.95	0.46
28:X:64:PRO:HB2	28:X:67:LEU:HD12	1.97	0.46
29:a:139:U:H4'	29:a:140:A:OP1	2.15	0.46
29:a:1277:C:H2'	29:a:1278:C:H6	1.79	0.46
29:a:2063:U:H2'	29:a:2064:U:C6	2.50	0.46
6:A:493:A:H2'	6:A:494:U:H5	1.79	0.46
6:A:605:A:H2'	6:A:606:A:O4'	2.15	0.46
6:A:1187:G:H4'	6:A:1188:A:OP2	2.14	0.46
7:B:85:GLN:HG2	7:B:216:ALA:C	2.41	0.46
29:a:52:A:H2'	29:a:53:A:C8	2.50	0.46
29:a:285:U:H2'	29:a:286:U:H6	1.79	0.46
29:a:299:U:H2'	29:a:300:C:C6	2.49	0.46
29:a:925:U:H2'	29:a:926:C:H6	1.80	0.46
29:a:2300:A:C2	34:f:77:PHE:HB3	2.51	0.46
35:g:38:HIS:HB3	35:g:41:VAL:HG23	1.97	0.46
6:A:1235:A:N7	6:A:1300:C:H1'	2.30	0.46
8:C:129:MET:HE3	8:C:129:MET:HB2	1.82	0.46
9:D:139:VAL:HG11	9:D:145:ILE:HD11	1.97	0.46
29:a:17:G:H4'	44:p:25:TYR:HE1	1.80	0.46
29:a:388:G:H1'	51:w:29:PHE:HB3	1.96	0.46
29:a:787:C:H2'	29:a:788:U:C6	2.49	0.46
29:a:986:A:H4'	44:p:91:ASP:OD2	2.15	0.46
29:a:2222:U:H2'	29:a:2223:G:H8	1.81	0.46
29:a:2437:A:H3'	29:a:2438:H2U:H2'	1.98	0.46
29:a:2580:C:H2'	29:a:2581:G:H8	1.78	0.46
29:a:2586:G:H2'	29:a:2587:A:C8	2.50	0.46
35:g:64:GLN:O	35:g:67:THR:HG22	2.15	0.46
1:0:25:THR:HG21	29:a:2275:G:OP1	2.16	0.46
6:A:86:C:H3'	6:A:87:U:C6	2.51	0.46
6:A:1509:U:H2'	6:A:1510:A:C8	2.50	0.46
13:H:3:MET:HE2	13:H:3:MET:HB2	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:86:TYR:O	18:M:90:ARG:HG2	2.14	0.46
26:V:23:G:H2'	26:V:24:C:C6	2.51	0.46
29:a:150:U:H2'	29:a:151:U:C6	2.49	0.46
29:a:680:A:H2'	29:a:681:U:C6	2.50	0.46
29:a:1394:U:H2'	29:a:1395:C:C6	2.50	0.46
31:c:75:PRO:HA	31:c:117:GLN:HG3	1.98	0.46
37:i:36:LEU:HD11	37:i:122:MET:HB2	1.97	0.46
6:A:1224:A:H5"	24:S:83:HIS:HD2	1.81	0.46
6:A:1474:C:H2'	6:A:1475:C:C6	2.50	0.46
9:D:156:ARG:HG3	9:D:157:ILE:N	2.30	0.46
19:N:72:GLY:O	19:N:80:SER:HA	2.15	0.46
29:a:151:U:H2'	29:a:152:G:H8	1.80	0.46
29:a:406:C:H2'	29:a:407:A:H8	1.80	0.46
29:a:1266:C:H2'	29:a:1267:G:H8	1.80	0.46
29:a:1943:G:N3	29:a:2540:C:H5"	2.31	0.46
30:b:27:A:H2'	30:b:28:C:C6	2.51	0.46
31:c:115:LYS:HB3	31:c:115:LYS:HE3	1.59	0.46
34:f:27:GLU:HG2	34:f:161:ARG:NH1	2.30	0.46
40:l:67:ARG:HD2	40:l:105:GLU:OE1	2.16	0.46
6:A:262:G:H3'	22:Q:70:LYS:HB2	1.97	0.46
6:A:892:G:H2'	6:A:893:U:C6	2.50	0.46
6:A:899:G:H2'	6:A:900:A:C8	2.50	0.46
6:A:1407:A:H2'	6:A:1408:C:C6	2.51	0.46
16:K:66:ALA:HB3	16:K:98:ALA:HB3	1.98	0.46
17:L:79:VAL:HG12	17:L:102:LEU:HD13	1.98	0.46
19:N:73:TYR:CE2	19:N:75:ARG:HA	2.51	0.46
29:a:1404:G:H2'	29:a:1405:C:C6	2.50	0.46
29:a:1845:U:H2'	29:a:1846:G:O4'	2.16	0.46
29:a:2121:U:H5'	29:a:2122:G:C4	2.51	0.46
40:l:6:ARG:HB3	40:l:6:ARG:HH11	1.81	0.46
50:v:41:ARG:HA	50:v:41:ARG:HD3	1.67	0.46
6:A:1460:U:H2'	6:A:1461:U:C6	2.51	0.46
9:D:161:ILE:HG23	9:D:177:HIS:ND1	2.31	0.46
21:P:52:GLU:HG2	21:P:54:ILE:HG23	1.98	0.46
29:a:963:A:H5"	45:q:81:LYS:HD2	1.98	0.46
29:a:2104:G:H2'	29:a:2106:A:N7	2.30	0.46
29:a:2689:A:H2'	29:a:2690:C:H6	1.81	0.46
29:a:2773:U:H2'	29:a:2774:U:C6	2.51	0.46
6:A:599:A:H2'	6:A:600:U:C6	2.51	0.46
6:A:1432:G:H2'	6:A:1433:U:C6	2.50	0.46
28:X:87:ILE:O	28:X:91:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2113:G:H2'	29:a:2114:G:O4'	2.15	0.46
29:a:2532:G:H2'	29:a:2533:G:C8	2.51	0.46
53:y:5:LYS:HB2	53:y:57:GLU:HB3	1.97	0.46
6:A:175:A:H2'	6:A:176:U:C6	2.50	0.46
6:A:327:G:O2'	25:T:2:ALA:HB1	2.16	0.46
6:A:378:A:H2'	6:A:379:A:C8	2.51	0.46
6:A:743:A:H2'	6:A:744:A:C8	2.51	0.46
6:A:1235:A:H2	6:A:1238:G:N3	2.13	0.46
6:A:1443:A:H1'	6:A:1444:A:H5'	1.98	0.46
7:B:168:VAL:HG21	7:B:189:VAL:HG13	1.98	0.46
8:C:15:VAL:HB	8:C:207:ILE:HD12	1.97	0.46
29:a:273:A:H2'	29:a:274:A:H8	1.81	0.46
29:a:2353:C:H2'	29:a:2354:G:O4'	2.16	0.46
29:a:2837:G:O2'	29:a:2838:G:H5'	2.16	0.46
1:0:34:LYS:HB2	1:0:45:PHE:CD1	2.51	0.46
6:A:37:G:H2'	6:A:38:C:C6	2.51	0.46
6:A:947:U:H2'	6:A:948:G:C8	2.51	0.46
6:A:1115:U:H2'	6:A:1116:C:C6	2.51	0.46
6:A:1118:U:H2'	6:A:1119:U:C6	2.51	0.46
6:A:1325:C:C2	6:A:1326:A:C8	3.04	0.46
9:D:8:LYS:HB3	9:D:21:LEU:HB3	1.98	0.46
15:J:90:LEU:HD12	15:J:90:LEU:HA	1.73	0.46
25:T:67:ILE:HB	25:T:71:LYS:HD2	1.98	0.46
29:a:1066:C:C2	29:a:1067:A:C8	3.04	0.46
29:a:1159:A:H2'	29:a:1160:U:C6	2.51	0.46
29:a:1349:G:H2'	29:a:1350:C:C6	2.50	0.46
29:a:2094:U:H2'	29:a:2095:A:H8	1.80	0.46
29:a:2885:C:H2'	29:a:2886:U:H6	1.81	0.46
30:b:37:U:H2'	30:b:38:U:C6	2.51	0.46
32:d:128:TRP:CD1	32:d:163:LYS:HB3	2.51	0.46
39:k:81:LEU:HD21	39:k:118:ILE:HG12	1.98	0.46
6:A:590:U:H2'	6:A:591:U:C6	2.51	0.45
6:A:1315:A:H1'	24:S:37:ARG:NH2	2.31	0.45
29:a:244:A:H5"	39:k:69:THR:HG21	1.98	0.45
29:a:1474:U:H2'	29:a:1475:C:H6	1.80	0.45
29:a:2019:6MZ:C2	29:a:2488:C:H5"	2.47	0.45
29:a:2105:G:O2'	29:a:2106:A:H5'	2.17	0.45
6:A:75:A:H1'	6:A:92:G:H22	1.81	0.45
6:A:497:G:H2'	6:A:498:C:C6	2.52	0.45
6:A:1144:C:H2'	6:A:1145:U:C6	2.51	0.45
9:D:199:GLU:H	9:D:199:GLU:HG3	1.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:89:ARG:HB2	20:O:89:ARG:NH1	2.30	0.45
29:a:208:C:H2'	29:a:209:C:H6	1.81	0.45
29:a:1337:C:C2	29:a:1338:C:C5	3.05	0.45
29:a:1671:U:H2'	29:a:1672:G:O4'	2.16	0.45
29:a:2775:U:H2'	29:a:2776:C:H6	1.81	0.45
5:4:42:HIS:HB3	5:4:45:TYR:CD1	2.52	0.45
6:A:559:U:H1'	17:L:12:ARG:HD2	1.98	0.45
19:N:45:MET:HE1	24:S:7:LYS:HB3	1.97	0.45
29:a:197:A:H62	29:a:2419:A:H2'	1.80	0.45
6:A:418:A:H1'	6:A:419:U:N3	2.32	0.45
9:D:64:ARG:HG3	9:D:74:PHE:CD1	2.52	0.45
11:F:26:ILE:HG23	11:F:36:ILE:HG13	1.98	0.45
15:J:8:ILE:HG21	15:J:25:ILE:HD13	1.97	0.45
20:O:56:LEU:O	20:O:60:VAL:HG13	2.16	0.45
29:a:1307:C:O2'	29:a:1308:C:H5'	2.17	0.45
29:a:1430:U:H2'	29:a:1431:C:C6	2.52	0.45
29:a:1526:U:H5"	29:a:1527:G:C8	2.51	0.45
2:1:1:MET:N	29:a:1610:G:H21	2.13	0.45
6:A:232:A:H2'	6:A:233:A:C8	2.51	0.45
6:A:1259:C:H2'	6:A:1260:A:H8	1.81	0.45
29:a:568:G:H2'	29:a:569:G:C8	2.52	0.45
29:a:1187:U:H2'	29:a:1188:C:C6	2.51	0.45
29:a:1424:G:H2'	29:a:1425:C:O4'	2.17	0.45
29:a:2638:C:H2'	29:a:2639:U:C6	2.51	0.45
29:a:2737:A:H5'	35:g:4:VAL:HG21	1.98	0.45
38:j:7:MET:HE3	38:j:7:MET:HB3	1.81	0.45
38:j:44:LYS:HA	38:j:44:LYS:HD2	1.76	0.45
41:m:87:TYR:OH	41:m:115:LEU:HB3	2.17	0.45
11:F:39:LEU:HD22	11:F:39:LEU:HA	1.80	0.45
21:P:74:ARG:HA	21:P:74:ARG:HD2	1.73	0.45
26:V:10:G:C2	26:V:27:G:H1'	2.51	0.45
29:a:303:G:H2'	29:a:304:G:C8	2.52	0.45
29:a:775:G:H5'	29:a:776:G:OP1	2.16	0.45
29:a:1277:C:H2'	29:a:1278:C:C6	2.52	0.45
29:a:2105:G:H2'	29:a:2106:A:C8	2.51	0.45
37:i:104:ALA:O	37:i:108:MET:HG3	2.17	0.45
6:A:220:A:H2'	6:A:221:U:C6	2.52	0.45
6:A:659:G:H2'	6:A:660:A:C8	2.51	0.45
6:A:978:U:H5"	19:N:6:MET:HE1	1.98	0.45
6:A:1355:U:P	19:N:75:ARG:HD2	2.56	0.45
29:a:514:G:H2'	29:a:515:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:5:ALA:O	4:3:38:GLY:HA2	2.16	0.45
6:A:78:G:H2'	6:A:79:U:C6	2.52	0.45
6:A:493:A:H2'	6:A:494:U:C5	2.52	0.45
6:A:999:G:H3'	6:A:1000:A:H8	1.82	0.45
6:A:1240:U:H2'	6:A:1241:C:C6	2.51	0.45
7:B:21:GLN:HB2	7:B:24:PHE:HD2	1.81	0.45
29:a:635:A:H2'	29:a:637:A:C8	2.51	0.45
29:a:1418:G:H2'	29:a:1419:A:O4'	2.17	0.45
29:a:1742:G:H5"	43:o:96:ARG:HG3	1.98	0.45
29:a:1836:A:O2'	29:a:1837:A:H8	1.98	0.45
29:a:2083:A:H2'	29:a:2084:A:C8	2.51	0.45
29:a:2696:U:H2'	29:a:2697:C:C6	2.52	0.45
6:A:242:A:C2	6:A:278:A:C5	3.05	0.45
6:A:395:G:H2'	6:A:396:C:C6	2.52	0.45
6:A:716:C:O2'	23:R:38:LYS:HB3	2.17	0.45
6:A:1140:G:H2'	6:A:1141:G:C8	2.51	0.45
6:A:1340:G:O3'	14:I:122:ARG:HG2	2.17	0.45
6:A:1534:U:H2'	6:A:1535:C:C6	2.52	0.45
18:M:89:LEU:HA	18:M:92:ARG:HD3	1.98	0.45
29:a:263:U:H2'	29:a:264:C:O4'	2.16	0.45
29:a:590:A:H2'	29:a:591:G:C8	2.51	0.45
29:a:671:A:H2'	29:a:672:G:C8	2.52	0.45
29:a:862:U:OP1	40:l:5:LYS:HG3	2.17	0.45
29:a:1078:A:H5'	29:a:1079:A:OP1	2.17	0.45
29:a:2846:G:H5'	29:a:2847:U:OP2	2.17	0.45
37:i:17:VAL:HG23	37:i:137:PRO:HB2	1.99	0.45
6:A:1406:C:H2'	6:A:1407:A:C8	2.52	0.45
8:C:119:ALA:O	8:C:123:GLN:HG3	2.16	0.45
14:I:39:ARG:HE	14:I:39:ARG:HB3	1.65	0.45
29:a:227:A:C2	29:a:2396:A:H1'	2.52	0.45
29:a:631:C:H2'	29:a:632:U:C6	2.52	0.45
29:a:662:C:H2'	29:a:663:C:H6	1.82	0.45
29:a:1054:C:N3	29:a:1059:A:H8	2.15	0.45
29:a:1429:A:H2'	29:a:1430:U:C6	2.52	0.45
48:t:70:ILE:HG21	48:t:81:VAL:HG23	1.99	0.45
6:A:1521:C:H2'	6:A:1522:G:C8	2.52	0.44
8:C:35:LYS:HB2	8:C:35:LYS:HE3	1.83	0.44
8:C:134:MET:HE3	8:C:168:TYR:CE1	2.51	0.44
12:G:89:MET:HE2	12:G:89:MET:HB3	1.82	0.44
19:N:20:TYR:HD2	19:N:55:ALA:HB2	1.81	0.44
29:a:629:G:H2'	29:a:630:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:937:A:H2'	29:a:938:C:C6	2.52	0.44
42:n:51:GLN:HG2	42:n:52:ALA:N	2.32	0.44
6:A:81:G:H5"	6:A:82:C:H5	1.82	0.44
6:A:1352:G:H2'	6:A:1353:G:C8	2.53	0.44
12:G:25:LYS:HB3	12:G:101:MET:HE1	1.97	0.44
18:M:79:ARG:CZ	18:M:79:ARG:HB3	2.46	0.44
29:a:194:G:H2'	29:a:195:A:O4'	2.17	0.44
29:a:1168:A:H2'	29:a:1169:U:C6	2.52	0.44
29:a:1420:G:H2'	29:a:1421:A:H8	1.82	0.44
45:q:15:VAL:HA	45:q:101:ILE:HD11	1.98	0.44
9:D:50:GLN:HE21	9:D:55:LEU:HD23	1.82	0.44
10:E:68:ARG:HE	10:E:68:ARG:HB3	1.57	0.44
24:S:63:THR:HG23	24:S:66:MET:HE3	1.98	0.44
29:a:684:A:H2'	29:a:685:U:C6	2.52	0.44
29:a:804:U:H2'	29:a:805:C:H6	1.81	0.44
29:a:1219:U:H2'	29:a:1220:G:H8	1.82	0.44
29:a:2639:U:H2'	29:a:2640:C:H6	1.81	0.44
6:A:745:U:C2	6:A:746:A:C8	3.05	0.44
6:A:1124:G:H1'	6:A:1277:A:C5	2.52	0.44
6:A:1534:U:H2'	6:A:1535:C:H6	1.82	0.44
25:T:34:ARG:HG2	25:T:34:ARG:HH11	1.82	0.44
29:a:491:U:H2'	29:a:492:G:O4'	2.17	0.44
29:a:1074:A:H1'	29:a:1095:U:O3'	2.17	0.44
29:a:1314:U:H2'	29:a:1315:A:C8	2.52	0.44
29:a:2164:C:H2'	29:a:2165:A:H8	1.79	0.44
32:d:187:ARG:NH1	43:o:10:ALA:HB1	2.33	0.44
4:3:36:ARG:HG2	4:3:37:GLN:N	2.31	0.44
6:A:367:A:H2'	6:A:368:C:O4'	2.18	0.44
6:A:595:U:H4'	13:H:87:TYR:CG	2.53	0.44
6:A:625:G:H2'	6:A:626:A:C8	2.52	0.44
6:A:734:A:H2'	6:A:735:U:H6	1.83	0.44
6:A:821:U:H2'	6:A:822:A:C8	2.52	0.44
6:A:1379:C:H1'	12:G:79:ARG:NH2	2.33	0.44
24:S:63:THR:H	24:S:66:MET:HE3	1.81	0.44
29:a:1304:A:H2'	29:a:1305:G:H8	1.82	0.44
29:a:2745:U:H1'	29:a:2746:A:H5"	1.99	0.44
30:b:11:A:H8	30:b:67:G:H21	1.64	0.44
34:f:50:LEU:HD23	34:f:50:LEU:HA	1.72	0.44
6:A:1233:A:H4'	6:A:1301:G:H4'	2.00	0.44
10:E:114:LEU:HD13	10:E:122:VAL:HG11	1.99	0.44
15:J:42:MET:HG3	15:J:71:LYS:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:66:C:C2	26:V:67:C:C5	3.06	0.44
28:X:25:LEU:HD11	28:X:41:VAL:HG21	1.99	0.44
29:a:589:U:H2'	29:a:590:A:C8	2.52	0.44
29:a:1342:A:H2'	29:a:1343:G:O4'	2.18	0.44
6:A:385:A:H3'	6:A:386:U:H6	1.82	0.44
6:A:776:C:H2'	6:A:777:A:O4'	2.17	0.44
6:A:1145:U:O3'	14:I:14:THR:HG21	2.17	0.44
9:D:199:GLU:HA	9:D:202:ILE:HD12	2.00	0.44
29:a:1099:C:H2'	29:a:1100:G:C4	2.52	0.44
46:r:1:MET:HA	46:r:1:MET:HE2	1.99	0.44
10:E:44:ARG:NH1	10:E:70:MET:HG2	2.33	0.44
11:F:22:VAL:HG11	11:F:39:LEU:HD11	1.99	0.44
29:a:72:A:C8	52:x:54:LYS:HD3	2.53	0.44
29:a:335:A:H2'	29:a:336:C:O4'	2.17	0.44
29:a:853:G:H2'	29:a:854:A:O4'	2.18	0.44
29:a:1328:U:H3'	29:a:1329:G:H5'	2.00	0.44
29:a:1960:U:O2'	31:c:223:MET:HE1	2.18	0.44
31:c:19:VAL:HG12	31:c:21:HIS:CD2	2.53	0.44
48:t:63:LEU:HB2	55:t:201:K:K	2.10	0.44
6:A:1421:U:H2'	6:A:1422:U:C6	2.53	0.44
6:A:1497:A:H5"	6:A:1505:G:H5"	1.98	0.44
24:S:10:PHE:CE2	24:S:37:ARG:HG3	2.49	0.44
29:a:1316:A:H2'	29:a:1318:C:C4	2.53	0.44
29:a:1917:A:H2'	29:a:1918:G:O4'	2.18	0.44
36:h:15:LEU:HD23	36:h:56:LYS:HD2	2.00	0.44
37:i:2:LYS:HB3	37:i:2:LYS:HE2	1.67	0.44
39:k:2:THR:HG22	39:k:3:LEU:H	1.83	0.44
50:v:72:LYS:HE3	50:v:72:LYS:HB2	1.65	0.44
6:A:470:A:H2'	6:A:471:G:C8	2.52	0.43
6:A:1022:U:H5"	6:A:1023:G:H5'	1.99	0.43
18:M:33:ILE:O	18:M:37:VAL:HG23	2.18	0.43
24:S:20:GLU:HA	24:S:23:VAL:HG12	2.01	0.43
29:a:197:A:N6	29:a:2419:A:H2'	2.33	0.43
29:a:1538:U:O2'	29:a:1539:G:H8	2.02	0.43
34:f:47:LYS:HE2	34:f:47:LYS:HB2	1.62	0.43
34:f:146:ILE:HG21	34:f:149:ILE:HD12	1.99	0.43
6:A:720:U:C4	27:W:10:G:H1'	2.54	0.43
6:A:1154:A:H4'	6:A:1155:C:O4'	2.18	0.43
16:K:97:ARG:HE	16:K:97:ARG:HB2	1.57	0.43
29:a:520:A:C2	29:a:2031:A:H2'	2.52	0.43
29:a:1869:U:H2'	29:a:1870:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:34:VAL:HG13	31:c:61:HIS:HB3	2.00	0.43
42:n:78:ALA:HB2	42:n:109:ALA:HA	1.98	0.43
6:A:189:A:H2'	6:A:190:G:C8	2.53	0.43
6:A:401:U:H3'	6:A:402:G:H5'	2.00	0.43
6:A:840:U:H3'	6:A:841:G:H8	1.83	0.43
7:B:22:THR:HA	7:B:41:HIS:CD2	2.54	0.43
12:G:76:LYS:HE3	12:G:76:LYS:HB3	1.63	0.43
16:K:13:ARG:O	16:K:15:VAL:HG13	2.18	0.43
16:K:16:SER:HA	16:K:78:LEU:HA	2.00	0.43
29:a:1561:A:H2'	29:a:1562:A:C8	2.53	0.43
45:q:14:VAL:HB	45:q:98:ILE:HG13	1.99	0.43
6:A:881:U:H4'	6:A:882:G:H5"	2.01	0.43
6:A:1339:C:H2'	6:A:1340:G:C8	2.53	0.43
13:H:109:LYS:HZ2	13:H:120:ALA:HB1	1.82	0.43
18:M:39:ILE:HG21	18:M:48:LEU:HD21	2.01	0.43
19:N:11:LEU:HD12	19:N:11:LEU:HA	1.81	0.43
29:a:154:A:H2'	29:a:155:A:H8	1.83	0.43
29:a:207:A:H2'	29:a:208:C:O4'	2.19	0.43
29:a:823:U:H2'	29:a:824:A:H8	1.82	0.43
29:a:969:A:H2'	29:a:972:C:H41	1.83	0.43
29:a:1872:U:H2'	29:a:1873:G:O4'	2.18	0.43
29:a:2432:U:OP1	33:e:62:LYS:HD3	2.18	0.43
29:a:2637:G:H2'	29:a:2638:C:C6	2.54	0.43
34:f:132:LEU:HD23	34:f:132:LEU:HA	1.82	0.43
42:n:87:THR:O	42:n:115:GLU:HG3	2.18	0.43
6:A:185:C:H4'	6:A:186:G:O5'	2.18	0.43
6:A:1148:A:HO2'	6:A:1149:A:H8	1.64	0.43
6:A:1424:C:H2'	6:A:1425:A:C8	2.54	0.43
26:V:62:C:H2'	26:V:63:C:C6	2.53	0.43
29:a:222:A:N1	29:a:233:A:H5"	2.33	0.43
29:a:463:A:H2'	29:a:464:A:O4'	2.19	0.43
29:a:1095:U:C2	29:a:1096:A:C8	3.06	0.43
29:a:1417:G:H2'	29:a:1418:G:C8	2.52	0.43
33:e:136:LYS:HB3	33:e:136:LYS:HE3	1.86	0.43
34:f:67:VAL:CG1	34:f:84:PRO:HB3	2.48	0.43
50:v:31:VAL:HG22	50:v:35:ASN:HB2	2.01	0.43
1:0:21:LYS:HD2	1:0:26:MET:HB3	2.01	0.43
6:A:673:A:H2'	6:A:674:U:H6	1.83	0.43
6:A:717:C:H2'	6:A:718:G:C8	2.54	0.43
6:A:1316:A:C8	6:A:1320:G:C5	3.06	0.43
9:D:181:GLU:HG2	9:D:182:GLY:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:26:C:H2'	26:V:27:G:O4'	2.19	0.43
29:a:162:U:H1'	29:a:163:A:N7	2.34	0.43
29:a:843:A:H5'	53:y:45:GLY:HA3	2.01	0.43
29:a:2160:A:H1'	29:a:2161:U:C5	2.53	0.43
32:d:57:ARG:O	32:d:61:VAL:HG23	2.18	0.43
34:f:120:LYS:HB2	34:f:120:LYS:HE3	1.78	0.43
6:A:908:U:H2'	6:A:909:C:C6	2.53	0.43
6:A:1127:A:H2'	6:A:1128:G:H8	1.84	0.43
6:A:1398:G:H2'	6:A:1399:4OC:O4'	2.19	0.43
24:S:41:LEU:HB2	24:S:44:PHE:CE1	2.54	0.43
26:V:33:OMC:HM23	26:V:39:A:H61	1.84	0.43
29:a:662:C:H2'	29:a:663:C:C6	2.54	0.43
29:a:842:C:H2'	29:a:843:A:C8	2.54	0.43
29:a:1060:A:H4'	29:a:1061:G:OP1	2.18	0.43
29:a:1473:A:H2'	29:a:1474:U:C6	2.53	0.43
29:a:2307:G:H3'	29:a:2308:U:C6	2.53	0.43
29:a:2339:C:H2'	29:a:2340:G:O4'	2.18	0.43
29:a:2876:C:H2'	29:a:2877:U:C6	2.53	0.43
30:b:66:C:H2'	30:b:67:G:O4'	2.19	0.43
52:x:32:LYS:HG3	52:x:37:LEU:HD22	2.01	0.43
6:A:177:A:N6	6:A:191:A:C8	2.87	0.43
6:A:467:U:H2'	6:A:468:A:H8	1.83	0.43
6:A:1316:A:C8	6:A:1320:G:C6	3.07	0.43
12:G:26:PHE:HZ	12:G:120:LEU:HD11	1.84	0.43
26:V:43:G:H2'	26:V:44:A:O4'	2.18	0.43
29:a:2112:G:H2'	29:a:2113:G:C8	2.54	0.43
29:a:2217:G:H2'	29:a:2218:U:C6	2.54	0.43
34:f:4:LEU:HG	34:f:101:ASP:HB2	2.00	0.43
35:g:4:VAL:O	35:g:69:ARG:HD2	2.17	0.43
40:l:33:ALA:HB2	40:l:105:GLU:HG3	2.01	0.43
46:r:55:ILE:O	46:r:59:GLU:HG3	2.18	0.43
6:A:1268:G:H2'	6:A:1269:U:C6	2.54	0.43
6:A:1349:C:H2'	6:A:1350:G:C8	2.53	0.43
14:I:63:ILE:HG21	14:I:77:ILE:HG12	2.01	0.43
25:T:28:VAL:HG23	25:T:61:MET:HG3	2.00	0.43
25:T:86:LEU:HD12	25:T:86:LEU:HA	1.76	0.43
29:a:658:U:H2'	29:a:659:A:O4'	2.19	0.43
29:a:1253:A:OP1	29:a:1253:A:H8	2.02	0.43
29:a:1483:A:H2'	29:a:1484:A:C8	2.54	0.43
29:a:1838:G:H2'	29:a:1839:G:H8	1.83	0.43
42:n:40:VAL:HB	42:n:50:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:76:TYR:CZ	44:p:80:ILE:HG13	2.54	0.43
46:r:80:MET:HE3	46:r:80:MET:HB2	1.75	0.43
1:0:32:ILE:HG23	1:0:34:LYS:HG3	2.01	0.43
3:2:30:HIS:CD2	3:2:31:ILE:HG13	2.53	0.43
6:A:422:U:H2'	6:A:423:U:C6	2.54	0.43
6:A:1326:A:C5	6:A:1327:U:C5	3.06	0.43
6:A:1407:A:H2'	6:A:1408:C:H6	1.84	0.43
11:F:6:ILE:HG23	11:F:89:ILE:HG12	2.01	0.43
23:R:29:LEU:O	23:R:33:ILE:HG23	2.19	0.43
25:T:39:ILE:HD11	25:T:83:VAL:HG23	2.01	0.43
29:a:457:G:H2'	29:a:458:A:C8	2.54	0.43
29:a:1075:A:H4'	29:a:1076:A:OP1	2.19	0.43
29:a:1170:A:H2'	29:a:1171:C:C6	2.54	0.43
29:a:1396:U:H2'	29:a:1397:G:H8	1.83	0.43
29:a:2334:A:N3	29:a:2370:A:H2'	2.34	0.43
29:a:2374:C:H2'	29:a:2375:U:C6	2.53	0.43
30:b:22:G:N7	30:b:54:G:H2'	2.34	0.43
31:c:38:LYS:HB2	31:c:38:LYS:HE2	1.84	0.43
6:A:760:A:H2'	6:A:761:C:C6	2.54	0.42
6:A:1187:G:H5'	8:C:176:HIS:NE2	2.34	0.42
7:B:72:VAL:HB	7:B:165:VAL:HG22	2.00	0.42
23:R:35:GLU:H	23:R:35:GLU:HG2	1.53	0.42
23:R:65:LEU:HD23	23:R:65:LEU:HA	1.83	0.42
23:R:70:TYR:HB2	23:R:74:HIS:NE2	2.34	0.42
24:S:19:VAL:O	24:S:23:VAL:HG12	2.19	0.42
29:a:1760:C:H2'	29:a:1761:A:C8	2.54	0.42
29:a:1912:U:H2'	29:a:1913:C:C6	2.54	0.42
29:a:2458:A:H2'	29:a:2459:G:O4'	2.19	0.42
29:a:2687:U:H2'	29:a:2688:G:C8	2.54	0.42
37:i:116:TYR:O	37:i:119:ILE:HG22	2.19	0.42
4:3:7:VAL:HG22	4:3:38:GLY:HA3	2.00	0.42
6:A:35:A:H2'	6:A:36:C:H6	1.83	0.42
6:A:542:C:P	9:D:64:ARG:HH12	2.42	0.42
11:F:42:TRP:HB2	11:F:59:TYR:HB2	2.00	0.42
12:G:86:GLN:HE22	26:V:33:OMC:H4'	1.84	0.42
15:J:14:ASP:HB2	15:J:17:LEU:HB2	2.01	0.42
15:J:26:VAL:HG23	15:J:74:ILE:HD13	2.00	0.42
25:T:39:ILE:HD13	25:T:82:GLN:HB3	2.01	0.42
29:a:383:A:H1'	29:a:403:G:O4'	2.20	0.42
29:a:475:A:C8	48:t:43:HIS:HD2	2.37	0.42
29:a:1043:U:H2'	29:a:1044:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:108:ILE:HG21	34:f:176:PRO:HG3	2.01	0.42
34:f:160:ALA:HB1	34:f:165:GLU:HB2	2.01	0.42
35:g:8:PRO:HB3	35:g:51:GLN:HG2	2.01	0.42
6:A:134:A:H2'	6:A:135:U:C6	2.53	0.42
6:A:947:U:OP2	18:M:101:ARG:HD2	2.19	0.42
6:A:1123:U:O2'	6:A:1124:G:H8	2.02	0.42
6:A:1237:U:O4	12:G:116:MET:HE2	2.19	0.42
12:G:92:ARG:O	12:G:96:ARG:HG3	2.19	0.42
12:G:131:LYS:HE2	12:G:131:LYS:HB3	1.76	0.42
26:V:11:A:H2'	26:V:12:G:H8	1.84	0.42
29:a:30:G:H2'	29:a:31:C:H6	1.84	0.42
29:a:963:A:H5'	29:a:1176:U:H1'	2.01	0.42
29:a:1484:A:H2'	29:a:1486:C:C5	2.53	0.42
29:a:2110:G:H2'	29:a:2111:U:C6	2.54	0.42
29:a:2126:C:H2'	29:a:2127:U:C6	2.55	0.42
5:4:68:MET:C	5:4:70:ARG:H	2.27	0.42
6:A:792:C:H5"	16:K:127:ARG:HH21	1.84	0.42
6:A:1188:A:H2'	6:A:1189:C:C6	2.54	0.42
29:a:589:U:H2'	29:a:590:A:H8	1.84	0.42
29:a:2089:G:H2'	29:a:2090:A:C8	2.55	0.42
38:j:4:THR:O	38:j:5:GLU:HB2	2.20	0.42
41:m:72:ASN:HB3	41:m:75:THR:HB	2.00	0.42
3:2:54:VAL:O	3:2:58:ARG:HG3	2.20	0.42
6:A:185:C:H1'	6:A:186:G:OP2	2.20	0.42
6:A:1007:C:H2'	6:A:1009:A:C8	2.54	0.42
7:B:34:PHE:HD1	7:B:44:ASN:HD22	1.67	0.42
7:B:138:GLU:HG3	7:B:139:ARG:HE	1.84	0.42
8:C:132:ARG:HA	8:C:132:ARG:HD3	1.82	0.42
19:N:6:MET:HE3	19:N:6:MET:HB3	1.83	0.42
29:a:170:G:H2'	29:a:171:U:C6	2.55	0.42
29:a:938:C:H1'	29:a:974:A:C8	2.55	0.42
29:a:1577:A:H2'	29:a:1578:G:O4'	2.20	0.42
29:a:2384:C:H2'	29:a:2385:G:O4'	2.19	0.42
29:a:2604:U:H2'	29:a:2605:C:H6	1.84	0.42
41:m:8:VAL:HG23	41:m:17:ARG:HD2	2.00	0.42
49:u:31:PRO:HB2	49:u:92:HIS:HD2	1.83	0.42
6:A:208:G:H2'	6:A:209:A:C8	2.55	0.42
7:B:63:ALA:HB3	7:B:226:GLY:HA3	2.02	0.42
13:H:29:SER:HB2	13:H:60:LEU:HB2	2.02	0.42
19:N:73:TYR:CZ	19:N:78:GLY:HA2	2.54	0.42
26:V:26:C:C4	26:V:27:G:C8	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:247:G:H4'	29:a:378:G:C4	2.55	0.42
29:a:733:G:H2'	29:a:734:U:H6	1.81	0.42
29:a:845:A:H2'	29:a:846:G:H8	1.84	0.42
29:a:1048:G:C8	29:a:1050:U:H5	2.37	0.42
29:a:1836:A:O2'	29:a:1837:A:H5'	2.18	0.42
29:a:2669:C:O2'	29:a:2670:C:H5'	2.20	0.42
34:f:4:LEU:HD23	34:f:4:LEU:HA	1.79	0.42
40:l:35:LYS:HG2	40:l:130:THR:HG22	2.01	0.42
45:q:60:THR:HG22	45:q:99:THR:OG1	2.20	0.42
6:A:347:G:OP1	25:T:2:ALA:HB3	2.19	0.42
12:G:46:ALA:O	12:G:50:VAL:HG13	2.20	0.42
18:M:106:ALA:O	18:M:110:LYS:HB2	2.20	0.42
22:Q:9:LEU:HB3	22:Q:26:ILE:HG12	2.02	0.42
29:a:291:U:H2'	29:a:292:G:C8	2.55	0.42
29:a:830:U:H2'	29:a:831:C:C6	2.55	0.42
29:a:842:C:H2'	29:a:843:A:H8	1.84	0.42
29:a:856:C:H42	29:a:900:A:H2	1.63	0.42
29:a:1339:C:H2'	29:a:1340:U:C6	2.54	0.42
57:a:2958:MG:MG	55:a:3189:K:K	1.56	0.42
35:g:85:ARG:HD2	35:g:85:ARG:HA	1.68	0.42
51:w:51:LEU:HD11	51:w:56:MET:HG3	2.02	0.42
6:A:579:U:H2'	6:A:580:A:H8	1.84	0.42
6:A:601:G:H2'	6:A:602:U:O4'	2.19	0.42
6:A:1116:C:H2'	6:A:1117:C:H6	1.85	0.42
23:R:45:THR:HG23	23:R:47:THR:H	1.85	0.42
28:X:29:PHE:CZ	28:X:90:LEU:HD23	2.55	0.42
29:a:1058:G:N1	29:a:1085:A:H1'	2.35	0.42
29:a:1299:G:HO2'	29:a:1300:U:H5	1.68	0.42
29:a:1500:G:H2'	29:a:1501:C:C6	2.55	0.42
29:a:2260:G:H5"	50:v:18:PRO:HB2	2.02	0.42
29:a:2772:A:H2'	29:a:2773:U:C6	2.54	0.42
34:f:26:MET:HB3	34:f:26:MET:HE3	1.76	0.42
6:A:182:C:H2'	6:A:183:U:O4'	2.19	0.42
6:A:329:C:H2'	6:A:330:C:H6	1.85	0.42
6:A:559:U:H5'	6:A:560:A:C5	2.54	0.42
9:D:19:LEU:HD22	9:D:66:ILE:HG13	2.01	0.42
18:M:71:ARG:NH2	34:f:115:ARG:HD3	2.35	0.42
19:N:60:LEU:HD12	19:N:60:LEU:HA	1.93	0.42
29:a:365:U:H2'	29:a:366:A:H8	1.84	0.42
29:a:1522:U:C4	29:a:1523:A:H1'	2.54	0.42
29:a:1605:A:C2	46:r:93:ALA:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1943:G:C2	29:a:2540:C:H5”	2.55	0.42
29:a:2240:OMG:HM23	29:a:2240:OMG:H1’	1.65	0.42
29:a:2841:G:H2’	29:a:2842:C:O4’	2.19	0.42
34:f:36:LEU:HD22	34:f:154:ILE:HG12	2.00	0.42
3:2:61:CYS:HB3	3:2:64:ILE:HG13	2.02	0.42
6:A:388:C:H2’	6:A:389:A:H8	1.85	0.42
6:A:861:A:H2’	6:A:862:A:C8	2.55	0.42
6:A:1264:C:O2	6:A:1324:C:H4’	2.20	0.42
6:A:1335:G:H2’	6:A:1336:A:C8	2.55	0.42
18:M:15:ALA:HB3	18:M:34:LEU:HD21	2.02	0.42
26:V:23:G:H2’	26:V:24:C:H6	1.85	0.42
26:V:38:A:H2’	26:V:39:A:O4’	2.20	0.42
28:X:38:HIS:HB3	28:X:63:ARG:HD2	2.01	0.42
29:a:208:C:H2’	29:a:209:C:C6	2.54	0.42
29:a:1716:A:H2’	29:a:1717:C:O4’	2.20	0.42
29:a:2773:U:H2’	29:a:2774:U:H6	1.85	0.42
6:A:88:A:H5”	6:A:89:C:C5	2.55	0.41
6:A:331:C:H2’	6:A:332:A:H8	1.84	0.41
6:A:675:U:H2’	6:A:676:C:H6	1.85	0.41
6:A:1213:G:OP1	19:N:3:LYS:HD2	2.20	0.41
13:H:18:GLN:HG3	13:H:71:PRO:CB	2.49	0.41
29:a:135:A:H2’	29:a:136:C:C6	2.55	0.41
29:a:605:A:H5’	29:a:607:A:C6	2.55	0.41
29:a:670:C:H2’	29:a:671:A:C8	2.55	0.41
29:a:1701:G:H2’	29:a:1702:U:C6	2.55	0.41
29:a:1764:U:O4	29:a:1778:A:H2	2.03	0.41
29:a:2140:C:H2’	29:a:2141:C:C6	2.54	0.41
29:a:2780:A:O2’	29:a:2781:G:H5”	2.19	0.41
33:e:104:MET:HE3	33:e:174:ILE:HD12	2.02	0.41
3:2:9:GLY:O	3:2:13:ARG:HD3	2.20	0.41
6:A:176:U:C2’	6:A:177:A:H5’	2.49	0.41
6:A:204:U:H1’	6:A:207:G:N2	2.35	0.41
6:A:979:U:H4’	6:A:980:A:O4’	2.21	0.41
7:B:29:MET:HE3	7:B:29:MET:HB3	1.74	0.41
15:J:76:ILE:HG22	15:J:79:PRO:HG3	2.02	0.41
28:X:68:LYS:HE3	28:X:68:LYS:HB3	1.82	0.41
29:a:123:G:H4’	29:a:1364:C:O5’	2.20	0.41
29:a:1831:G:H2’	29:a:1832:C:C6	2.55	0.41
29:a:2193:G:H4’	31:c:150:LYS:HG3	2.01	0.41
29:a:2281:G:H2’	29:a:2282:C:C6	2.55	0.41
29:a:2303:A:H1’	34:f:155:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2305:G:H2'	29:a:2306:C:H6	1.85	0.41
43:o:36:LYS:HB3	43:o:36:LYS:NZ	2.35	0.41
6:A:105:A:C6	6:A:322:G:C6	3.08	0.41
6:A:256:G:H2'	6:A:257:U:C6	2.55	0.41
8:C:39:VAL:HG23	8:C:94:ILE:HG21	2.01	0.41
11:F:42:TRP:N	11:F:42:TRP:CD1	2.88	0.41
26:V:25:U:H2'	26:V:26:C:C6	2.55	0.41
29:a:244:A:H2'	29:a:245:G:O4'	2.20	0.41
29:a:332:C:H2'	29:a:333:G:O4'	2.21	0.41
29:a:471:A:N3	29:a:473:G:H5"	2.35	0.41
29:a:614:C:H2'	29:a:615:C:C6	2.56	0.41
29:a:1144:C:H2'	29:a:1145:G:O4'	2.20	0.41
29:a:1266:C:H2'	29:a:1267:G:C8	2.55	0.41
29:a:2760:C:H2'	29:a:2761:C:C6	2.55	0.41
34:f:57:MET:HE3	34:f:65:PRO:HB3	2.02	0.41
50:v:75:PHE:HB2	50:v:77:ARG:HG3	2.02	0.41
52:x:14:LEU:HD23	52:x:14:LEU:HA	1.87	0.41
4:3:1:MET:HE2	4:3:1:MET:HB2	1.85	0.41
6:A:744:A:C4	6:A:745:U:C5	3.08	0.41
6:A:821:U:H2'	6:A:822:A:H8	1.85	0.41
6:A:1466:C:H2'	6:A:1467:G:O4'	2.21	0.41
6:A:1501:G:H4'	6:A:1502:G:C4	2.56	0.41
12:G:57:ASP:OD2	12:G:59:VAL:HG12	2.21	0.41
15:J:7:ARG:HD3	15:J:73:LEU:HD11	2.02	0.41
26:V:65:G:C4	26:V:66:C:C5	3.09	0.41
29:a:247:G:H4'	29:a:378:G:C5	2.55	0.41
29:a:567:U:H2'	29:a:568:G:C8	2.56	0.41
29:a:1303:C:H2'	29:a:1304:A:H8	1.86	0.41
29:a:1476:U:H2'	29:a:1477:U:C6	2.55	0.41
29:a:1984:U:H3'	29:a:1985:C:H2'	2.02	0.41
29:a:2059:A:H2'	29:a:2060:A:O4'	2.21	0.41
29:a:2365:A:H2'	29:a:2366:A:O4'	2.20	0.41
29:a:2501:C:H2'	29:a:2502:A:O4'	2.20	0.41
30:b:11:A:O2'	30:b:12:U:H3'	2.20	0.41
38:j:98:ILE:HD13	38:j:114:ILE:HG23	2.03	0.41
40:l:43:THR:HG22	40:l:94:VAL:HG12	2.01	0.41
47:s:81:LYS:HB3	47:s:81:LYS:HE2	1.78	0.41
48:t:25:LEU:HD21	48:t:35:GLU:HG3	2.03	0.41
6:A:211:C:H2'	6:A:212:U:O4'	2.20	0.41
6:A:476:U:H2'	6:A:477:G:C8	2.55	0.41
6:A:529:A:H5'	6:A:529:A:N3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:639:A:N7	13:H:108:SER:HA	2.35	0.41
6:A:684:A:C2	6:A:701:A:C5	3.08	0.41
6:A:1421:U:H2'	6:A:1422:U:H6	1.85	0.41
6:A:1425:A:H2'	6:A:1426:C:O4'	2.20	0.41
7:B:145:LYS:HE3	7:B:148:ARG:HH21	1.86	0.41
29:a:805:C:H2'	29:a:806:C:H6	1.85	0.41
29:a:2306:C:C4	29:a:2307:G:C5	3.09	0.41
29:a:2541:OMU:OP2	29:a:2541:OMU:H6	2.21	0.41
53:y:15:ARG:HG3	53:y:53:MET:SD	2.60	0.41
6:A:240:U:O4	6:A:903:A:H1'	2.20	0.41
6:A:1051:C:C2	28:X:47:ASN:HB3	2.56	0.41
7:B:21:GLN:HB2	7:B:24:PHE:CD2	2.56	0.41
9:D:32:THR:C	9:D:34:LYS:H	2.29	0.41
12:G:86:GLN:OE1	12:G:144:MET:HE1	2.20	0.41
16:K:58:THR:HG22	16:K:60:PHE:H	1.85	0.41
18:M:77:ILE:HG22	18:M:81:MET:SD	2.61	0.41
29:a:64:G:H2'	29:a:65:C:H6	1.86	0.41
29:a:747:A:H2'	29:a:748:G:O4'	2.20	0.41
29:a:1202:A:H61	29:a:1223:G:H1'	1.84	0.41
29:a:2297:G:N3	29:a:2297:G:H2'	2.36	0.41
30:b:49:G:H2'	30:b:50:A:C8	2.55	0.41
30:b:64:A:H61	30:b:104:U:H2'	1.84	0.41
35:g:3:ARG:HA	35:g:6:LYS:HE2	2.01	0.41
40:l:54:ILE:HG13	40:l:121:ALA:HB2	2.02	0.41
46:r:84:ARG:C	46:r:85:ILE:HD12	2.45	0.41
6:A:1379:C:H1'	12:G:79:ARG:HH22	1.86	0.41
7:B:52:LEU:HA	7:B:202:ILE:HD12	2.02	0.41
7:B:115:ARG:HD3	7:B:115:ARG:HA	1.87	0.41
8:C:22:TRP:HB3	8:C:59:ARG:HB2	2.03	0.41
10:E:73:VAL:HG11	10:E:143:LEU:HB3	2.02	0.41
17:L:42:PRO:HG3	17:L:50:ARG:HE	1.86	0.41
23:R:34:THR:HG22	23:R:38:LYS:N	2.36	0.41
28:X:16:ARG:HG3	28:X:17:LEU:N	2.35	0.41
29:a:805:C:H2'	29:a:806:C:C6	2.56	0.41
29:a:1261:C:H4'	29:a:1263:A:OP1	2.21	0.41
29:a:1336:C:C5	29:a:1337:C:C5	3.08	0.41
29:a:2801:A:H2'	29:a:2802:G:O4'	2.21	0.41
34:f:162:THR:HG22	34:f:163:ASP:N	2.36	0.41
6:A:1433:U:H2'	6:A:1434:A:C8	2.56	0.41
9:D:120:VAL:O	9:D:133:ASN:HA	2.21	0.41
9:D:200:SER:O	9:D:204:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:43:TRP:CZ3	16:K:45:THR:HG23	2.56	0.41
19:N:20:TYR:HE2	19:N:52:PRO:HG2	1.86	0.41
24:S:36:ARG:HB3	24:S:72:GLY:HA3	2.02	0.41
24:S:53:ASN:O	24:S:77:THR:HG22	2.21	0.41
29:a:661:A:OP1	39:k:44:LYS:HE3	2.21	0.41
29:a:868:U:H2'	29:a:869:A:C8	2.55	0.41
29:a:1498:A:H2'	29:a:1499:U:C6	2.56	0.41
31:c:37:LYS:HE3	31:c:37:LYS:HB3	1.73	0.41
32:d:128:TRP:CG	32:d:163:LYS:HB3	2.56	0.41
37:i:15:TRP:CE2	37:i:135:GLN:HG2	2.55	0.41
38:j:111:PHE:HB3	38:j:114:ILE:HD12	2.03	0.41
45:q:77:MET:HE3	45:q:77:MET:HB3	1.97	0.41
6:A:76:A:H62	6:A:92:G:H21	1.69	0.41
6:A:150:A:H2'	6:A:151:U:C6	2.55	0.41
6:A:156:A:H2'	6:A:157:A:O4'	2.20	0.41
6:A:299:A:H2'	6:A:300:U:O4'	2.21	0.41
6:A:498:C:H1'	6:A:546:C:H1'	2.03	0.41
6:A:880:C:O2'	6:A:881:U:H5'	2.21	0.41
6:A:920:A:H2'	6:A:921:C:C6	2.55	0.41
6:A:1011:A:H5"	24:S:14:HIS:CG	2.56	0.41
6:A:1034:U:H2'	6:A:1035:C:C6	2.55	0.41
6:A:1259:C:H2'	6:A:1260:A:C8	2.55	0.41
6:A:1516:MA6:OP2	6:A:1516:MA6:H8	2.21	0.41
8:C:92:THR:HG22	8:C:99:ALA:H	1.85	0.41
8:C:118:GLU:HG2	8:C:187:MET:HE2	2.03	0.41
12:G:7:VAL:HG13	12:G:8:ALA:H	1.86	0.41
26:V:20:G:N2	26:V:58:A:H1'	2.35	0.41
29:a:27:G:H22	29:a:504:G:C2'	2.34	0.41
29:a:87:C:H5"	29:a:88:G:H5'	2.03	0.41
29:a:233:A:H8	29:a:233:A:OP2	2.03	0.41
29:a:274:A:H2'	29:a:275:G:O4'	2.21	0.41
29:a:283:U:H2'	29:a:284:G:H5'	2.03	0.41
29:a:296:C:H1'	29:a:297:G:C8	2.56	0.41
29:a:1184:C:H2'	29:a:1185:G:C8	2.55	0.41
29:a:1396:U:H2'	29:a:1397:G:C8	2.56	0.41
29:a:1663:A:C2	29:a:2571:G:H5'	2.56	0.41
29:a:1863:C:H2'	29:a:1864:G:O4'	2.21	0.41
29:a:2104:G:H4'	29:a:2155:U:O2'	2.21	0.41
29:a:2109:G:H2'	29:a:2110:G:C8	2.47	0.41
29:a:2503:U:H2'	29:a:2504:C:H6	1.85	0.41
29:a:2666:G:H2'	29:a:2667:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2736:G:O6	29:a:2744:C:H5”	2.21	0.41
32:d:127:ARG:HG3	32:d:168:LEU:HD13	2.03	0.41
38:j:38:ILE:HD13	38:j:91:LYS:HD2	2.03	0.41
40:l:32:ILE:HG23	40:l:118:PHE:HE2	1.86	0.41
41:m:1:MET:HE3	41:m:1:MET:HB2	1.75	0.41
43:o:17:LYS:HD3	43:o:80:HIS:HA	2.02	0.41
45:q:50:GLY:HA3	45:q:53:VAL:C	2.45	0.41
46:r:18:ARG:HG3	46:r:76:VAL:HB	2.02	0.41
46:r:62:ASN:HB3	46:r:64:LEU:HD13	2.03	0.41
3:2:15:LYS:HZ2	3:2:15:LYS:HG2	1.76	0.41
6:A:127:U:H2’	6:A:128:C:C6	2.56	0.41
6:A:258:A:H2’	6:A:259:A:C8	2.55	0.41
6:A:316:G:H2’	6:A:317:A:O4’	2.21	0.41
6:A:1115:U:H1’	6:A:1176:A:C5	2.55	0.41
7:B:102:MET:HA	7:B:109:LEU:HG	2.03	0.41
9:D:3:ARG:HD2	9:D:117:ARG:HD3	2.02	0.41
9:D:198:ASN:ND2	9:D:201:LEU:HG	2.36	0.41
11:F:38:ARG:HB3	11:F:63:ASN:HB2	2.03	0.41
19:N:64:CYS:HB3	19:N:65:GLY:H	1.66	0.41
26:V:64:G:C4	26:V:65:G:C8	3.08	0.41
26:V:67:C:H2’	26:V:68:C:H6	1.86	0.41
29:a:681:U:H2’	29:a:682:C:O4’	2.21	0.41
29:a:852:A:H2’	29:a:853:G:O4’	2.21	0.41
29:a:970:A:N7	29:a:1126:G:H5”	2.35	0.41
29:a:1528:U:H2’	29:a:1529:A:O4’	2.20	0.41
29:a:1529:A:H2’	29:a:1530:C:C6	2.55	0.41
30:b:87:A:H2’	30:b:88:C:O4’	2.21	0.41
37:i:90:GLU:HG2	37:i:91:LYS:N	2.36	0.41
6:A:411:A:C4	6:A:412:G:C8	3.09	0.40
17:L:123:LYS:HA	17:L:123:LYS:HD2	1.86	0.40
19:N:31:ILE:O	19:N:41:ARG:HD2	2.21	0.40
26:V:33:OMC:HM22	26:V:34:U:H1’	2.02	0.40
28:X:59:MET:HE3	28:X:59:MET:HB3	1.86	0.40
29:a:573:A:H2’	29:a:574:G:C8	2.56	0.40
29:a:2003:A:H2’	29:a:2004:A:C8	2.56	0.40
29:a:2080:C:O3’	51:w:56:MET:HE1	2.21	0.40
29:a:2186:U:O3’	29:a:2187:A:H8	2.04	0.40
29:a:2557:A:H2’	29:a:2558:G:O4’	2.22	0.40
6:A:208:G:C4	6:A:209:A:C8	3.09	0.40
6:A:281:U:H2’	6:A:282:G:H8	1.86	0.40
6:A:451:U:H2’	6:A:452:A:C8	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:610:C:H2'	6:A:611:C:H6	1.84	0.40
6:A:1117:C:H2'	6:A:1118:U:C6	2.56	0.40
6:A:1396:C:H4'	6:A:1397:C:H3'	2.04	0.40
6:A:1536:C:H2'	6:A:1537:U:C6	2.57	0.40
7:B:76:ARG:HD3	7:B:76:ARG:H	1.86	0.40
22:Q:40:ARG:HB3	22:Q:40:ARG:HH11	1.85	0.40
29:a:128:C:H2'	29:a:129:C:C6	2.56	0.40
29:a:714:C:H2'	29:a:715:U:O4'	2.20	0.40
29:a:2566:A:H5"	29:a:2567:G:H5'	2.03	0.40
32:d:155:PRO:HG3	32:d:159:PHE:CZ	2.55	0.40
38:j:79:PHE:HE1	38:j:101:PRO:HG2	1.84	0.40
46:r:73:THR:HB	46:r:106:LYS:HB2	2.03	0.40
6:A:865:C:H2'	6:A:866:G:O4'	2.21	0.40
8:C:91:LEU:O	8:C:95:MET:HG3	2.21	0.40
8:C:134:MET:HE3	8:C:168:TYR:CD1	2.56	0.40
29:a:279:U:H2'	29:a:280:G:C8	2.56	0.40
29:a:348:C:O2'	29:a:349:A:H5'	2.21	0.40
29:a:1674:U:H2'	29:a:1675:A:C8	2.57	0.40
29:a:1938:G:H2'	29:a:1939:G:C8	2.56	0.40
29:a:2541:OMU:HM23	29:a:2543:U:C6	2.56	0.40
29:a:2814:U:H3'	29:a:2815:A:H8	1.85	0.40
35:g:26:VAL:HG12	35:g:79:VAL:HG11	2.03	0.40
35:g:99:LYS:NZ	35:g:99:LYS:HB2	2.36	0.40
35:g:135:SER:HB3	35:g:141:LEU:HB2	2.02	0.40
5:4:70:ARG:HD2	5:4:70:ARG:HA	1.55	0.40
6:A:491:G:H2'	6:A:492:A:H5"	2.03	0.40
6:A:510:C:H2'	6:A:511:U:C6	2.57	0.40
6:A:549:U:H2'	6:A:550:A:C8	2.56	0.40
6:A:1290:G:H2'	6:A:1291:A:C8	2.56	0.40
15:J:28:THR:O	15:J:32:THR:HG22	2.21	0.40
17:L:114:ARG:HG2	17:L:119:ALA:HB3	2.03	0.40
26:V:33:OMC:HM23	26:V:33:OMC:H1'	1.96	0.40
29:a:26:G:H2'	29:a:27:G:O4'	2.21	0.40
29:a:485:G:H2'	29:a:486:G:O4'	2.22	0.40
29:a:1004:A:H2'	29:a:1005:U:C6	2.55	0.40
29:a:1316:A:H2'	29:a:1318:C:C5	2.57	0.40
29:a:1373:A:H1'	29:a:1374:A:C8	2.57	0.40
29:a:1516:A:O2'	29:a:1517:A:H8	2.03	0.40
29:a:1582:C:H2'	29:a:1583:A:H8	1.83	0.40
33:e:167:ASP:HB2	33:e:182:PHE:CZ	2.57	0.40
34:f:33:LYS:HG2	34:f:157:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:10:LYS:HB3	36:h:10:LYS:HE2	1.76	0.40
41:m:55:ALA:HA	41:m:80:PHE:CE1	2.56	0.40
43:o:43:LEU:HD23	43:o:43:LEU:HA	1.93	0.40
2:1:3:ARG:HD3	2:1:3:ARG:HA	1.82	0.40
5:4:5:ILE:HD12	34:f:64:LYS:HD2	2.02	0.40
6:A:533:C:H2'	6:A:534:A:C8	2.57	0.40
6:A:975:A:C4	6:A:1316:A:C2	3.10	0.40
6:A:1235:A:C8	6:A:1300:C:H1'	2.57	0.40
7:B:175:ILE:HG22	7:B:197:ASN:HB2	2.04	0.40
9:D:74:PHE:CE1	9:D:96:LEU:HD11	2.56	0.40
17:L:86:ARG:H	17:L:86:ARG:HG3	1.75	0.40
18:M:11:ASP:HB3	18:M:46:ARG:HB3	2.02	0.40
29:a:437:C:H2'	29:a:438:G:O4'	2.21	0.40
29:a:638:G:H2'	29:a:639:G:O4'	2.22	0.40
29:a:1054:C:C4	29:a:1059:A:H5"	2.56	0.40
29:a:1285:C:OP1	29:a:2699:C:H4'	2.21	0.40
29:a:1342:A:C4'	31:c:38:LYS:HE3	2.50	0.40
29:a:1416:C:C5	29:a:1560:A:H5"	2.57	0.40
29:a:1507:U:H2'	29:a:1508:C:C6	2.57	0.40
29:a:2105:G:H3'	29:a:2106:A:H2'	2.04	0.40
29:a:2289:C:H2'	29:a:2290:G:H8	1.87	0.40
33:e:47:SER:O	33:e:51:VAL:HG23	2.21	0.40
35:g:88:GLN:HB3	35:g:163:ARG:HG2	2.03	0.40
47:s:47:GLU:HG2	47:s:52:VAL:O	2.21	0.40
50:v:46:HIS:NE2	50:v:77:ARG:HD2	2.36	0.40
52:x:37:LEU:HD23	52:x:40:SER:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
2	1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	2	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
5	4	69/74 (93%)	61 (88%)	8 (12%)	0	100	100
7	B	227/250 (91%)	212 (93%)	14 (6%)	1 (0%)	30	49
8	C	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
9	D	205/208 (99%)	198 (97%)	7 (3%)	0	100	100
10	E	153/165 (93%)	152 (99%)	1 (1%)	0	100	100
11	F	104/127 (82%)	102 (98%)	2 (2%)	0	100	100
12	G	151/156 (97%)	141 (93%)	10 (7%)	0	100	100
13	H	128/131 (98%)	123 (96%)	5 (4%)	0	100	100
14	I	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
15	J	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
16	K	113/128 (88%)	105 (93%)	8 (7%)	0	100	100
17	L	119/124 (96%)	114 (96%)	5 (4%)	0	100	100
18	M	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
19	N	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
20	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
21	P	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
22	Q	77/85 (91%)	76 (99%)	1 (1%)	0	100	100
23	R	64/75 (85%)	64 (100%)	0	0	100	100
24	S	82/91 (90%)	81 (99%)	1 (1%)	0	100	100
25	T	84/88 (96%)	84 (100%)	0	0	100	100
28	X	102/116 (88%)	100 (98%)	2 (2%)	0	100	100
31	c	270/274 (98%)	260 (96%)	10 (4%)	0	100	100
32	d	208/212 (98%)	202 (97%)	5 (2%)	1 (0%)	24	43
33	e	197/200 (98%)	196 (100%)	1 (0%)	0	100	100
34	f	175/178 (98%)	158 (90%)	17 (10%)	0	100	100
35	g	173/177 (98%)	167 (96%)	5 (3%)	1 (1%)	21	38
36	h	58/148 (39%)	53 (91%)	5 (9%)	0	100	100
37	i	140/142 (99%)	137 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	j	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
39	k	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
40	l	133/137 (97%)	131 (98%)	2 (2%)	0	100	100
41	m	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
42	n	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
43	o	115/122 (94%)	113 (98%)	2 (2%)	0	100	100
44	p	115/119 (97%)	115 (100%)	0	0	100	100
45	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
46	r	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
47	s	90/106 (85%)	89 (99%)	1 (1%)	0	100	100
48	t	101/105 (96%)	98 (97%)	3 (3%)	0	100	100
49	u	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
50	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
51	w	75/78 (96%)	75 (100%)	0	0	100	100
52	x	60/64 (94%)	59 (98%)	1 (2%)	0	100	100
53	y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
54	z	52/61 (85%)	50 (96%)	2 (4%)	0	100	100
All	All	5571/5937 (94%)	5384 (97%)	184 (3%)	3 (0%)	49	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	B	128	PHE
32	d	152	ASN
35	g	86	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	47 (100%)	0	100	100
2	1	36/36 (100%)	35 (97%)	1 (3%)	38	66
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	32 (97%)	1 (3%)	36	64
5	4	60/63 (95%)	60 (100%)	0	100	100
7	B	188/200 (94%)	177 (94%)	11 (6%)	18	37
8	C	175/175 (100%)	167 (95%)	8 (5%)	24	48
9	D	170/171 (99%)	167 (98%)	3 (2%)	51	77
10	E	113/120 (94%)	109 (96%)	4 (4%)	32	58
11	F	95/111 (86%)	93 (98%)	2 (2%)	47	74
12	G	125/128 (98%)	123 (98%)	2 (2%)	55	79
13	H	108/109 (99%)	104 (96%)	4 (4%)	30	57
14	I	99/100 (99%)	97 (98%)	2 (2%)	48	75
15	J	89/91 (98%)	85 (96%)	4 (4%)	24	49
16	K	87/97 (90%)	84 (97%)	3 (3%)	32	60
17	L	103/105 (98%)	101 (98%)	2 (2%)	50	76
18	M	96/98 (98%)	96 (100%)	0	100	100
19	N	81/82 (99%)	78 (96%)	3 (4%)	30	57
20	O	71/72 (99%)	68 (96%)	3 (4%)	26	52
21	P	63/63 (100%)	63 (100%)	0	100	100
22	Q	71/76 (93%)	67 (94%)	4 (6%)	19	39
23	R	58/66 (88%)	57 (98%)	1 (2%)	53	78
24	S	71/78 (91%)	68 (96%)	3 (4%)	26	52
25	T	65/67 (97%)	63 (97%)	2 (3%)	35	62
28	X	92/102 (90%)	90 (98%)	2 (2%)	45	73
31	c	218/220 (99%)	216 (99%)	2 (1%)	70	87
32	d	165/166 (99%)	159 (96%)	6 (4%)	31	58
33	e	155/155 (100%)	151 (97%)	4 (3%)	40	68
34	f	146/147 (99%)	141 (97%)	5 (3%)	32	60
35	g	140/142 (99%)	134 (96%)	6 (4%)	26	51
36	h	45/112 (40%)	41 (91%)	4 (9%)	9	20
37	i	118/118 (100%)	117 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	j	103/103 (100%)	103 (100%)	0	100	100
39	k	108/108 (100%)	106 (98%)	2 (2%)	50	76
40	l	111/111 (100%)	111 (100%)	0	100	100
41	m	96/101 (95%)	96 (100%)	0	100	100
42	n	84/85 (99%)	81 (96%)	3 (4%)	31	58
43	o	99/102 (97%)	97 (98%)	2 (2%)	48	75
44	p	85/86 (99%)	85 (100%)	0	100	100
45	q	84/84 (100%)	83 (99%)	1 (1%)	63	83
46	r	88/88 (100%)	88 (100%)	0	100	100
47	s	78/87 (90%)	78 (100%)	0	100	100
48	t	83/85 (98%)	80 (96%)	3 (4%)	31	58
49	u	79/80 (99%)	77 (98%)	2 (2%)	42	69
50	v	60/64 (94%)	56 (93%)	4 (7%)	15	31
51	w	69/70 (99%)	67 (97%)	2 (3%)	37	65
52	x	54/55 (98%)	52 (96%)	2 (4%)	30	57
53	y	54/54 (100%)	53 (98%)	1 (2%)	50	76
54	z	46/50 (92%)	44 (96%)	2 (4%)	26	51
All	All	4616/4816 (96%)	4499 (98%)	117 (2%)	42	69

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	43	THR
4	3	17	ILE
7	B	40	ILE
7	B	48	THR
7	B	76	ARG
7	B	85	GLN
7	B	134	ARG
7	B	140	THR
7	B	163	LEU
7	B	173	ILE
7	B	183	ILE
7	B	198	VAL
7	B	201	VAL
8	C	39	VAL

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Mol	Chain	Res	Type
8	C	80	LYS
8	C	86	LYS
8	C	97	VAL
8	C	165	THR
8	C	182	ILE
8	C	195	THR
8	C	212	LYS
9	D	5	ILE
9	D	174	GLU
9	D	199	GLU
10	E	33	THR
10	E	45	VAL
10	E	72	THR
10	E	155	LYS
11	F	39	LEU
11	F	70	THR
12	G	7	VAL
12	G	75	VAL
13	H	74	GLU
13	H	76	VAL
13	H	81	ARG
13	H	86	GLN
14	I	27	VAL
14	I	89	ASP
15	J	18	ILE
15	J	57	VAL
15	J	77	VAL
15	J	80	THR
16	K	32	THR
16	K	78	LEU
16	K	110	THR
17	L	34	CYS
17	L	98	VAL
19	N	39	GLU
19	N	45	MET
19	N	58	VAL
20	O	10	GLU
20	O	54	ARG
20	O	68	ASP
22	Q	5	THR
22	Q	30	VAL
22	Q	39	ILE

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Mol	Chain	Res	Type
22	Q	61	THR
23	R	25	ASP
24	S	5	LEU
24	S	60	VAL
24	S	61	ILE
25	T	3	ASN
25	T	30	THR
28	X	24	GLU
28	X	100	LYS
31	c	108	LYS
31	c	186	VAL
32	d	36	THR
32	d	79	LEU
32	d	81	LYS
32	d	101	VAL
32	d	140	SER
32	d	207	ARG
33	e	13	LEU
33	e	15	GLU
33	e	32	THR
33	e	172	THR
34	f	24	ASN
34	f	101	ASP
34	f	104	ILE
34	f	137	VAL
34	f	149	ILE
35	g	9	VAL
35	g	10	THR
35	g	15	VAL
35	g	24	VAL
35	g	79	VAL
35	g	149	ARG
36	h	15	LEU
36	h	37	VAL
36	h	50	ARG
36	h	57	GLN
37	i	93	VAL
39	k	2	THR
39	k	19	ARG
42	n	68	GLU
42	n	87	THR
42	n	89	VAL

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Mol	Chain	Res	Type
43	o	18	THR
43	o	36	LYS
45	q	19	THR
48	t	5	LYS
48	t	23	THR
48	t	50	THR
49	u	69	VAL
49	u	76	VAL
50	v	10	THR
50	v	31	VAL
50	v	64	ASP
50	v	70	GLU
51	w	2	SER
51	w	22	ASN
52	x	5	ASP
52	x	20	GLU
53	y	49	LYS
54	z	35	GLU
54	z	54	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
7	B	38	ASN
7	B	61	GLN
7	B	80	ASN
7	B	197	ASN
8	C	21	ASN
8	C	216	ASN
9	D	50	GLN
9	D	154	GLN
9	D	166	GLN
13	H	4	GLN
14	I	48	GLN
15	J	15	HIS
15	J	58	ASN
17	L	112	GLN
20	O	48	HIS
20	O	50	HIS
20	O	62	GLN
21	P	62	GLN
28	X	30	GLN

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Mol	Chain	Res	Type
31	c	128	ASN
32	d	129	ASN
33	e	89	GLN
33	e	93	GLN
33	e	138	ASN
35	g	23	GLN
35	g	36	ASN
35	g	38	HIS
35	g	137	ASN
36	h	11	ASN
36	h	57	GLN
37	i	12	GLN
37	i	47	HIS
37	i	67	ASN
37	i	138	GLN
38	j	89	ASN
39	k	71	GLN
40	l	85	ASN
41	m	5	ASN
44	p	52	GLN
44	p	87	GLN
45	q	87	GLN
46	r	62	ASN
47	s	29	GLN
47	s	90	GLN
48	t	21	GLN
48	t	47	ASN
49	u	58	ASN
50	v	12	ASN
50	v	57	HIS
54	z	4	GLN
54	z	19	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	V	76/77 (98%)	35 (46%)	1 (1%)
27	W	9/15 (60%)	1 (11%)	0
29	a	2889/2893 (99%)	540 (18%)	0
30	b	114/115 (99%)	15 (13%)	0
6	A	1534/1537 (99%)	275 (17%)	13 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4622/4637 (99%)	866 (18%)	14 (0%)

All (866) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	6	C
6	A	9	A
6	A	10	A
6	A	11	G
6	A	24	G
6	A	34	A
6	A	41	G
6	A	49	C
6	A	50	U
6	A	52	A
6	A	53	A
6	A	64	U
6	A	74	G
6	A	75	A
6	A	76	A
6	A	77	G
6	A	82	C
6	A	83	U
6	A	86	C
6	A	88	A
6	A	90	C
6	A	91	G
6	A	92	G
6	A	105	A
6	A	106	C
6	A	107	G
6	A	112	A
6	A	126	A
6	A	127	U
6	A	140	G
6	A	160	G
6	A	167	A
6	A	169	U
6	A	170	A
6	A	177	A
6	A	184	A
6	A	186	G

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Mol	Chain	Res	Type
6	A	187	G
6	A	193	A
6	A	205	U
6	A	206	C
6	A	207	G
6	A	208	G
6	A	214	G
6	A	216	G
6	A	237	G
6	A	241	U
6	A	243	G
6	A	247	G
6	A	262	G
6	A	263	C
6	A	272	G
6	A	276	C
6	A	277	G
6	A	285	G
6	A	317	A
6	A	324	C
6	A	325	A
6	A	326	C
6	A	336	U
6	A	340	A
6	A	347	G
6	A	348	C
6	A	350	G
6	A	351	C
6	A	359	A
6	A	363	U
6	A	368	C
6	A	373	G
6	A	394	U
6	A	402	G
6	A	408	A
6	A	409	G
6	A	410	A
6	A	414	C
6	A	418	A
6	A	419	U
6	A	425	U
6	A	435	U

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Mol	Chain	Res	Type
6	A	442	G
6	A	448	G
6	A	459	U
6	A	461	A
6	A	463	U
6	A	465	C
6	A	469	G
6	A	470	A
6	A	474	A
6	A	479	A
6	A	481	G
6	A	482	U
6	A	483	U
6	A	493	A
6	A	494	U
6	A	497	G
6	A	506	A
6	A	508	C
6	A	511	U
6	A	515	C
6	A	518	G
6	A	521	G
6	A	524	G7M
6	A	529	A
6	A	532	A
6	A	544	A
6	A	556	A
6	A	559	U
6	A	561	C
6	A	567	G
6	A	569	A
6	A	570	A
6	A	571	A
6	A	572	G
6	A	573	C
6	A	574	G
6	A	585	G
6	A	598	G
6	A	630	G
6	A	639	A
6	A	648	C
6	A	649	U

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Mol	Chain	Res	Type
6	A	650	A
6	A	654	U
6	A	662	A
6	A	684	A
6	A	700	G
6	A	720	U
6	A	721	G
6	A	728	G
6	A	731	G
6	A	744	A
6	A	745	U
6	A	752	G
6	A	756	A
6	A	774	A
6	A	778	A
6	A	790	U
6	A	791	A
6	A	809	G
6	A	812	A
6	A	814	C
6	A	816	A
6	A	818	G
6	A	829	G
6	A	839	U
6	A	840	U
6	A	841	G
6	A	842	A
6	A	843	G
6	A	852	G
6	A	867	A
6	A	873	A
6	A	884	G
6	A	899	G
6	A	907	C
6	A	911	A
6	A	931	C
6	A	932	A
6	A	957	U
6	A	958	U
6	A	963	2MG
6	A	965	A
6	A	966	A

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Mol	Chain	Res	Type
6	A	968	G
6	A	972	A
6	A	973	G
6	A	974	A
6	A	990	G
6	A	991	A
6	A	992	C
6	A	996	C
6	A	1000	A
6	A	1001	A
6	A	1002	A
6	A	1003	C
6	A	1004	U
6	A	1007	C
6	A	1008	C
6	A	1010	G
6	A	1013	A
6	A	1015	G
6	A	1016	G
6	A	1023	G
6	A	1025	C
6	A	1027	U
6	A	1028	C
6	A	1029	G
6	A	1030	G
6	A	1031	G
6	A	1033	A
6	A	1034	U
6	A	1039	A
6	A	1042	C
6	A	1043	A
6	A	1062	U
6	A	1091	G
6	A	1092	U
6	A	1096	G
6	A	1098	A
6	A	1101	G
6	A	1115	U
6	A	1121	C
6	A	1123	U
6	A	1124	G
6	A	1130	A

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Mol	Chain	Res	Type
6	A	1134	C
6	A	1136	G
6	A	1137	A
6	A	1142	A
6	A	1156	U
6	A	1157	G
6	A	1161	G
6	A	1162	U
6	A	1165	C
6	A	1166	A
6	A	1167	A
6	A	1168	A
6	A	1180	C
6	A	1185	A
6	A	1188	A
6	A	1193	A
6	A	1194	A
6	A	1209	U
6	A	1210	A
6	A	1211	C
6	A	1217	G
6	A	1223	C
6	A	1224	A
6	A	1226	A
6	A	1235	A
6	A	1238	G
6	A	1247	A
6	A	1249	A
6	A	1255	G
6	A	1257	U
6	A	1259	C
6	A	1277	A
6	A	1282	A
6	A	1284	A
6	A	1285	A
6	A	1294	G
6	A	1295	U
6	A	1296	A
6	A	1297	G
6	A	1299	C
6	A	1302	G
6	A	1317	C

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Mol	Chain	Res	Type
6	A	1328	G
6	A	1332	U
6	A	1335	G
6	A	1343	A
6	A	1350	G
6	A	1360	A
6	A	1361	U
6	A	1367	G
6	A	1376	G
6	A	1384	G
6	A	1394	C
6	A	1395	A
6	A	1416	G
6	A	1429	G
6	A	1438	A
6	A	1444	A
6	A	1450	A
6	A	1488	G
6	A	1490	A
6	A	1494	G
6	A	1499	A
6	A	1500	A
6	A	1503	U
6	A	1514	G
6	A	1516	MA6
6	A	1517	C
6	A	1526	G
6	A	1527	G
26	V	2	G
26	V	3	C
26	V	4	G
26	V	7	G
26	V	9	G
26	V	10	G
26	V	12	G
26	V	16	C
26	V	17	C
26	V	18	U
26	V	19	G
26	V	20	G
26	V	21	H2U
26	V	22	A

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Mol	Chain	Res	Type
26	V	23	G
26	V	24	C
26	V	27	G
26	V	29	C
26	V	30	G
26	V	32	G
26	V	33	OMC
26	V	34	U
26	V	43	G
26	V	46	G
26	V	47	A
26	V	52	C
26	V	53	G
26	V	54	G
26	V	59	A
26	V	64	G
26	V	65	G
26	V	72	C
26	V	75	C
26	V	76	C
26	V	77	A
27	W	7	U
29	a	3	U
29	a	15	G
29	a	27	G
29	a	34	U
29	a	46	G
29	a	51	G
29	a	71	A
29	a	74	A
29	a	75	G
29	a	79	C
29	a	85	G
29	a	86	G
29	a	91	A
29	a	94	U
29	a	95	A
29	a	96	U
29	a	97	C
29	a	99	U
29	a	102	G
29	a	118	A

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Mol	Chain	Res	Type
29	a	119	A
29	a	120	U
29	a	125	G
29	a	140	A
29	a	141	A
29	a	142	G
29	a	143	G
29	a	162	U
29	a	163	A
29	a	165	A
29	a	178	G
29	a	181	A
29	a	196	A
29	a	199	A
29	a	215	G
29	a	216	A
29	a	222	A
29	a	225	C
29	a	228	U
29	a	229	U
29	a	233	A
29	a	248	G
29	a	255	A
29	a	265	A
29	a	266	G
29	a	268	C
29	a	271	U
29	a	272	U
29	a	276	U
29	a	277	U
29	a	278	A
29	a	282	G
29	a	283	U
29	a	284	G
29	a	286	U
29	a	290	G
29	a	296	C
29	a	306	A
29	a	311	G
29	a	324	G
29	a	325	A
29	a	344	G

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Mol	Chain	Res	Type
29	a	350	C
29	a	352	U
29	a	359	G
29	a	362	G
29	a	364	G
29	a	378	G
29	a	379	U
29	a	380	G
29	a	388	G
29	a	396	A
29	a	397	U
29	a	403	G
29	a	416	G
29	a	443	U
29	a	447	C
29	a	472	A
29	a	473	G
29	a	486	G
29	a	496	U
29	a	497	A
29	a	500	U
29	a	505	A
29	a	519	C
29	a	522	G
29	a	524	A
29	a	535	C
29	a	537	U
29	a	538	C
29	a	541	G
29	a	546	G
29	a	547	A
29	a	554	A
29	a	564	U
29	a	566	A
29	a	594	A
29	a	605	A
29	a	606	U
29	a	618	A
29	a	619	G
29	a	626	C
29	a	628	A
29	a	630	U

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Mol	Chain	Res	Type
29	a	636	U
29	a	642	G
29	a	644	U
29	a	645	U
29	a	646	A
29	a	647	G
29	a	654	G
29	a	668	A
29	a	677	U
29	a	685	U
29	a	686	G
29	a	717	G
29	a	721	A
29	a	738	U
29	a	755	A
29	a	756	C
29	a	766	G
29	a	767	G
29	a	773	A
29	a	774	A
29	a	775	G
29	a	776	G
29	a	780	A
29	a	783	A
29	a	785	G
29	a	796	G
29	a	803	C
29	a	810	A
29	a	818	U
29	a	819	U
29	a	821	G
29	a	836	G
29	a	838	A
29	a	848	G
29	a	850	G
29	a	857	A
29	a	868	U
29	a	869	A
29	a	873	G
29	a	875	U
29	a	876	C
29	a	877	A

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Mol	Chain	Res	Type
29	a	882	G
29	a	884	C
29	a	886	U
29	a	887	A
29	a	888	C
29	a	891	A
29	a	894	C
29	a	898	G
29	a	901	A
29	a	905	C
29	a	916	U
29	a	919	G
29	a	922	C
29	a	931	A
29	a	935	A
29	a	936	G
29	a	948	U
29	a	951	C
29	a	964	G
29	a	973	A
29	a	979	G
29	a	986	A
29	a	999	A
29	a	1002	U
29	a	1003	C
29	a	1007	G
29	a	1016	G
29	a	1023	U
29	a	1029	A
29	a	1030	A
29	a	1036	A
29	a	1037	G
29	a	1050	U
29	a	1052	G
29	a	1053	G
29	a	1054	C
29	a	1055	U
29	a	1056	U
29	a	1057	A
29	a	1060	A
29	a	1061	G
29	a	1062	C

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Mol	Chain	Res	Type
29	a	1063	A
29	a	1065	C
29	a	1066	C
29	a	1068	C
29	a	1069	C
29	a	1070	C
29	a	1073	U
29	a	1075	A
29	a	1076	A
29	a	1077	G
29	a	1078	A
29	a	1079	A
29	a	1080	A
29	a	1084	U
29	a	1085	A
29	a	1087	U
29	a	1091	U
29	a	1094	C
29	a	1095	U
29	a	1096	A
29	a	1100	G
29	a	1101	A
29	a	1102	G
29	a	1106	G
29	a	1112	G
29	a	1122	U
29	a	1123	A
29	a	1124	A
29	a	1125	C
29	a	1126	G
29	a	1133	A
29	a	1142	G
29	a	1163	U
29	a	1164	U
29	a	1165	U
29	a	1166	G
29	a	1193	A
29	a	1194	G
29	a	1235	A
29	a	1238	G
29	a	1241	A
29	a	1244	G

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Mol	Chain	Res	Type
29	a	1259	G
29	a	1260	A
29	a	1262	A
29	a	1263	A
29	a	1275	A
29	a	1289	A
29	a	1290	A
29	a	1294	C
29	a	1300	U
29	a	1302	C
29	a	1309	A
29	a	1317	U
29	a	1329	G
29	a	1332	U
29	a	1333	C
29	a	1340	U
29	a	1347	A
29	a	1353	A
29	a	1356	G
29	a	1366	A
29	a	1367	U
29	a	1371	A
29	a	1383	A
29	a	1404	G
29	a	1408	U
29	a	1413	G
29	a	1416	C
29	a	1420	G
29	a	1422	A
29	a	1423	G
29	a	1425	C
29	a	1426	U
29	a	1428	A
29	a	1440	G
29	a	1441	U
29	a	1448	U
29	a	1454	U
29	a	1455	G
29	a	1463	G
29	a	1467	G
29	a	1470	U
29	a	1478	A

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Mol	Chain	Res	Type
29	a	1479	G
29	a	1481	C
29	a	1485	U
29	a	1489	G
29	a	1497	U
29	a	1498	A
29	a	1513	A
29	a	1516	A
29	a	1519	C
29	a	1521	G
29	a	1522	U
29	a	1523	A
29	a	1524	C
29	a	1525	U
29	a	1526	U
29	a	1527	G
29	a	1530	C
29	a	1533	C
29	a	1536	A
29	a	1538	U
29	a	1539	G
29	a	1540	G
29	a	1551	G
29	a	1557	A
29	a	1560	A
29	a	1569	U
29	a	1574	U
29	a	1575	U
29	a	1576	C
29	a	1598	G
29	a	1599	A
29	a	1604	G
29	a	1609	A
29	a	1637	C
29	a	1638	U
29	a	1639	U
29	a	1658	G
29	a	1665	G
29	a	1666	C
29	a	1683	U
29	a	1684	U
29	a	1686	G

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Mol	Chain	Res	Type
29	a	1706	U
29	a	1707	G
29	a	1710	G
29	a	1718	U
29	a	1719	C
29	a	1721	C
29	a	1725	C
29	a	1726	U
29	a	1727	G
29	a	1739	G
29	a	1745	G
29	a	1753	G
29	a	1762	A
29	a	1768	U
29	a	1769	A
29	a	1771	U
29	a	1773	A
29	a	1777	C
29	a	1789	C
29	a	1790	A
29	a	1791	A
29	a	1798	A
29	a	1805	C
29	a	1818	A
29	a	1836	A
29	a	1837	A
29	a	1838	G
29	a	1846	G
29	a	1855	A
29	a	1858	G
29	a	1862	G
29	a	1863	C
29	a	1878	A
29	a	1888	A
29	a	1890	A
29	a	1892	G
29	a	1896	G
29	a	1902	A
29	a	1903	C
29	a	1908	A
29	a	1918	G
29	a	1919	G

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Mol	Chain	Res	Type
29	a	1926	A
29	a	1927	A
29	a	1929	U
29	a	1943	G
29	a	1944	U
29	a	1953	G
29	a	1956	C
29	a	1959	A
29	a	1960	U
29	a	1961	G
29	a	1971	U
29	a	1980	U
29	a	1982	U
29	a	1986	C
29	a	2011	U
29	a	2012	C
29	a	2019	6MZ
29	a	2020	A
29	a	2021	G
29	a	2022	A
29	a	2024	G
29	a	2025	C
29	a	2032	C
29	a	2044	C
29	a	2045	G
29	a	2049	A
29	a	2050	G
29	a	2051	A
29	a	2058	G7M
29	a	2082	G
29	a	2089	G
29	a	2093	U
29	a	2098	U
29	a	2100	U
29	a	2105	G
29	a	2106	A
29	a	2107	U
29	a	2108	A
29	a	2111	U
29	a	2113	G
29	a	2121	U
29	a	2122	G

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Mol	Chain	Res	Type
29	a	2123	A
29	a	2126	C
29	a	2128	G
29	a	2131	A
29	a	2134	C
29	a	2137	G
29	a	2146	G
29	a	2147	A
29	a	2151	G
29	a	2155	U
29	a	2165	A
29	a	2167	C
29	a	2171	G
29	a	2173	A
29	a	2174	A
29	a	2178	U
29	a	2179	G
29	a	2182	G
29	a	2187	A
29	a	2193	G
29	a	2201	A
29	a	2214	A
29	a	2227	G
29	a	2229	U
29	a	2257	A
29	a	2262	A
29	a	2267	A
29	a	2272	U
29	a	2276	A
29	a	2277	A
29	a	2293	G
29	a	2294	U
29	a	2297	G
29	a	2300	A
29	a	2301	U
29	a	2307	G
29	a	2308	U
29	a	2314	A
29	a	2316	A
29	a	2325	A
29	a	2333	U
29	a	2334	A

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Mol	Chain	Res	Type
29	a	2339	C
29	a	2343	A
29	a	2348	C
29	a	2350	A
29	a	2361	U
29	a	2371	G
29	a	2372	G
29	a	2373	U
29	a	2374	C
29	a	2385	G
29	a	2391	U
29	a	2392	C
29	a	2394	G
29	a	2395	U
29	a	2396	A
29	a	2409	C
29	a	2411	C
29	a	2412	U
29	a	2414	A
29	a	2418	G
29	a	2419	A
29	a	2429	C
29	a	2430	U
29	a	2436	G
29	a	2437	A
29	a	2438	H2U
29	a	2439	A
29	a	2448	A
29	a	2463	U
29	a	2465	A
29	a	2476	G
29	a	2483	G
29	a	2487	OMC
29	a	2491	G
29	a	2492	2MA
29	a	2494	G
29	a	2495	U
29	a	2506	C
29	a	2507	A
29	a	2509	C
29	a	2518	G
29	a	2523	A

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Mol	Chain	Res	Type
29	a	2536	A
29	a	2541	OMU
29	a	2543	U
29	a	2555	A
29	a	2556	G
29	a	2562	C
29	a	2575	U
29	a	2591	A
29	a	2592	G
29	a	2598	U
29	a	2599	C
29	a	2602	U
29	a	2618	U
29	a	2627	G
29	a	2635	C
29	a	2654	A
29	a	2678	U
29	a	2679	A
29	a	2703	G
29	a	2715	U
29	a	2722	A
29	a	2724	G
29	a	2728	U
29	a	2737	A
29	a	2746	A
29	a	2750	G
29	a	2754	A
29	a	2755	G
29	a	2767	A
29	a	2769	A
29	a	2770	A
29	a	2780	A
29	a	2785	U
29	a	2786	U
29	a	2787	U
29	a	2789	U
29	a	2790	G
29	a	2793	C
29	a	2797	A
29	a	2807	U
29	a	2809	G
29	a	2810	A

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Mol	Chain	Res	Type
29	a	2812	A
29	a	2822	U
29	a	2824	A
29	a	2825	U
29	a	2838	G
29	a	2844	U
29	a	2845	A
29	a	2850	U
29	a	2856	A
29	a	2861	G
29	a	2862	A
29	a	2868	A
29	a	2872	A
29	a	2873	U
29	a	2874	U
29	a	2882	A
30	b	2	C
30	b	7	G
30	b	11	A
30	b	14	G
30	b	16	A
30	b	18	G
30	b	22	G
30	b	38	U
30	b	39	C
30	b	42	G
30	b	54	G
30	b	86	U
30	b	87	A
30	b	106	A
30	b	109	G

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	139	U
6	A	185	C
6	A	481	G
6	A	492	A
6	A	618	A
6	A	683	U
6	A	775	G

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Mol	Chain	Res	Type
6	A	876	C
6	A	989	U
6	A	1123	U
6	A	1179	G
6	A	1187	G
6	A	1449	A
26	V	20	G

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

39 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	$\#\|Z\| > 2$
29	PSU	a	2569	29	18,21,22	2.14	8 (44%)	22,30,33	1.98	5 (22%)
26	PSU	V	56	26	18,21,22	1.91	7 (38%)	22,30,33	1.80	3 (13%)
32	MEQ	d	153	32	8,9,10	0.85	0	5,10,12	0.76	0
29	G7M	a	2058	29	23,26,27	2.17	5 (21%)	35,39,42	1.88	7 (20%)
40	4D4	l	82	40	9,11,12	0.79	0	8,13,15	1.66	2 (25%)
29	OMG	a	2240	29,55	23,26,27	2.34	6 (26%)	33,38,41	1.88	10 (30%)
29	PSU	a	945	29	18,21,22	2.08	7 (38%)	22,30,33	1.84	3 (13%)
26	OMC	V	33	26	19,22,23	1.76	3 (15%)	26,31,34	0.96	2 (7%)
6	5MC	A	964	6	18,22,23	1.90	6 (33%)	26,32,35	1.35	2 (7%)
29	3TD	a	1904	29	18,22,23	2.72	7 (38%)	22,32,35	1.74	2 (9%)
29	H2U	a	2438	29	18,21,22	4.09	5 (27%)	21,30,33	5.05	7 (33%)
29	1MG	a	736	29	22,26,27	2.47	6 (27%)	33,39,42	2.00	7 (21%)
40	MS6	l	83	40	5,7,8	0.60	0	2,7,9	1.73	1 (50%)
26	4SU	V	8	26	18,21,22	3.75	8 (44%)	26,30,33	2.17	4 (15%)
6	MA6	A	1516	6	23,26,27	1.23	3 (13%)	34,38,41	2.24	9 (26%)
29	PSU	a	1900	29	18,21,22	2.01	7 (38%)	22,30,33	1.82	3 (13%)
17	D2T	L	89	17	7,9,10	1.31	1 (14%)	6,11,13	1.46	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	6MZ	a	2019	29	22,25,26	2.34	3 (13%)	30,36,39	2.41	9 (30%)
29	OMC	a	2487	29,57	19,22,23	1.75	3 (15%)	26,31,34	1.05	2 (7%)
29	PSU	a	2594	29	18,21,22	2.11	7 (38%)	22,30,33	1.84	3 (13%)
6	PSU	A	513	57,6	18,21,22	2.01	7 (38%)	22,30,33	1.86	4 (18%)
29	PSU	a	737	29,57	18,21,22	2.10	8 (44%)	22,30,33	1.84	3 (13%)
29	PSU	a	2493	29,55	18,21,22	2.08	7 (38%)	22,30,33	1.77	5 (22%)
6	UR3	A	1495	6	19,22,23	2.54	6 (31%)	26,32,35	1.32	2 (7%)
26	H2U	V	21	26	18,21,22	4.33	5 (27%)	21,30,33	4.86	7 (33%)
29	PSU	a	2446	29	18,21,22	2.16	7 (38%)	22,30,33	1.90	5 (22%)
6	2MG	A	963	6	23,26,27	2.56	4 (17%)	32,38,41	2.10	10 (31%)
16	IAS	K	118	16	5,6,8	1.89	1 (20%)	3,6,10	3.31	1 (33%)
29	OMU	a	2541	29	19,22,23	2.61	7 (36%)	26,31,34	1.76	5 (19%)
6	MA6	A	1515	6	23,26,27	1.21	3 (13%)	34,38,41	2.24	9 (26%)
29	2MA	a	2492	29,55	22,25,26	1.34	3 (13%)	33,37,40	2.04	7 (21%)
6	2MG	A	1513	6	23,26,27	2.57	6 (26%)	32,38,41	2.15	11 (34%)
29	2MG	a	2434	29	23,26,27	2.58	7 (30%)	32,38,41	2.04	10 (31%)
6	2MG	A	1204	55,6	23,26,27	2.57	5 (21%)	32,38,41	2.13	11 (34%)
6	G7M	A	524	55,6	23,26,27	2.15	5 (21%)	35,39,42	1.83	7 (20%)
26	5MU	V	55	26	19,22,23	2.35	7 (36%)	28,32,35	3.74	10 (35%)
6	4OC	A	1399	6	20,23,24	2.20	4 (20%)	26,32,35	1.07	2 (7%)
29	PSU	a	1906	29	18,21,22	2.04	7 (38%)	22,30,33	1.83	3 (13%)
29	5MU	a	1928	29,55	19,22,23	2.54	7 (36%)	28,32,35	3.75	10 (35%)

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
29	PSU	a	2569	29	-	0/7/25/26	0/2/2/2
26	PSU	V	56	26	-	0/7/25/26	0/2/2/2
32	MEQ	d	153	32	-	4/8/9/11	-
29	G7M	a	2058	29	-	2/7/25/26	0/3/3/3
40	4D4	l	82	40	-	3/11/12/14	-
29	OMG	a	2240	29,55	-	1/9/27/28	0/3/3/3
29	PSU	a	945	29	-	0/7/25/26	0/2/2/2
26	OMC	V	33	26	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5MC	A	964	6	-	0/7/25/26	0/2/2/2
29	3TD	a	1904	29	-	0/7/25/26	0/2/2/2
29	H2U	a	2438	29	-	1/7/38/39	0/2/2/2
29	1MG	a	736	29	-	0/7/25/26	0/3/3/3
40	MS6	l	83	40	-	2/4/6/8	-
26	4SU	V	8	26	-	0/7/25/26	0/2/2/2
6	MA6	A	1516	6	-	1/11/29/30	0/3/3/3
29	PSU	a	1900	29	-	0/7/25/26	0/2/2/2
17	D2T	L	89	17	-	4/7/12/14	-
29	6MZ	a	2019	29	-	2/9/27/28	0/3/3/3
29	OMC	a	2487	29,57	-	0/9/27/28	0/2/2/2
29	PSU	a	2594	29	-	0/7/25/26	0/2/2/2
6	PSU	A	513	57,6	-	0/7/25/26	0/2/2/2
29	PSU	a	737	29,57	-	1/7/25/26	0/2/2/2
29	PSU	a	2493	29,55	-	2/7/25/26	0/2/2/2
6	UR3	A	1495	6	-	0/7/25/26	0/2/2/2
26	H2U	V	21	26	-	4/7/38/39	0/2/2/2
29	PSU	a	2446	29	-	0/7/25/26	0/2/2/2
6	2MG	A	963	6	-	0/9/27/28	0/3/3/3
16	IAS	K	118	16	-	2/3/5/8	-
29	OMU	a	2541	29	-	2/9/27/28	0/2/2/2
6	MA6	A	1515	6	-	0/11/29/30	0/3/3/3
29	2MA	a	2492	29,55	-	3/7/25/26	0/3/3/3
6	2MG	A	1513	6	-	0/9/27/28	0/3/3/3
29	2MG	a	2434	29	-	1/9/27/28	0/3/3/3
6	2MG	A	1204	55,6	-	2/9/27/28	0/3/3/3
6	G7M	A	524	55,6	-	3/7/25/26	0/3/3/3
26	5MU	V	55	26	-	0/7/25/26	0/2/2/2
6	4OC	A	1399	6	-	0/9/29/30	0/2/2/2
29	PSU	a	1906	29	-	0/7/25/26	0/2/2/2
29	5MU	a	1928	29,55	-	0/7/25/26	0/2/2/2

All (198) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	21	H2U	O4-C4	10.17	1.43	1.23
29	a	2438	H2U	O4-C4	9.84	1.43	1.23
29	a	2019	6MZ	C6-N6	9.55	1.44	1.34
6	A	1204	2MG	O6-C6	9.09	1.40	1.23
6	A	1513	2MG	O6-C6	8.99	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	963	2MG	O6-C6	8.92	1.40	1.23
29	a	2434	2MG	O6-C6	8.81	1.40	1.23
26	V	21	H2U	C2-N1	8.66	1.48	1.35
26	V	21	H2U	O2-C2	8.61	1.38	1.23
6	A	1495	UR3	O4-C4	8.60	1.42	1.23
29	a	2240	OMG	O6-C6	8.36	1.39	1.23
29	a	1904	3TD	O4-C4	8.24	1.40	1.23
29	a	2438	H2U	C2-N1	8.22	1.47	1.35
29	a	2438	H2U	O2-C2	7.97	1.37	1.23
6	A	524	G7M	O6-C6	7.89	1.38	1.23
29	a	736	1MG	O6-C6	7.87	1.39	1.23
29	a	2058	G7M	O6-C6	7.86	1.38	1.23
29	a	2541	OMU	O4-C4	7.80	1.39	1.24
26	V	8	4SU	C4-N3	7.72	1.45	1.37
26	V	21	H2U	C2-N3	7.29	1.51	1.38
26	V	8	4SU	C2-N3	7.13	1.50	1.38
26	V	8	4SU	C4-S4	-6.75	1.55	1.68
29	a	2438	H2U	C2-N3	6.74	1.50	1.38
6	A	1399	4OC	O2-C2	6.44	1.35	1.23
29	a	1928	5MU	C2-N1	-6.04	1.28	1.38
6	A	963	2MG	C2-N2	5.99	1.46	1.33
6	A	1204	2MG	C2-N2	5.96	1.46	1.33
29	a	736	1MG	C2-N2	5.95	1.45	1.34
6	A	1513	2MG	C2-N2	5.92	1.46	1.33
29	a	2434	2MG	C2-N2	5.79	1.46	1.33
26	V	55	5MU	C2-N1	-5.49	1.29	1.38
6	A	1399	4OC	C4-N4	5.44	1.47	1.35
26	V	21	H2U	C4-N3	5.37	1.46	1.37
26	V	8	4SU	C6-C5	5.10	1.46	1.35
26	V	33	OMC	C4-N4	5.04	1.45	1.33
29	a	2438	H2U	C4-N3	4.97	1.46	1.37
29	a	1928	5MU	C2-N3	-4.95	1.29	1.38
26	V	8	4SU	C2-N1	4.94	1.46	1.38
29	a	2487	OMC	C4-N4	4.67	1.44	1.33
26	V	55	5MU	C2-N3	-4.49	1.30	1.38
29	a	2492	2MA	C6-N6	4.37	1.45	1.34
29	a	1928	5MU	C6-N1	-4.25	1.30	1.38
26	V	55	5MU	C6-N1	-4.16	1.31	1.38
6	A	964	5MC	C4-N4	4.13	1.44	1.34
26	V	8	4SU	C5-C4	4.11	1.47	1.42
29	a	2240	OMG	C2-N2	4.08	1.43	1.34
26	V	8	4SU	C6-N1	4.03	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	2446	PSU	C4-N3	-4.01	1.31	1.38
29	a	2487	OMC	C2-N1	-3.97	1.31	1.40
29	a	2541	OMU	C2-N1	-3.97	1.32	1.38
29	a	2569	PSU	C2-N1	-3.96	1.31	1.36
29	a	1904	3TD	C2-N1	-3.95	1.32	1.37
26	V	33	OMC	C2-N1	-3.91	1.31	1.40
29	a	2240	OMG	C6-N1	-3.89	1.31	1.38
29	a	2594	PSU	C4-N3	-3.86	1.31	1.38
29	a	737	PSU	C4-N3	-3.85	1.31	1.38
29	a	945	PSU	C4-N3	-3.84	1.31	1.38
29	a	2446	PSU	C2-N1	-3.83	1.31	1.36
29	a	2541	OMU	C4-N3	-3.79	1.31	1.38
6	A	964	5MC	C2-N1	-3.77	1.31	1.40
29	a	1904	3TD	C4-N3	-3.77	1.32	1.40
6	A	513	PSU	C2-N1	-3.76	1.31	1.36
29	a	2493	PSU	C2-N1	-3.76	1.31	1.36
29	a	736	1MG	C6-N1	-3.75	1.32	1.40
29	a	2493	PSU	C4-N3	-3.74	1.31	1.38
29	a	2569	PSU	C4-N3	-3.71	1.32	1.38
29	a	1906	PSU	C4-N3	-3.70	1.32	1.38
6	A	1495	UR3	C4-N3	-3.70	1.32	1.40
29	a	2541	OMU	C2-N3	-3.69	1.31	1.38
29	a	737	PSU	C2-N1	-3.69	1.31	1.36
29	a	1900	PSU	C4-N3	-3.67	1.32	1.38
29	a	2594	PSU	C2-N3	-3.65	1.31	1.37
29	a	2446	PSU	C2-N3	-3.65	1.31	1.37
29	a	1928	5MU	C6-C5	3.64	1.40	1.34
26	V	55	5MU	C6-C5	3.63	1.40	1.34
16	K	118	IAS	OD1-CG	3.61	1.40	1.19
29	a	2594	PSU	C2-N1	-3.60	1.31	1.36
29	a	945	PSU	C2-N1	-3.58	1.31	1.36
29	a	737	PSU	C2-N3	-3.57	1.31	1.37
29	a	945	PSU	C2-N3	-3.52	1.31	1.37
26	V	8	4SU	O2-C2	-3.51	1.16	1.23
29	a	1906	PSU	C2-N1	-3.51	1.32	1.36
6	A	513	PSU	C4-N3	-3.51	1.32	1.38
29	a	1906	PSU	C2-N3	-3.49	1.31	1.37
29	a	1928	5MU	C4-N3	-3.49	1.32	1.38
29	a	1900	PSU	C2-N1	-3.48	1.32	1.36
6	A	1399	4OC	C2-N1	-3.47	1.32	1.40
29	a	2493	PSU	C2-N3	-3.44	1.31	1.37
26	V	56	PSU	C4-N3	-3.42	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	524	G7M	C5-N7	-3.41	1.35	1.39
6	A	1516	MA6	C6-N6	3.40	1.46	1.36
29	a	2569	PSU	C2-N3	-3.37	1.31	1.37
29	a	2058	G7M	C6-N1	-3.35	1.32	1.38
26	V	56	PSU	C6-C5	3.34	1.39	1.35
29	a	1900	PSU	C2-N3	-3.34	1.31	1.37
6	A	1515	MA6	C6-N6	3.33	1.46	1.36
29	a	2058	G7M	C5-N7	-3.33	1.35	1.39
6	A	1495	UR3	C2-N3	-3.32	1.32	1.39
6	A	1515	MA6	C8-N9	-3.24	1.31	1.37
6	A	524	G7M	C6-N1	-3.24	1.32	1.38
6	A	513	PSU	C2-N3	-3.21	1.32	1.37
26	V	56	PSU	C2-N1	-3.20	1.32	1.36
29	a	2434	2MG	C6-N1	-3.19	1.32	1.38
29	a	1904	3TD	C6-C5	3.18	1.39	1.35
29	a	2493	PSU	C6-C5	3.18	1.39	1.35
6	A	1516	MA6	C8-N9	-3.16	1.31	1.37
29	a	1900	PSU	C6-C5	3.14	1.39	1.35
6	A	524	G7M	C2-N2	3.14	1.41	1.34
26	V	55	5MU	C4-N3	-3.13	1.33	1.38
29	a	2019	6MZ	C8-N9	-3.12	1.31	1.37
29	a	2594	PSU	C6-C5	3.10	1.38	1.35
26	V	56	PSU	C2-N3	-3.09	1.32	1.37
29	a	1906	PSU	C6-C5	3.07	1.38	1.35
6	A	1513	2MG	C6-N1	-3.07	1.33	1.38
29	a	2058	G7M	C2-N2	3.06	1.41	1.34
29	a	945	PSU	C6-C5	3.06	1.38	1.35
6	A	1204	2MG	C6-N1	-3.03	1.33	1.38
6	A	964	5MC	C6-N1	-3.02	1.32	1.38
6	A	963	2MG	C6-N1	-3.02	1.33	1.38
29	a	2446	PSU	C6-C5	3.01	1.38	1.35
29	a	2569	PSU	C6-C5	3.00	1.38	1.35
29	a	1904	3TD	C2-N3	-2.96	1.32	1.38
29	a	737	PSU	C6-C5	2.95	1.38	1.35
29	a	1928	5MU	O4-C4	-2.92	1.18	1.23
29	a	2594	PSU	O4-C4	-2.92	1.18	1.23
6	A	1495	UR3	C2-N1	-2.92	1.34	1.38
6	A	964	5MC	O2-C2	-2.89	1.18	1.23
6	A	513	PSU	C6-C5	2.88	1.38	1.35
29	a	2240	OMG	C8-N9	-2.86	1.31	1.37
29	a	2434	2MG	C5-N7	-2.84	1.33	1.39
6	A	1204	2MG	C5-N7	-2.82	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	2019	6MZ	C5-N7	-2.81	1.33	1.39
6	A	963	2MG	C5-N7	-2.80	1.33	1.39
29	a	945	PSU	O4-C4	-2.78	1.18	1.23
29	a	2446	PSU	O4-C4	-2.74	1.18	1.23
29	a	2493	PSU	O4-C4	-2.73	1.18	1.23
29	a	2541	OMU	O2-C2	-2.72	1.18	1.23
29	a	2569	PSU	O4-C4	-2.72	1.18	1.23
6	A	964	5MC	C6-C5	2.71	1.39	1.34
29	a	1906	PSU	O4-C4	-2.71	1.18	1.23
29	a	737	PSU	O4-C4	-2.68	1.18	1.23
29	a	2569	PSU	C6-N1	-2.67	1.31	1.36
29	a	1900	PSU	O4-C4	-2.64	1.18	1.23
29	a	2446	PSU	C6-N1	-2.63	1.31	1.36
6	A	513	PSU	O4-C4	-2.62	1.18	1.23
6	A	1513	2MG	C5-N7	-2.61	1.34	1.39
29	a	2240	OMG	C5-N7	-2.59	1.34	1.39
29	a	2594	PSU	C6-N1	-2.59	1.31	1.36
29	a	1928	5MU	O2-C2	-2.56	1.18	1.23
29	a	737	PSU	C6-N1	-2.56	1.32	1.36
26	V	55	5MU	O4-C4	-2.55	1.18	1.23
29	a	945	PSU	O2-C2	-2.53	1.18	1.23
29	a	945	PSU	C6-N1	-2.52	1.32	1.36
29	a	2058	G7M	C2-N1	-2.52	1.31	1.37
29	a	2446	PSU	O2-C2	-2.50	1.18	1.23
29	a	2569	PSU	O2-C2	-2.50	1.18	1.23
6	A	513	PSU	C6-N1	-2.49	1.32	1.36
29	a	736	1MG	C5-N7	-2.47	1.34	1.39
29	a	736	1MG	C8-N9	-2.47	1.32	1.37
26	V	56	PSU	O4-C4	-2.46	1.18	1.23
29	a	2541	OMU	C6-N1	-2.46	1.32	1.38
29	a	2493	PSU	C6-N1	-2.43	1.32	1.36
29	a	2493	PSU	O2-C2	-2.42	1.18	1.23
29	a	1904	3TD	C6-N1	-2.38	1.32	1.36
29	a	2541	OMU	C5-C4	-2.38	1.38	1.43
29	a	1906	PSU	O2-C2	-2.37	1.18	1.23
29	a	1904	3TD	O2-C2	-2.36	1.18	1.23
29	a	737	PSU	O2-C2	-2.36	1.18	1.23
6	A	524	G7M	C2-N1	-2.36	1.31	1.37
29	a	2569	PSU	O4'-C1'	-2.35	1.40	1.43
29	a	2594	PSU	O2-C2	-2.35	1.18	1.23
29	a	1906	PSU	C6-N1	-2.33	1.32	1.36
29	a	1900	PSU	C6-N1	-2.31	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	55	5MU	O2-C2	-2.29	1.18	1.23
29	a	2434	2MG	C4-N9	-2.29	1.32	1.38
26	V	56	PSU	C6-N1	-2.28	1.32	1.36
29	a	1900	PSU	O2-C2	-2.26	1.18	1.23
6	A	513	PSU	O2-C2	-2.24	1.18	1.23
6	A	1515	MA6	C5-N7	-2.22	1.34	1.39
6	A	1495	UR3	C6-N1	-2.19	1.32	1.38
29	a	2240	OMG	C2-N1	-2.19	1.32	1.37
6	A	1516	MA6	C5-N7	-2.19	1.34	1.39
17	L	89	D2T	CB-CG	2.18	1.55	1.52
29	a	2434	2MG	CM2-N2	-2.18	1.41	1.45
26	V	33	OMC	C6-C5	2.17	1.40	1.35
29	a	2487	OMC	C5-C4	-2.14	1.38	1.42
26	V	56	PSU	O2-C2	-2.13	1.18	1.23
6	A	1495	UR3	O2-C2	2.12	1.26	1.22
6	A	1513	2MG	C4-N9	-2.10	1.32	1.38
6	A	964	5MC	C2-N3	-2.07	1.32	1.36
29	a	2492	2MA	C8-N9	-2.06	1.33	1.37
29	a	2492	2MA	C5-N7	-2.03	1.35	1.39
29	a	737	PSU	O4'-C1'	-2.03	1.41	1.43
6	A	1399	4OC	C2-N3	-2.03	1.32	1.36
29	a	2434	2MG	C8-N9	-2.01	1.33	1.37
6	A	1513	2MG	CM2-N2	-2.01	1.42	1.45
29	a	736	1MG	C5-C6	-2.01	1.40	1.45
6	A	1204	2MG	CM2-N2	-2.00	1.42	1.45

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	2438	H2U	C4-N3-C2	-14.75	113.55	125.79
26	V	21	H2U	C4-N3-C2	-13.64	114.48	125.79
26	V	21	H2U	O2-C2-N1	-11.70	108.42	123.11
29	a	2438	H2U	O2-C2-N1	-10.62	109.78	123.11
29	a	1928	5MU	C4-N3-C2	-8.74	116.04	127.35
26	V	55	5MU	C5M-C5-C4	8.52	128.15	118.77
29	a	1928	5MU	N3-C2-N1	8.45	126.10	114.89
26	V	55	5MU	C4-N3-C2	-8.28	116.62	127.35
29	a	2438	H2U	O4-C4-N3	-8.16	107.34	120.28
26	V	55	5MU	N3-C2-N1	8.06	125.59	114.89
29	a	1928	5MU	C5-C6-N1	-7.88	115.23	123.34
26	V	8	4SU	C4-N3-C2	-7.63	119.93	127.34
29	a	1928	5MU	C5M-C5-C4	7.43	126.95	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	21	H2U	O4-C4-N3	-7.37	108.60	120.28
6	A	1204	2MG	C2-N3-C4	7.35	121.15	112.04
6	A	1513	2MG	C2-N3-C4	7.35	121.15	112.04
6	A	963	2MG	C2-N3-C4	7.23	121.00	112.04
26	V	21	H2U	O2-C2-N3	-7.14	108.21	121.50
29	a	2492	2MA	C5-C4-N3	-7.13	119.17	127.19
26	V	55	5MU	C5-C6-N1	-7.13	116.01	123.34
29	a	2434	2MG	C2-N3-C4	6.99	120.71	112.04
29	a	2438	H2U	O2-C2-N3	-6.86	108.72	121.50
29	a	736	1MG	C5-C4-N3	-6.79	117.45	128.46
29	a	1928	5MU	C5-C4-N3	6.70	121.03	115.31
26	V	55	5MU	C5M-C5-C6	-6.69	113.91	122.85
29	a	1904	3TD	N1-C2-N3	6.68	121.41	116.14
26	V	21	H2U	O4-C4-C5	-6.50	108.29	122.17
29	a	2438	H2U	O4-C4-C5	-6.50	108.29	122.17
29	a	2438	H2U	N3-C2-N1	-6.44	109.84	116.65
26	V	55	5MU	C5-C4-N3	6.15	120.56	115.31
29	a	2446	PSU	N1-C2-N3	5.94	121.86	115.13
29	a	2569	PSU	N1-C2-N3	5.86	121.77	115.13
29	a	1928	5MU	C5M-C5-C6	-5.85	115.04	122.85
6	A	1515	MA6	C5-C4-N3	-5.77	119.22	126.75
29	a	737	PSU	N1-C2-N3	5.76	121.66	115.13
16	K	118	IAS	OD1-CG-CB	-5.71	108.80	125.43
29	a	2019	6MZ	C9-N6-C6	-5.62	118.03	122.87
6	A	1516	MA6	C5-C4-N3	-5.61	119.43	126.75
29	a	1906	PSU	N1-C2-N3	5.58	121.46	115.13
29	a	945	PSU	N1-C2-N3	5.57	121.44	115.13
29	a	2594	PSU	N1-C2-N3	5.57	121.44	115.13
6	A	1204	2MG	C5-C4-N3	-5.48	119.57	128.46
29	a	2541	OMU	N3-C2-N1	5.48	122.17	114.89
29	a	1900	PSU	N1-C2-N3	5.48	121.34	115.13
26	V	56	PSU	N1-C2-N3	5.44	121.30	115.13
6	A	513	PSU	N1-C2-N3	5.42	121.27	115.13
29	a	2240	OMG	C5-C4-N3	-5.40	119.71	128.46
26	V	8	4SU	C5-C4-N3	5.38	119.68	114.69
6	A	964	5MC	C5-C6-N1	-5.34	117.84	123.34
29	a	2493	PSU	N1-C2-N3	5.32	121.16	115.13
29	a	2058	G7M	C2-N3-C4	5.25	121.66	112.30
6	A	963	2MG	C5-C4-N3	-5.20	120.02	128.46
6	A	524	G7M	C2-N3-C4	5.19	121.55	112.30
29	a	2019	6MZ	C5-C4-N3	-5.15	120.04	126.75
29	a	736	1MG	C2-N3-C4	5.12	123.50	111.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	2492	2MA	N3-C4-N9	5.09	134.06	126.99
6	A	1513	2MG	C5-C4-N3	-4.97	120.40	128.46
29	a	2019	6MZ	N1-C2-N3	-4.95	120.87	128.60
6	A	1515	MA6	N1-C2-N3	-4.88	120.97	128.60
6	A	1516	MA6	N1-C2-N3	-4.87	120.99	128.60
29	a	2434	2MG	C5-C4-N3	-4.77	120.72	128.46
6	A	1495	UR3	C4-N3-C2	-4.72	120.12	124.56
29	a	2240	OMG	C2-N3-C4	4.69	120.66	112.30
29	a	736	1MG	N9-C4-N3	4.68	135.33	125.94
6	A	1515	MA6	N3-C4-N9	4.67	134.78	127.08
6	A	524	G7M	C5-C4-N3	-4.62	119.29	128.15
29	a	2058	G7M	C5-C4-N3	-4.32	119.86	128.15
6	A	524	G7M	C5-C6-N1	4.23	120.62	111.79
6	A	1516	MA6	N3-C4-N9	4.22	134.04	127.08
29	a	2541	OMU	C4-N3-C2	-4.22	121.02	126.58
6	A	1516	MA6	C2-N1-C6	4.20	121.68	111.75
29	a	2058	G7M	C5-C6-N1	4.18	120.52	111.79
6	A	1515	MA6	C2-N1-C6	4.16	121.59	111.75
6	A	1515	MA6	C2-N3-C4	4.15	121.55	111.75
6	A	1516	MA6	C2-N3-C4	4.12	121.48	111.75
29	a	2058	G7M	C6-C5-N7	4.02	137.11	132.25
29	a	2019	6MZ	C6-C5-N7	3.97	136.68	132.39
29	a	2019	6MZ	C2-N3-C4	3.95	121.09	111.75
26	V	55	5MU	O4-C4-N3	-3.91	112.63	120.12
29	a	1928	5MU	O4-C4-N3	-3.89	112.65	120.12
29	a	1928	5MU	O2-C2-N1	-3.86	117.65	122.79
26	V	8	4SU	N3-C2-N1	3.84	119.99	114.89
29	a	2240	OMG	N9-C4-N3	3.83	133.64	125.94
6	A	1516	MA6	N9-C8-N7	-3.81	108.71	113.91
29	a	2594	PSU	C4-N3-C2	-3.80	120.86	126.34
29	a	737	PSU	C4-N3-C2	-3.77	120.91	126.34
26	V	21	H2U	N3-C2-N1	-3.74	112.70	116.65
29	a	1906	PSU	C4-N3-C2	-3.69	121.03	126.34
6	A	524	G7M	N9-C4-N3	3.68	133.33	125.94
29	a	2446	PSU	C4-N3-C2	-3.68	121.03	126.34
6	A	1516	MA6	C5-N7-C8	3.67	108.73	103.51
29	a	1900	PSU	C4-N3-C2	-3.67	121.05	126.34
6	A	1515	MA6	N9-C8-N7	-3.65	108.93	113.91
29	a	945	PSU	C4-N3-C2	-3.64	121.09	126.34
29	a	2019	6MZ	C5-N7-C8	3.64	108.68	103.51
6	A	1204	2MG	N9-C4-N3	3.64	133.24	125.94
6	A	963	2MG	N9-C4-N3	3.62	133.21	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	56	PSU	C4-N3-C2	-3.61	121.13	126.34
29	a	2019	6MZ	C4-C5-N7	-3.60	106.24	110.62
29	a	2569	PSU	O2-C2-N1	-3.59	118.84	122.79
6	A	513	PSU	C4-N3-C2	-3.59	121.17	126.34
29	a	2569	PSU	C4-N3-C2	-3.57	121.20	126.34
6	A	1515	MA6	C4-N9-C8	3.49	109.51	105.73
6	A	1515	MA6	C5-N7-C8	3.49	108.46	103.51
6	A	524	G7M	O6-C6-C5	-3.49	120.20	128.06
6	A	513	PSU	O2-C2-N1	-3.42	119.03	122.79
29	a	2058	G7M	O6-C6-C5	-3.38	120.44	128.06
6	A	1516	MA6	C4-N9-C8	3.33	109.33	105.73
6	A	1513	2MG	C6-C5-N7	3.32	136.43	130.25
29	a	737	PSU	O2-C2-N1	-3.30	119.16	122.79
29	a	2493	PSU	C4-N3-C2	-3.28	121.62	126.34
29	a	2434	2MG	N9-C4-N3	3.28	132.52	125.94
29	a	2058	G7M	N9-C4-N3	3.25	132.47	125.94
6	A	1516	MA6	C4-C5-N7	-3.23	106.69	110.62
29	a	945	PSU	O2-C2-N1	-3.20	119.26	122.79
6	A	524	G7M	C6-C5-N7	3.20	136.12	132.25
40	l	82	4D4	NE-CZ-NH2	3.19	126.31	120.70
26	V	8	4SU	C5-C4-S4	-3.12	120.45	124.47
6	A	1513	2MG	N9-C4-N3	3.12	132.20	125.94
26	V	55	5MU	O2-C2-N3	-3.11	115.71	121.50
29	a	2019	6MZ	N9-C8-N7	-3.09	109.69	113.91
26	V	55	5MU	O2-C2-N1	-3.08	118.69	122.79
29	a	2019	6MZ	N3-C4-N9	3.06	132.12	127.08
29	a	1900	PSU	O2-C2-N1	-3.05	119.43	122.79
29	a	2434	2MG	C6-C5-N7	3.05	135.91	130.25
29	a	2492	2MA	N9-C8-N7	-3.00	109.81	113.91
29	a	2492	2MA	C5-N7-C8	2.99	107.76	103.51
29	a	2487	OMC	O2-C2-N3	-2.98	117.48	122.33
29	a	2594	PSU	O2-C2-N1	-2.96	119.53	122.79
29	a	2446	PSU	O2-C2-N1	-2.95	119.54	122.79
26	V	56	PSU	O2-C2-N1	-2.92	119.58	122.79
6	A	1515	MA6	C4-C5-N7	-2.89	107.10	110.62
6	A	1399	4OC	O2-C2-N3	-2.83	117.73	122.33
29	a	1928	5MU	O2-C2-N3	-2.82	116.24	121.50
29	a	1906	PSU	O2-C2-N1	-2.81	119.69	122.79
29	a	2493	PSU	O2-C2-N1	-2.81	119.70	122.79
6	A	963	2MG	C6-C5-N7	2.77	135.39	130.25
29	a	2240	OMG	C6-C5-N7	2.77	135.39	130.25
6	A	1204	2MG	C6-C5-N7	2.72	135.30	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	2492	2MA	C4-C5-N7	-2.70	107.33	110.62
6	A	1513	2MG	C4-C5-N7	-2.67	106.49	110.72
6	A	524	G7M	C2-N1-C6	-2.62	120.31	125.10
29	a	1904	3TD	C4-N3-C2	-2.62	121.77	124.61
26	V	33	OMC	O2-C2-N3	-2.59	118.12	122.33
29	a	2569	PSU	O4'-C1'-C2'	2.58	108.78	105.14
29	a	2541	OMU	C5-C4-N3	2.56	118.67	114.84
29	a	736	1MG	C5-C6-N1	2.55	119.84	114.91
26	V	55	5MU	C1'-N1-C6	-2.55	116.88	121.12
17	L	89	D2T	OD1-CG-CB	-2.54	117.11	122.44
29	a	2240	OMG	C8-N7-C5	2.52	108.81	104.24
29	a	2058	G7M	C2-N1-C6	-2.51	120.51	125.10
6	A	1204	2MG	C4-C5-N7	-2.46	106.83	110.72
29	a	736	1MG	C4-C5-N7	-2.46	106.83	110.72
29	a	2240	OMG	C4-C5-N7	-2.46	106.83	110.72
29	a	2240	OMG	C5-C6-N1	2.42	119.34	113.19
29	a	2492	2MA	N3-C2-N1	-2.40	121.30	125.72
40	l	83	MS6	CE-SD-CG	2.40	108.65	100.40
29	a	736	1MG	C6-C5-N7	2.40	134.78	129.35
40	l	82	4D4	NH1-CZ-NE	-2.40	113.66	119.19
29	a	2492	2MA	C4-N9-C8	2.39	108.32	105.73
29	a	2541	OMU	O4-C4-C5	-2.39	120.96	125.16
29	a	2434	2MG	O6-C6-C5	-2.36	120.34	126.60
29	a	2240	OMG	O6-C6-C5	-2.36	120.35	126.60
29	a	2240	OMG	N9-C8-N7	-2.35	108.97	113.39
6	A	1495	UR3	C5-C6-N1	-2.34	117.89	121.81
29	a	2569	PSU	C6-N1-C2	-2.31	120.32	122.68
29	a	2434	2MG	C4-C5-N7	-2.30	107.07	110.72
6	A	1204	2MG	C2-N1-C6	-2.30	121.83	124.48
6	A	1513	2MG	N1-C2-N3	-2.30	120.40	123.95
6	A	1513	2MG	C8-N7-C5	2.29	108.39	104.24
29	a	2487	OMC	N1-C2-N3	2.29	122.97	118.81
6	A	1513	2MG	C5-C6-N1	2.28	118.97	113.19
6	A	963	2MG	C5-C6-N1	2.27	118.96	113.19
6	A	963	2MG	C4-C5-N7	-2.26	107.14	110.72
29	a	1928	5MU	C6-N1-C2	2.26	123.59	121.30
6	A	513	PSU	O4'-C1'-C2'	2.26	108.33	105.14
6	A	964	5MC	C5-C4-N3	-2.26	119.24	121.67
6	A	963	2MG	O6-C6-C5	-2.23	120.67	126.60
29	a	2434	2MG	N1-C2-N3	-2.21	120.53	123.95
29	a	2438	H2U	C5-C4-N3	-2.21	114.17	116.65
6	A	963	2MG	C2-N1-C6	-2.20	121.94	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1513	2MG	O6-C6-C5	-2.19	120.79	126.60
29	a	2434	2MG	C5-C6-N1	2.19	118.75	113.19
6	A	1204	2MG	C5-C6-N1	2.19	118.74	113.19
29	a	2541	OMU	O2-C2-N1	-2.18	119.89	122.79
6	A	1204	2MG	C8-N7-C5	2.17	108.16	104.24
6	A	963	2MG	N1-C2-N3	-2.17	120.60	123.95
29	a	2446	PSU	O4'-C1'-C2'	2.17	108.20	105.14
6	A	1204	2MG	CM2-N2-C2	-2.16	119.09	123.86
6	A	1513	2MG	C2-N1-C6	-2.16	122.00	124.48
29	a	736	1MG	C8-N7-C5	2.16	108.14	104.24
26	V	33	OMC	N1-C2-N3	2.15	122.72	118.81
29	a	2240	OMG	C2-N1-C6	-2.13	121.22	125.10
6	A	1204	2MG	O6-C6-C5	-2.12	120.97	126.60
6	A	1513	2MG	N9-C8-N7	-2.12	109.40	113.39
6	A	1399	4OC	C5-C4-N3	-2.12	119.19	122.59
29	a	2434	2MG	C8-N7-C5	2.11	108.06	104.24
29	a	2493	PSU	C6-N1-C2	-2.11	120.53	122.68
29	a	2434	2MG	N9-C8-N7	-2.09	109.45	113.39
6	A	963	2MG	C8-N7-C5	2.07	107.98	104.24
29	a	2493	PSU	C6-C5-C4	-2.04	116.77	118.20
29	a	2446	PSU	C6-N1-C2	-2.03	120.61	122.68
26	V	21	H2U	C5-C4-N3	-2.01	114.39	116.65
6	A	1204	2MG	N1-C2-N3	-2.01	120.84	123.95

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD1
17	L	89	D2T	CA-CB-CG-OD2
17	L	89	D2T	SB-CB-CG-OD2
32	d	153	MEQ	O-C-CA-CB
6	A	524	G7M	C3'-C4'-C5'-O5'
6	A	1204	2MG	N1-C2-N2-CM2
6	A	1204	2MG	N3-C2-N2-CM2
16	K	118	IAS	N-CA-CB-CG
26	V	21	H2U	O4'-C4'-C5'-O5'
26	V	21	H2U	C3'-C4'-C5'-O5'
26	V	21	H2U	O4'-C1'-N1-C2
26	V	21	H2U	O4'-C1'-N1-C6
29	a	2240	OMG	C1'-C2'-O2'-CM2
29	a	2541	OMU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
29	a	2541	OMU	O4'-C4'-C5'-O5'
29	a	2019	6MZ	O4'-C4'-C5'-O5'
29	a	2019	6MZ	C3'-C4'-C5'-O5'
29	a	2493	PSU	O4'-C4'-C5'-O5'
32	d	153	MEQ	NE2-CD-CG-CB
32	d	153	MEQ	OE1-CD-CG-CB
29	a	2493	PSU	C3'-C4'-C5'-O5'
6	A	524	G7M	O4'-C4'-C5'-O5'
29	a	2492	2MA	O4'-C4'-C5'-O5'
40	l	83	MS6	CA-CB-CG-SD
40	l	83	MS6	CB-CG-SD-CE
29	a	2492	2MA	C3'-C4'-C5'-O5'
17	L	89	D2T	CG-CB-SB-CB1
40	l	82	4D4	OB-CB-CG-CD
6	A	1516	MA6	C4'-C5'-O5'-P
29	a	2434	2MG	C3'-C4'-C5'-O5'
6	A	524	G7M	C4'-C5'-O5'-P
29	a	737	PSU	O4'-C1'-C5-C6
29	a	2492	2MA	C4'-C5'-O5'-P
29	a	2058	G7M	O4'-C4'-C5'-O5'
40	l	82	4D4	CG-CD-NE-CZ
16	K	118	IAS	CA-CB-CG-OD1
32	d	153	MEQ	CA-CB-CG-CD
40	l	82	4D4	O-C-CA-CB
29	a	2058	G7M	C4'-C5'-O5'-P
29	a	2438	H2U	O4'-C1'-N1-C2

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	2240	OMG	1	0
26	V	33	OMC	5	0
29	a	1904	3TD	1	0
29	a	2438	H2U	1	0
6	A	1516	MA6	1	0
29	a	2019	6MZ	2	0
26	V	21	H2U	2	0
29	a	2541	OMU	2	0
6	A	1515	MA6	1	0
6	A	1513	2MG	1	0
26	V	55	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1399	4OC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 531 ligands modelled in this entry, 531 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1530:C	O3'	1531:A	P	4.72

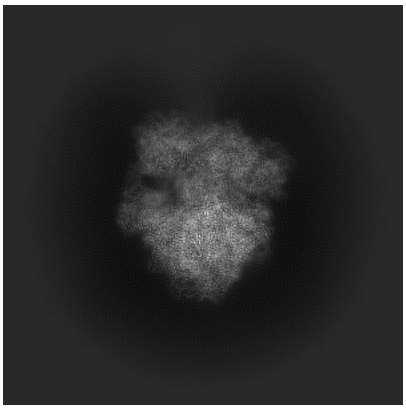
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55260. These allow visual inspection of the internal detail of the map and identification of artifacts.

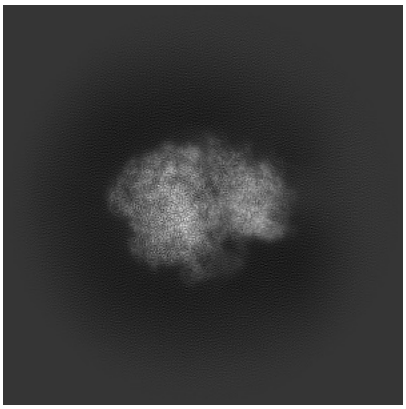
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

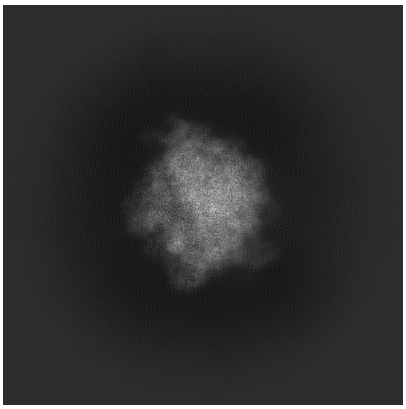
6.1.1 Primary map



X

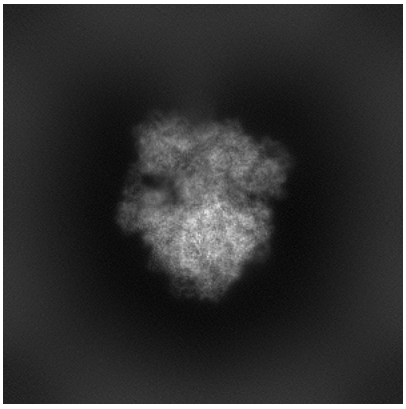


Y

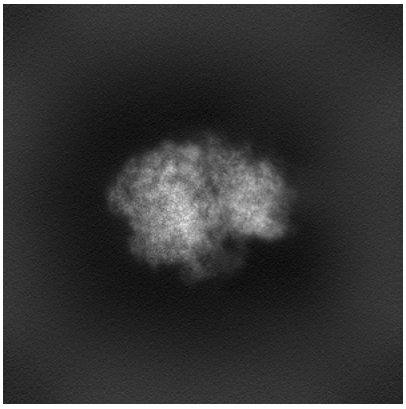


Z

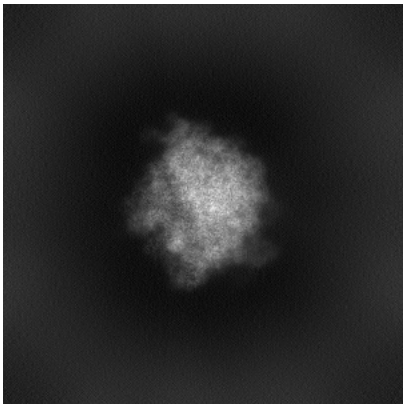
6.1.2 Raw map



X



Y

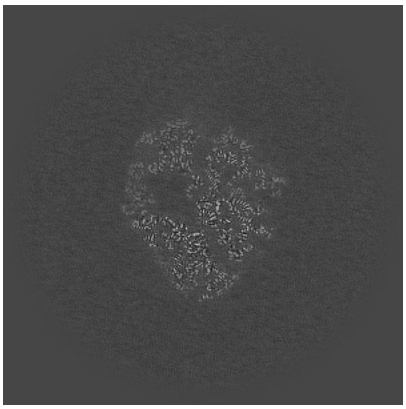


Z

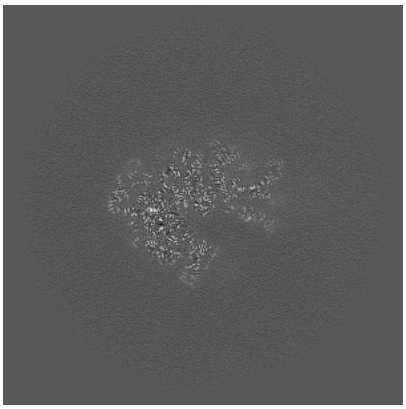
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

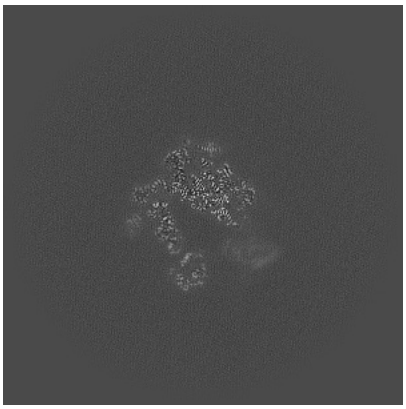
6.2.1 Primary map



X Index: 256

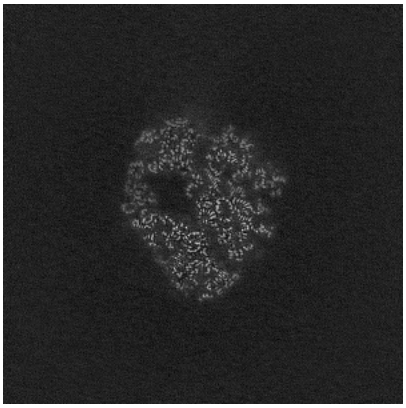


Y Index: 256

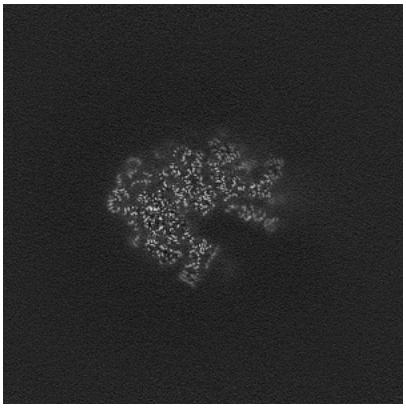


Z Index: 256

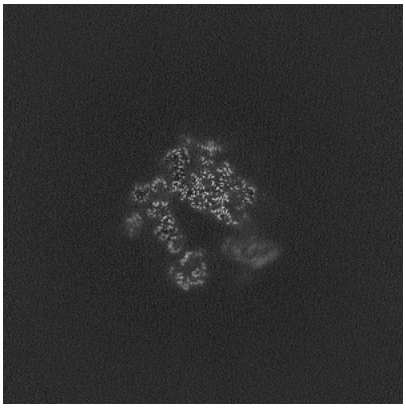
6.2.2 Raw map



X Index: 256



Y Index: 256

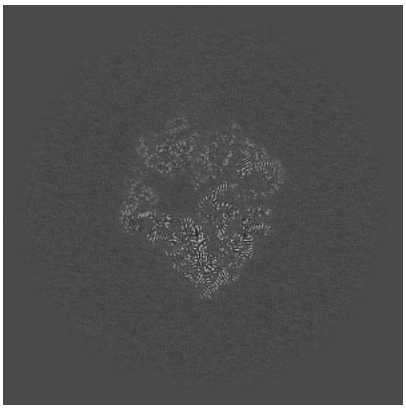


Z Index: 256

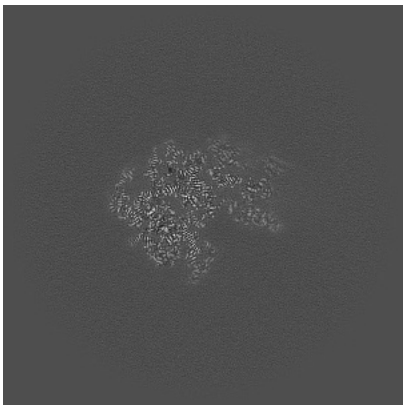
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

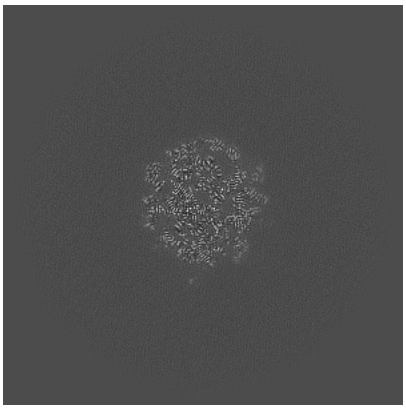
6.3.1 Primary map



X Index: 248

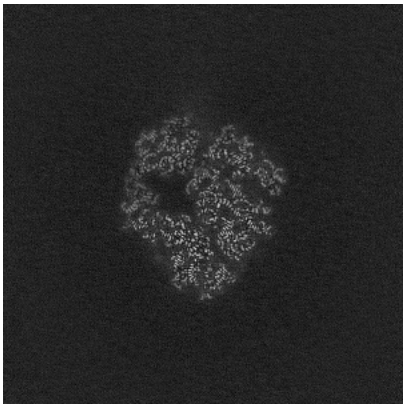


Y Index: 262

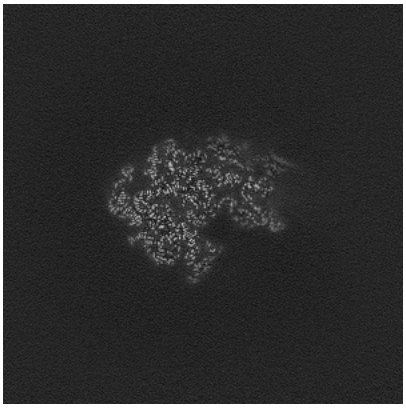


Z Index: 216

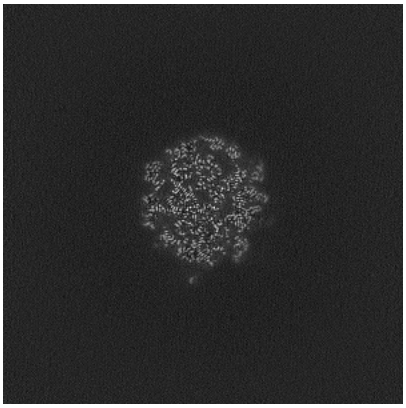
6.3.2 Raw map



X Index: 253



Y Index: 263

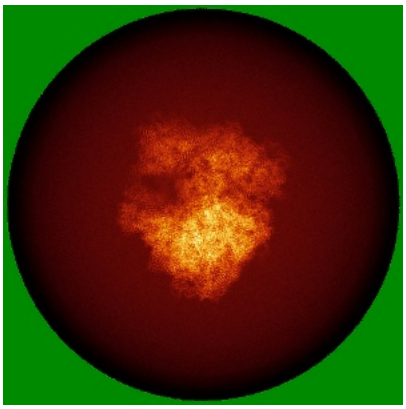


Z Index: 216

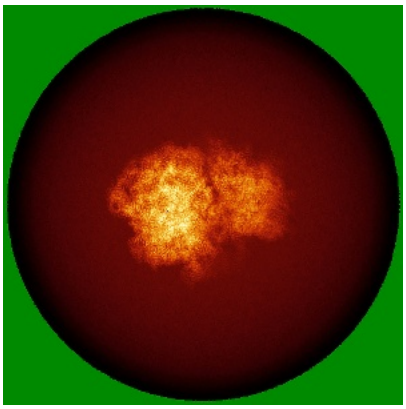
The images above show the largest variance slices of the map in three orthogonal directions.

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

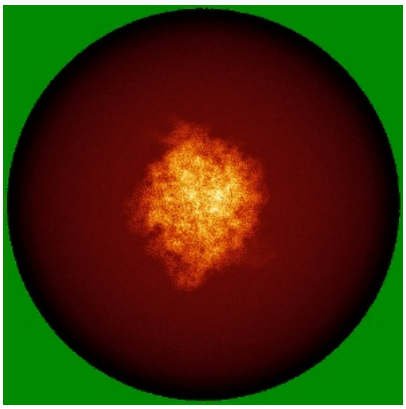
6.4.1 Primary map



X

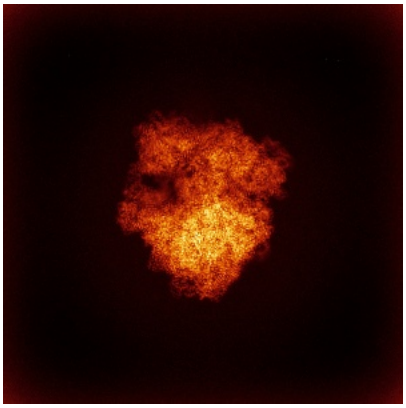


Y

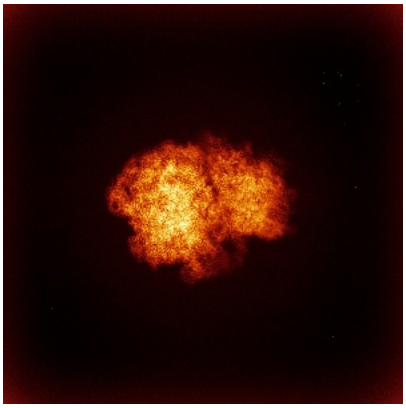


Z

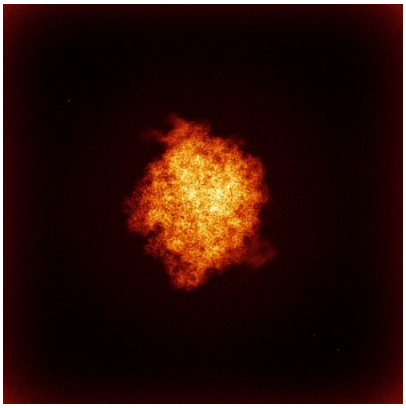
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

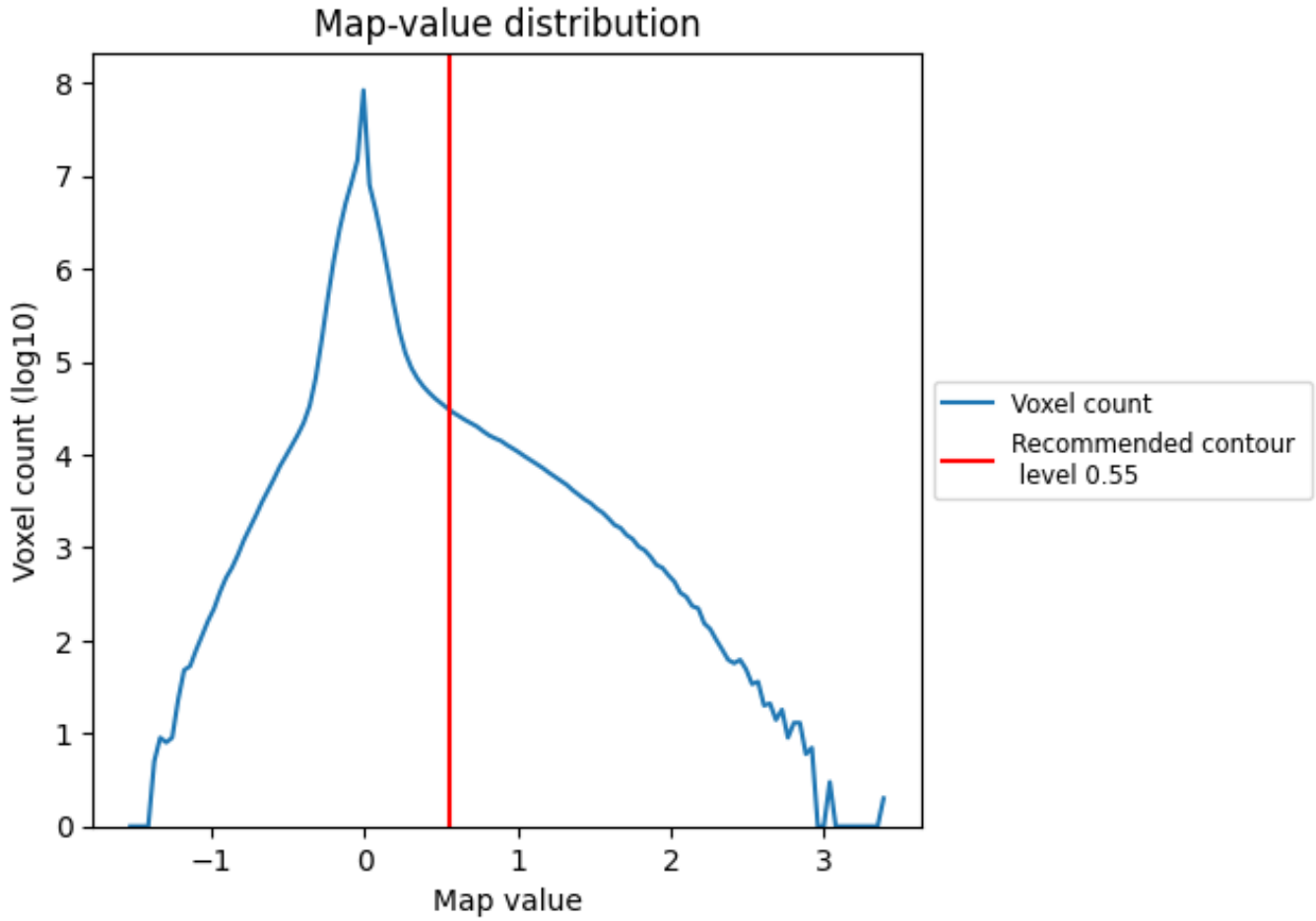
6.6 Mask visualisation (i)

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

7 Map analysis

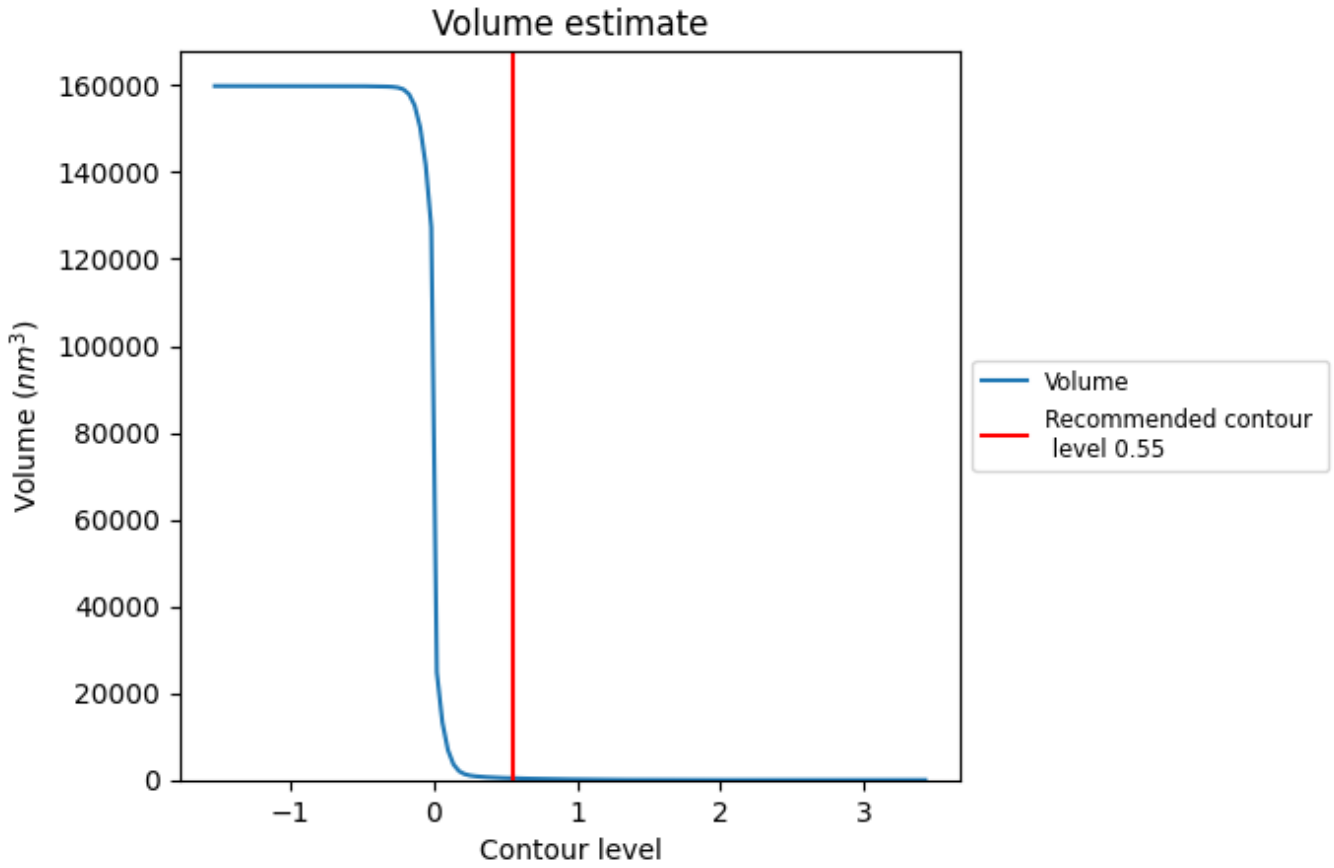
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

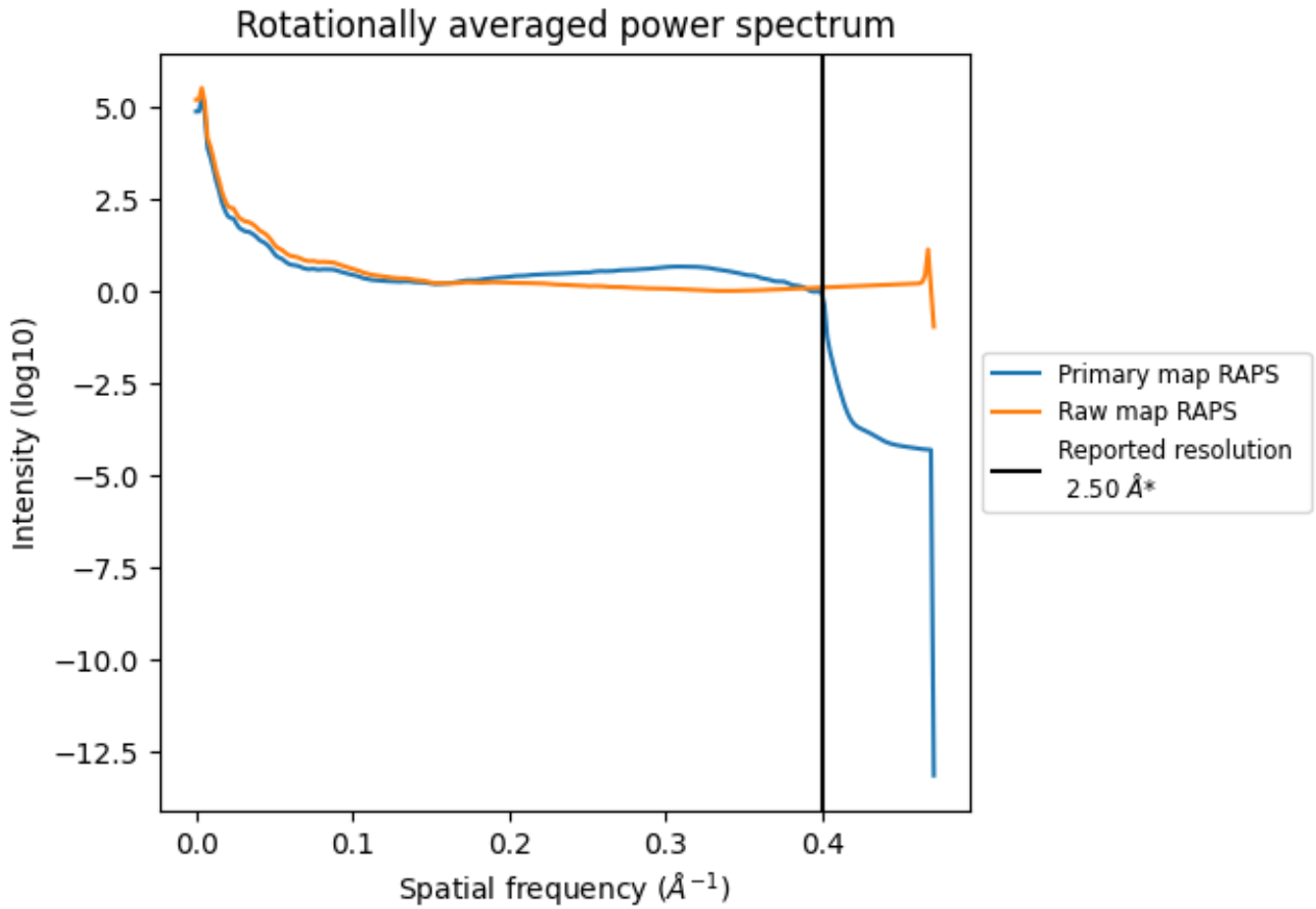
7.2 Volume estimate



The volume at the recommended contour level is 397 nm^3; this corresponds to an approximate mass of 359 kDa.

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

7.3 Rotationally averaged power spectrum (i)

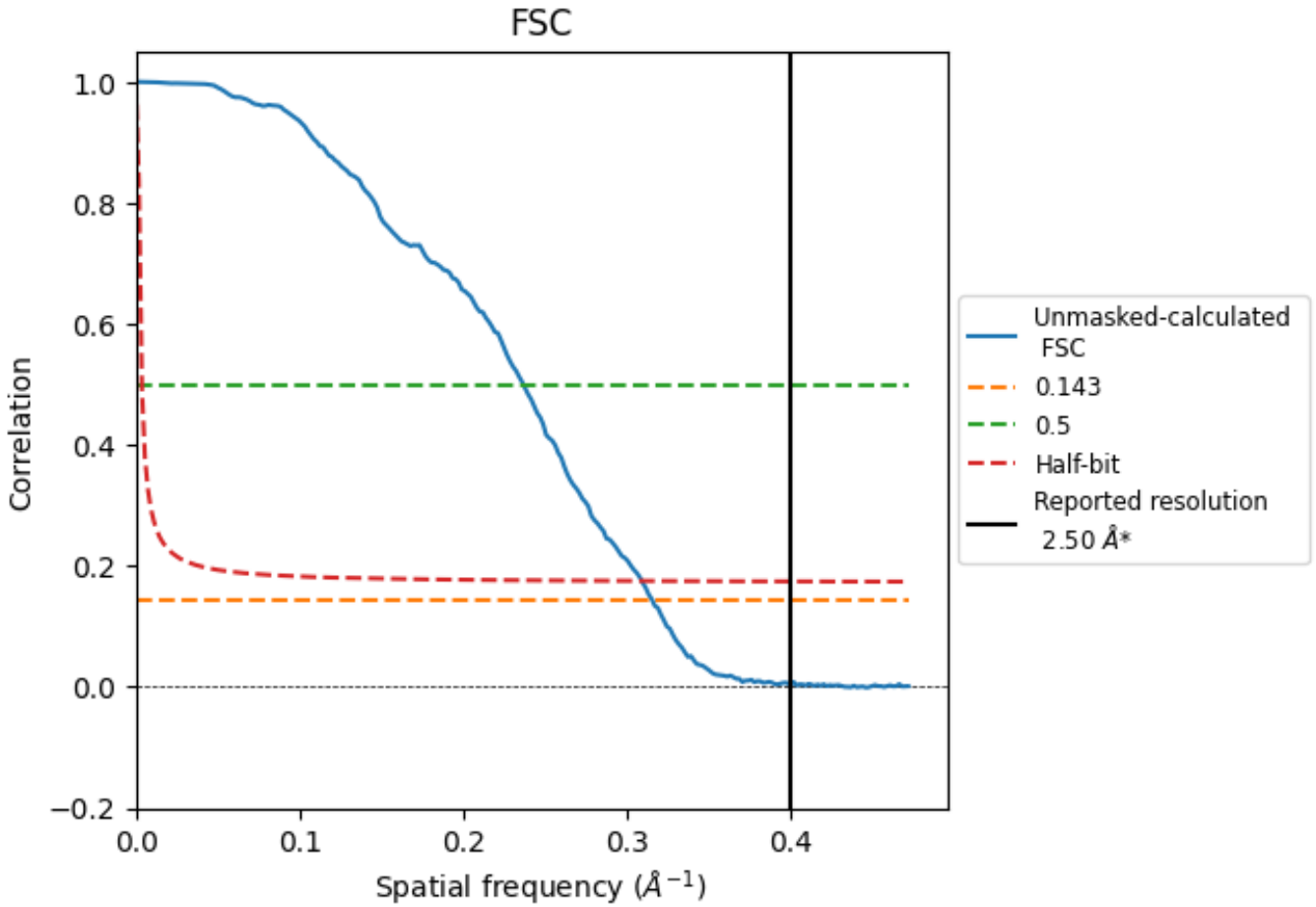


*Reported resolution corresponds to spatial frequency of 0.400 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

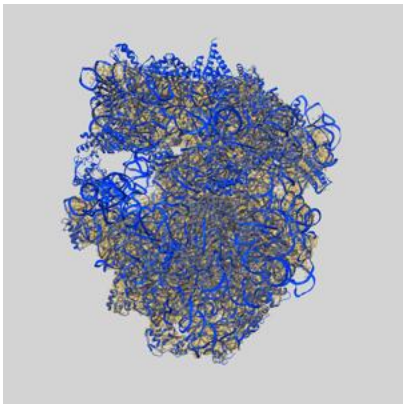
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.17	4.23	3.24

*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 3.17 differs from the reported value 2.5 by more than 10 %

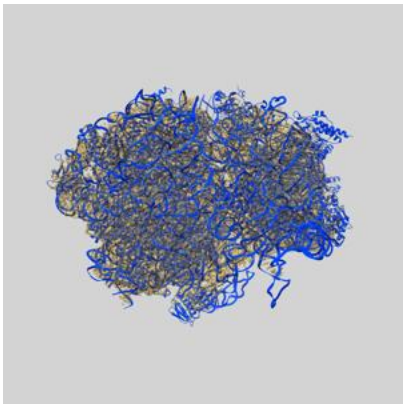
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55260 and PDB model 9SVJ. Per-residue inclusion information can be found in section 3 on page 16.

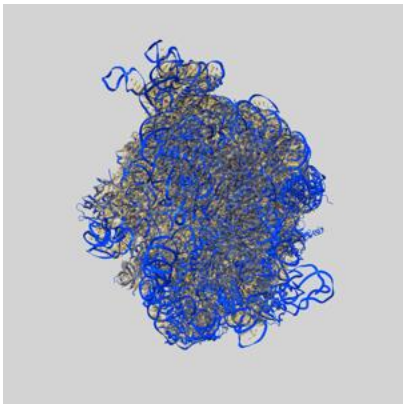
9.1 Map-model overlay



X



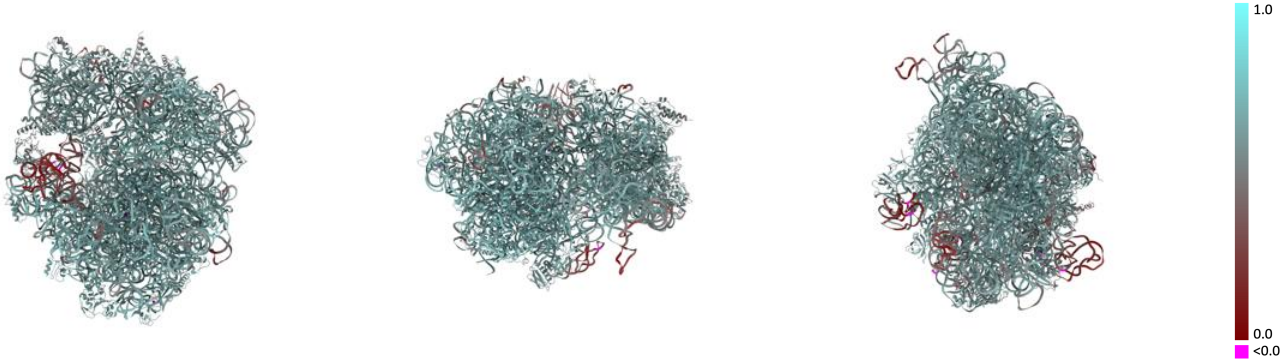
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

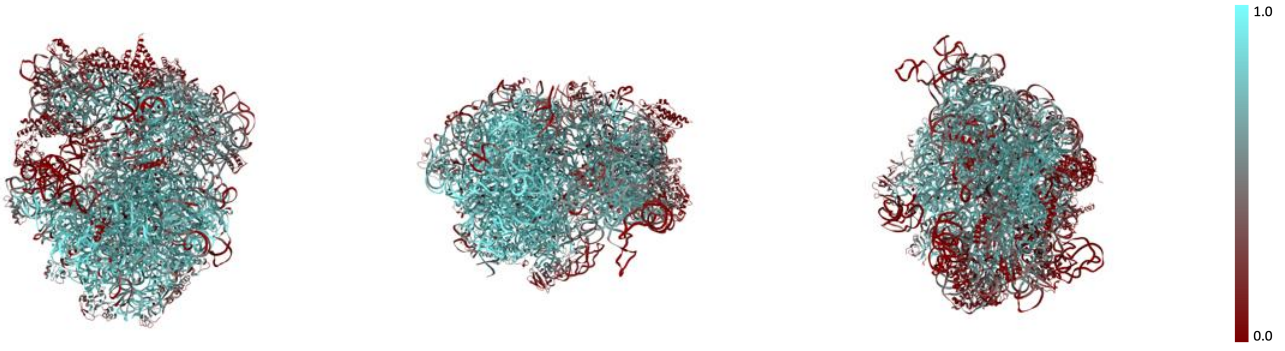
9.2 Q-score mapped to coordinate model



X Y Z

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

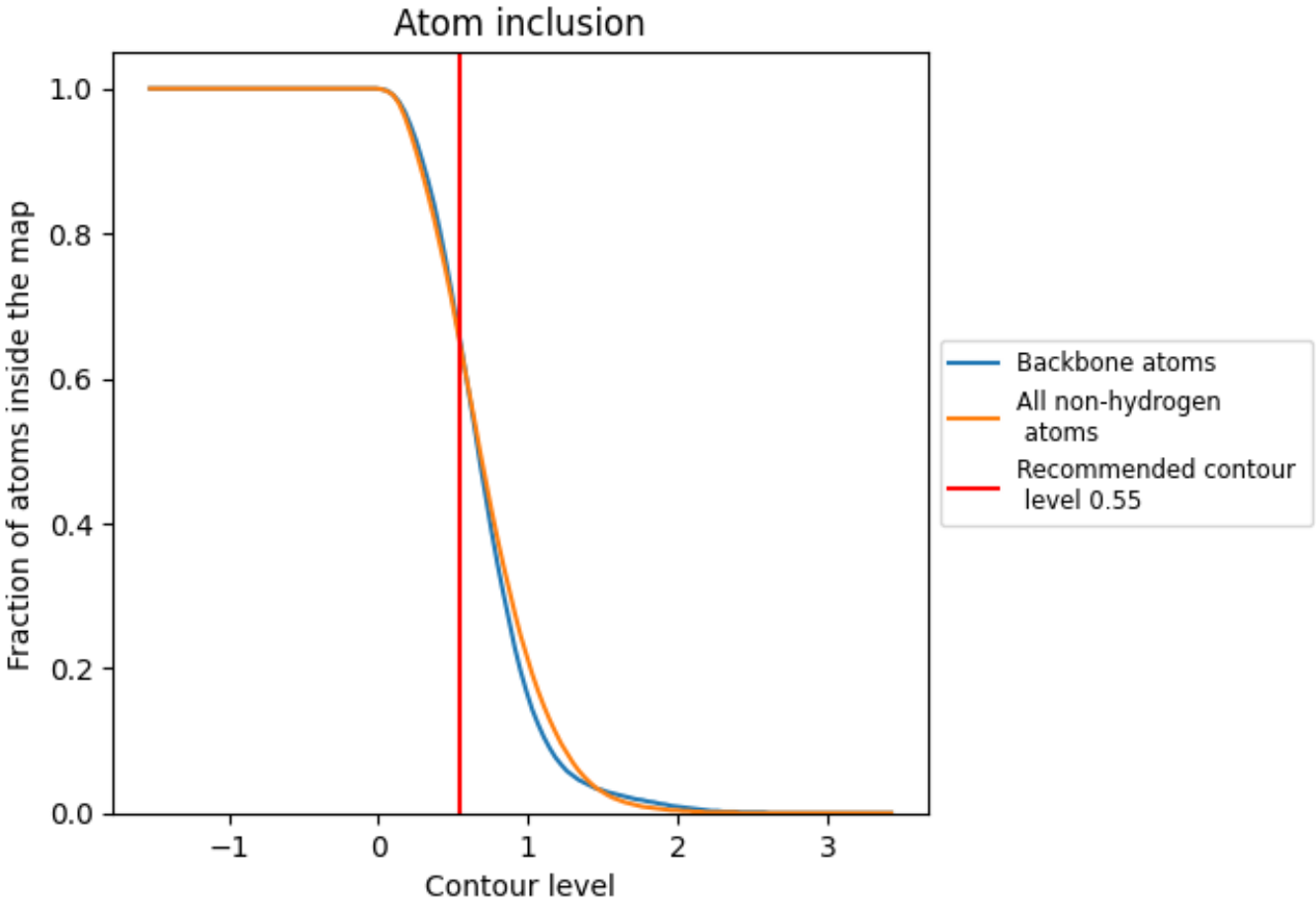
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 64% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.6160
0	0.6040	0.6470
1	0.8690	0.6750
2	0.8710	0.6840
3	0.7140	0.6590
4	0.0060	0.4620
A	0.6290	0.6060
B	0.0420	0.5440
C	0.3540	0.6030
D	0.2580	0.5880
E	0.5920	0.6450
F	0.1780	0.5830
G	0.1850	0.5690
H	0.5220	0.6430
I	0.3270	0.5980
J	0.2910	0.5750
K	0.3730	0.6080
L	0.5010	0.6350
M	0.1960	0.5800
N	0.3410	0.5900
O	0.5120	0.6340
P	0.4650	0.6180
Q	0.3570	0.6160
R	0.2550	0.6000
S	0.1540	0.5660
T	0.4770	0.6320
V	0.0100	0.3630
W	0.0320	0.4320
X	0.4280	0.6230
a	0.7770	0.6230
b	0.6540	0.6210
c	0.7980	0.6740
d	0.7850	0.6700
e	0.6540	0.6590
f	0.1430	0.5580



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Chain	Atom inclusion	Q-score
g	0.2950	0.6010
h	0.0040	0.4380
i	0.7760	0.6670
j	0.6890	0.6650
k	0.7170	0.6630
l	0.6630	0.6600
m	0.8320	0.6800
n	0.5410	0.6340
o	0.6640	0.6610
p	0.8460	0.6840
q	0.7180	0.6630
r	0.7490	0.6700
s	0.6060	0.6480
t	0.4390	0.6130
u	0.5140	0.6300
v	0.7930	0.6740
w	0.6930	0.6640
x	0.4320	0.6200
y	0.7220	0.6620
z	0.7280	0.6650