



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 07:58 PM UTC

PDB ID : 6VWN / pdb_00006vwn
EMDB ID : EMD-21422
Title : 70S ribosome bound to HIV frameshifting stem-loop (FSS) and P-site tRNA (non-rotated conformation, Structure II)
Authors : Loerch, S.; Bao, C.; Ling, C.; Korostelev, A.A.; Grigorieff, N.; Ermolenko, D.M.
Deposited on : 2020-02-20
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

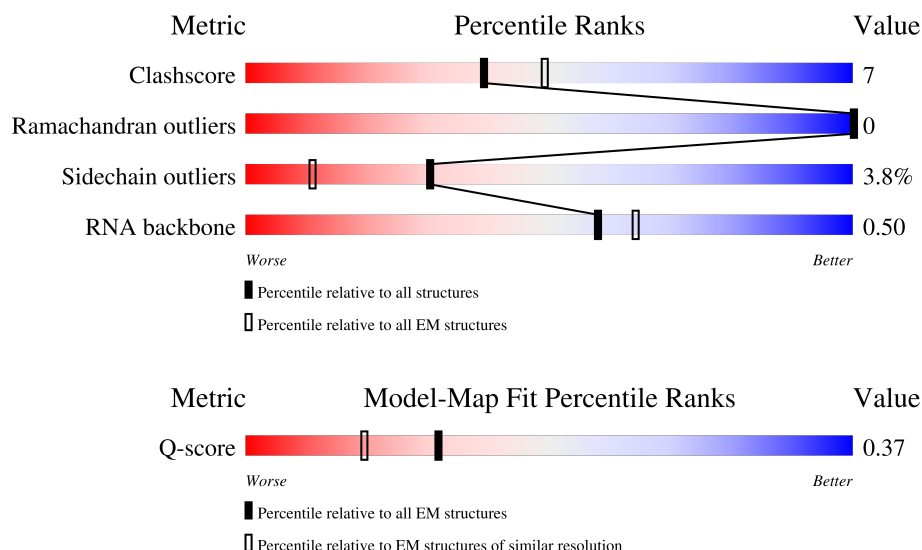
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	3	120	
2	5	76	
3	A	273	

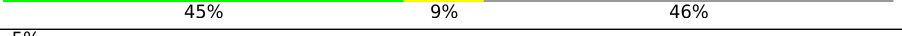
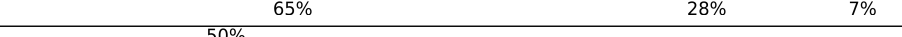
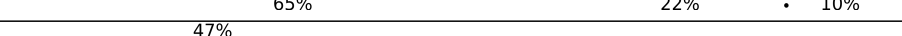
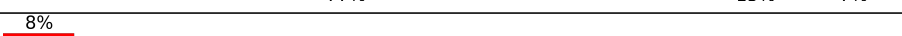
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Mol	Chain	Length	Quality of chain
4	B	209	
5	C	201	
6	D	179	
7	E	177	
8	F	149	
9	G	142	
10	I	123	
11	J	144	
12	K	136	
13	L	127	
14	M	117	
15	N	115	
16	O	118	
17	P	103	
18	Q	110	
19	R	100	
20	S	104	
21	T	94	
22	U	85	
23	V	78	
24	W	63	
25	X	59	
26	Y	57	
27	Z	55	
28	AA	46	

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Mol	Chain	Length	Quality of chain
29	AB	65	
30	AC	38	
31	2	2903	
32	a	241	
33	b	233	
34	c	206	
35	d	167	
36	e	135	
37	f	179	
38	g	130	
39	h	130	
40	i	103	
41	j	129	
42	k	124	
43	l	118	
44	m	101	
45	n	89	
46	o	82	
47	p	84	
48	q	75	
49	r	92	
50	s	87	
51	t	71	
52	1	1540	
53	4	93	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 140036 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	120	A	U	conflict	GB 984297099

- Molecule 2 is a RNA chain called tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	173	Total	C	N	O	S	0	0
			1298	817	238	241	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	48	Total	C	N	O	S	0	0
			368	238	63	66	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	114	Total	C	N	O	S	0	0
			875	542	175	158			

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	90	Total	C	N	O	S	0	0
			714	449	136	128	1		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	S	96	Total	C	N	O		
			735	464	138	133	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	93	Total	C	N	O	S		
			745	474	136	133	2	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	75	Total	C	N	O	S		
			575	356	116	102	1	0	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	60	Total	C	N	O	S		
			491	303	96	91	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	55	Total	C	N	O	S		
			434	263	92	78	1	0	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	48	Total	C	N	O	0	0
			396	255	72	69		

- Molecule 28 is a protein called 50S ribosomal protein L34.

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

- Molecule 29 is a protein called 50S ribosomal protein L35.

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

- Molecule 30 is a protein called 50S ribosomal protein L36.

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

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	2833	Total	C	N	O	P	0	0
			60819	27131	11192	19664	2832		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	208	C	-	insertion	GB 984297099
2	284	U	C	conflict	GB 984297099
2	285	G	A	conflict	GB 984297099
2	356	G	A	conflict	GB 984297099
2	542	C	U	conflict	GB 984297099
2	747	C	U	conflict	GB 984297099
2	1174	U	G	conflict	GB 984297099
2	1211	C	U	conflict	GB 984297099
2	1513	U	C	conflict	GB 984297099
2	1723	G	A	conflict	GB 984297099
2	1730	C	U	conflict	GB 984297099
2	1865	U	C	conflict	GB 984297099
2	2163	A	G	conflict	GB 984297099

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Chain	Residue	Modelled	Actual	Comment	Reference
2	2712	C	U	conflict	GB 984297099
2	2794	C	U	conflict	GB 984297099
2	2796	U	C	conflict	GB 984297099
2	2797	U	C	conflict	GB 984297099
2	2799	A	G	conflict	GB 984297099
2	2802	G	A	conflict	GB 984297099

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	220	Total	C	N	O	S	0	0
			1672	1062	293	310	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	197	Total	C	N	O	S	0	0
			1502	957	276	266	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	159	Total	C	N	O	S	0	0
			1273	796	240	234	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	157	Total	C	N	O	S	0	0
			1146	714	215	211	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	97	Total	C	N	O	S	0	0
			742	467	133	139	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	121	Total	C	N	O	S	0	0
			950	591	189	168	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	89	Total	C	N	O	S	0	0
			726	455	141	129	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	111	Total	C	N	O	S	0	0
			867	535	180	148	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	111	Total	C	N	O	S	0	0
			859	531	172	153	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	87	Total	C	N	O	S	0	0
			702	433	140	128	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	78	Total	C	N	O	S	0	0
			632	400	118	111	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
48	q	54	Total	C	N	O	0	0
			443	281	81	81		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	84	Total	C	N	O	S	0	0
			655	406	136	110	3		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	68	Total	C	N	O	S	0	0
			566	351	120	94	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	1508	Total	C	N	O	P	0	0
			32365	14434	5945	10478	1508		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1517	A	G	conflict	GB 1726036237

- Molecule 53 is a RNA chain called HIV1 frameshift stimulating sequence mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	43	Total	C	N	O	P	0	0
			926	413	174	296	43		

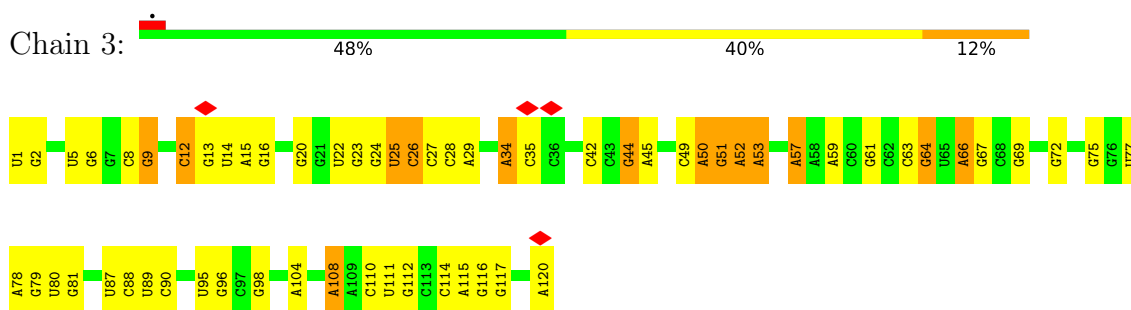
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	2	Total	Mg	0
			2	2	
54	Y	1	Total	Mg	0
			1	1	
54	2	45	Total	Mg	0
			45	45	
54	1	7	Total	Mg	0
			7	7	

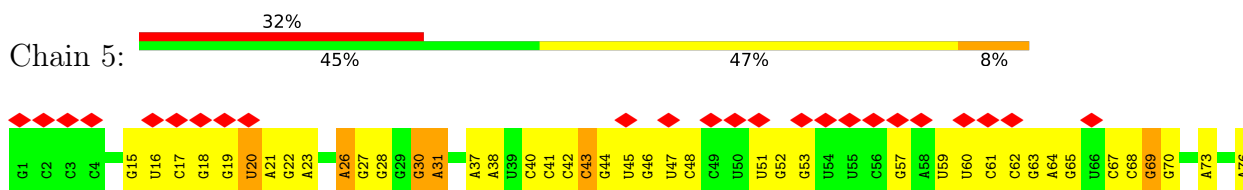
3 Residue-property plots [i](#)

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.

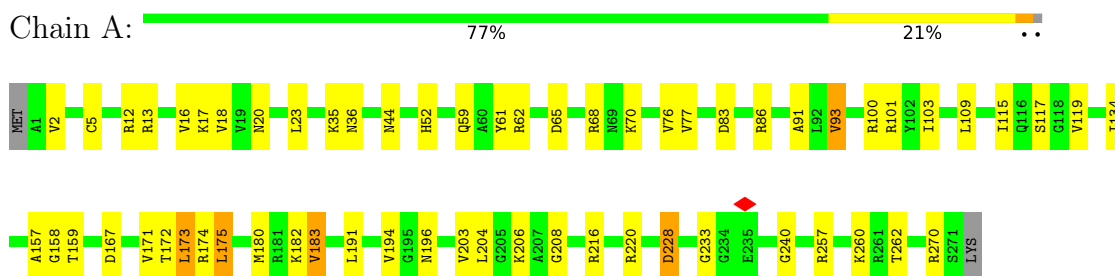
- Molecule 1: 5S ribosomal RNA



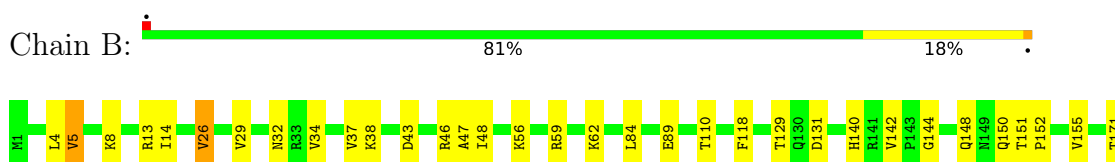
- Molecule 2: tRNA^{Phe}



- Molecule 3: 50S ribosomal protein L2

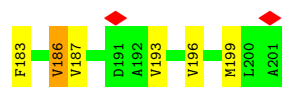
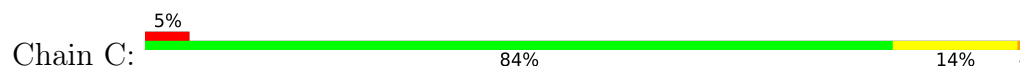


- Molecule 4: 50S ribosomal protein L3

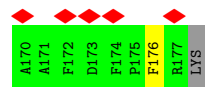
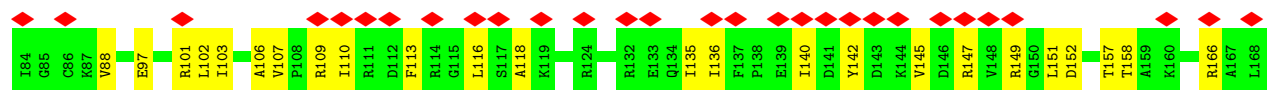
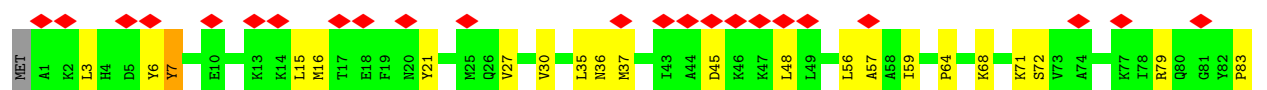




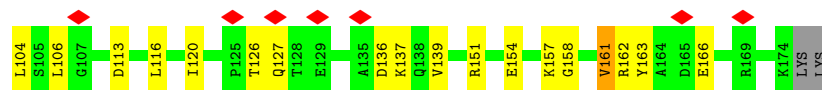
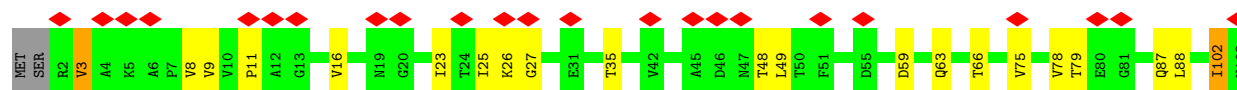
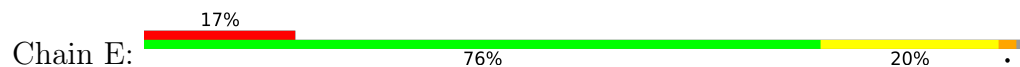
- Molecule 5: 50S ribosomal protein L4



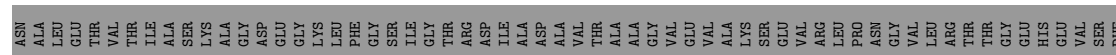
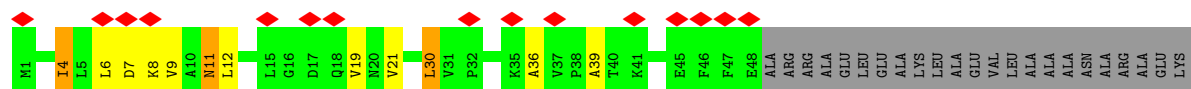
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



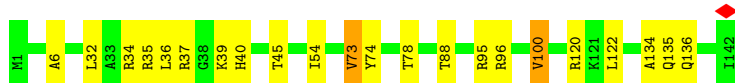
- Molecule 8: 50S ribosomal protein L9



GLN
VAL
HIS
SER
GLU
VAL
PHE
ALA
LYS
VAL
ILE
VAL
ASN
VAL
VAL
ALA
GLU

• Molecule 9: 50S ribosomal protein L13

Chain G:  85% 14%



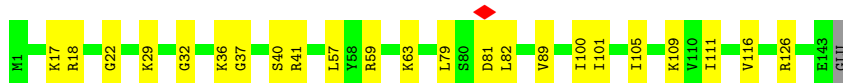
• Molecule 10: 50S ribosomal protein L14

Chain I:  76% 24%



• Molecule 11: 50S ribosomal protein L15

Chain J:  83% 16%



• Molecule 12: 50S ribosomal protein L16

Chain K:  79% 21%



• Molecule 13: 50S ribosomal protein L17

Chain L:  77% 16% 6%



• Molecule 14: 50S ribosomal protein L18

Chain M:  5% 78% 19%



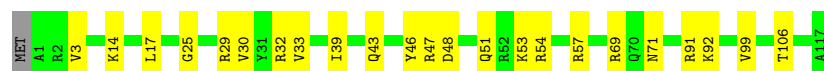
• Molecule 15: 50S ribosomal protein L19

Chain N:  67% 29%



- Molecule 16: 50S ribosomal protein L20

Chain O: 80% 19% .



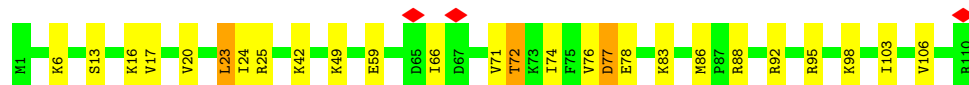
- Molecule 17: 50S ribosomal protein L21

Chain P: 5% 82% 18% .



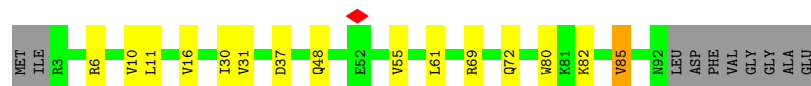
- Molecule 18: 50S ribosomal protein L22

Chain Q: 76% 21% .



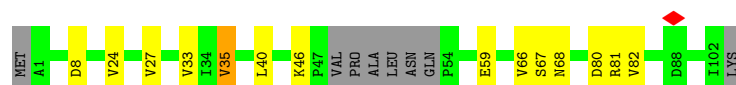
- Molecule 19: 50S ribosomal protein L23

Chain R: 75% 14% 10% .



- Molecule 20: 50S ribosomal protein L24

Chain S: 79% 12% 8% .



- Molecule 21: 50S ribosomal protein L25

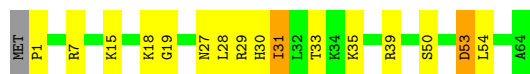
Chain T: 5% 72% 26% ..

Chain AA:  83% 17%



- Molecule 29: 50S ribosomal protein L35

Chain AB:  74% 22%



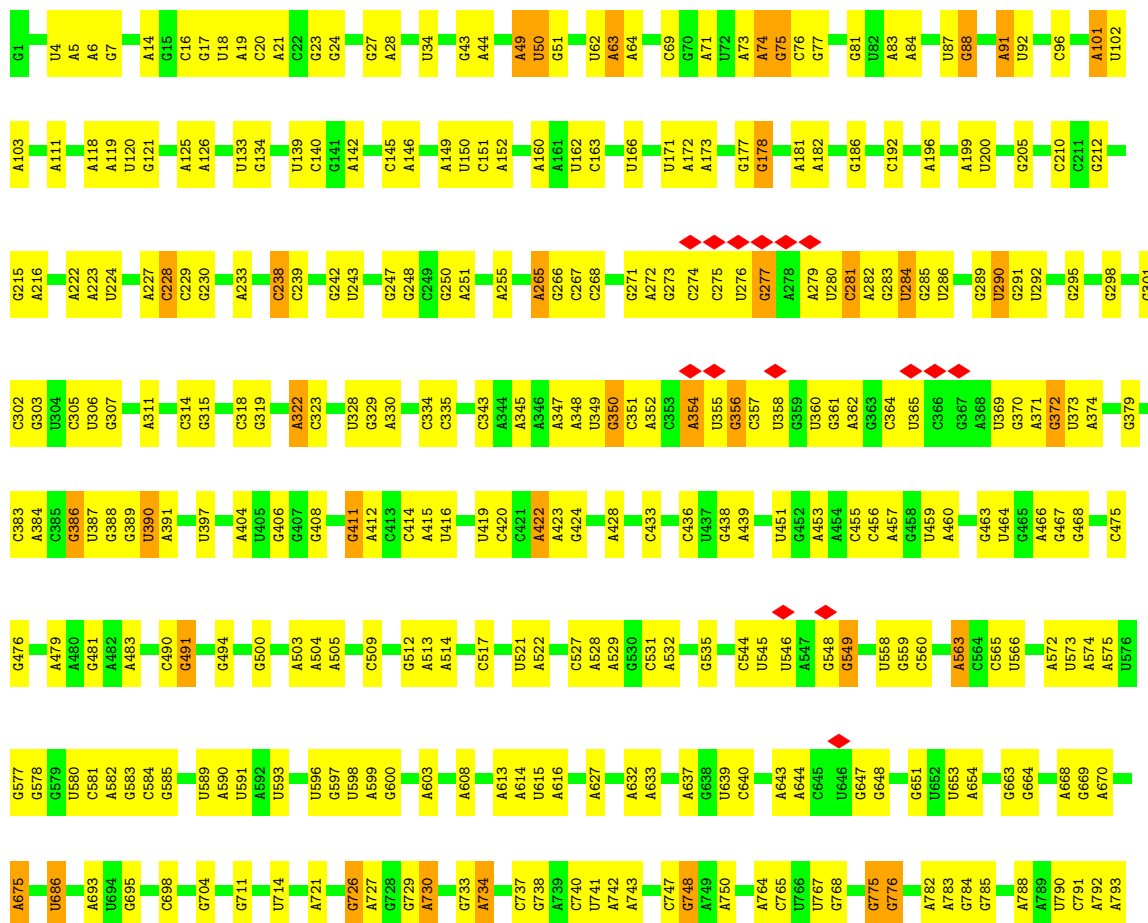
- Molecule 30: 50S ribosomal protein L36

Chain AC:  66% 32%

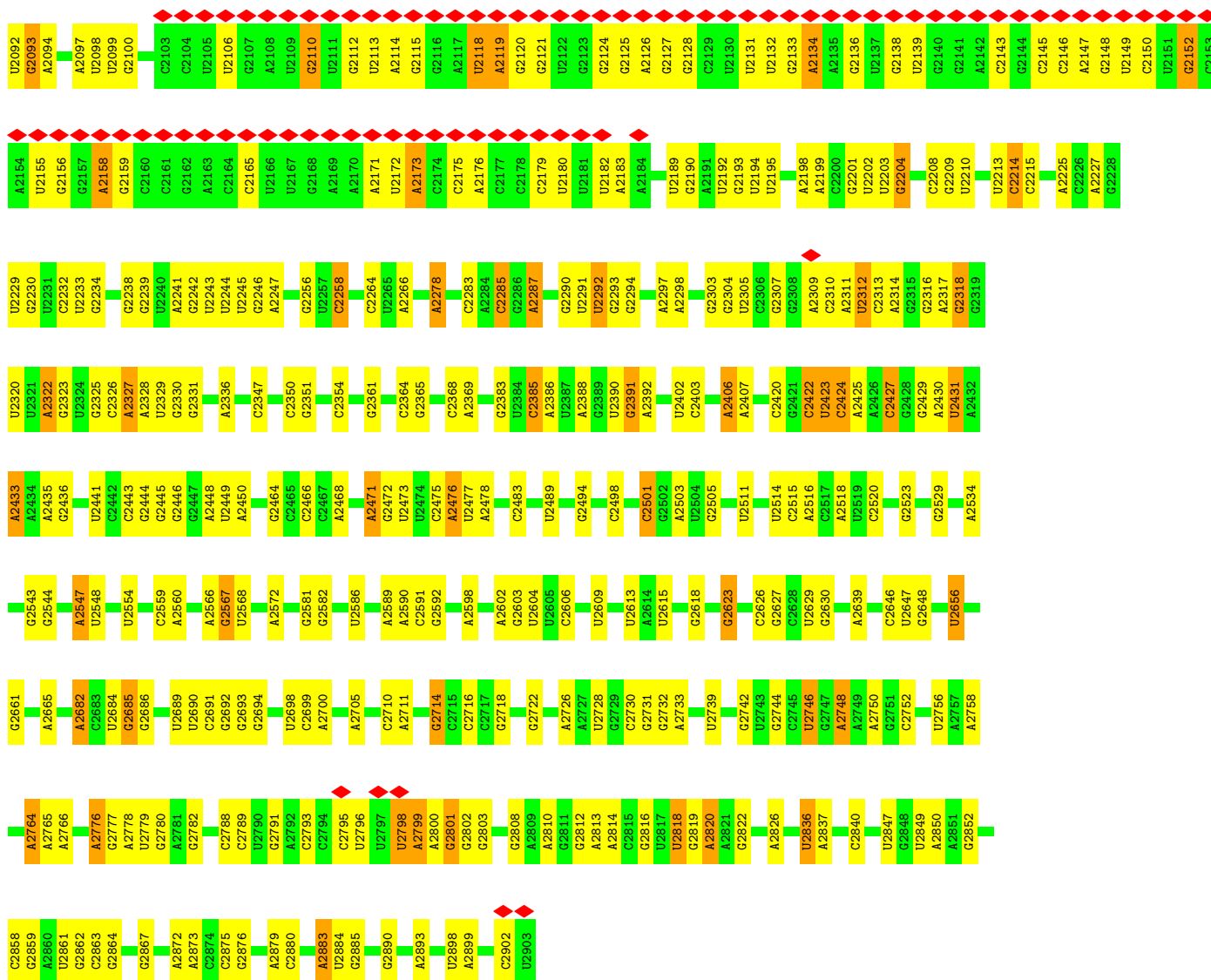


- Molecule 31: 23S ribosomal RNA

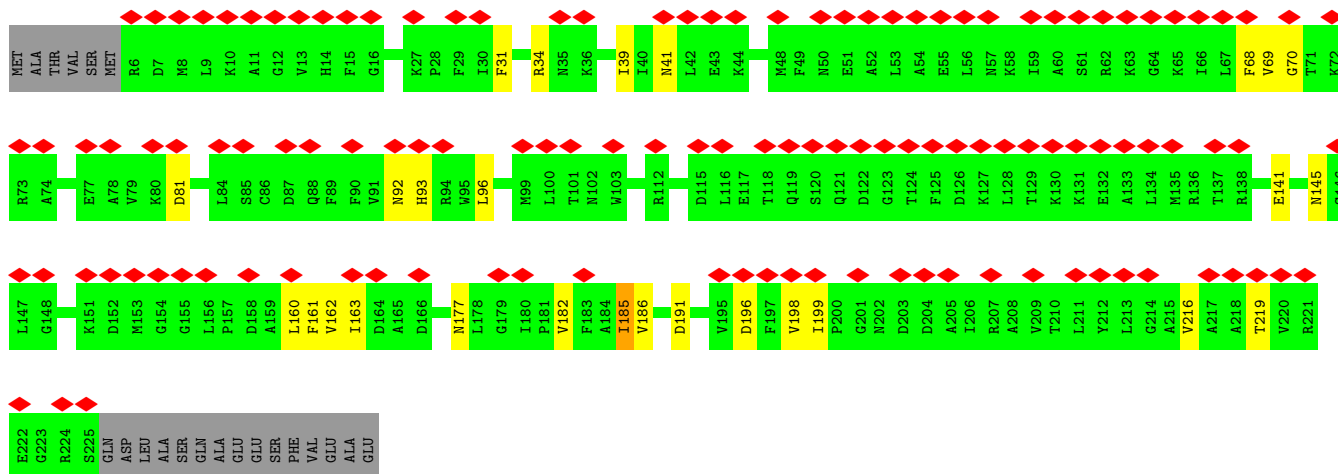
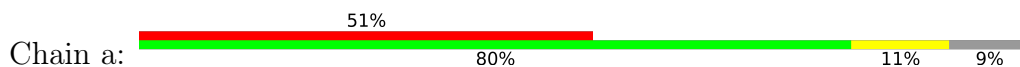
Chain 2:  6% 58% 35% 5%



C1990	A1876	G1769	G1695	G1587	C1498	G1421	C1306	C1211	G	U1113	C	A973	C888	A802
U1991	A1877	C1790	G1699	G1588	C1499	A1427	A1307	C1212		G1115	C	G974	C889	G805
U1992	G1878	A1791		A1570	G1500	C1428	G1311	G1217			A	A975	C890	C906
U1993	U1880		G1702	A1571	G1501		U1312	U1218		U1119	G	A979	G891	U807
U1995	G1883	C1795	U1709	A1572	A1502	A1431	U1313	G1219			U	A980	A992	G808
C1996	U1796	G1797	G1710	A1573	A1503	A1432	U1316	U1220		G1122	G		C993	G809
C1997	U1884	U1798	G1711	A1574	A1504	A1433	G1317	G1223		G1123	U	A983	U894	U811
U1998	G1885			A1575	A1505	A1434	C1323	U1224		G1124	U	A984	U895	C812
G2010	A1889	G1799	U1714		U1506	G1436	U1329	G1225		G1128	G	C986	A996	U813
U2011	A1890	A1801	G1715		U1507	G1437		G1226		G1129	C	C987	C987	C814
G2012		A1802	G1716		C1507	U1438	U1329			U1130	U		C998	
	C1893	A1803	A1717		A1508	A1439		G1236		U1131	U		A899	A819
U2022					A1509	U1440	G1333			U1132	U		A902	A827
C2023	G1902	G1807	G1721		G1510	U1441	G1334	U1242		U1133	A		G993	U828
G2024		A1808	U1722		G1511	U1442	C1335	U1247		A1134	G		C994	
C2025	G1906	A1809	G1723		G1512	U1443	A1336	A1248		C1135	A		C995	
		A1810	G1724		U1513	G1444		U1249			G		G997	U832
A2031	C1909		U1725		G1514	G1445	U1340	G1250		U1141	C		A905	A833
G2032	G1910	C1816	U1726		A1515	C1446	G1341	G1251		A1142	A		U999	G834
A2033	U1911	G1817	C1726		G1516	G1447	C1345	G1252		A1143	A		A910	C835
U2034	A1912	U1818	C1727		G1517	G1448	G1346	A1253			G		A911	G836
G2035	A1913	A1819	C1728		C1518			A1260			C		A1000	C837
C2036			G1728		G1519	G1452				U1148	U		A1009	
A2037	G1924	G1826	U1729		A1522	A1453	A1353	A1264		G1161	A		A1020	C851
G2038	C1925		C1730		U1523	C1454	A1354	G1265		A1162	A		A1021	U852
U2039	G1926	A1829	G1731		G1524	G1455		G1266		G1163	A		G1022	G857
G2040	A1927	C1830	C1732		G1525	G1456	G1360	A1267		G1164	G		A1026	G858
	G1928	G1831	G1733		A1526	U1457	C1361	G1270		A1165	A		A1027	G859
G2043	G1929		G1734		C1526		C1362	G1271			A		A1028	U860
	G1930	G1835	A1735		G1527		G1363	A1272		G1168	A		A1029	A863
			U1736		A1528		A1365	A1275		C1170	G		C1030	C864
C2047	A1936	G1839	G1737		G1529		A1367	G1278		U1172	C		A1032	C865
G2048	A1937		U1738		G1530		G1368	G1279		U1173	U		U1033	A866
A2052	G1938	G1845	C1739		C1531		G1369			U1174	A		G1036	G869
	U1939		A1739		A1532					A1175	U		G1037	
C2055	U1940	A1848	A1744		C1533		A1378			U1176	A		A1038	C873
G2056	C1942	G1849	A1745		U1534		U1379			U1177	G		A1039	G874
A2060		G1850	A1746		A1535					G1178	C		A1040	G875
G2061	G1954	U1851	U1747		C1536		C1386			G1179	U		G1041	A878
A2062	U1955	A1852			G1537		A1387			U1180	C		C	G879
	U1956	A1853	C1752		G1538		G1388			G1186	U		C	G880
G2069			G1753		U1539		A1395				G		C	G881
A2070	A1960	U1856	G1754		G1540		G1407			G1190	U		G	G882
A2071		G1857	A1755		C1541		G1408			U1198	C		A	G883
C2072	G1964	U1858	G1756		A1544		U1409			U1199	U		C	U884
		A1859	U1756		A1545		U1410			G1199	C		A	C885
C2073	G1964	G1859	G1756		G1546		U1411			G1186	U		G	A886
U2074		G1860			G1547		U1412				G		A	
U2075	C1967		A1759		A1548		A1413			G1190	U		C	U887
		U1864			A1549		G1416			U1301	C		C	
U2081	A1970	U1865	A1762		A1554					U1303	A		G	
U2082	U1971	A1866	G1763		A1545		A1419				U		A	
A2083	G1972	G1867	C1764		G1546		A1493				C		C	
		U1868			G1547		A1496				G		A	
U2086	G1983		A1773		A1548						U		C	
G2087		G1869			A1549		G1416				G		A	
A2088	A1987	C1870	U1779		U1554		A1419				U		C	
		A1871			U1559		A1493				C		A	
C2091	G1989	A1872	A1784		G1560		A1420				G		A	
					C1561						C		A	
					U1562						U		C	
					U1563						C		A	
					C1564						G		A	
					G1565						A			
					A1566									



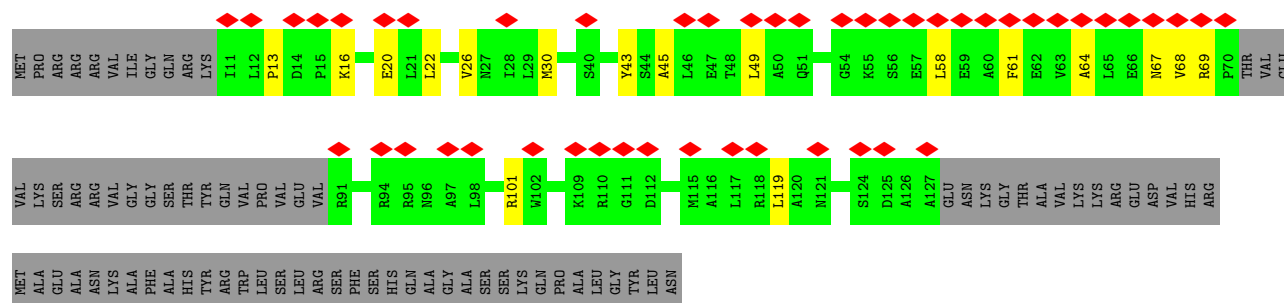
• Molecule 32: 30S ribosomal protein S2



ARG
ASP
ASP
PHE
ALA
ASN
GLU
THR
ASP
ASP
ALA
GLU
GLY
ALA
GLY
SER
SER
GLU
GLU
GLU
GLU
GLU

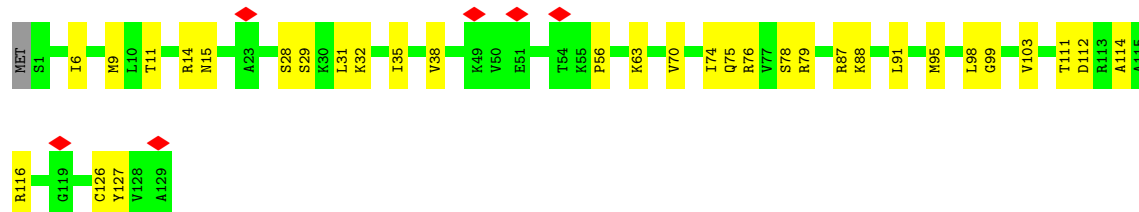
• Molecule 37: 30S ribosomal protein S7

Chain f:



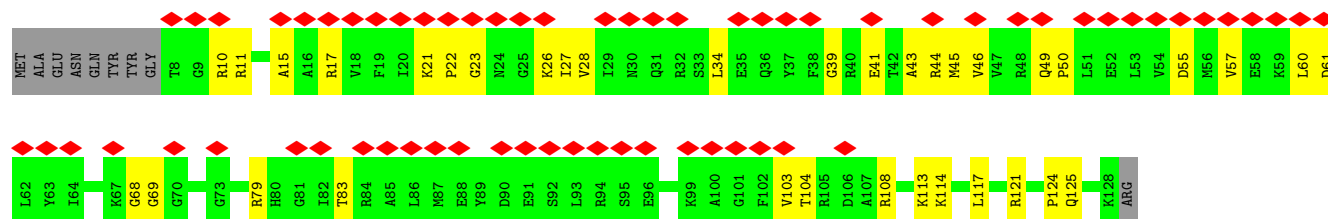
• Molecule 38: 30S ribosomal protein S8

Chain g:



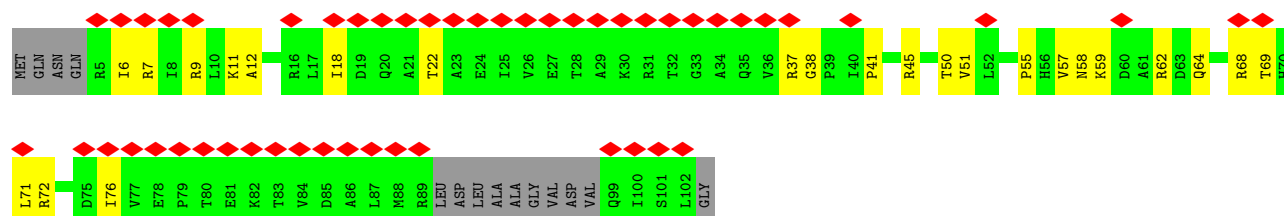
• Molecule 39: 30S ribosomal protein S9

Chain h:

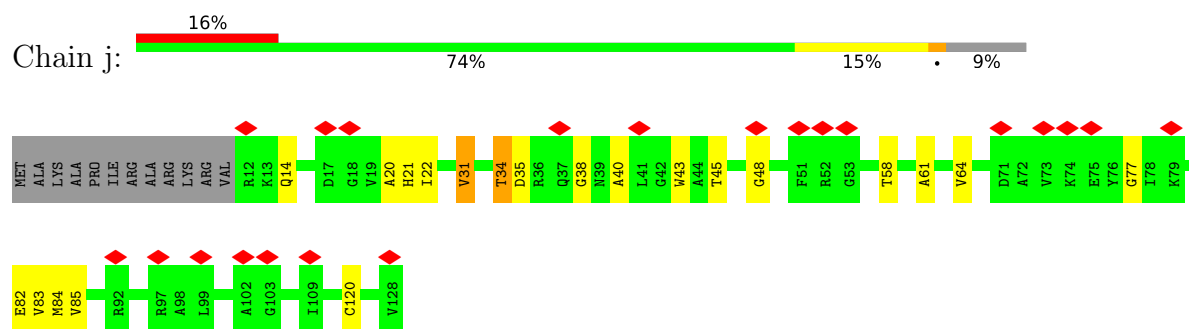


• Molecule 40: 30S ribosomal protein S10

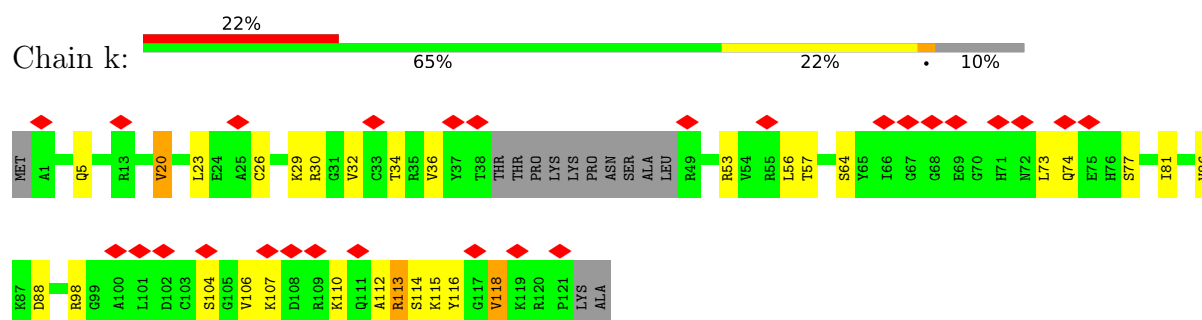
Chain i:



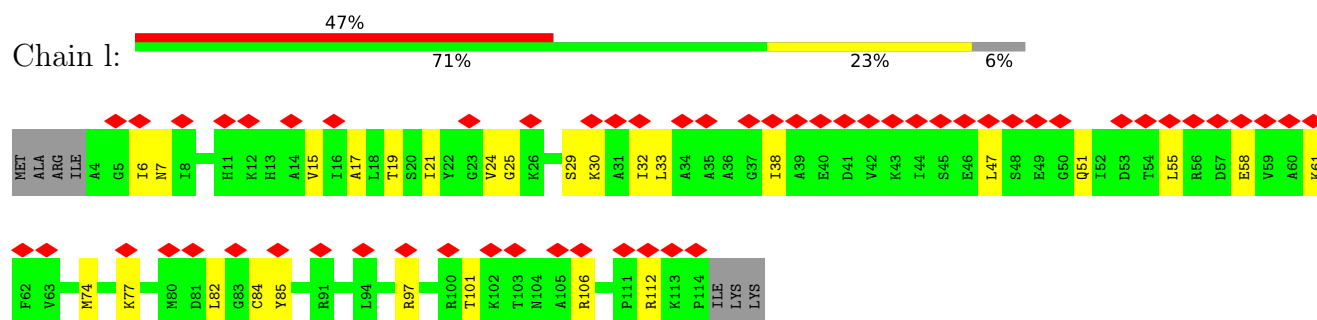
- Molecule 41: 30S ribosomal protein S11



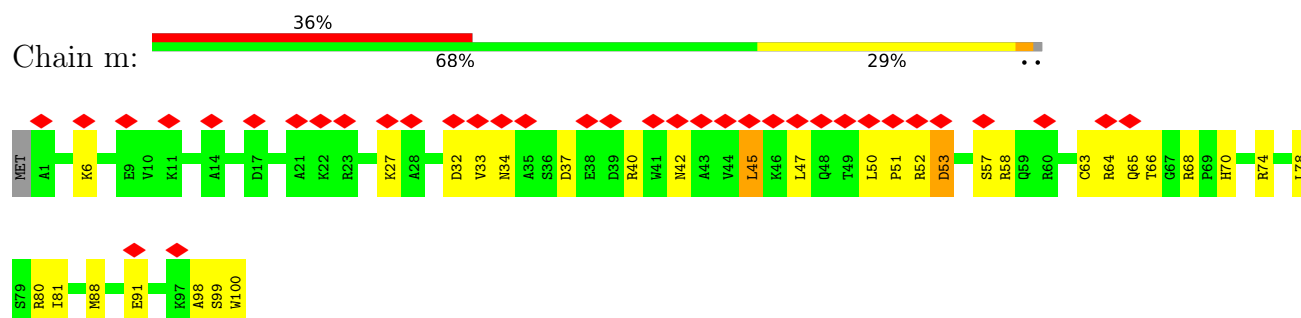
- Molecule 42: 30S ribosomal protein S12



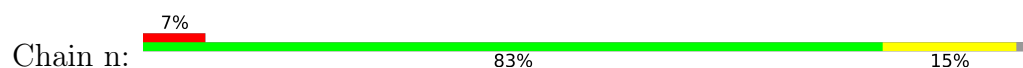
- Molecule 43: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S14

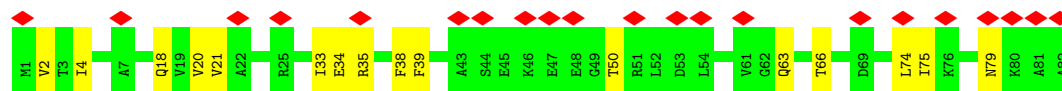
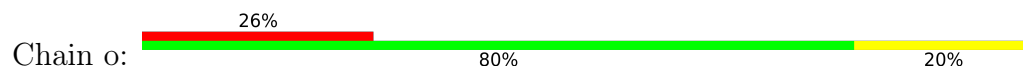


- Molecule 45: 30S ribosomal protein S15

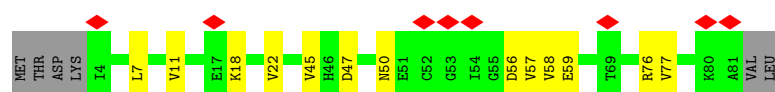
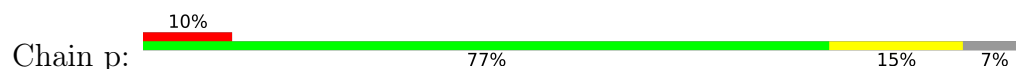




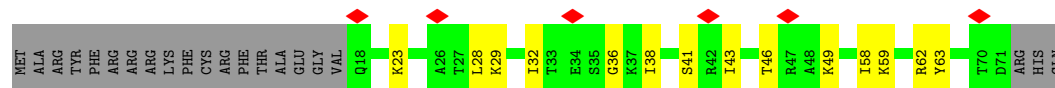
- Molecule 46: 30S ribosomal protein S16



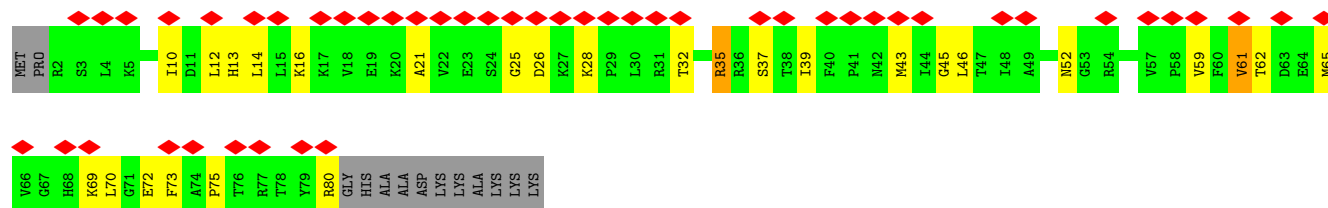
- Molecule 47: 30S ribosomal protein S17



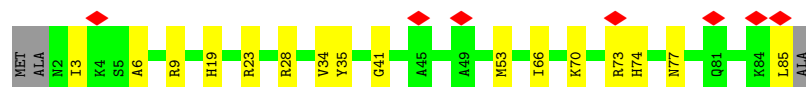
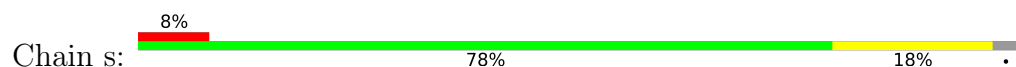
- Molecule 48: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S19

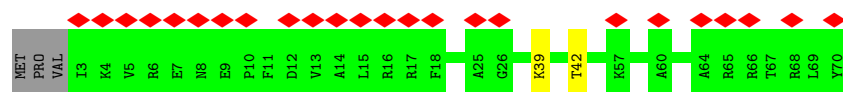


- Molecule 50: 30S ribosomal protein S20

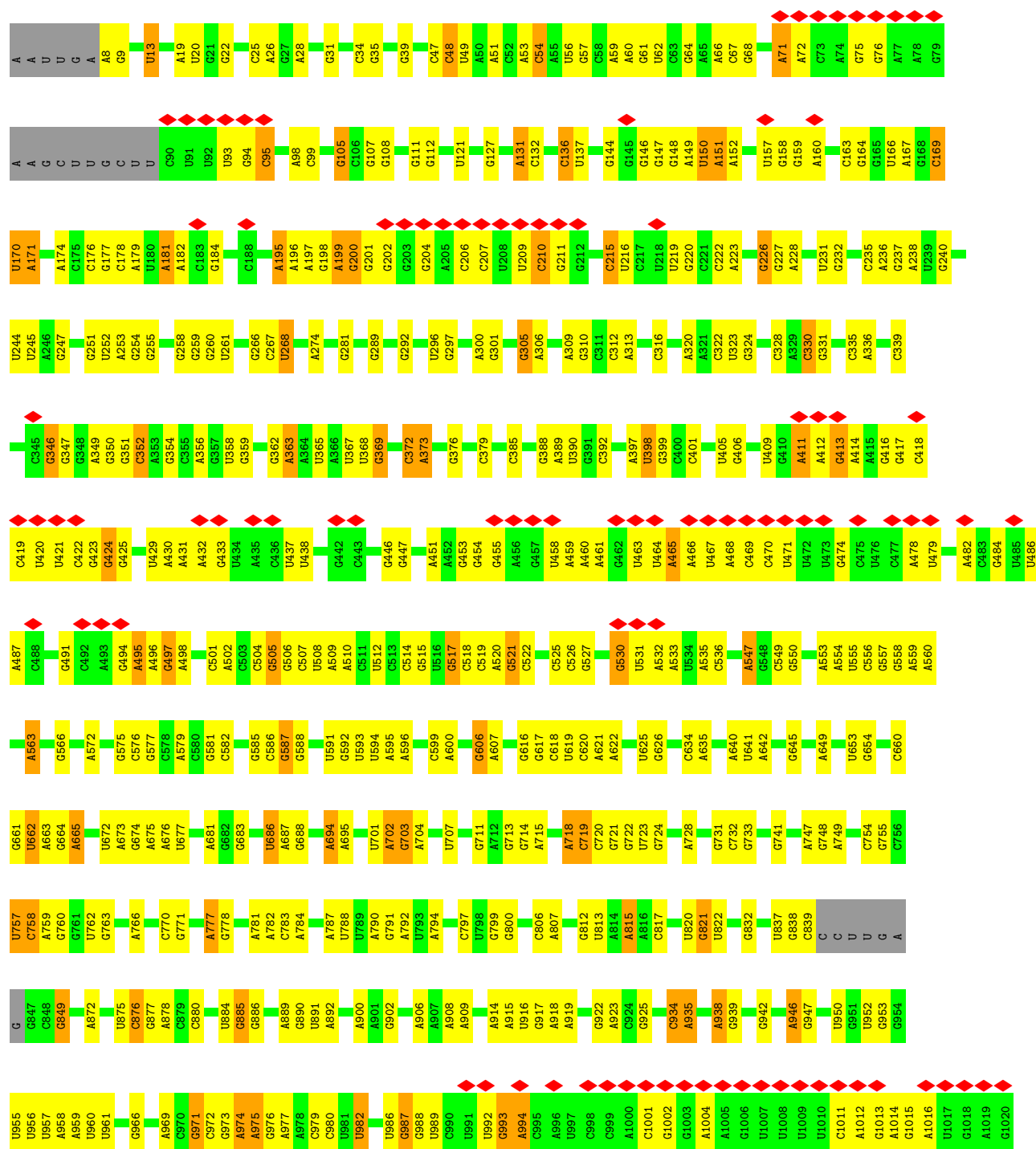


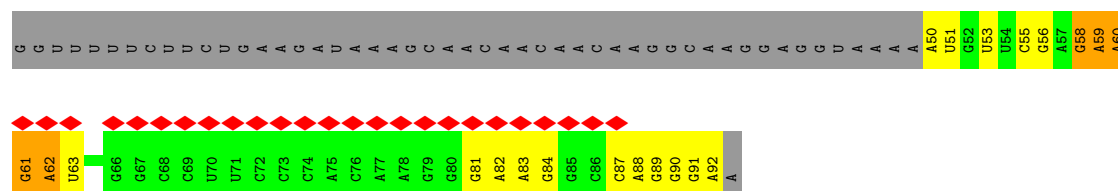
- Molecule 51: 30S ribosomal protein S21





• Molecule 52: 16S ribosomal RNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	640261	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	27.710	Depositor
Minimum map value	-8.896	Depositor
Average map value	0.203	Depositor
Map value standard deviation	1.100	Depositor
Recommended contour level	5.8	Depositor
Map size ($\text{\AA}$)	654.48, 654.48, 654.48	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	3	0.12	0/2872	0.27	0/4479
2	5	0.13	0/1809	0.31	0/2819
3	A	0.13	0/2121	0.33	0/2852
4	B	0.12	0/1586	0.33	0/2134
5	C	0.12	0/1571	0.31	0/2113
6	D	0.14	0/1434	0.40	0/1926
7	E	0.12	0/1318	0.33	0/1786
8	F	0.13	0/373	0.40	0/502
9	G	0.12	0/1152	0.31	0/1551
10	I	0.12	0/956	0.34	0/1279
11	J	0.11	0/1052	0.31	0/1401
12	K	0.12	0/1093	0.33	0/1460
13	L	0.17	0/964	0.41	0/1289
14	M	0.13	0/885	0.38	0/1187
15	N	0.12	0/929	0.36	0/1242
16	O	0.14	0/960	0.32	0/1278
17	P	0.14	0/829	0.38	0/1107
18	Q	0.12	0/864	0.35	0/1156
19	R	0.11	0/720	0.32	0/962
20	S	0.11	0/741	0.30	0/984
21	T	0.12	0/758	0.36	0/1015
22	U	0.12	0/582	0.34	0/769
23	V	0.13	0/635	0.35	0/848
24	W	0.12	0/492	0.31	0/655
25	X	0.13	0/453	0.31	0/605
26	Y	0.12	0/440	0.33	0/588
27	Z	0.10	0/403	0.29	0/538
28	AA	0.12	0/380	0.35	0/498
29	AB	0.14	0/513	0.34	0/676
30	AC	0.14	0/303	0.35	0/397
31	2	0.12	0/68117	0.27	0/106268
32	a	0.12	0/1703	0.35	0/2305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.15	0/1528	0.35	0/2069
34	c	0.14	0/1289	0.41	0/1729
35	d	0.14	0/1159	0.38	0/1561
36	e	0.14	0/843	0.40	0/1140
37	f	0.15	0/750	0.41	0/1009
38	g	0.11	0/989	0.33	0/1326
39	h	0.22	0/960	0.46	0/1280
40	i	0.14	0/735	0.38	0/991
41	j	0.13	0/893	0.40	0/1205
42	k	0.17	0/878	0.46	0/1176
43	l	0.13	0/868	0.37	0/1161
44	m	0.13	0/817	0.37	0/1088
45	n	0.13	0/710	0.32	0/950
46	o	0.14	0/659	0.35	0/884
47	p	0.13	0/641	0.37	0/860
48	q	0.12	0/449	0.36	0/604
49	r	0.20	0/652	0.44	0/877
50	s	0.14	0/661	0.32	0/876
51	t	0.13	0/573	0.34	0/759
52	1	0.12	0/36240	0.28	0/56532
53	4	0.15	0/1037	0.28	0/1616
All	All	0.13	0/152339	0.30	0/228362

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	2568	0	1303	37	0
2	5	1619	0	822	25	0
3	A	2082	0	2157	41	0
4	B	1565	0	1616	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1552	0	1619	19	0
6	D	1410	0	1447	23	0
7	E	1298	0	1340	23	0
8	F	368	0	387	7	0
9	G	1129	0	1162	14	0
10	I	947	0	1023	17	0
11	J	1043	0	1123	17	0
12	K	1074	0	1157	19	0
13	L	951	0	994	12	0
14	M	875	0	906	11	0
15	N	917	0	965	25	0
16	O	947	0	1022	16	0
17	P	816	0	839	13	0
18	Q	857	0	922	20	0
19	R	714	0	773	6	0
20	S	735	0	788	10	0
21	T	745	0	768	15	0
22	U	575	0	592	2	0
23	V	625	0	655	9	0
24	W	491	0	523	2	0
25	X	449	0	491	9	0
26	Y	434	0	448	6	0
27	Z	396	0	424	9	0
28	AA	377	0	418	6	0
29	AB	504	0	574	11	0
30	AC	302	0	343	11	0
31	2	60819	0	30591	587	0
32	a	1672	0	1649	15	0
33	b	1502	0	1534	31	0
34	c	1273	0	1304	23	0
35	d	1146	0	1184	19	0
36	e	824	0	815	11	0
37	f	742	0	762	11	0
38	g	979	0	1034	22	0
39	h	950	0	993	23	0
40	i	726	0	766	21	0
41	j	877	0	887	14	0
42	k	867	0	917	24	0
43	l	859	0	912	21	0
44	m	805	0	847	25	0
45	n	702	0	724	6	0
46	o	649	0	666	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	p	632	0	669	5	0
48	q	443	0	466	10	0
49	r	637	0	665	21	0
50	s	655	0	705	12	0
51	t	566	0	597	1	0
52	1	32365	0	16288	466	0
53	4	926	0	467	20	0
54	1	7	0	0	0	0
54	2	45	0	0	0	0
54	A	2	0	0	0	0
54	Y	1	0	0	0	0
All	All	140036	0	93043	1621	0

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

All (1621) 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)
52:1:412:A:H62	52:1:431:A:N6	1.36	1.24
53:4:62:A:N6	53:4:91:G:H1	1.47	1.11
52:1:412:A:N6	52:1:431:A:H61	1.52	1.08
31:2:2114:A:C6	31:2:2119:A:N6	2.26	1.02
31:2:1527:G:H21	31:2:1545:A:N6	1.59	1.01
52:1:447:G:H21	52:1:487:A:H62	1.11	0.99
31:2:1527:G:N2	31:2:1545:A:H62	1.63	0.97
52:1:75:G:H1	52:1:95:C:H42	0.98	0.95
31:2:1858:A:N6	31:2:1884:G:H21	1.63	0.95
1:3:72:G:N2	1:3:104:A:H62	1.64	0.94
2:5:51:U:H3	2:5:63:G:H1	1.02	0.93
31:2:1858:A:N6	31:2:1884:G:N2	2.16	0.93
31:2:1360:G:H22	31:2:2214:C:H42	1.17	0.93
52:1:76:G:H1	52:1:93:U:H3	1.03	0.93
52:1:202:G:H1	52:1:215:C:H42	1.16	0.93
52:1:75:G:H1	52:1:95:C:N4	1.67	0.92
1:3:72:G:H21	1:3:104:A:H62	0.92	0.92
52:1:447:G:N2	52:1:487:A:H62	1.67	0.92
52:1:1088:G:N2	52:1:1167:A:H61	1.66	0.91
1:3:72:G:H21	1:3:104:A:N6	1.69	0.90
52:1:575:G:H1	52:1:880:C:H42	1.19	0.90
52:1:1088:G:H21	52:1:1167:A:H61	1.14	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:1360:G:H22	31:2:2214:C:N4	1.70	0.89
52:1:925:G:H1	52:1:1391:U:H3	1.21	0.89
31:2:1483:G:H1	31:2:1506:U:H3	0.98	0.88
1:3:9:G:H1	1:3:111:U:H3	1.20	0.88
52:1:1088:G:H21	52:1:1167:A:N6	1.72	0.88
52:1:463:U:H3	52:1:469:C:H42	0.91	0.88
2:5:20:U:C4	2:5:59:U:O4	2.27	0.87
52:1:447:G:H21	52:1:487:A:N6	1.70	0.87
31:2:2099:U:H3	31:2:2190:G:H1	0.88	0.87
52:1:1445:U:H3	52:1:1457:G:H1	1.15	0.87
31:2:280:U:H3	31:2:360:U:H3	1.16	0.86
53:4:62:A:N6	53:4:91:G:N1	2.23	0.86
31:2:1858:A:C6	31:2:1884:G:N2	2.44	0.85
52:1:463:U:H3	52:1:469:C:N4	1.74	0.85
52:1:1238:A:H62	52:1:1301:U:H3	1.24	0.85
31:2:1527:G:H21	31:2:1545:A:H62	0.89	0.84
31:2:1360:G:N2	31:2:2214:C:H42	1.74	0.83
52:1:686:U:C2	52:1:704:A:N6	2.46	0.83
52:1:687:A:C6	52:1:703:G:N2	2.46	0.83
52:1:13:U:O4	52:1:20:U:O4	1.95	0.83
18:Q:42:LYS:HB2	31:2:2010:G:H5"	1.62	0.82
52:1:409:U:H3	52:1:433:G:H1	1.24	0.82
31:2:1858:A:N6	31:2:1884:G:C2	2.47	0.81
53:4:62:A:H61	53:4:91:G:H1	1.28	0.81
52:1:458:U:H3	52:1:474:G:H1	1.30	0.80
2:5:26:A:N6	2:5:44:G:C6	2.51	0.79
53:4:62:A:H62	53:4:91:G:H1	1.31	0.78
52:1:437:U:H3	52:1:495:A:H62	1.32	0.78
52:1:686:U:N3	52:1:704:A:N6	2.32	0.77
31:2:2114:A:C5	31:2:2119:A:N6	2.52	0.77
52:1:923:A:H61	52:1:1393:U:H3	1.30	0.77
17:P:1:MET:HA	17:P:42:ALA:O	1.83	0.77
31:2:2114:A:N6	31:2:2119:A:C6	2.53	0.77
29:AB:50:SER:O	29:AB:54:LEU:HB2	1.84	0.76
52:1:686:U:N3	52:1:704:A:C6	2.54	0.76
31:2:1858:A:C5	31:2:1884:G:N2	2.54	0.76
52:1:412:A:N6	52:1:431:A:N6	2.20	0.76
52:1:934:C:N3	52:1:938:A:N1	2.34	0.76
52:1:1242:G:H1	52:1:1295:U:H3	1.33	0.75
31:2:160:A:H62	31:2:166:U:H3	1.32	0.75
52:1:687:A:C5	52:1:703:G:N2	2.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:202:G:H1	52:1:215:C:N4	1.85	0.74
52:1:950:U:H3	52:1:1231:G:H1	1.35	0.74
1:3:29:A:H1'	1:3:57:A:H61	1.52	0.74
52:1:1239:A:H62	52:1:1299:A:H2	1.34	0.73
52:1:198:G:H1	52:1:219:U:H3	1.36	0.72
52:1:111:G:H1	52:1:330:C:H41	1.35	0.72
52:1:202:G:N2	52:1:215:C:N3	2.37	0.72
52:1:292:G:N7	52:1:305:G:N2	2.38	0.72
53:4:61:G:O6	53:4:92:A:N1	2.23	0.71
31:2:2431:U:C4	31:2:2433:A:N7	2.59	0.71
31:2:1858:A:H62	31:2:1884:G:N2	1.78	0.70
52:1:1304:G:H21	52:1:1333:A:H62	1.39	0.70
31:2:285:G:H1	31:2:355:U:H3	1.38	0.70
31:2:2110:G:H1	31:2:2179:C:H42	1.40	0.70
44:m:53:ASP:HA	44:m:58:ARG:HG3	1.75	0.69
31:2:837:C:N3	31:2:941:A:N6	2.41	0.69
52:1:157:U:H3	52:1:164:G:H1	1.41	0.68
43:l:7:ASN:HD22	43:l:21:ILE:HG13	1.57	0.68
31:2:1478:G:H1	31:2:1513:U:H3	1.39	0.68
33:b:53:ARG:HB2	33:b:68:HIS:HB2	1.76	0.68
52:1:1356:G:H2'	52:1:1357:A:H8	1.59	0.68
31:2:1428:C:H42	31:2:1570:A:H62	1.43	0.67
52:1:1403:C:N4	53:4:55:C:OP1	2.27	0.67
8:F:30:LEU:HD13	8:F:36:ALA:HB3	1.77	0.67
31:2:265:A:H5'	31:2:428:A:H61	1.59	0.67
36:e:42:TRP:HB2	36:e:59:TYR:HB2	1.76	0.66
4:B:4:LEU:HD23	4:B:29:VAL:HG11	1.78	0.66
11:J:59:ARG:HH11	31:2:250:G:H5'	1.61	0.66
49:r:43:MET:HG3	49:r:46:LEU:HD22	1.76	0.66
52:1:412:A:H62	52:1:431:A:H61	0.68	0.66
52:1:1239:A:N6	52:1:1299:A:C2	2.60	0.66
52:1:1175:G:H2'	52:1:1176:A:H8	1.61	0.66
2:5:26:A:N6	2:5:44:G:N1	2.44	0.66
1:3:22:U:H3	1:3:61:G:H1	1.43	0.65
31:2:274:C:H42	31:2:364:C:H42	1.44	0.65
31:2:698:C:O2'	31:2:734:A:N6	2.29	0.65
31:2:1801:A:N6	31:2:2201:G:O2'	2.28	0.65
7:E:11:PRO:HG2	7:E:79:THR:HG21	1.78	0.65
31:2:1433:A:N1	31:2:1560:G:O6	2.29	0.65
52:1:575:G:N2	52:1:880:C:N3	2.41	0.65
2:5:20:U:C5	2:5:59:U:O4	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:517:G:H21	52:1:530:G:H5''	1.61	0.65
52:1:837:U:H3	52:1:849:G:H1	1.45	0.65
31:2:1036:G:H1	31:2:1119:U:H3	1.42	0.65
31:2:1779:U:OP2	31:2:1784:A:N6	2.30	0.65
42:k:98:ARG:HB3	42:k:116:TYR:HA	1.78	0.65
48:q:36:GLY:O	48:q:62:ARG:NH2	2.30	0.65
52:1:181:A:H2'	52:1:182:A:H8	1.63	0.64
52:1:520:A:H61	52:1:533:A:H61	1.45	0.64
15:N:28:LYS:HB2	15:N:82:SER:HB3	1.78	0.64
52:1:454:G:H2'	52:1:455:G:H8	1.62	0.64
52:1:575:G:H1	52:1:880:C:N4	1.93	0.64
1:3:66:A:N6	1:3:108:A:OP2	2.30	0.64
31:2:200:U:H3	31:2:250:G:H1	1.46	0.64
3:A:159:THR:HG21	31:2:1819:A:H5''	1.79	0.64
31:2:832:U:H2'	31:2:833:A:H8	1.62	0.64
31:2:1597:A:H5''	31:2:1598:A:H5'	1.80	0.64
52:1:1433:A:N6	52:1:1467:C:O2	2.30	0.64
1:3:28:C:H2'	1:3:29:A:H8	1.63	0.64
52:1:519:C:OP1	53:4:59:A:N6	2.31	0.64
52:1:674:G:H2'	52:1:675:A:H8	1.62	0.64
31:2:668:A:H2'	31:2:670:A:H62	1.62	0.64
29:AB:53:ASP:OD1	29:AB:53:ASP:N	2.27	0.63
52:1:1345:U:O2	52:1:1376:U:O2	2.16	0.63
31:2:251:A:H61	31:2:386:G:H1	1.46	0.63
3:A:257:ARG:NH2	31:2:1799:G:OP1	2.31	0.63
34:c:151:GLN:HG2	34:c:155:LYS:HG2	1.79	0.63
31:2:2682:A:H61	31:2:2728:U:H1'	1.63	0.63
31:2:2114:A:N6	31:2:2119:A:N6	2.46	0.63
33:b:64:ARG:HG2	33:b:99:GLN:HE21	1.64	0.63
52:1:582:C:OP2	52:1:758:C:N4	2.32	0.63
31:2:514:A:N3	31:2:581:C:O2'	2.28	0.63
38:g:14:ARG:NH1	52:1:875:U:O2'	2.32	0.63
52:1:1160:G:H1	52:1:1176:A:H61	1.47	0.62
52:1:1239:A:N6	52:1:1299:A:H2	1.94	0.62
7:E:136:ASP:HB3	7:E:139:VAL:HG12	1.80	0.62
52:1:606:G:H5''	52:1:607:A:H5'	1.81	0.62
3:A:5:CYS:SG	3:A:17:LYS:NZ	2.73	0.62
2:5:42:C:H1'	52:1:1338:G:H21	1.64	0.62
10:I:69:VAL:HG11	10:I:106:GLU:HG3	1.79	0.62
33:b:75:VAL:HG22	33:b:76:ILE:HG13	1.80	0.62
4:B:151:THR:OG1	31:2:2032:G:N2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:1408:G:H1	31:2:1594:U:H3	1.45	0.62
42:k:26:CYS:SG	42:k:29:LYS:NZ	2.72	0.62
31:2:1723:G:O6	31:2:1738:G:N2	2.33	0.62
52:1:373:A:O2'	52:1:451:A:N7	2.33	0.62
31:2:1303:G:N7	31:2:1607:C:N4	2.46	0.61
31:2:1858:A:N7	31:2:1884:G:N2	2.48	0.61
12:K:36:VAL:HG23	21:T:82:TYR:HB2	1.82	0.61
31:2:1433:A:H2'	31:2:1434:A:H8	1.65	0.61
31:2:1475:G:O2'	31:2:1732:C:N4	2.33	0.61
39:h:45:MET:SD	39:h:49:GLN:NE2	2.72	0.61
15:N:92:ARG:HD3	31:2:1753:G:H5''	1.82	0.61
33:b:110:LEU:HG	33:b:143:LEU:HD23	1.81	0.61
41:j:34:THR:HB	41:j:40:ALA:HA	1.81	0.61
13:L:53:THR:HG21	31:2:2840:C:H5''	1.82	0.61
31:2:290:U:O2	31:2:350:G:N2	2.34	0.61
14:M:64:TYR:O	14:M:67:ASN:ND2	2.33	0.61
52:1:454:G:N2	52:1:479:U:O2	2.34	0.61
3:A:172:THR:HG22	3:A:182:LYS:HB3	1.82	0.61
11:J:18:ARG:NH1	31:2:1250:G:N7	2.48	0.61
31:2:62:U:H3'	31:2:63:A:H5''	1.83	0.61
23:V:57:VAL:HG23	31:2:372:G:H5'	1.82	0.61
31:2:463:G:N2	31:2:466:A:OP2	2.30	0.61
31:2:2229:U:H2'	31:2:2230:G:H8	1.66	0.61
48:q:38:ILE:HD12	48:q:58:ILE:HD13	1.83	0.61
32:a:70:GLY:HA3	32:a:163:ILE:HG12	1.83	0.60
50:s:41:GLY:HA2	50:s:85:LEU:HD21	1.81	0.60
10:I:76:VAL:H	15:N:72:VAL:HG22	1.65	0.60
16:O:48:ASP:OD1	31:2:559:G:N2	2.29	0.60
3:A:134:ILE:HD11	3:A:191:LEU:HD21	1.83	0.60
31:2:767:U:H2'	31:2:768:G:H8	1.66	0.60
39:h:83:THR:HG21	39:h:104:THR:HG21	1.83	0.60
52:1:766:A:N6	52:1:813:U:C2	2.70	0.60
6:D:59:ILE:O	6:D:101:ARG:NH1	2.34	0.60
52:1:876:C:H2'	52:1:877:G:H8	1.65	0.60
30:AC:16:ILE:HG22	30:AC:25:VAL:HB	1.83	0.60
29:AB:7:ARG:NH1	31:2:243:U:OP2	2.34	0.60
31:2:383:C:N3	31:2:391:A:N6	2.50	0.60
6:D:109:ARG:NH1	6:D:136:ILE:O	2.35	0.60
41:j:43:TRP:HE1	52:1:686:U:H1'	1.66	0.60
52:1:687:A:N7	52:1:703:G:N1	2.50	0.60
16:O:32:ARG:O	31:2:1252:G:N2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:987:C:O2'	31:2:1000:A:N3	2.33	0.60
52:1:553:A:H2'	52:1:554:A:H8	1.66	0.60
15:N:50:ARG:NH1	31:2:2684:U:OP2	2.35	0.59
17:P:71:LYS:NZ	31:2:1225:G:OP1	2.34	0.59
31:2:2258:C:O2'	31:2:2427:C:OP2	2.20	0.59
52:1:687:A:N6	52:1:703:G:N2	2.49	0.59
48:q:41:SER:HG	48:q:46:THR:HG1	1.44	0.59
17:P:79:ARG:NH2	31:2:563:A:OP2	2.35	0.59
31:2:475:C:O2	31:2:479:A:N6	2.35	0.59
31:2:2114:A:N6	31:2:2119:A:C5	2.70	0.59
53:4:87:C:H2'	53:4:88:A:H8	1.68	0.59
31:2:2134:A:N6	31:2:2158:A:O2'	2.36	0.59
52:1:1160:G:H1	52:1:1176:A:N6	2.01	0.59
10:I:19:VAL:HG21	10:I:41:ILE:HD12	1.84	0.59
31:2:848:C:H2'	31:2:849:A:H8	1.66	0.59
31:2:2515:C:H2'	31:2:2516:A:H8	1.67	0.59
37:f:101:ARG:NH2	52:1:1375:A:O2'	2.36	0.59
52:1:1266:G:N2	52:1:1269:A:OP2	2.36	0.59
38:g:11:THR:HG22	38:g:14:ARG:HH12	1.68	0.59
50:s:73:ARG:O	50:s:77:ASN:ND2	2.34	0.59
5:C:196:VAL:HA	5:C:199:MET:HG2	1.83	0.58
15:N:102:ARG:NH1	31:2:1754:A:O2'	2.37	0.58
23:V:15:ASN:OD1	23:V:15:ASN:N	2.36	0.58
35:d:11:GLN:NE2	35:d:116:VAL:O	2.36	0.58
40:i:38:GLY:HA3	52:1:1123:U:H4'	1.84	0.58
1:3:50:A:N1	1:3:51:G:N2	2.51	0.58
43:l:85:TYR:N	49:r:72:GLU:O	2.35	0.58
20:S:67:SER:OG	31:2:335:C:O2	2.20	0.58
52:1:362:G:N2	52:1:365:U:OP2	2.36	0.58
33:b:35:ASP:HB3	33:b:58:ARG:HH22	1.69	0.58
41:j:22:ILE:HD11	41:j:85:VAL:HG22	1.85	0.58
18:Q:86:MET:HE3	18:Q:88:ARG:HD3	1.85	0.58
52:1:664:G:H22	52:1:741:G:H1	1.52	0.58
52:1:1060:U:H2'	52:1:1061:G:H8	1.69	0.58
31:2:1826:G:O2'	31:2:1971:U:OP2	2.21	0.58
38:g:11:THR:O	38:g:15:ASN:ND2	2.36	0.58
21:T:30:ILE:HG12	21:T:91:PHE:HB2	1.85	0.58
31:2:1032:A:N1	31:2:1122:G:O6	2.37	0.58
31:2:2471:A:N6	31:2:2476:A:O2'	2.36	0.58
35:d:16:ALA:HB3	35:d:35:LEU:HB3	1.83	0.58
52:1:411:A:H2	52:1:430:A:H62	1.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AC:19:ARG:HD2	30:AC:24:ARG:HD2	1.85	0.58
31:2:2298:A:H62	31:2:2318:G:H21	1.52	0.58
35:d:84:VAL:HG12	35:d:95:MET:HB2	1.85	0.58
52:1:231:U:H2'	52:1:232:G:H8	1.69	0.58
11:J:81:ASP:HB3	11:J:100:ILE:HD13	1.85	0.58
31:2:2233:U:H2'	31:2:2234:G:H8	1.69	0.58
42:k:98:ARG:HG2	42:k:106:VAL:HG23	1.86	0.58
46:o:75:ILE:O	46:o:79:ASN:ND2	2.37	0.58
52:1:258:G:H1	52:1:268:U:H3	1.50	0.58
52:1:1241:G:H2'	52:1:1242:G:C8	2.39	0.58
31:2:476:G:N1	31:2:479:A:OP2	2.36	0.57
39:h:11:ARG:NH2	52:1:1347:G:N7	2.52	0.57
9:G:120:ARG:NE	31:2:2780:G:OP2	2.35	0.57
12:K:26:VAL:HG11	12:K:133:LYS:HA	1.86	0.57
31:2:1040:A:N1	31:2:1115:G:O6	2.36	0.57
35:d:134:ASN:ND2	52:1:19:A:OP1	2.37	0.57
52:1:1304:G:N2	52:1:1333:A:H62	2.01	0.57
31:2:121:G:H4'	31:2:149:A:H5'	1.86	0.57
31:2:807:U:O2'	31:2:2060:A:N1	2.36	0.57
52:1:934:C:C2	52:1:938:A:N6	2.71	0.57
52:1:971:G:OP2	52:1:1231:G:N2	2.37	0.57
3:A:86:ARG:NH1	31:2:1817:G:OP1	2.37	0.57
9:G:32:LEU:HD22	9:G:54:ILE:HG21	1.85	0.57
31:2:950:G:H1	31:2:967:U:H3	1.51	0.57
31:2:1830:C:H2'	31:2:1831:G:H8	1.70	0.57
31:2:1386:C:H2'	31:2:1387:A:H8	1.70	0.57
52:1:157:U:O2	52:1:164:G:N2	2.31	0.57
52:1:993:G:O2'	52:1:994:A:N7	2.38	0.57
1:3:78:A:H62	1:3:98:G:H21	1.53	0.57
9:G:135:GLN:NE2	31:2:6:A:N3	2.52	0.57
27:Z:25:ASN:ND2	31:2:2285:C:OP1	2.37	0.57
52:1:687:A:N7	52:1:703:G:C2	2.72	0.57
27:Z:29:LYS:NZ	31:2:2287:A:OP1	2.36	0.57
31:2:2446:G:N2	31:2:2449:U:O2	2.34	0.57
42:k:86:VAL:HG13	42:k:88:ASP:H	1.70	0.57
52:1:1347:G:H21	52:1:1373:G:H3'	1.69	0.57
4:B:37:VAL:HG12	4:B:48:ILE:HG22	1.86	0.57
31:2:814:C:H1'	31:2:1225:G:H21	1.70	0.56
32:a:92:ASN:OD1	32:a:93:HIS:ND1	2.38	0.56
10:I:26:GLY:HA3	10:I:30:ARG:HH11	1.70	0.56
17:P:80:ARG:NH2	31:2:572:A:OP2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:1668:A:N3	31:2:1670:C:N4	2.53	0.56
50:s:3:ILE:HG22	50:s:6:ALA:H	1.70	0.56
1:3:80:U:O2'	31:2:918:A:N3	2.37	0.56
4:B:148:GLN:HB2	4:B:152:PRO:HG2	1.87	0.56
7:E:16:VAL:HG12	7:E:25:ILE:HG12	1.86	0.56
11:J:79:LEU:HB3	11:J:116:VAL:HG13	1.87	0.56
12:K:123:LYS:NZ	31:2:2483:C:N3	2.51	0.56
17:P:91:GLN:NE2	31:2:993:G:N3	2.53	0.56
31:2:284:U:N3	31:2:356:G:N1	2.52	0.56
31:2:2304:G:N1	31:2:2312:U:O4	2.38	0.56
42:k:20:VAL:HG21	52:1:553:A:H5''	1.87	0.56
50:s:35:TYR:OH	52:1:259:G:OP1	2.23	0.56
5:C:117:ARG:NH2	5:C:183:PHE:O	2.36	0.56
16:O:91:ARG:NH2	31:2:1153:C:OP1	2.38	0.56
7:E:154:GLU:OE1	7:E:157:LYS:N	2.37	0.56
31:2:2368:C:H2'	31:2:2369:A:H8	1.70	0.56
32:a:141:GLU:O	32:a:145:ASN:ND2	2.38	0.56
42:k:114:SER:N	52:1:502:A:OP1	2.32	0.56
49:r:10:ILE:HD11	49:r:14:LEU:HD22	1.87	0.56
4:B:129:THR:OG1	4:B:140:HIS:O	2.24	0.56
16:O:47:ARG:NH2	31:2:560:C:O2'	2.39	0.56
31:2:2692:G:N3	31:2:2847:U:O2'	2.36	0.56
31:2:2798:U:H5'	31:2:2799:A:H5'	1.88	0.56
31:2:160:A:N3	31:2:2208:C:O2'	2.38	0.56
39:h:69:GLY:O	52:1:1249:C:O2'	2.23	0.56
52:1:673:A:H2'	52:1:674:G:C8	2.41	0.56
13:L:72:ASP:HB3	13:L:75:ILE:HB	1.87	0.56
40:i:57:VAL:HG13	52:1:972:C:H1'	1.86	0.56
17:P:59:ILE:HG12	17:P:101:ILE:HG22	1.87	0.56
22:U:39:THR:H	31:2:2331:G:H4'	1.69	0.56
13:L:28:LEU:HD23	13:L:48:VAL:HG21	1.88	0.56
52:1:766:A:N6	52:1:813:U:N3	2.52	0.56
3:A:220:ARG:NH1	31:2:1789:A:OP2	2.38	0.55
8:F:11:ASN:ND2	31:2:2094:A:O3'	2.39	0.55
43:l:97:ARG:NH1	52:1:1308:U:OP2	2.39	0.55
11:J:63:LYS:O	29:AB:29:ARG:NH1	2.39	0.55
31:2:581:C:H2'	31:2:582:A:H8	1.71	0.55
29:AB:18:LYS:HG3	31:2:651:G:H5'	1.88	0.55
31:2:1128:G:N7	31:2:2489:U:O2'	2.38	0.55
36:e:3:HIS:ND1	36:e:65:GLU:OE1	2.39	0.55
6:D:36:ASN:ND2	31:2:2312:U:O2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:47:GLU:OE2	12:K:50:ARG:NH1	2.37	0.55
14:M:50:ALA:O	14:M:81:ARG:NH2	2.37	0.55
31:2:277:G:OP1	31:2:277:G:N2	2.39	0.55
31:2:282:A:N6	31:2:283:G:O6	2.40	0.55
18:Q:72:THR:HB	18:Q:106:VAL:HG23	1.88	0.55
43:l:82:LEU:HD13	49:r:65:MET:HB3	1.89	0.55
44:m:50:LEU:HD12	44:m:51:PRO:HD2	1.88	0.55
52:1:618:C:C2	52:1:622:A:N6	2.71	0.55
52:1:1356:G:H2'	52:1:1357:A:C8	2.40	0.55
23:V:9:LYS:NZ	31:2:397:U:OP2	2.40	0.55
33:b:168:ARG:NH1	52:1:1106:G:O2'	2.40	0.55
34:c:99:ASN:OD1	34:c:110:ARG:NH1	2.39	0.55
49:r:32:THR:HG21	49:r:70:LEU:HD21	1.88	0.55
52:1:151:A:H62	52:1:170:U:H3	1.52	0.55
52:1:1241:G:H2'	52:1:1242:G:H8	1.71	0.55
3:A:100:ARG:HH12	31:2:1500:G:H4'	1.71	0.55
31:2:810:U:H5'	31:2:811:U:H5'	1.89	0.55
38:g:14:ARG:NH2	38:g:74:ILE:O	2.38	0.55
52:1:591:U:H2'	52:1:592:G:H8	1.70	0.55
1:3:77:U:OP1	21:T:21:ARG:NH1	2.36	0.55
4:B:38:LYS:O	4:B:46:ARG:HA	2.05	0.55
7:E:113:ASP:OD1	7:E:113:ASP:N	2.39	0.55
31:2:1481:U:H3	31:2:1510:G:H1	1.53	0.55
12:K:110:GLU:OE2	12:K:114:ARG:NH1	2.40	0.55
16:O:57:ARG:NH2	31:2:998:C:OP2	2.40	0.55
38:g:28:SER:HB2	38:g:56:PRO:HB2	1.86	0.55
52:1:71:A:N1	52:1:99:C:O2'	2.38	0.55
52:1:356:A:N3	52:1:368:U:O2'	2.40	0.55
52:1:414:A:N6	52:1:430:A:C2	2.74	0.55
52:1:788:U:O2'	53:4:50:A:N1	2.35	0.55
31:2:1483:G:O6	31:2:1506:U:O4	2.25	0.55
34:c:57:LYS:HE2	34:c:199:ILE:HD12	1.89	0.55
52:1:76:G:N2	52:1:93:U:O2	2.35	0.55
15:N:21:PRO:HD3	15:N:49:ILE:HD12	1.89	0.54
40:i:37:ARG:HB3	52:1:1124:G:H5''	1.89	0.54
40:i:50:THR:OG1	52:1:975:A:N6	2.40	0.54
52:1:335:C:H2'	52:1:336:A:H8	1.72	0.54
2:5:27:G:H2'	2:5:28:G:C8	2.42	0.54
33:b:55:VAL:HB	33:b:66:THR:HG23	1.89	0.54
33:b:189:HIS:NE2	52:1:1204:A:O2'	2.40	0.54
52:1:416:G:H2'	52:1:417:G:H8	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:517:G:H1	52:1:532:A:H5'	1.72	0.54
1:3:52:A:O2'	1:3:53:A:O5'	2.23	0.54
21:T:17:SER:OG	21:T:21:ARG:NH1	2.40	0.54
31:2:1178:C:H2'	31:2:1179:G:C8	2.42	0.54
42:k:110:LYS:O	42:k:113:ARG:NE	2.32	0.54
25:X:40:THR:HG22	25:X:42:ALA:H	1.72	0.54
31:2:284:U:O2	31:2:356:G:N2	2.40	0.54
31:2:750:A:OP1	31:2:1615:C:N4	2.39	0.54
31:2:793:A:OP2	31:2:2071:A:O2'	2.26	0.54
31:2:2523:G:O2'	31:2:2764:A:O2'	2.25	0.54
36:e:71:ILE:HD13	36:e:74:LEU:HD21	1.89	0.54
52:1:31:G:O2'	52:1:48:C:N4	2.41	0.54
52:1:563:A:HO2'	52:1:566:G:HO2'	1.51	0.54
52:1:582:C:O2	52:1:759:A:N6	2.40	0.54
52:1:585:G:N2	52:1:757:U:O2	2.40	0.54
52:1:1370:G:H2'	52:1:1371:G:H8	1.71	0.54
1:3:79:G:N7	21:T:14:LYS:NZ	2.55	0.54
7:E:9:VAL:HG12	7:E:48:THR:HG22	1.88	0.54
25:X:10:ARG:HB2	25:X:53:MET:HB2	1.89	0.54
28:AA:24:THR:HG23	28:AA:27:GLY:H	1.73	0.54
31:2:2099:U:O2	31:2:2190:G:N2	2.38	0.54
44:m:32:ASP:OD1	44:m:34:ASN:ND2	2.41	0.54
52:1:195:A:O2'	52:1:222:C:O2'	2.25	0.54
52:1:401:C:O2'	52:1:621:A:N3	2.41	0.54
31:2:1995:U:H3'	31:2:1996:C:H2'	1.90	0.54
31:2:2081:U:H2'	31:2:2082:A:H8	1.73	0.54
52:1:28:A:O2'	52:1:296:U:OP1	2.26	0.54
52:1:514:C:H2'	52:1:515:G:H8	1.73	0.54
31:2:279:A:C5	31:2:361:G:N2	2.76	0.54
52:1:1041:G:H2'	52:1:1042:A:C8	2.43	0.54
12:K:20:LEU:HD13	21:T:81:PRO:HG2	1.89	0.54
20:S:33:VAL:HG23	20:S:66:VAL:HG22	1.89	0.54
30:AC:38:GLY:HA3	31:2:1124:G:H1'	1.90	0.54
31:2:411:G:OP2	31:2:2406:A:O2'	2.25	0.54
31:2:2139:U:O2	31:2:2152:G:O6	2.25	0.54
33:b:45:GLU:HG3	33:b:46:LEU:HG	1.89	0.54
40:i:55:PRO:O	52:1:973:G:O2'	2.25	0.54
52:1:137:U:H3	52:1:226:G:H1	1.56	0.54
31:2:247:G:O2'	31:2:250:G:O6	2.26	0.53
31:2:1275:A:OP2	31:2:1646:C:N4	2.41	0.53
35:d:155:LYS:NZ	38:g:70:VAL:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:g:95:MET:HB2	38:g:99:GLY:H	1.72	0.53
52:1:94:G:H4'	52:1:95:C:H5'	1.90	0.53
52:1:925:G:O6	52:1:1391:U:O4	2.26	0.53
52:1:1096:C:O2	52:1:1170:A:O2'	2.24	0.53
52:1:1414:U:H2'	52:1:1415:G:H8	1.72	0.53
3:A:228:ASP:OD1	3:A:228:ASP:N	2.35	0.53
31:2:693:A:O2'	31:2:1353:A:N3	2.40	0.53
31:2:1754:A:N1	31:2:2716:C:O2'	2.40	0.53
40:i:7:ARG:NH2	52:1:1125:U:O2'	2.41	0.53
41:j:58:THR:HG23	41:j:61:ALA:H	1.74	0.53
52:1:309:A:O2'	52:1:607:A:N1	2.37	0.53
52:1:414:A:H62	52:1:430:A:H2	1.55	0.53
52:1:1251:A:N3	52:1:1369:C:O2'	2.38	0.53
3:A:20:ASN:HB3	3:A:23:LEU:HD23	1.90	0.53
4:B:150:GLN:NE2	31:2:2032:G:O2'	2.41	0.53
31:2:1724:G:O6	31:2:1737:G:N2	2.42	0.53
31:2:2245:U:H5''	31:2:2246:G:H5'	1.89	0.53
39:h:68:GLY:HA2	52:1:1250:A:H4'	1.90	0.53
46:o:4:ILE:HG12	46:o:21:VAL:HG12	1.91	0.53
50:s:28:ARG:HH12	52:1:1437:A:H5'	1.71	0.53
52:1:54:C:OP1	52:1:351:G:N2	2.41	0.53
32:a:96:LEU:HD21	52:1:1103:C:H4'	1.90	0.53
5:C:176:ASP:N	5:C:176:ASP:OD1	2.40	0.53
37:f:68:VAL:HG13	37:f:69:ARG:HG2	1.91	0.53
52:1:1086:U:H3	52:1:1099:G:H1	1.56	0.53
3:A:208:GLY:HA2	31:2:764:A:H5''	1.91	0.53
31:2:598:U:H2'	31:2:599:A:H8	1.74	0.53
52:1:1238:A:N7	52:1:1301:U:O4	2.42	0.53
31:2:1852:U:O2	31:2:1890:A:N6	2.41	0.53
31:2:2297:A:O2'	31:2:2322:A:N3	2.40	0.53
44:m:6:LYS:NZ	44:m:63:CYS:O	2.37	0.53
52:1:683:G:H1	52:1:707:U:H3	1.56	0.53
12:K:134:THR:OG1	21:T:79:ARG:NH2	2.42	0.53
31:2:1386:C:H2'	31:2:1387:A:C8	2.44	0.53
52:1:1071:C:H2'	52:1:1072:G:H8	1.73	0.53
4:B:56:LYS:HD3	4:B:59:ARG:HH22	1.74	0.53
5:C:148:ILE:HB	5:C:169:VAL:HG12	1.90	0.53
7:E:26:LYS:NZ	7:E:27:GLY:O	2.42	0.53
9:G:6:ALA:H	9:G:45:THR:HG21	1.74	0.53
15:N:81:ASP:OD1	15:N:81:ASP:N	2.41	0.53
16:O:39:ILE:HG22	16:O:43:GLN:HE21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:81:ARG:NH1	31:2:301:G:OP2	2.42	0.53
31:2:581:C:H2'	31:2:582:A:C8	2.43	0.53
4:B:5:VAL:H	4:B:32:ASN:HD21	1.56	0.53
21:T:6:ALA:HB3	21:T:65:VAL:HB	1.91	0.53
31:2:979:A:H5'	31:2:980:A:H5''	1.91	0.53
31:2:1796:U:H2'	31:2:1797:G:H8	1.74	0.53
52:1:75:G:N2	52:1:95:C:N3	2.47	0.53
52:1:1013:G:N2	52:1:1016:A:OP2	2.42	0.53
3:A:174:ARG:HG2	3:A:180:MET:HG2	1.91	0.52
31:2:2110:G:N2	31:2:2179:C:N3	2.57	0.52
35:d:82:HIS:HB3	38:g:98:LEU:HD12	1.90	0.52
52:1:766:A:N7	52:1:813:U:O4	2.43	0.52
31:2:16:C:H2'	31:2:17:G:H8	1.74	0.52
31:2:1178:C:H2'	31:2:1179:G:H8	1.75	0.52
31:2:1571:A:H2'	31:2:1572:A:H8	1.75	0.52
32:a:177:ASN:ND2	52:1:1075:U:OP1	2.42	0.52
42:k:26:CYS:SG	52:1:363:A:N6	2.83	0.52
52:1:1081:A:H2'	52:1:1082:A:H8	1.74	0.52
13:L:44:LEU:HD23	13:L:113:ILE:HD13	1.89	0.52
31:2:2801:G:H2'	31:2:2802:G:C8	2.44	0.52
52:1:372:C:H42	52:1:389:A:H62	1.57	0.52
52:1:520:A:N6	52:1:533:A:H61	2.06	0.52
52:1:618:C:O2	52:1:622:A:N6	2.43	0.52
52:1:1083:U:O2'	52:1:1102:A:OP2	2.24	0.52
52:1:1238:A:N6	52:1:1301:U:H3	2.01	0.52
12:K:29:GLY:HA2	12:K:106:ASP:HB3	1.91	0.52
31:2:1466:U:HO2'	31:2:1546:G:HO2'	1.52	0.52
41:j:14:GLN:NE2	41:j:77:GLY:O	2.41	0.52
2:5:43:C:H2'	2:5:44:G:H8	1.75	0.52
31:2:2246:G:H2'	31:2:2247:A:H8	1.74	0.52
49:r:10:ILE:HA	49:r:37:SER:HB2	1.92	0.52
52:1:210:C:O2'	52:1:211:G:N2	2.42	0.52
52:1:454:G:H1	52:1:479:U:H3	1.57	0.52
52:1:1410:A:N6	52:1:1491:G:O6	2.43	0.52
10:I:65:THR:HG22	10:I:67:LYS:H	1.74	0.52
10:I:81:GLY:N	15:N:67:GLU:OE2	2.38	0.52
31:2:1570:A:H2'	31:2:1571:A:C8	2.44	0.52
36:e:86:ARG:NH1	48:q:63:TYR:O	2.43	0.52
49:r:52:ASN:ND2	49:r:75:PRO:O	2.39	0.52
52:1:147:G:H2'	52:1:148:G:C8	2.45	0.52
6:D:15:LEU:HG	6:D:27:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:31:ARG:NH2	31:2:1995:U:O2'	2.43	0.52
36:e:7:VAL:HG22	36:e:61:LEU:HB3	1.90	0.52
40:i:62:ARG:NH1	52:1:1366:C:O2'	2.43	0.52
20:S:68:ASN:ND2	31:2:328:U:O2'	2.42	0.52
30:AC:5:ALA:HA	30:AC:37:GLN:HG2	1.92	0.52
40:i:72:ARG:NH2	52:1:1151:A:O2'	2.41	0.52
31:2:1454:C:N4	31:2:1457:U:O4	2.40	0.52
34:c:201:GLU:O	52:1:8:A:N6	2.41	0.52
47:p:18:LYS:H	47:p:50:ASN:HD21	1.58	0.52
52:1:1412:C:H2'	52:1:1413:A:C8	2.45	0.52
53:4:90:G:H2'	53:4:91:G:C8	2.45	0.52
2:5:52:G:H2'	2:5:53:G:H8	1.75	0.52
31:2:704:G:O2'	31:2:726:G:N2	2.37	0.52
34:c:53:GLN:HG2	34:c:202:LEU:HB2	1.92	0.52
52:1:54:C:H2'	52:1:352:C:H41	1.73	0.52
52:1:677:U:O2	52:1:777:A:O2'	2.24	0.52
11:J:82:LEU:HD23	11:J:116:VAL:HG11	1.92	0.51
16:O:25:GLY:O	16:O:29:ARG:NH1	2.43	0.51
17:P:68:ARG:NH2	31:2:1223:G:OP1	2.42	0.51
19:R:6:ARG:NH2	19:R:37:ASP:O	2.43	0.51
31:2:388:G:O2'	31:2:389:G:N7	2.39	0.51
33:b:13:ILE:HD12	52:1:1113:C:H4'	1.91	0.51
33:b:175:HIS:ND1	52:1:1109:C:OP2	2.42	0.51
52:1:459:A:H2'	52:1:460:A:H8	1.75	0.51
2:5:18:G:OP2	2:5:60:U:O2'	2.28	0.51
30:AC:2:LYS:HE3	30:AC:4:ARG:HE	1.75	0.51
31:2:1469:A:OP2	31:2:1522:A:N6	2.41	0.51
33:b:56:ILE:HG12	33:b:65:VAL:HG12	1.92	0.51
41:j:34:THR:OG1	41:j:35:ASP:N	2.43	0.51
49:r:69:LYS:NZ	52:1:1320:C:OP1	2.38	0.51
7:E:158:GLY:O	7:E:162:ARG:NH1	2.43	0.51
31:2:574:A:N6	31:2:2034:U:OP1	2.44	0.51
31:2:2776:A:O2'	31:2:2782:G:N7	2.38	0.51
33:b:41:TYR:HA	33:b:44:LYS:HE3	1.93	0.51
34:c:53:GLN:HA	34:c:198:LEU:HD13	1.91	0.51
40:i:55:PRO:HB3	44:m:81:ILE:HD11	1.93	0.51
52:1:1066:C:C2	52:1:1191:A:N6	2.78	0.51
52:1:677:U:H3	52:1:713:G:H22	1.59	0.51
7:E:137:LYS:HE3	31:2:2746:U:H5'	1.93	0.51
31:2:84:A:H62	31:2:101:A:H2	1.57	0.51
31:2:318:C:H2'	31:2:319:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:i:9:ARG:HH21	40:i:71:LEU:HD11	1.74	0.51
52:1:662:U:H2'	52:1:663:A:C8	2.46	0.51
16:O:30:VAL:HG12	16:O:33:VAL:H	1.75	0.51
31:2:280:U:O4	31:2:360:U:O4	2.29	0.51
34:c:120:LYS:O	34:c:145:ARG:NE	2.38	0.51
43:l:84:CYS:HA	49:r:73:PHE:HA	1.93	0.51
52:1:1066:C:O2	52:1:1191:A:N6	2.43	0.51
6:D:16:MET:HE1	6:D:21:TYR:HB2	1.92	0.51
31:2:76:C:H2'	31:2:77:G:H8	1.76	0.51
39:h:23:GLY:HA3	39:h:26:LYS:HE2	1.92	0.51
41:j:21:HIS:NE2	41:j:84:MET:SD	2.84	0.51
52:1:960:U:O2	52:1:1222:G:O2'	2.22	0.51
52:1:1355:G:H2'	52:1:1356:G:H8	1.76	0.51
53:4:88:A:H2'	53:4:89:G:H8	1.75	0.51
4:B:14:ILE:HG23	15:N:11:GLN:HE22	1.76	0.51
27:Z:39:ASP:HB3	27:Z:42:VAL:HG22	1.92	0.51
31:2:1270:C:H5''	31:2:1271:G:H5'	1.92	0.51
31:2:1539:U:H2'	31:2:1540:G:C8	2.46	0.51
31:2:2202:U:O2'	31:2:2204:G:OP1	2.26	0.51
33:b:10:ARG:NH2	33:b:176:THR:O	2.38	0.51
36:e:38:ARG:HH11	36:e:99:ALA:HA	1.76	0.51
49:r:35:ARG:HA	49:r:70:LEU:HD23	1.93	0.51
52:1:437:U:O4	52:1:495:A:N7	2.44	0.51
52:1:1270:G:H2'	52:1:1271:A:C8	2.46	0.51
52:1:1304:G:H21	52:1:1333:A:N6	2.08	0.51
1:3:5:U:H2'	1:3:6:G:H8	1.76	0.51
2:5:31:A:O2'	52:1:1340:A:O2'	2.27	0.51
52:1:309:A:H2'	52:1:310:G:H8	1.76	0.51
52:1:687:A:N6	52:1:703:G:C2	2.78	0.51
1:3:5:U:O2'	1:3:26:C:O2'	2.28	0.51
2:5:68:C:H2'	2:5:69:G:H8	1.74	0.51
11:J:17:LYS:HE3	31:2:663:G:H5''	1.93	0.51
11:J:41:ARG:NH1	31:2:807:U:OP2	2.39	0.51
29:AB:33:THR:OG1	31:2:2420:C:OP1	2.28	0.51
31:2:1130:U:N3	31:2:2025:C:OP1	2.36	0.51
44:m:74:ARG:NH2	52:1:1360:A:OP2	2.43	0.51
50:s:28:ARG:NH1	52:1:1438:G:OP1	2.44	0.51
7:E:163:TYR:HB2	7:E:166:GLU:HB2	1.94	0.50
12:K:42:THR:HG22	12:K:93:VAL:HG12	1.93	0.50
14:M:27:VAL:HG13	14:M:38:GLN:HG3	1.92	0.50
31:2:414:C:H1'	31:2:1864:U:H1'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:558:U:H2'	31:2:559:G:H8	1.76	0.50
31:2:1992:G:O2'	31:2:1997:C:N4	2.43	0.50
31:2:2591:C:H2'	31:2:2592:G:H8	1.77	0.50
33:b:1:GLY:N	52:1:1191:A:OP1	2.41	0.50
49:r:13:HIS:NE2	52:1:1015:G:OP1	2.44	0.50
52:1:412:A:H3'	52:1:413:G:H4'	1.94	0.50
2:5:30:G:OP1	52:1:1229:A:O2'	2.27	0.50
6:D:3:LEU:O	6:D:7:TYR:HB3	2.11	0.50
20:S:46:LYS:HD2	31:2:483:A:H5''	1.93	0.50
31:2:151:C:H2'	31:2:152:A:H8	1.77	0.50
31:2:2233:U:H2'	31:2:2234:G:C8	2.46	0.50
31:2:2647:U:H2'	31:2:2648:G:H8	1.76	0.50
52:1:1130:A:H61	52:1:1144:G:H1'	1.75	0.50
52:1:1342:C:H2'	52:1:1343:G:C8	2.46	0.50
12:K:11:LYS:NZ	31:2:2278:A:OP1	2.38	0.50
31:2:1264:A:H5''	31:2:1265:A:H2'	1.93	0.50
31:2:2646:C:OP2	31:2:2732:G:O2'	2.23	0.50
39:h:108:ARG:HB3	52:1:1347:G:H8	1.76	0.50
46:o:63:GLN:OE1	52:1:227:G:O2'	2.28	0.50
52:1:49:U:H3	52:1:362:G:H1'	1.76	0.50
52:1:1260:G:H21	52:1:1275:A:H62	1.58	0.50
31:2:1443:U:H2'	31:2:1444:G:H8	1.75	0.50
31:2:1638:C:O2	31:2:2698:U:O2'	2.28	0.50
31:2:1876:A:H3'	31:2:1877:A:C8	2.46	0.50
34:c:100:VAL:HG21	34:c:136:VAL:HG21	1.93	0.50
40:i:6:ILE:HB	40:i:76:ILE:HB	1.92	0.50
49:r:21:ALA:HA	49:r:25:GLY:HA3	1.94	0.50
52:1:252:U:C2	52:1:253:A:N7	2.79	0.50
52:1:694:A:N1	52:1:787:A:O2'	2.42	0.50
52:1:1507:A:H2'	52:1:1508:A:C8	2.46	0.50
1:3:75:G:O2'	21:T:88:HIS:NE2	2.41	0.50
31:2:775:G:H4'	31:2:776:G:H5'	1.93	0.50
35:d:100:GLU:O	35:d:121:ASN:ND2	2.44	0.50
38:g:111:THR:HG23	38:g:114:ALA:H	1.76	0.50
46:o:18:GLN:HA	46:o:38:PHE:HA	1.94	0.50
52:1:20:U:H3	52:1:915:A:N6	2.09	0.50
13:L:56:LYS:NZ	13:L:87:PHE:O	2.44	0.50
14:M:53:THR:HB	14:M:65:THR:HB	1.94	0.50
52:1:1464:U:H2'	52:1:1465:A:H8	1.76	0.50
52:1:1467:C:H2'	52:1:1468:A:H8	1.77	0.50
3:A:65:ASP:OD2	3:A:101:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:13:ARG:HH11	15:N:55:HIS:HA	1.76	0.50
26:Y:31:LYS:HG3	26:Y:32:THR:HG23	1.94	0.50
28:AA:39:ARG:NH2	31:2:468:G:N7	2.60	0.50
31:2:500:G:N1	31:2:503:A:OP2	2.37	0.50
31:2:639:U:H2'	31:2:640:C:H6	1.75	0.50
31:2:2731:G:N1	31:2:2732:G:C6	2.80	0.50
36:e:90:MET:SD	36:e:91:ARG:N	2.84	0.50
52:1:147:G:H2'	52:1:148:G:H8	1.76	0.50
3:A:62:ARG:NH1	31:2:1568:G:OP2	2.45	0.50
31:2:1278:C:H2'	31:2:1279:G:H8	1.76	0.50
7:E:63:GLN:HE22	31:2:2758:A:H1'	1.77	0.50
13:L:38:LEU:HG	13:L:42:LYS:HE2	1.93	0.50
31:2:2656:U:O2	31:2:2665:A:N7	2.45	0.50
33:b:109:GLU:HB3	33:b:143:LEU:HD22	1.94	0.50
53:4:81:G:H2'	53:4:82:A:H8	1.77	0.50
31:2:74:A:O2'	31:2:88:G:OP2	2.25	0.49
31:2:807:U:H2'	31:2:808:G:C8	2.47	0.49
31:2:2039:U:H2'	31:2:2040:G:C8	2.47	0.49
31:2:2810:A:H62	31:2:2890:G:H21	1.59	0.49
39:h:27:ILE:HB	39:h:34:LEU:HD22	1.94	0.49
46:o:20:VAL:HG23	46:o:35:ARG:HA	1.94	0.49
52:1:599:C:H2'	52:1:600:A:H8	1.76	0.49
3:A:157:ALA:HB1	3:A:196:ASN:HB3	1.95	0.49
6:D:118:ALA:O	6:D:166:ARG:NH1	2.45	0.49
18:Q:83:LYS:HG2	18:Q:95:ARG:HD3	1.93	0.49
31:2:1681:G:H21	31:2:1762:A:H3'	1.77	0.49
52:1:76:G:O6	52:1:93:U:O4	2.30	0.49
52:1:908:A:H2'	52:1:909:A:H8	1.76	0.49
52:1:1342:C:H2'	52:1:1343:G:H8	1.77	0.49
18:Q:78:GLU:O	31:2:24:G:O2'	2.27	0.49
52:1:1042:A:H2'	52:1:1043:G:C8	2.47	0.49
10:I:56:ASP:N	10:I:56:ASP:OD1	2.44	0.49
20:S:8:ASP:H	20:S:24:VAL:HG22	1.76	0.49
25:X:5:LYS:HB2	25:X:57:GLU:HB2	1.94	0.49
25:X:15:ARG:O	25:X:20:LYS:NZ	2.44	0.49
31:2:81:G:HO2'	31:2:295:G:HO2'	1.56	0.49
31:2:2047:C:H2'	31:2:2048:G:H8	1.77	0.49
35:d:37:VAL:HG21	35:d:113:VAL:HG23	1.93	0.49
52:1:59:A:H5'	52:1:60:A:H5''	1.94	0.49
26:Y:12:ARG:NH2	31:2:517:C:OP1	2.45	0.49
27:Z:5:ARG:NH2	27:Z:23:THR:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:742:A:H2'	31:2:743:A:C8	2.48	0.49
44:m:57:SER:HA	52:1:1360:A:C8	2.48	0.49
48:q:59:LYS:NZ	52:1:719:C:N3	2.52	0.49
52:1:1001:C:H2'	52:1:1002:G:H8	1.76	0.49
53:4:88:A:H2'	53:4:89:G:C8	2.48	0.49
14:M:12:THR:OG1	14:M:16:ARG:NH1	2.46	0.49
47:p:11:VAL:HA	47:p:22:VAL:HA	1.95	0.49
52:1:459:A:H2'	52:1:460:A:C8	2.48	0.49
52:1:806:C:H2'	52:1:807:A:H8	1.78	0.49
2:5:20:U:H5	2:5:48:C:H42	1.59	0.49
25:X:40:THR:HB	25:X:43:ILE:HG12	1.95	0.49
31:2:1020:A:N1	31:2:1141:U:O2'	2.32	0.49
39:h:117:LEU:HA	39:h:124:PRO:HD3	1.94	0.49
52:1:202:G:N1	52:1:215:C:N4	2.40	0.49
52:1:1085:U:OP1	52:1:1094:G:N2	2.45	0.49
52:1:1115:U:H3	52:1:1185:G:H1	1.61	0.49
52:1:1243:C:H2'	52:1:1244:G:H8	1.78	0.49
4:B:131:ASP:OD1	4:B:131:ASP:N	2.41	0.49
14:M:89:ASP:OD1	14:M:89:ASP:N	2.45	0.49
31:2:832:U:H2'	31:2:833:A:C8	2.45	0.49
2:5:64:A:H2'	2:5:65:G:H8	1.76	0.49
31:2:83:A:O2'	31:2:103:A:N6	2.46	0.49
31:2:160:A:N7	31:2:166:U:O4	2.46	0.49
31:2:584:C:N4	31:2:585:G:O6	2.46	0.49
31:2:835:C:H2'	31:2:836:G:H8	1.77	0.49
31:2:879:G:H2'	31:2:880:G:H8	1.78	0.49
31:2:935:C:H2'	31:2:936:A:H8	1.78	0.49
36:e:42:TRP:HE1	36:e:61:LEU:HD11	1.78	0.49
42:k:98:ARG:NE	42:k:104:SER:O	2.39	0.49
4:B:62:LYS:HD2	31:2:2810:A:H4'	1.94	0.49
10:I:64:ARG:HB2	10:I:83:ALA:HB3	1.95	0.49
31:2:1636:U:H2'	31:2:1637:A:C8	2.47	0.49
31:2:2392:A:N6	31:2:2424:C:O2	2.46	0.49
52:1:181:A:H2'	52:1:182:A:C8	2.46	0.49
52:1:235:C:H2'	52:1:236:A:C8	2.48	0.49
53:4:62:A:N6	53:4:92:A:C6	2.81	0.49
9:G:34:ARG:HG3	9:G:39:LYS:HB2	1.95	0.48
9:G:136:GLN:NE2	31:2:2898:U:O3'	2.46	0.48
9:G:136:GLN:HE21	31:2:2899:A:H5'	1.77	0.48
16:O:71:ASN:HD21	16:O:106:THR:HG22	1.78	0.48
34:c:56:GLU:HB2	34:c:198:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:g:75:GLN:HG2	38:g:127:TYR:HB2	1.95	0.48
42:k:112:ALA:HB1	42:k:115:LYS:HB3	1.95	0.48
52:1:25:C:H41	52:1:559:A:H61	1.59	0.48
52:1:112:G:H21	52:1:354:G:H5'	1.78	0.48
52:1:1300:G:O2'	52:1:1303:C:N4	2.44	0.48
31:2:2036:C:H2'	31:2:2037:A:H8	1.78	0.48
35:d:46:GLY:HA3	35:d:70:MET:HA	1.95	0.48
52:1:1450:U:H3	52:1:1453:G:H22	1.61	0.48
53:4:87:C:H2'	53:4:88:A:C8	2.46	0.48
2:5:27:G:H2'	2:5:28:G:H8	1.78	0.48
31:2:926:G:H2'	31:2:927:A:C8	2.49	0.48
31:2:2092:U:OP1	31:2:2199:A:O2'	2.26	0.48
42:k:113:ARG:NH1	42:k:118:VAL:O	2.40	0.48
43:l:19:THR:HG23	43:l:25:GLY:HA2	1.95	0.48
52:1:419:C:O3'	52:1:512:U:O2'	2.31	0.48
52:1:521:G:HO2'	52:1:536:C:HO2'	1.58	0.48
52:1:585:G:C2	52:1:757:U:O2	2.66	0.48
52:1:1178:G:N2	52:1:1181:G:OP2	2.47	0.48
8:F:9:VAL:HG23	8:F:12:LEU:H	1.78	0.48
15:N:20:ARG:NH2	31:2:2849:U:O4	2.45	0.48
18:Q:77:ASP:OD1	18:Q:77:ASP:N	2.42	0.48
44:m:99:SER:OG	52:1:1186:G:N2	2.46	0.48
52:1:59:A:H3'	52:1:331:G:H22	1.79	0.48
52:1:151:A:N7	52:1:170:U:O4	2.47	0.48
52:1:202:G:H21	52:1:466:A:H61	1.58	0.48
52:1:916:U:H2'	52:1:917:G:H8	1.79	0.48
52:1:1238:A:OP1	52:1:1335:U:O2'	2.30	0.48
4:B:46:ARG:NH2	4:B:89:GLU:OE2	2.47	0.48
31:2:954:G:H1	31:2:963:U:H3	1.60	0.48
31:2:2691:C:H2'	31:2:2692:G:H8	1.78	0.48
52:1:1015:G:H21	52:1:1218:C:H2'	1.78	0.48
2:5:68:C:H2'	2:5:69:G:C8	2.48	0.48
11:J:29:LYS:HA	31:2:810:U:H3'	1.95	0.48
15:N:38:ARG:NH1	52:1:346:G:OP1	2.46	0.48
31:2:20:C:H2'	31:2:21:A:H8	1.77	0.48
47:p:47:ASP:OD1	47:p:47:ASP:N	2.47	0.48
52:1:1305:G:H22	52:1:1331:G:H2'	1.78	0.48
1:3:8:C:OP1	14:M:15:ARG:NH2	2.46	0.48
6:D:135:ILE:HD11	6:D:145:VAL:HG11	1.95	0.48
10:I:123:LEU:HA	15:N:40:GLN:HE22	1.78	0.48
16:O:46:TYR:OH	31:2:992:C:OP1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:48:GLN:HE21	19:R:55:VAL:H	1.61	0.48
31:2:1518:C:H2'	31:2:1519:G:H8	1.78	0.48
31:2:1571:A:H2'	31:2:1572:A:C8	2.48	0.48
31:2:1830:C:H2'	31:2:1831:G:C8	2.49	0.48
46:o:66:THR:HG1	52:1:136:C:HO2'	1.59	0.48
52:1:1088:G:N2	52:1:1167:A:N6	2.40	0.48
52:1:1200:C:O2'	52:1:1205:U:O4	2.26	0.48
1:3:1:U:H2'	1:3:2:G:H8	1.77	0.48
18:Q:23:LEU:HD12	18:Q:24:ILE:HG23	1.96	0.48
29:AB:35:LYS:HB3	29:AB:39:ARG:HD3	1.96	0.48
31:2:18:U:H2'	31:2:19:A:H8	1.78	0.48
31:2:272:A:H2'	31:2:273:G:C8	2.49	0.48
31:2:675:A:N3	31:2:2443:C:O2'	2.45	0.48
31:2:1913:A:C8	52:1:1494:G:H1'	2.48	0.48
31:2:2246:G:H2'	31:2:2247:A:C8	2.48	0.48
31:2:2802:G:H2'	31:2:2803:G:C8	2.49	0.48
40:i:22:THR:HG21	40:i:72:ARG:HD2	1.95	0.48
43:l:7:ASN:ND2	43:l:17:ALA:O	2.42	0.48
52:1:60:A:N6	52:1:107:G:O2'	2.46	0.48
15:N:46:VAL:HA	15:N:60:VAL:HA	1.95	0.48
27:Z:16:THR:HG21	27:Z:41:VAL:HG21	1.95	0.48
31:2:2816:G:N3	31:2:2883:A:O2'	2.43	0.48
43:l:74:MET:HA	43:l:77:LYS:HG2	1.95	0.48
44:m:27:LYS:NZ	52:1:1317:C:OP2	2.47	0.48
52:1:1351:U:H3	52:1:1371:G:H1	1.61	0.48
3:A:158:GLY:H	3:A:194:VAL:HB	1.78	0.48
17:P:55:ASP:OD1	17:P:55:ASP:N	2.42	0.48
18:Q:76:VAL:HG22	18:Q:103:ILE:HG23	1.95	0.48
23:V:33:HIS:NE2	31:2:2091:C:O2	2.47	0.48
32:a:34:ARG:HE	32:a:39:ILE:HG13	1.78	0.48
37:f:16:LYS:HB2	39:h:45:MET:HE2	1.95	0.48
42:k:114:SER:OG	52:1:35:G:N2	2.39	0.48
5:C:131:THR:HG22	5:C:160:ALA:HA	1.95	0.47
6:D:71:LYS:NZ	6:D:72:SER:O	2.47	0.47
7:E:59:ASP:OD1	7:E:59:ASP:N	2.44	0.47
31:2:1311:G:OP2	31:2:1311:G:N2	2.43	0.47
31:2:1853:A:N3	31:2:2233:U:O2'	2.44	0.47
31:2:1869:G:O2'	31:2:1872:A:N6	2.47	0.47
31:2:2422:C:O2'	31:2:2423:U:O5'	2.32	0.47
31:2:2810:A:H62	31:2:2890:G:N2	2.11	0.47
44:m:100:TRP:NE1	52:1:1369:C:OP1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:34:VAL:HG21	50:s:53:MET:HG2	1.95	0.47
52:1:1513:A:H2'	52:1:1514:G:C8	2.49	0.47
9:G:95:ARG:HG3	9:G:96:ARG:HD3	1.96	0.47
31:2:1421:G:H1'	31:2:1495:A:H61	1.78	0.47
31:2:1796:U:H2'	31:2:1797:G:C8	2.49	0.47
32:a:196:ASP:OD1	32:a:196:ASP:N	2.45	0.47
32:a:216:VAL:HA	32:a:219:THR:HG22	1.96	0.47
34:c:201:GLU:OE1	35:d:111:ARG:NH2	2.47	0.47
52:1:1512:U:H2'	52:1:1513:A:C8	2.49	0.47
12:K:6:ARG:NH2	31:2:869:G:O3'	2.47	0.47
24:W:3:ALA:HB2	24:W:52:ARG:HD3	1.96	0.47
28:AA:18:PHE:HB2	28:AA:43:THR:HG21	1.96	0.47
31:2:379:G:O2'	31:2:2232:C:OP1	2.32	0.47
31:2:599:A:H2'	31:2:600:G:H8	1.79	0.47
31:2:1437:C:O2'	31:2:1516:G:O2'	2.25	0.47
31:2:2623:G:O5'	31:2:2826:A:O2'	2.32	0.47
35:d:24:VAL:HG13	35:d:26:GLY:H	1.80	0.47
52:1:411:A:H1'	52:1:413:G:H1'	1.96	0.47
52:1:1516:G:N2	52:1:1519:A:OP2	2.44	0.47
31:2:355:U:H2'	31:2:356:G:C8	2.50	0.47
31:2:1538:G:H2'	31:2:1539:U:H6	1.79	0.47
31:2:2182:U:H2'	31:2:2183:A:C8	2.50	0.47
32:a:69:VAL:HG23	32:a:162:VAL:HG23	1.97	0.47
52:1:416:G:H2'	52:1:417:G:C8	2.50	0.47
6:D:57:ALA:HB2	6:D:64:PRO:HD3	1.96	0.47
14:M:10:ARG:NH2	14:M:96:GLY:O	2.39	0.47
31:2:5:A:H2'	31:2:6:A:H8	1.80	0.47
31:2:578:G:OP1	31:2:1255:U:O2'	2.30	0.47
38:g:111:THR:OG1	38:g:112:ASP:N	2.47	0.47
44:m:42:ASN:HA	44:m:45:LEU:HB2	1.96	0.47
52:1:369:G:O6	52:1:392:C:N3	2.48	0.47
52:1:634:C:H2'	52:1:635:A:H8	1.80	0.47
52:1:1233:G:O2'	52:1:1365:G:OP1	2.32	0.47
52:1:1237:C:O2'	52:1:1300:G:N2	2.42	0.47
53:4:89:G:H2'	53:4:90:G:H8	1.79	0.47
1:3:22:U:H2'	1:3:23:G:C8	2.50	0.47
3:A:240:GLY:O	31:2:1902:C:O2'	2.31	0.47
18:Q:98:LYS:NZ	31:2:1323:C:OP1	2.48	0.47
31:2:577:G:O2'	31:2:1254:A:OP1	2.32	0.47
31:2:807:U:H2'	31:2:808:G:H8	1.79	0.47
31:2:2115:G:N1	31:2:2118:U:OP2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:91:ALA:HB3	3:A:103:ILE:HG22	1.97	0.47
4:B:8:LYS:HB2	4:B:201:LEU:HD11	1.97	0.47
4:B:26:VAL:HG11	15:N:4:ILE:HG12	1.97	0.47
4:B:142:VAL:HG12	4:B:144:GLY:H	1.80	0.47
7:E:151:ARG:HB3	7:E:161:VAL:HG13	1.97	0.47
10:I:80:ASP:OD2	15:N:61:ARG:NH1	2.40	0.47
12:K:25:ASP:N	12:K:25:ASP:OD1	2.46	0.47
18:Q:49:LYS:NZ	31:2:491:G:O6	2.38	0.47
31:2:145:C:H2'	31:2:146:A:C8	2.50	0.47
31:2:741:U:H2'	31:2:742:A:C8	2.50	0.47
31:2:968:C:H2'	31:2:969:G:C8	2.49	0.47
37:f:26:VAL:O	37:f:30:MET:HB2	2.14	0.47
38:g:76:ARG:NE	38:g:78:SER:O	2.47	0.47
39:h:10:ARG:HG2	39:h:15:ALA:HA	1.96	0.47
41:j:20:ALA:HB3	41:j:83:VAL:HA	1.96	0.47
50:s:19:HIS:CE1	50:s:23:ARG:HE	2.31	0.47
52:1:505:G:H2'	52:1:506:G:C8	2.50	0.47
3:A:70:LYS:O	3:A:117:SER:OG	2.33	0.47
16:O:69:ARG:NH1	31:2:1012:U:OP2	2.47	0.47
31:2:414:C:H2'	31:2:415:A:C8	2.50	0.47
31:2:1544:A:H2'	31:2:1545:A:C8	2.50	0.47
31:2:1954:G:O2'	31:2:1956:U:O4	2.25	0.47
31:2:2086:U:H2'	31:2:2087:G:C8	2.49	0.47
31:2:2385:C:H2'	31:2:2386:A:C8	2.49	0.47
52:1:297:G:N2	52:1:300:A:OP2	2.47	0.47
2:5:60:U:OP1	2:5:62:C:N4	2.45	0.47
9:G:134:ALA:O	31:2:2898:U:O2'	2.27	0.47
31:2:741:U:H2'	31:2:742:A:H8	1.79	0.47
31:2:1527:G:H2'	31:2:1544:A:H61	1.80	0.47
52:1:770:C:H2'	52:1:771:G:H8	1.79	0.47
17:P:78:ARG:HB3	17:P:81:LYS:HB2	1.97	0.47
28:AA:43:THR:OG1	28:AA:44:VAL:N	2.48	0.47
31:2:18:U:H2'	31:2:19:A:C8	2.50	0.47
31:2:177:G:H5'	31:2:178:G:C8	2.50	0.47
31:2:976:G:HO2'	31:2:1155:A:HO2'	1.57	0.47
42:k:23:LEU:HD22	42:k:29:LYS:HZ1	1.80	0.47
4:B:197:THR:OG1	31:2:2820:A:N1	2.48	0.46
31:2:274:C:H42	31:2:364:C:N4	2.12	0.46
31:2:318:C:H2'	31:2:319:G:C8	2.51	0.46
31:2:1518:C:H2'	31:2:1519:G:C8	2.50	0.46
31:2:2328:A:H2'	31:2:2329:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:15:LYS:HE3	33:b:182:ASP:HB3	1.97	0.46
44:m:37:ASP:OD1	44:m:40:ARG:NH1	2.47	0.46
52:1:222:C:H2'	52:1:223:A:H8	1.81	0.46
52:1:312:C:H2'	52:1:313:A:H8	1.80	0.46
3:A:260:LYS:HB2	31:2:2227:A:H4'	1.96	0.46
11:J:109:LYS:HG2	11:J:126:ARG:HB2	1.97	0.46
31:2:171:U:H2'	31:2:172:A:H8	1.80	0.46
31:2:598:U:H2'	31:2:599:A:C8	2.50	0.46
31:2:2692:G:H1'	31:2:2847:U:H1'	1.96	0.46
52:1:1124:G:N2	52:1:1125:U:O4	2.38	0.46
6:D:110:ILE:HB	6:D:113:PHE:HB2	1.98	0.46
17:P:68:ARG:HB2	17:P:90:ARG:HH21	1.80	0.46
20:S:24:VAL:HA	20:S:35:VAL:HA	1.98	0.46
31:2:513:A:H2'	31:2:514:A:H8	1.79	0.46
31:2:1161:C:H2'	31:2:1162:G:H8	1.81	0.46
33:b:57:GLU:HG3	33:b:59:PRO:HD3	1.97	0.46
43:l:25:GLY:H	52:1:1329:A:H5''	1.80	0.46
52:1:782:A:H62	52:1:800:G:H21	1.63	0.46
6:D:103:ILE:HD12	6:D:107:VAL:HG21	1.98	0.46
12:K:50:ARG:HG3	12:K:65:ILE:HD11	1.98	0.46
18:Q:88:ARG:NH1	31:2:748:G:OP1	2.39	0.46
31:2:1291:C:H2'	31:2:1292:G:H8	1.79	0.46
31:2:2192:U:H2'	31:2:2193:G:C8	2.50	0.46
37:f:49:LEU:HD23	37:f:58:LEU:HA	1.97	0.46
38:g:6:ILE:HD11	38:g:31:LEU:HG	1.96	0.46
40:i:11:LYS:HD3	40:i:71:LEU:HD12	1.98	0.46
45:n:64:LYS:HZ1	52:1:581:G:H5''	1.79	0.46
52:1:34:C:H2'	52:1:35:G:H8	1.80	0.46
52:1:253:A:N6	52:1:274:A:C6	2.83	0.46
52:1:1524:C:H2'	52:1:1525:G:C8	2.50	0.46
6:D:102:LEU:HD12	6:D:106:ALA:HB3	1.98	0.46
9:G:73:VAL:HA	9:G:88:THR:HA	1.98	0.46
18:Q:25:ARG:NH1	18:Q:74:ILE:O	2.48	0.46
31:2:1738:G:H2'	31:2:1739:A:H8	1.81	0.46
31:2:2450:A:N6	31:2:2501:C:O2	2.48	0.46
31:2:2705:A:O2'	31:2:2852:G:OP1	2.31	0.46
33:b:50:SER:O	33:b:69:THR:OG1	2.29	0.46
34:c:69:ARG:O	34:c:73:ASN:ND2	2.49	0.46
38:g:91:LEU:O	38:g:116:ARG:NH2	2.48	0.46
51:t:39:LYS:NZ	52:1:1526:G:N7	2.61	0.46
52:1:62:U:OP1	52:1:385:C:O2'	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:322:C:H2'	52:1:323:U:C6	2.50	0.46
52:1:713:G:H2'	52:1:714:G:C8	2.50	0.46
52:1:1376:U:H2'	52:1:1377:A:H8	1.80	0.46
10:I:88:ASN:ND2	10:I:91:SER:OG	2.42	0.46
27:Z:41:VAL:HG23	27:Z:42:VAL:HG13	1.98	0.46
31:2:145:C:H2'	31:2:146:A:H8	1.80	0.46
31:2:596:U:H2'	31:2:597:G:H8	1.80	0.46
44:m:70:HIS:HB3	52:1:974:A:H5'	1.96	0.46
52:1:312:C:H2'	52:1:313:A:C8	2.50	0.46
31:2:5:A:H2'	31:2:6:A:C8	2.51	0.46
31:2:768:G:N2	31:2:1379:U:H1'	2.31	0.46
31:2:927:A:H2'	31:2:928:A:C8	2.50	0.46
31:2:1526:C:H2'	31:2:1527:G:C8	2.51	0.46
31:2:2087:G:H2'	31:2:2088:A:H8	1.81	0.46
35:d:104:ILE:O	35:d:111:ARG:NH2	2.49	0.46
41:j:38:GLY:O	52:1:683:G:N2	2.48	0.46
49:r:59:VAL:HG11	49:r:73:PHE:HB3	1.97	0.46
52:1:202:G:N2	52:1:466:A:H61	2.14	0.46
9:G:36:LEU:HD11	9:G:122:LEU:HB2	1.97	0.46
10:I:19:VAL:HG23	10:I:43:ILE:HA	1.98	0.46
31:2:373:U:H2'	31:2:374:A:H8	1.79	0.46
31:2:1179:G:H2'	31:2:1180:U:C6	2.50	0.46
50:s:66:ILE:HB	50:s:70:LYS:HD2	1.97	0.46
52:1:152:A:H62	52:1:169:C:H42	1.64	0.46
52:1:987:G:N2	52:1:1015:G:H22	2.13	0.46
52:1:1270:G:H2'	52:1:1271:A:H8	1.79	0.46
8:F:6:LEU:HD23	8:F:7:ASP:HB2	1.98	0.46
30:AC:4:ARG:NH2	31:2:2466:C:OP2	2.49	0.46
31:2:302:C:H2'	31:2:303:G:H8	1.80	0.46
31:2:639:U:H2'	31:2:640:C:C6	2.51	0.46
31:2:1683:U:H2'	31:2:1684:G:H8	1.80	0.46
31:2:1940:U:O2	31:2:1942:C:N4	2.49	0.46
40:i:41:PRO:HA	40:i:72:ARG:HG2	1.97	0.46
40:i:50:THR:HG1	52:1:975:A:N6	2.13	0.46
42:k:30:ARG:HB2	52:1:363:A:H5'	1.97	0.46
52:1:13:U:C4	52:1:20:U:O4	2.67	0.46
52:1:297:G:N2	52:1:301:G:N7	2.64	0.46
31:2:281:C:H2'	31:2:282:A:C8	2.52	0.46
31:2:285:G:N2	31:2:355:U:O2	2.40	0.46
31:2:788:A:OP1	31:2:791:C:N4	2.43	0.46
31:2:1807:G:N2	31:2:1810:A:OP2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:2691:C:H2'	31:2:2692:G:C8	2.51	0.46
32:a:31:PHE:HB2	32:a:41:ASN:HA	1.97	0.46
32:a:191:ASP:OD1	32:a:191:ASP:N	2.39	0.46
52:1:67:C:H2'	52:1:68:G:C8	2.51	0.46
52:1:71:A:H61	52:1:99:C:H1'	1.81	0.46
10:I:21:CYS:HA	10:I:41:ILE:HG22	1.98	0.45
11:J:36:LYS:HA	11:J:41:ARG:HH22	1.81	0.45
18:Q:16:LYS:NZ	31:2:2011:U:OP2	2.41	0.45
31:2:302:C:H2'	31:2:303:G:C8	2.51	0.45
31:2:1716:U:H2'	31:2:1717:A:H8	1.81	0.45
44:m:63:CYS:HB3	44:m:68:ARG:H	1.81	0.45
44:m:63:CYS:SG	44:m:66:THR:OG1	2.64	0.45
52:1:227:G:H2'	52:1:228:A:C8	2.51	0.45
52:1:431:A:H2'	52:1:432:A:H8	1.79	0.45
52:1:587:G:N1	52:1:754:C:OP2	2.47	0.45
52:1:1173:U:H2'	52:1:1174:G:C8	2.52	0.45
1:3:1:U:H2'	1:3:2:G:C8	2.52	0.45
1:3:5:U:H2'	1:3:6:G:C8	2.51	0.45
1:3:5:U:OP1	1:3:61:G:O2'	2.30	0.45
1:3:115:A:H2'	1:3:116:G:H8	1.81	0.45
10:I:8:LEU:N	10:I:19:VAL:O	2.42	0.45
10:I:112:PHE:HD1	10:I:115:ILE:HD12	1.81	0.45
21:T:72:VAL:HG23	21:T:93:ARG:HA	1.98	0.45
31:2:2099:U:O4	31:2:2190:G:O6	2.34	0.45
31:2:2125:G:C6	31:2:2173:A:N1	2.84	0.45
31:2:2626:C:H2'	31:2:2627:G:C8	2.51	0.45
33:b:183:TYR:HE1	33:b:198:LYS:HB3	1.80	0.45
37:f:22:LEU:HD21	37:f:61:PHE:HE2	1.80	0.45
42:k:64:SER:HB2	42:k:81:ILE:HD11	1.97	0.45
52:1:105:G:N2	52:1:379:C:O3'	2.50	0.45
52:1:166:U:H2'	52:1:167:A:C8	2.52	0.45
52:1:520:A:H61	52:1:533:A:N6	2.10	0.45
52:1:553:A:H2'	52:1:554:A:C8	2.49	0.45
52:1:982:U:O2	52:1:1222:G:O6	2.35	0.45
5:C:111:GLU:OE2	5:C:115:GLN:NE2	2.49	0.45
31:2:298:G:O2'	31:2:322:A:N1	2.48	0.45
31:2:1709:U:H2'	31:2:1710:G:H8	1.81	0.45
31:2:2316:G:H2'	31:2:2317:A:H8	1.80	0.45
31:2:2836:U:H2'	31:2:2837:A:C8	2.52	0.45
49:r:80:ARG:NH1	52:1:955:U:O2'	2.42	0.45
52:1:922:G:H2'	52:1:923:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1261:A:N6	52:1:1274:A:O2'	2.49	0.45
6:D:45:ASP:OD2	6:D:48:LEU:N	2.49	0.45
31:2:934:U:H2'	31:2:935:C:H6	1.82	0.45
31:2:2567:G:H2'	31:2:2568:U:C6	2.51	0.45
43:l:106:ARG:HG2	43:l:112:ARG:HH21	1.81	0.45
52:1:519:C:O5'	53:4:61:G:N2	2.50	0.45
52:1:672:U:H2'	52:1:673:A:C8	2.51	0.45
52:1:938:A:H2'	52:1:939:G:C8	2.52	0.45
52:1:1098:C:H2'	52:1:1099:G:C8	2.52	0.45
52:1:1175:G:H2'	52:1:1176:A:C8	2.48	0.45
1:3:116:G:H2'	1:3:117:G:H8	1.81	0.45
3:A:270:ARG:HH22	31:2:1797:G:H3'	1.81	0.45
5:C:97:ASN:ND2	5:C:100:MET:SD	2.89	0.45
16:O:51:GLN:OE1	31:2:559:G:N2	2.49	0.45
16:O:92:LYS:NZ	31:2:996:A:OP2	2.41	0.45
20:S:40:LEU:HD12	20:S:59:GLU:HG3	1.97	0.45
31:2:648:G:O2'	31:2:2351:G:OP1	2.32	0.45
31:2:968:C:H2'	31:2:969:G:H8	1.80	0.45
39:h:17:ARG:NH2	52:1:1130:A:OP1	2.49	0.45
52:1:460:A:H2'	52:1:461:A:C8	2.52	0.45
52:1:890:G:O2'	52:1:906:A:N6	2.50	0.45
52:1:935:A:O2'	52:1:1383:C:N3	2.49	0.45
1:3:116:G:H2'	1:3:117:G:C8	2.52	0.45
5:C:154:ASP:HB3	5:C:157:LEU:HB2	1.98	0.45
26:Y:8:THR:OG1	26:Y:9:ARG:N	2.49	0.45
31:2:20:C:H2'	31:2:21:A:C8	2.51	0.45
31:2:1028:A:H2'	31:2:1029:A:C8	2.51	0.45
31:2:1278:C:H2'	31:2:1279:G:C8	2.52	0.45
31:2:1440:U:H2'	31:2:1441:G:H8	1.81	0.45
31:2:2099:U:H2'	31:2:2100:G:C8	2.51	0.45
31:2:2194:U:H2'	31:2:2195:U:H6	1.81	0.45
31:2:2710:C:H2'	31:2:2711:A:C8	2.52	0.45
42:k:74:GLN:HB2	42:k:77:SER:HB2	1.98	0.45
47:p:11:VAL:HG22	47:p:56:ASP:H	1.82	0.45
52:1:885:G:H2'	52:1:886:G:H8	1.81	0.45
52:1:1166:G:C6	52:1:1168:U:H5''	2.51	0.45
52:1:1412:C:H2'	52:1:1413:A:H8	1.81	0.45
23:V:36:ARG:NH2	31:2:2199:A:OP1	2.49	0.45
31:2:69:C:O2	31:2:73:A:O2'	2.33	0.45
31:2:459:U:H2'	31:2:460:A:H8	1.81	0.45
31:2:1130:U:C2	31:2:2025:C:H5''	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:1997:C:H2'	31:2:1998:A:H8	1.80	0.45
52:1:1236:A:O2'	52:1:1334:G:N2	2.48	0.45
52:1:1300:G:O2'	52:1:1301:U:OP2	2.31	0.45
3:A:233:GLY:HA3	31:2:2598:A:H5''	1.97	0.45
5:C:193:VAL:HA	5:C:196:VAL:HG12	1.98	0.45
13:L:100:CYS:HA	26:Y:42:ILE:HG12	1.99	0.45
31:2:1509:A:H2'	31:2:1510:G:H8	1.82	0.45
52:1:335:C:H2'	52:1:336:A:C8	2.52	0.45
1:3:49:C:H2'	1:3:50:A:C8	2.52	0.45
14:M:29:HIS:HB3	14:M:36:TYR:HB2	1.98	0.45
31:2:238:C:O2'	31:2:608:A:N3	2.49	0.45
31:2:1734:G:H2'	31:2:1735:A:H8	1.82	0.45
31:2:2023:C:H2'	31:2:2024:G:H8	1.82	0.45
31:2:2693:G:H2'	31:2:2694:G:H8	1.81	0.45
52:1:68:G:N2	52:1:152:A:O2'	2.49	0.45
52:1:591:U:H2'	52:1:592:G:C8	2.50	0.45
52:1:1200:C:H1'	52:1:1205:U:H3	1.80	0.45
3:A:257:ARG:NH1	3:A:262:THR:OG1	2.50	0.45
13:L:11:ASN:OD1	31:2:1653:G:N1	2.46	0.45
29:AB:1:PRO:HD2	31:2:591:U:H1'	1.99	0.45
31:2:351:C:H2'	31:2:352:A:C8	2.52	0.45
31:2:354:A:H2'	31:2:355:U:C6	2.52	0.45
31:2:1667:G:O2'	31:2:1991:U:O4	2.32	0.45
31:2:1744:A:H3'	31:2:1745:A:H8	1.81	0.45
31:2:1939:U:OP1	31:2:2604:U:O2'	2.31	0.45
31:2:2385:C:H2'	31:2:2386:A:H8	1.81	0.45
31:2:2591:C:H2'	31:2:2592:G:C8	2.52	0.45
34:c:200:VAL:O	34:c:204:SER:HB2	2.16	0.45
52:1:67:C:H2'	52:1:68:G:H8	1.81	0.45
12:K:41:LEU:HD13	12:K:96:ILE:HG13	1.99	0.44
31:2:438:G:H2'	31:2:439:A:C8	2.53	0.44
43:l:15:VAL:HG11	43:l:30:LYS:HE3	1.99	0.44
46:o:39:PHE:HD1	46:o:50:THR:HG22	1.81	0.44
49:r:28:LYS:HE3	49:r:28:LYS:HB3	1.79	0.44
52:1:397:A:N7	52:1:547:A:O2'	2.45	0.44
52:1:1162:C:H2'	52:1:1163:A:C8	2.53	0.44
4:B:197:THR:O	31:2:2820:A:N6	2.49	0.44
5:C:119:ILE:HB	5:C:187:VAL:HG12	1.99	0.44
10:I:60:ALA:HA	10:I:87:LEU:HB2	1.99	0.44
18:Q:6:LYS:HB2	31:2:494:G:H4'	1.99	0.44
31:2:2836:U:H2'	31:2:2837:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:f:67:ASN:ND2	37:f:69:ARG:O	2.51	0.44
52:1:254:G:H2'	52:1:255:G:H8	1.82	0.44
52:1:414:A:N6	52:1:430:A:H2	2.13	0.44
52:1:496:A:H2'	52:1:497:G:C8	2.53	0.44
52:1:687:A:C5	52:1:703:G:C2	3.05	0.44
52:1:1200:C:H5''	52:1:1201:A:H3'	1.99	0.44
1:3:95:U:H2'	1:3:96:G:H8	1.81	0.44
17:P:78:ARG:HH11	31:2:974:G:H4'	1.83	0.44
31:2:1983:G:H4'	31:2:2606:C:H4'	1.97	0.44
39:h:22:PRO:HA	39:h:60:LEU:HA	1.98	0.44
52:1:26:A:H61	52:1:558:G:H1'	1.81	0.44
2:5:20:U:O4	2:5:59:U:O4	2.35	0.44
4:B:184:ARG:NH2	15:N:6:GLN:OE1	2.50	0.44
18:Q:92:ARG:O	31:2:1614:A:N6	2.41	0.44
31:2:6:A:H2'	31:2:7:G:C8	2.53	0.44
31:2:873:C:H2'	31:2:874:G:H8	1.81	0.44
31:2:904:G:H2'	31:2:905:A:H8	1.81	0.44
31:2:1255:U:H5''	31:2:1256:G:H5''	2.00	0.44
31:2:1510:G:H2'	31:2:1511:G:C8	2.53	0.44
31:2:1960:A:HO2'	52:1:1484:C:HO2'	1.63	0.44
31:2:2125:G:O6	31:2:2173:A:N1	2.50	0.44
34:c:109:THR:HG22	34:c:111:ALA:H	1.82	0.44
34:c:118:SER:O	34:c:130:ASN:ND2	2.51	0.44
43:l:84:CYS:HB2	49:r:72:GLU:HB3	1.98	0.44
44:m:63:CYS:SG	44:m:64:ARG:N	2.90	0.44
52:1:150:U:O2	52:1:171:A:N7	2.51	0.44
52:1:616:G:H2'	52:1:617:G:C8	2.52	0.44
52:1:702:A:H8	52:1:703:G:H4'	1.81	0.44
52:1:1001:C:H2'	52:1:1002:G:C8	2.53	0.44
52:1:1149:C:O2'	52:1:1280:A:N1	2.50	0.44
52:1:1157:A:H62	52:1:1178:G:H1'	1.82	0.44
52:1:1363:A:H2'	52:1:1365:G:N7	2.33	0.44
15:N:91:VAL:HG21	15:N:96:LEU:HD11	1.99	0.44
19:R:80:TRP:HZ3	19:R:82:LYS:HB3	1.82	0.44
38:g:79:ARG:NH1	52:1:878:A:OP1	2.47	0.44
39:h:121:ARG:HD3	52:1:1348:U:H4'	1.99	0.44
49:r:45:GLY:N	49:r:61:VAL:O	2.51	0.44
52:1:1089:G:O6	52:1:1097:C:N4	2.50	0.44
52:1:1269:A:N1	52:1:1312:G:O2'	2.42	0.44
52:1:1399:C:H4'	52:1:1400:C:H3'	1.98	0.44
1:3:1:U:O4	1:3:120:A:N6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:64:A:H2'	2:5:65:G:C8	2.52	0.44
31:2:1476:U:H2'	31:2:1477:A:H8	1.82	0.44
31:2:1510:G:H2'	31:2:1511:G:H8	1.81	0.44
31:2:1689:A:H2'	31:2:1690:A:C8	2.53	0.44
31:2:2070:A:H2'	31:2:2071:A:H8	1.82	0.44
31:2:2093:G:H2'	31:2:2094:A:H8	1.82	0.44
31:2:2229:U:H2'	31:2:2230:G:C8	2.49	0.44
33:b:26:LYS:NZ	33:b:27:GLU:OE2	2.48	0.44
33:b:149:LYS:HB3	33:b:200:TRP:HB2	2.00	0.44
49:r:13:HIS:CD2	52:1:1014:A:H5''	2.53	0.44
52:1:201:G:H21	52:1:469:C:H1'	1.83	0.44
52:1:555:U:H2'	52:1:556:C:C6	2.53	0.44
3:A:5:CYS:SG	3:A:12:ARG:NH2	2.88	0.44
4:B:118:PHE:O	31:2:1654:A:O2'	2.31	0.44
13:L:96:ARG:HH22	13:L:116:VAL:HA	1.82	0.44
14:M:30:ARG:HH11	14:M:102:ARG:HH11	1.65	0.44
15:N:23:ASP:HA	15:N:89:GLY:H	1.83	0.44
23:V:58:ILE:HG12	23:V:66:VAL:HG21	1.99	0.44
29:AB:31:ILE:O	29:AB:35:LYS:NZ	2.50	0.44
31:2:75:G:H22	31:2:111:A:H2	1.65	0.44
31:2:422:A:H3'	31:2:423:A:H8	1.83	0.44
31:2:879:G:H2'	31:2:880:G:C8	2.53	0.44
31:2:1149:G:H2'	31:2:1150:C:C6	2.53	0.44
31:2:1266:G:O2'	31:2:2012:G:O6	2.32	0.44
31:2:2303:G:O6	31:2:2314:A:N6	2.51	0.44
31:2:2788:C:H2'	31:2:2789:C:C6	2.52	0.44
34:c:70:GLN:HA	34:c:73:ASN:HD21	1.82	0.44
35:d:148:SER:OG	35:d:150:GLU:OE1	2.34	0.44
42:k:5:GLN:HE21	52:1:880:C:H3'	1.83	0.44
43:l:38:ILE:HG13	43:l:55:LEU:HD21	1.99	0.44
43:l:101:THR:O	52:1:1226:C:O2'	2.34	0.44
44:m:47:LEU:HD21	52:1:1317:C:H4'	2.00	0.44
1:3:78:A:H62	1:3:98:G:N2	2.13	0.44
3:A:44:ASN:N	3:A:44:ASN:OD1	2.50	0.44
9:G:37:ARG:HG3	9:G:39:LYS:HG3	1.99	0.44
31:2:742:A:H2'	31:2:743:A:H8	1.81	0.44
31:2:1683:U:H2'	31:2:1684:G:C8	2.52	0.44
31:2:2303:G:H2'	31:2:2304:G:C8	2.52	0.44
31:2:2329:U:H2'	31:2:2330:G:C8	2.52	0.44
39:h:45:MET:HE3	39:h:45:MET:HB3	1.82	0.44
44:m:52:ARG:HD3	52:1:1317:C:H42	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:131:A:H2'	52:1:132:C:C6	2.53	0.44
52:1:235:C:H2'	52:1:236:A:H8	1.82	0.44
52:1:497:G:H2'	52:1:498:A:C8	2.53	0.44
52:1:934:C:O2	52:1:938:A:N6	2.50	0.44
14:M:115:LEU:HD23	14:M:115:LEU:HA	1.83	0.44
25:X:8:GLN:HB2	25:X:28:LEU:HD22	1.98	0.44
31:2:1447:C:H2'	31:2:1448:G:C8	2.53	0.44
31:2:2039:U:H2'	31:2:2040:G:H8	1.82	0.44
31:2:2320:U:O2'	31:2:2322:A:N7	2.47	0.44
32:a:160:LEU:HB3	32:a:182:VAL:HG12	2.00	0.44
33:b:36:PHE:HE1	44:m:91:GLU:HG3	1.82	0.44
44:m:99:SER:OG	52:1:1187:G:N3	2.46	0.44
30:AC:19:ARG:NE	31:2:2756:U:OP2	2.41	0.43
31:2:582:A:H2'	31:2:583:G:C8	2.53	0.43
31:2:1031:G:H2'	31:2:1032:A:C8	2.53	0.43
31:2:1387:A:H5'	31:2:1469:A:H1'	2.00	0.43
31:2:1682:G:OP2	31:2:1699:G:N2	2.46	0.43
31:2:2093:G:H2'	31:2:2094:A:C8	2.53	0.43
31:2:2391:G:H1	31:2:2424:C:H3'	1.82	0.43
36:e:9:MET:HG2	36:e:86:ARG:HB3	1.99	0.43
45:n:57:ARG:NH1	45:n:61:GLN:OE1	2.51	0.43
50:s:9:ARG:HG2	52:1:108:G:N1	2.33	0.43
52:1:507:C:OP2	52:1:508:U:O2'	2.29	0.43
52:1:575:G:O2'	52:1:821:G:OP2	2.31	0.43
52:1:1354:U:H2'	52:1:1355:G:H8	1.83	0.43
53:4:58:G:N2	53:4:60:A:N1	2.66	0.43
5:C:69:ARG:NH1	31:2:2445:G:OP1	2.50	0.43
6:D:35:LEU:HG	6:D:88:VAL:HB	2.00	0.43
7:E:87:GLN:HE21	7:E:162:ARG:HD2	1.83	0.43
31:2:874:G:H2'	31:2:875:G:H8	1.83	0.43
31:2:1198:U:H2'	31:2:1199:U:H6	1.83	0.43
31:2:1440:U:H2'	31:2:1441:G:C8	2.53	0.43
31:2:1710:G:H2'	31:2:1711:A:C8	2.53	0.43
31:2:2590:A:H2'	31:2:2591:C:H6	1.83	0.43
40:i:12:ALA:HB3	40:i:18:ILE:HB	2.01	0.43
41:j:45:THR:HG23	41:j:48:GLY:H	1.83	0.43
42:k:30:ARG:N	52:1:363:A:OP1	2.49	0.43
52:1:815:A:N7	52:1:1509:C:O2'	2.40	0.43
52:1:1291:U:H2'	52:1:1292:G:H8	1.84	0.43
52:1:1355:G:H2'	52:1:1356:G:C8	2.53	0.43
6:D:68:LYS:HA	6:D:83:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:8:VAL:O	7:E:49:LEU:N	2.50	0.43
30:AC:25:VAL:HG13	30:AC:35:GLN:HB2	2.00	0.43
31:2:314:C:H2'	31:2:315:G:C8	2.54	0.43
31:2:733:G:N2	31:2:734:A:N7	2.66	0.43
31:2:2514:U:H2'	31:2:2515:C:C6	2.53	0.43
31:2:2589:A:N1	31:2:2606:C:N4	2.66	0.43
33:b:21:TRP:HB3	33:b:58:ARG:HB2	1.99	0.43
42:k:107:LYS:HA	42:k:107:LYS:HD3	1.80	0.43
52:1:405:U:H1'	52:1:498:A:H2'	1.99	0.43
52:1:549:C:H2'	52:1:550:G:H8	1.83	0.43
52:1:1162:C:H2'	52:1:1163:A:H8	1.84	0.43
52:1:1513:A:H2'	52:1:1514:G:H8	1.82	0.43
9:G:35:ARG:HA	9:G:40:HIS:HD2	1.83	0.43
16:O:14:LYS:HE2	16:O:14:LYS:HB2	1.84	0.43
26:Y:37:HIS:ND1	26:Y:38:LEU:O	2.45	0.43
31:2:1361:G:HO2'	31:2:2215:C:HO2'	1.62	0.43
31:2:1794:A:H2'	31:2:1795:C:C6	2.54	0.43
31:2:1987:A:H2'	31:2:1988:G:H8	1.82	0.43
31:2:2818:U:H2'	31:2:2819:G:C8	2.53	0.43
31:2:2818:U:H2'	31:2:2819:G:H8	1.82	0.43
32:a:81:ASP:N	32:a:81:ASP:OD1	2.52	0.43
35:d:149:PRO:HA	35:d:152:VAL:HG12	2.00	0.43
40:i:64:GLN:HB3	44:m:98:ALA:HB3	2.00	0.43
52:1:236:A:H2'	52:1:237:G:C8	2.53	0.43
52:1:411:A:H2	52:1:430:A:N6	2.16	0.43
52:1:748:G:H2'	52:1:749:A:H8	1.84	0.43
52:1:762:U:H2'	52:1:763:G:H8	1.83	0.43
52:1:1524:C:H2'	52:1:1525:G:H8	1.83	0.43
15:N:32:VAL:HG12	15:N:37:LYS:HB2	1.99	0.43
30:AC:36:ARG:NE	31:2:2742:G:OP1	2.52	0.43
31:2:632:A:H2'	31:2:633:A:C8	2.53	0.43
31:2:1164:C:H2'	31:2:1165:A:H8	1.84	0.43
31:2:1443:U:H2'	31:2:1444:G:C8	2.53	0.43
31:2:1592:C:H2'	31:2:1593:A:H8	1.82	0.43
31:2:1716:U:O2	31:2:1744:A:N7	2.52	0.43
31:2:2547:A:H2'	31:2:2548:U:C6	2.53	0.43
33:b:35:ASP:HA	33:b:38:VAL:HG22	2.00	0.43
34:c:119:HIS:O	34:c:145:ARG:NH2	2.50	0.43
3:A:36:ASN:HB2	3:A:61:TYR:HB2	1.99	0.43
3:A:83:ASP:OD2	3:A:86:ARG:NH2	2.45	0.43
6:D:35:LEU:HA	6:D:152:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:75:VAL:HA	7:E:78:VAL:HG12	2.01	0.43
12:K:35:ALA:HB2	12:K:102:LEU:HD11	1.99	0.43
21:T:32:GLY:O	21:T:93:ARG:NH1	2.42	0.43
31:2:6:A:H2'	31:2:7:G:H8	1.83	0.43
31:2:390:U:OP1	31:2:412:A:O2'	2.36	0.43
31:2:408:G:H1	31:2:419:U:H3	1.67	0.43
31:2:882:G:H2'	31:2:883:G:H8	1.83	0.43
31:2:1509:A:H2'	31:2:1510:G:C8	2.54	0.43
39:h:113:LYS:NZ	39:h:114:LYS:O	2.45	0.43
40:i:59:LYS:NZ	52:1:973:G:OP1	2.48	0.43
50:s:73:ARG:NH1	52:1:260:G:N7	2.67	0.43
52:1:260:G:H2'	52:1:261:U:C6	2.53	0.43
52:1:358:U:H2'	52:1:359:G:C8	2.54	0.43
52:1:1068:G:H1	52:1:1108:G:H1'	1.83	0.43
52:1:1305:G:N2	52:1:1331:G:H2'	2.34	0.43
7:E:3:VAL:HG21	31:2:2748:A:H4'	2.01	0.43
31:2:91:A:H1'	31:2:92:U:C2	2.54	0.43
31:2:848:C:H2'	31:2:849:A:C8	2.49	0.43
31:2:2291:U:H2'	31:2:2292:U:C6	2.53	0.43
31:2:2875:C:H2'	31:2:2876:G:H8	1.84	0.43
33:b:196:GLY:H	52:1:1057:G:H4'	1.83	0.43
41:j:22:ILE:HG22	41:j:31:VAL:HB	2.00	0.43
52:1:791:G:O6	52:1:792:A:N6	2.51	0.43
52:1:1011:C:H2'	52:1:1012:A:H8	1.83	0.43
52:1:1288:A:H2'	52:1:1289:A:C8	2.53	0.43
52:1:1345:U:O2	52:1:1376:U:C2	2.71	0.43
52:1:1457:G:H2'	52:1:1458:G:H8	1.83	0.43
4:B:155:VAL:HG11	31:2:2618:G:H21	1.83	0.43
31:2:1432:G:H2'	31:2:1433:A:C8	2.54	0.43
31:2:2087:G:H2'	31:2:2088:A:C8	2.54	0.43
31:2:2192:U:H2'	31:2:2193:G:H8	1.84	0.43
35:d:155:LYS:HD2	38:g:70:VAL:HA	1.99	0.43
39:h:39:GLY:HA2	39:h:44:ARG:HE	1.84	0.43
39:h:108:ARG:HB3	52:1:1347:G:C8	2.52	0.43
44:m:65:GLN:HG2	44:m:78:LEU:HD22	2.01	0.43
52:1:783:C:H2'	52:1:784:A:H8	1.83	0.43
52:1:1074:G:H1	52:1:1083:U:H3	1.67	0.43
52:1:1118:U:H1'	52:1:1179:A:C5	2.54	0.43
2:5:38:A:O2'	52:1:790:A:OP1	2.27	0.43
5:C:18:THR:HG23	5:C:106:LYS:HG2	2.01	0.43
5:C:156:ASN:OD1	5:C:156:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:30:VAL:HA	6:D:157:THR:HG22	2.00	0.43
7:E:120:ILE:HD11	7:E:139:VAL:HG13	2.00	0.43
31:2:172:A:H2'	31:2:173:A:C8	2.53	0.43
31:2:513:A:O2'	31:2:1217:U:OP1	2.35	0.43
31:2:833:A:H2'	31:2:834:G:C8	2.54	0.43
31:2:2070:A:H2'	31:2:2071:A:C8	2.54	0.43
31:2:2071:A:H2'	31:2:2072:C:C6	2.54	0.43
31:2:2110:G:N1	31:2:2179:C:N4	2.64	0.43
48:q:49:LYS:HD3	52:1:663:A:H5''	1.99	0.43
52:1:922:G:H2'	52:1:923:A:C8	2.54	0.43
25:X:15:ARG:HG3	25:X:53:MET:HE1	2.01	0.43
27:Z:35:LEU:HD12	27:Z:35:LEU:HA	1.93	0.43
31:2:582:A:H2'	31:2:583:G:H8	1.83	0.43
31:2:1219:U:H2'	31:2:1220:G:C8	2.54	0.43
31:2:1709:U:H2'	31:2:1710:G:C8	2.54	0.43
31:2:1866:A:N3	31:2:1876:A:N6	2.67	0.43
31:2:2875:C:H2'	31:2:2876:G:C8	2.53	0.43
34:c:104:MET:HE3	34:c:170:LEU:HD22	2.01	0.43
37:f:13:PRO:HB3	37:f:20:GLU:HG3	2.01	0.43
52:1:199:A:H2'	52:1:200:G:C8	2.54	0.43
1:3:63:C:H2'	1:3:64:G:C8	2.54	0.42
3:A:13:ARG:NH1	31:2:1693:U:O2'	2.46	0.42
11:J:37:GLY:H	11:J:40:SER:HB3	1.84	0.42
12:K:17:ASN:HD21	12:K:95:LEU:HD22	1.84	0.42
28:AA:25:LYS:NZ	31:2:210:C:OP1	2.47	0.42
31:2:1746:A:H2'	31:2:1747:U:C6	2.54	0.42
31:2:2114:A:C6	31:2:2119:A:C6	2.98	0.42
31:2:2559:C:H2'	31:2:2560:A:H8	1.84	0.42
35:d:146:MET:HE3	35:d:146:MET:HB3	1.87	0.42
52:1:56:U:H2'	52:1:57:G:C8	2.54	0.42
52:1:952:U:H2'	52:1:953:G:H8	1.84	0.42
52:1:1268:G:HO2'	52:1:1326:U:HO2'	1.66	0.42
2:5:18:G:O2'	2:5:57:G:N2	2.52	0.42
4:B:110:THR:HB	4:B:171:THR:HG23	2.00	0.42
7:E:16:VAL:HB	7:E:23:ILE:HD11	2.01	0.42
9:G:74:TYR:HE2	9:G:100:VAL:HG12	1.84	0.42
13:L:79:LEU:HD12	13:L:83:LEU:HD12	2.01	0.42
31:2:976:G:O2'	31:2:1155:A:O2'	2.31	0.42
31:2:1427:A:H4'	31:2:1428:C:O4'	2.19	0.42
31:2:1909:C:H2'	31:2:1910:G:C8	2.53	0.42
31:2:1913:A:H62	52:1:1408:A:H61	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:g:63:LYS:HB3	38:g:70:VAL:HG21	2.00	0.42
40:i:68:ARG:HH22	52:1:1115:U:H5'	1.84	0.42
43:l:32:ILE:HD12	43:l:58:GLU:HG3	2.00	0.42
49:r:45:GLY:H	49:r:62:THR:HA	1.84	0.42
52:1:13:U:O4	52:1:20:U:C4	2.69	0.42
52:1:1316:G:N1	52:1:1319:A:OP2	2.47	0.42
52:1:1454:G:H2'	52:1:1455:G:H8	1.85	0.42
52:1:1492:A:H4'	53:4:92:A:H3'	2.01	0.42
1:3:66:A:N1	1:3:108:A:N6	2.67	0.42
2:5:15:G:H2'	2:5:16:U:C6	2.54	0.42
6:D:116:LEU:HB2	6:D:176:PHE:HD1	1.84	0.42
31:2:49:A:H4'	31:2:50:U:H5'	2.01	0.42
31:2:1164:C:H2'	31:2:1165:A:C8	2.55	0.42
31:2:1258:U:H2'	31:2:1259:G:C8	2.55	0.42
3:A:35:LYS:NZ	31:2:1354:A:OP1	2.50	0.42
3:A:167:ASP:N	3:A:167:ASP:OD1	2.51	0.42
3:A:206:LYS:HB2	31:2:729:G:C5	2.54	0.42
5:C:126:VAL:HG22	5:C:157:LEU:HD22	2.01	0.42
8:F:12:LEU:HD13	8:F:19:VAL:HG21	2.00	0.42
30:AC:7:VAL:O	31:2:1031:G:O2'	2.38	0.42
31:2:859:G:H1'	31:2:860:U:H5	1.84	0.42
31:2:1368:G:H2'	31:2:1369:G:H8	1.85	0.42
31:2:1434:A:H2'	31:2:1435:G:C8	2.54	0.42
31:2:1877:A:H2'	31:2:1878:G:H8	1.85	0.42
31:2:2861:U:H2'	31:2:2862:G:C8	2.55	0.42
42:k:73:LEU:HD22	42:k:98:ARG:HH12	1.85	0.42
46:o:33:ILE:HG22	46:o:34:GLU:HG3	2.01	0.42
52:1:72:A:H61	52:1:98:A:H2	1.67	0.42
52:1:549:C:H2'	52:1:550:G:C8	2.54	0.42
52:1:762:U:H2'	52:1:763:G:C8	2.54	0.42
52:1:1242:G:N2	52:1:1295:U:O2	2.48	0.42
19:R:30:ILE:HG23	19:R:85:VAL:HG13	2.01	0.42
19:R:69:ARG:HH11	19:R:72:GLN:HA	1.83	0.42
25:X:47:ILE:O	25:X:51:SER:HB3	2.18	0.42
28:AA:3:ARG:HD3	28:AA:3:ARG:HA	1.87	0.42
31:2:593:U:H3	31:2:664:G:H1	1.66	0.42
31:2:813:U:H2'	31:2:814:C:H6	1.84	0.42
31:2:851:C:H2'	31:2:852:U:H6	1.84	0.42
31:2:1476:U:H3	31:2:1515:A:H62	1.67	0.42
31:2:2175:C:H2'	31:2:2176:A:C8	2.55	0.42
31:2:2863:C:H2'	31:2:2864:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:120:LYS:HE3	34:c:130:ASN:HD22	1.84	0.42
42:k:110:LYS:HA	42:k:113:ARG:HH21	1.85	0.42
52:1:663:A:H2'	52:1:664:G:C8	2.55	0.42
52:1:1467:C:H2'	52:1:1468:A:C8	2.55	0.42
52:1:1522:U:H2'	52:1:1523:G:C8	2.55	0.42
3:A:175:LEU:HD23	31:2:1799:G:C5	2.55	0.42
5:C:130:LYS:HD3	5:C:130:LYS:HA	1.85	0.42
12:K:12:MET:HA	31:2:910:A:H62	1.84	0.42
13:L:13:ASN:OD1	13:L:14:SER:N	2.50	0.42
31:2:151:C:H2'	31:2:152:A:C8	2.54	0.42
31:2:596:U:H2'	31:2:597:G:C8	2.54	0.42
31:2:1431:A:H2'	31:2:1432:G:C8	2.54	0.42
31:2:2812:G:H2'	31:2:2813:A:H8	1.84	0.42
33:b:175:HIS:O	52:1:1111:A:N6	2.51	0.42
36:e:6:ILE:HG21	36:e:78:PHE:HE2	1.85	0.42
43:l:47:LEU:HD11	43:l:51:GLN:HB2	2.02	0.42
52:1:424:G:H2'	52:1:425:G:C8	2.55	0.42
52:1:674:G:H2'	52:1:675:A:C8	2.48	0.42
52:1:714:G:H2'	52:1:715:A:C8	2.55	0.42
52:1:1314:C:H2'	52:1:1315:U:C6	2.55	0.42
52:1:1472:U:H2'	52:1:1473:G:C8	2.55	0.42
3:A:77:VAL:HA	3:A:93:VAL:HA	2.02	0.42
6:D:37:MET:HG3	6:D:56:LEU:HD11	2.01	0.42
6:D:79:ARG:HA	6:D:79:ARG:HD3	1.74	0.42
23:V:60:LYS:NZ	31:2:371:A:N3	2.63	0.42
31:2:224:U:O4	31:2:419:U:O2'	2.36	0.42
31:2:453:A:N3	31:2:457:A:O2'	2.53	0.42
31:2:2118:U:H3	31:2:2143:C:H42	1.68	0.42
31:2:2128:G:H1'	31:2:2173:A:H1'	2.02	0.42
31:2:2627:G:N2	31:2:2777:G:OP2	2.52	0.42
38:g:88:LYS:HE2	38:g:88:LYS:HB3	1.90	0.42
52:1:676:A:H2'	52:1:677:U:H6	1.85	0.42
52:1:1491:G:H2'	52:1:1492:A:C4	2.55	0.42
5:C:65:THR:HG23	5:C:67:ARG:H	1.84	0.42
5:C:173:THR:HA	5:C:199:MET:HE1	2.02	0.42
15:N:104:GLY:O	15:N:108:ARG:NH2	2.52	0.42
16:O:53:LYS:NZ	31:2:994:C:OP2	2.35	0.42
18:Q:17:VAL:HG12	18:Q:76:VAL:HG21	2.02	0.42
31:2:1306:C:H2'	31:2:1307:A:H8	1.85	0.42
31:2:1445:G:O6	31:2:1466:U:O2	2.38	0.42
31:2:2293:G:H2'	31:2:2294:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:185:ILE:HA	32:a:199:ILE:HG23	2.02	0.42
33:b:69:THR:OG1	33:b:70:ALA:N	2.52	0.42
37:f:45:ALA:HB1	37:f:119:LEU:HD13	2.02	0.42
49:r:13:HIS:HA	49:r:16:LYS:HG2	2.02	0.42
52:1:533:A:O2'	52:1:535:A:OP2	2.32	0.42
52:1:1140:C:H2'	52:1:1141:C:C6	2.55	0.42
3:A:173:LEU:HD21	3:A:183:VAL:HG23	2.02	0.42
21:T:3:THR:HG22	21:T:62:THR:HB	2.01	0.42
31:2:851:C:H2'	31:2:852:U:C6	2.55	0.42
31:2:974:G:H1'	31:2:975:A:C8	2.55	0.42
31:2:1592:C:H2'	31:2:1593:A:C8	2.55	0.42
35:d:141:ASP:HA	35:d:144:GLU:HG2	2.01	0.42
38:g:9:MET:HE2	38:g:9:MET:HB3	1.94	0.42
39:h:43:ALA:HA	39:h:46:VAL:HG22	2.01	0.42
52:1:458:U:H2'	52:1:459:A:C8	2.55	0.42
52:1:757:U:H5'	52:1:822:U:H1'	2.01	0.42
52:1:1266:G:H21	52:1:1268:G:H3'	1.85	0.42
1:3:25:U:O2	1:3:117:G:O2'	2.33	0.42
1:3:80:U:H2'	1:3:81:G:H8	1.85	0.42
2:5:40:C:H2'	2:5:41:C:C6	2.55	0.42
21:T:76:ASP:N	21:T:90:ASP:OD1	2.50	0.42
21:T:77:VAL:HG22	21:T:89:ILE:HD12	2.02	0.42
31:2:414:C:H2'	31:2:415:A:H8	1.84	0.42
31:2:1013:C:H2'	31:2:1014:A:H8	1.85	0.42
31:2:1335:C:H2'	31:2:1336:A:H8	1.85	0.42
31:2:1447:C:H2'	31:2:1448:G:H8	1.84	0.42
31:2:1563:U:H2'	31:2:1564:C:C6	2.55	0.42
31:2:1801:A:H5''	31:2:2203:U:H2'	2.02	0.42
31:2:2443:C:H2'	31:2:2444:G:C8	2.55	0.42
38:g:35:ILE:HA	38:g:38:VAL:HG12	2.01	0.42
40:i:51:VAL:HG13	44:m:80:ARG:HB3	2.02	0.42
52:1:505:G:H2'	52:1:506:G:H8	1.85	0.42
3:A:68:ARG:HH12	3:A:115:ILE:HD12	1.84	0.41
4:B:186:LEU:HD12	4:B:186:LEU:HA	1.86	0.41
8:F:7:ASP:OD1	8:F:8:LYS:N	2.53	0.41
31:2:2626:C:H2'	31:2:2627:G:H8	1.85	0.41
31:2:2863:C:H2'	31:2:2864:G:C8	2.55	0.41
32:a:68:PHE:HD1	32:a:161:PHE:HB3	1.85	0.41
33:b:5:HIS:CE1	33:b:7:ASN:HB3	2.55	0.41
36:e:74:LEU:HA	36:e:77:THR:HG22	2.02	0.41
52:1:952:U:H2'	52:1:953:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:16:VAL:HB	3:A:203:VAL:HB	2.02	0.41
7:E:106:LEU:HD13	7:E:151:ARG:HB2	2.01	0.41
21:T:36:ALA:O	21:T:93:ARG:NH2	2.52	0.41
31:2:192:C:O2	31:2:802:A:O2'	2.35	0.41
31:2:306:U:H2'	31:2:307:G:O4'	2.20	0.41
31:2:548:G:N7	31:2:549:G:O2'	2.53	0.41
31:2:729:G:H5'	31:2:730:A:H5''	2.01	0.41
42:k:116:TYR:OH	52:1:522:C:OP1	2.38	0.41
43:l:25:GLY:N	52:1:1329:A:H5''	2.35	0.41
52:1:358:U:H2'	52:1:359:G:H8	1.85	0.41
52:1:634:C:H2'	52:1:635:A:C8	2.55	0.41
52:1:1500:A:H5''	52:1:1508:A:H5''	2.02	0.41
1:3:12:C:H41	22:U:70:PRO:HD3	1.85	0.41
11:J:18:ARG:NH2	31:2:1250:G:OP2	2.52	0.41
31:2:182:A:N3	31:2:433:C:O2'	2.52	0.41
31:2:1219:U:H2'	31:2:1220:G:H8	1.84	0.41
31:2:1409:U:H2'	31:2:1410:G:H8	1.86	0.41
34:c:144:ILE:HB	34:c:177:MET:HB3	2.01	0.41
35:d:45:VAL:O	35:d:71:ILE:N	2.47	0.41
41:j:20:ALA:N	41:j:82:GLU:O	2.54	0.41
42:k:23:LEU:HD13	42:k:29:LYS:HG3	2.02	0.41
45:n:48:ASP:OD1	45:n:48:ASP:N	2.41	0.41
52:1:176:C:H2'	52:1:177:G:N3	2.36	0.41
52:1:195:A:H2'	52:1:196:A:C4	2.55	0.41
52:1:558:G:OP2	52:1:559:A:O2'	2.35	0.41
52:1:806:C:H2'	52:1:807:A:C8	2.54	0.41
52:1:1076:U:H2'	52:1:1077:G:C8	2.54	0.41
52:1:1173:U:H2'	52:1:1174:G:H8	1.85	0.41
53:4:83:A:H2'	53:4:84:G:H8	1.86	0.41
3:A:77:VAL:HG12	3:A:93:VAL:HG12	2.02	0.41
18:Q:17:VAL:HB	18:Q:76:VAL:HG11	2.03	0.41
31:2:133:U:H2'	31:2:134:G:H8	1.85	0.41
31:2:895:U:H2'	31:2:897:C:H5	1.85	0.41
31:2:1038:G:H2'	31:2:1039:A:C8	2.55	0.41
34:c:58:GLN:OE1	34:c:61:ARG:NH2	2.53	0.41
38:g:29:SER:HB2	38:g:32:LYS:HG3	2.01	0.41
43:l:61:LYS:HE2	43:l:61:LYS:HB3	1.93	0.41
52:1:453:G:H2'	52:1:454:G:C8	2.55	0.41
52:1:960:U:H4'	52:1:961:U:H5''	2.02	0.41
52:1:1313:U:H2'	52:1:1314:C:C6	2.55	0.41
52:1:1388:C:H2'	52:1:1389:C:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:112:LEU:HD13	5:C:186:VAL:HG11	2.03	0.41
15:N:23:ASP:OD1	15:N:89:GLY:N	2.54	0.41
15:N:59:THR:HA	15:N:72:VAL:HA	2.01	0.41
27:Z:25:ASN:OD1	27:Z:25:ASN:N	2.52	0.41
31:2:415:A:H2'	31:2:416:U:C6	2.56	0.41
31:2:863:A:H2'	31:2:864:G:C8	2.55	0.41
31:2:2037:A:H2'	31:2:2038:G:C8	2.55	0.41
31:2:2241:A:H2'	31:2:2242:G:C8	2.55	0.41
31:2:2424:C:H5'	31:2:2425:A:H5''	2.02	0.41
31:2:2543:G:H2'	31:2:2544:G:C8	2.56	0.41
38:g:87:ARG:HA	52:1:599:C:H5''	2.02	0.41
43:l:25:GLY:O	43:l:29:SER:OG	2.25	0.41
48:q:29:LYS:HA	48:q:32:ILE:HG22	2.03	0.41
50:s:53:MET:HE2	50:s:53:MET:HB2	1.91	0.41
31:2:290:U:O2	31:2:350:G:C2	2.73	0.41
31:2:1176:U:H3'	31:2:1177:G:H8	1.85	0.41
33:b:181:ILE:HD11	33:b:200:TRP:HB3	2.02	0.41
37:f:61:PHE:HB3	37:f:64:ALA:HB3	2.03	0.41
52:1:254:G:H2'	52:1:255:G:C8	2.55	0.41
52:1:259:G:H2'	52:1:260:G:C8	2.55	0.41
52:1:501:C:H2'	52:1:502:A:C8	2.54	0.41
52:1:525:C:H2'	52:1:526:C:C6	2.56	0.41
3:A:204:LEU:O	31:2:1791:A:O2'	2.31	0.41
5:C:58:LYS:NZ	5:C:70:SER:O	2.43	0.41
16:O:54:ARG:NH2	31:2:1155:A:O3'	2.45	0.41
20:S:80:ASP:OD1	20:S:81:ARG:N	2.53	0.41
27:Z:36:LYS:HE2	27:Z:45:HIS:HB3	2.02	0.41
31:2:565:C:H2'	31:2:566:U:C6	2.55	0.41
31:2:599:A:H2'	31:2:600:G:C8	2.56	0.41
31:2:1752:C:H2'	31:2:1753:G:C8	2.56	0.41
31:2:1802:A:H2'	31:2:1803:A:H8	1.86	0.41
31:2:2081:U:H2'	31:2:2082:A:C8	2.55	0.41
31:2:2143:C:O2	31:2:2147:A:N6	2.54	0.41
31:2:2699:C:H2'	31:2:2700:A:C8	2.55	0.41
43:l:33:LEU:HG	43:l:38:ILE:HB	2.02	0.41
44:m:45:LEU:HA	49:r:12:LEU:HD11	2.02	0.41
52:1:625:U:H2'	52:1:626:G:H8	1.86	0.41
52:1:1250:A:H2'	52:1:1251:A:C8	2.55	0.41
19:R:11:LEU:O	24:W:29:ARG:NH1	2.54	0.41
31:2:521:U:H2'	31:2:522:A:H8	1.85	0.41
31:2:1283:G:N2	31:2:1286:A:OP2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:1940:U:H1'	31:2:1942:C:H41	1.86	0.41
31:2:2208:C:H2'	31:2:2209:G:C8	2.56	0.41
35:d:110:MET:HA	35:d:113:VAL:HG12	2.03	0.41
52:1:593:U:H2'	52:1:594:U:C6	2.55	0.41
52:1:718:A:OP2	52:1:720:C:N4	2.54	0.41
52:1:1386:G:H2'	52:1:1387:G:H8	1.86	0.41
3:A:52:HIS:HA	3:A:216:ARG:HB2	2.02	0.41
4:B:47:ALA:HA	4:B:84:LEU:HD13	2.03	0.41
6:D:140:ILE:HD11	6:D:145:VAL:HB	2.02	0.41
7:E:102:ILE:HD11	7:E:116:LEU:HG	2.03	0.41
8:F:4:ILE:HG22	8:F:39:ALA:HB2	2.03	0.41
11:J:36:LYS:NZ	31:2:808:G:OP2	2.41	0.41
17:P:2:TYR:HE2	17:P:40:MET:HE1	1.85	0.41
26:Y:6:LYS:HE3	26:Y:6:LYS:HB2	1.90	0.41
29:AB:15:LYS:HE2	29:AB:19:GLY:HA2	2.02	0.41
29:AB:27:ASN:HB3	29:AB:35:LYS:HE2	2.03	0.41
30:AC:37:GLN:HG3	30:AC:38:GLY:H	1.86	0.41
31:2:16:C:H2'	31:2:17:G:C8	2.54	0.41
31:2:305:C:H2'	31:2:306:U:C6	2.56	0.41
31:2:475:C:N3	31:2:479:A:N7	2.69	0.41
31:2:589:U:H2'	31:2:590:A:C8	2.56	0.41
31:2:806:C:O2	31:2:2444:G:O2'	2.39	0.41
31:2:934:U:H2'	31:2:935:C:C6	2.56	0.41
31:2:970:U:O2	31:2:984:A:O2'	2.35	0.41
31:2:1148:U:H2'	31:2:1149:G:C8	2.55	0.41
31:2:1161:C:H2'	31:2:1162:G:C8	2.55	0.41
31:2:1652:A:O2'	31:2:2822:G:N2	2.54	0.41
31:2:1759:A:O2'	31:2:2714:G:O2'	2.37	0.41
31:2:2074:U:H2'	31:2:2075:U:C6	2.56	0.41
31:2:2243:U:H2'	31:2:2244:U:C6	2.56	0.41
31:2:2290:G:H2'	31:2:2291:U:C6	2.56	0.41
31:2:2685:G:H2'	31:2:2686:G:H8	1.85	0.41
33:b:5:HIS:HB2	44:m:88:MET:HG3	2.02	0.41
42:k:34:THR:OG1	42:k:53:ARG:NH1	2.54	0.41
43:l:101:THR:OG1	52:1:1226:C:OP2	2.35	0.41
48:q:43:ILE:HD12	48:q:43:ILE:HA	1.95	0.41
48:q:59:LYS:HD3	48:q:59:LYS:HA	1.81	0.41
52:1:349:A:H2'	52:1:350:G:C8	2.56	0.41
52:1:585:G:N1	52:1:757:U:N3	2.68	0.41
52:1:722:G:H1	52:1:733:G:H1	1.69	0.41
52:1:946:A:H2'	52:1:947:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:946:A:H2'	52:1:947:G:H8	1.86	0.41
2:5:67:C:H2'	2:5:68:C:H6	1.86	0.41
18:Q:13:SER:O	18:Q:17:VAL:HG23	2.20	0.41
18:Q:78:GLU:OE1	31:2:24:G:N2	2.54	0.41
31:2:1204:A:N6	31:2:1242:U:O4	2.54	0.41
31:2:1259:G:H2'	31:2:1260:A:C8	2.56	0.41
31:2:1316:U:H2'	31:2:1317:G:C8	2.56	0.41
31:2:1335:C:H2'	31:2:1336:A:C8	2.56	0.41
31:2:1387:A:H2'	31:2:1388:G:C8	2.56	0.41
31:2:2327:A:H2'	31:2:2328:A:C8	2.56	0.41
34:c:186:GLU:HG3	34:c:188:SER:H	1.85	0.41
45:n:6:ALA:HA	45:n:9:LYS:HE2	2.02	0.41
52:1:211:G:H21	52:1:211:G:P	2.43	0.41
52:1:1248:A:N7	52:1:1290:G:N1	2.69	0.41
11:J:22:GLY:HA2	31:2:811:U:H3'	2.03	0.40
15:N:13:LYS:HE3	15:N:76:HIS:HA	2.02	0.40
17:P:14:VAL:HB	17:P:98:ILE:HG13	2.03	0.40
23:V:70:LEU:HD23	23:V:70:LEU:HA	1.96	0.40
31:2:228:C:N4	31:2:2407:A:N3	2.68	0.40
31:2:419:U:H2'	31:2:420:C:C6	2.57	0.40
31:2:464:U:H1'	31:2:686:U:H5	1.85	0.40
31:2:521:U:H2'	31:2:522:A:C8	2.56	0.40
31:2:1361:G:H2'	31:2:1362:C:C6	2.56	0.40
39:h:125:GLN:HG3	52:1:1342:C:H1'	2.02	0.40
40:i:45:ARG:NH2	52:1:1255:G:OP2	2.50	0.40
52:1:215:C:H2'	52:1:216:U:O4'	2.21	0.40
52:1:323:U:H2'	52:1:324:G:O4'	2.21	0.40
52:1:470:C:H2'	52:1:471:U:C6	2.56	0.40
52:1:579:A:H5'	52:1:728:A:H1'	2.02	0.40
52:1:1160:G:N2	52:1:1176:A:N1	2.69	0.40
1:3:114:C:H2'	1:3:115:A:C8	2.56	0.40
3:A:59:GLN:HA	31:2:1568:G:H5'	2.02	0.40
13:L:35:LYS:HD2	13:L:112:TYR:CZ	2.56	0.40
18:Q:59:GLU:HB2	18:Q:66:ILE:HD11	2.03	0.40
31:2:1148:U:H2'	31:2:1149:G:H8	1.86	0.40
31:2:1363:C:O2'	31:2:1809:A:N3	2.50	0.40
31:2:1364:G:N2	31:2:1367:A:OP2	2.47	0.40
31:2:1412:U:H2'	31:2:1413:A:C8	2.55	0.40
41:j:120:CYS:HB2	52:1:778:G:H1'	2.03	0.40
45:n:25:GLU:HG3	45:n:80:LEU:HD22	2.02	0.40
45:n:71:ARG:NH2	52:1:754:C:OP1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:206:C:H2'	52:1:207:C:C6	2.56	0.40
52:1:918:A:H2'	52:1:919:A:C8	2.56	0.40
52:1:1118:U:H2'	52:1:1119:C:H6	1.87	0.40
6:D:147:ARG:HG3	6:D:149:ARG:H	1.86	0.40
7:E:126:THR:OG1	7:E:127:GLN:N	2.55	0.40
31:2:535:G:H1	31:2:558:U:H3	1.70	0.40
31:2:1412:U:H2'	31:2:1413:A:H8	1.86	0.40
31:2:2364:C:H2'	31:2:2365:G:O4'	2.22	0.40
31:2:2730:C:H2'	31:2:2731:G:C8	2.56	0.40
31:2:2861:U:H2'	31:2:2862:G:H8	1.86	0.40
41:j:21:HIS:CG	52:1:707:U:H4'	2.56	0.40
52:1:237:G:H2'	52:1:238:A:C8	2.57	0.40
52:1:465:A:H3'	52:1:466:A:C8	2.56	0.40
1:3:34:A:H2'	1:3:44:G:O6	2.20	0.40
7:E:66:THR:HG22	31:2:2748:A:H1'	2.04	0.40
11:J:101:ILE:HB	11:J:105:ILE:HG13	2.04	0.40
15:N:28:LYS:HB3	15:N:39:LEU:HD23	2.02	0.40
20:S:81:ARG:NH2	31:2:334:C:O2'	2.54	0.40
23:V:66:VAL:HA	23:V:69:GLU:HG2	2.04	0.40
25:X:19:HIS:HA	25:X:22:THR:HG22	2.03	0.40
31:2:2813:A:H2'	31:2:2814:A:H8	1.86	0.40
34:c:63:ILE:HD13	34:c:63:ILE:HA	1.97	0.40
34:c:72:ARG:HA	34:c:203:TYR:HE2	1.85	0.40
39:h:26:LYS:N	39:h:61:ASP:OD2	2.46	0.40
39:h:50:PRO:HG2	39:h:79:ARG:HG3	2.03	0.40
52:1:398:U:H2'	52:1:399:G:H8	1.85	0.40
3:A:103:ILE:HD12	3:A:103:ILE:HA	1.86	0.40
11:J:32:GLY:HA2	31:2:1190:G:H5''	2.03	0.40
12:K:7:THR:HG21	12:K:92:TRP:HH2	1.86	0.40
12:K:75:GLU:HG3	31:2:957:C:H5'	2.03	0.40
31:2:910:A:N3	31:2:2264:C:O2'	2.45	0.40
31:2:910:A:H2'	31:2:911:A:C8	2.56	0.40
31:2:1435:G:H2'	31:2:1436:G:C8	2.56	0.40
31:2:2322:A:H3'	31:2:2323:G:H8	1.87	0.40
37:f:43:TYR:CE2	39:h:41:GLU:HG3	2.57	0.40
47:p:59:GLU:OE1	47:p:76:ARG:NH2	2.54	0.40
48:q:23:LYS:HB2	48:q:23:LYS:HE2	1.90	0.40
52:1:556:C:H2'	52:1:557:G:C8	2.57	0.40
52:1:665:A:N3	52:1:732:C:H2'	2.37	0.40
52:1:891:U:H2'	52:1:892:A:H8	1.86	0.40
52:1:1440:U:H2'	52:1:1441:A:C4	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
4	B	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
5	C	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
6	D	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
7	E	171/177 (97%)	160 (94%)	11 (6%)	0	100	100
8	F	46/149 (31%)	39 (85%)	7 (15%)	0	100	100
9	G	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
10	I	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
11	J	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
12	K	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
13	L	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
14	M	112/117 (96%)	106 (95%)	6 (5%)	0	100	100
15	N	112/115 (97%)	103 (92%)	9 (8%)	0	100	100
16	O	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
17	P	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
18	Q	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
19	R	88/100 (88%)	86 (98%)	2 (2%)	0	100	100
20	S	92/104 (88%)	92 (100%)	0	0	100	100
21	T	91/94 (97%)	87 (96%)	4 (4%)	0	100	100
22	U	73/85 (86%)	73 (100%)	0	0	100	100
23	V	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
24	W	58/63 (92%)	58 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	X	56/59 (95%)	56 (100%)	0	0	100	100
26	Y	53/57 (93%)	53 (100%)	0	0	100	100
27	Z	46/55 (84%)	45 (98%)	1 (2%)	0	100	100
28	AA	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
29	AB	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	AC	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
32	a	218/241 (90%)	208 (95%)	10 (5%)	0	100	100
33	b	193/233 (83%)	188 (97%)	5 (3%)	0	100	100
34	c	157/206 (76%)	148 (94%)	9 (6%)	0	100	100
35	d	155/167 (93%)	152 (98%)	3 (2%)	0	100	100
36	e	99/135 (73%)	90 (91%)	9 (9%)	0	100	100
37	f	93/179 (52%)	86 (92%)	7 (8%)	0	100	100
38	g	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
39	h	119/130 (92%)	104 (87%)	15 (13%)	0	100	100
40	i	85/103 (82%)	80 (94%)	5 (6%)	0	100	100
41	j	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
42	k	107/124 (86%)	93 (87%)	14 (13%)	0	100	100
43	l	109/118 (92%)	101 (93%)	8 (7%)	0	100	100
44	m	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
45	n	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
46	o	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
47	p	76/84 (90%)	67 (88%)	9 (12%)	0	100	100
48	q	52/75 (69%)	50 (96%)	2 (4%)	0	100	100
49	r	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
50	s	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
51	t	66/71 (93%)	65 (98%)	1 (2%)	0	100	100
All	All	5235/5843 (90%)	5008 (96%)	227 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	216/218 (99%)	205 (95%)	11 (5%)	21	48
4	B	164/164 (100%)	158 (96%)	6 (4%)	30	55
5	C	165/165 (100%)	161 (98%)	4 (2%)	43	62
6	D	148/150 (99%)	142 (96%)	6 (4%)	27	52
7	E	134/138 (97%)	128 (96%)	6 (4%)	24	51
8	F	39/114 (34%)	35 (90%)	4 (10%)	7	24
9	G	116/116 (100%)	113 (97%)	3 (3%)	40	61
10	I	104/104 (100%)	100 (96%)	4 (4%)	29	54
11	J	102/103 (99%)	99 (97%)	3 (3%)	37	60
12	K	109/109 (100%)	107 (98%)	2 (2%)	51	67
13	L	99/103 (96%)	98 (99%)	1 (1%)	68	75
14	M	84/87 (97%)	79 (94%)	5 (6%)	17	43
15	N	99/100 (99%)	90 (91%)	9 (9%)	9	30
16	O	89/90 (99%)	86 (97%)	3 (3%)	32	57
17	P	84/84 (100%)	82 (98%)	2 (2%)	43	62
18	Q	93/93 (100%)	88 (95%)	5 (5%)	20	47
19	R	77/84 (92%)	72 (94%)	5 (6%)	15	42
20	S	78/85 (92%)	75 (96%)	3 (4%)	29	54
21	T	77/78 (99%)	72 (94%)	5 (6%)	15	42
22	U	57/63 (90%)	55 (96%)	2 (4%)	32	56
23	V	67/68 (98%)	64 (96%)	3 (4%)	24	51
24	W	54/55 (98%)	54 (100%)	0	100	100
25	X	48/49 (98%)	46 (96%)	2 (4%)	26	52
26	Y	46/48 (96%)	44 (96%)	2 (4%)	26	51
27	Z	44/49 (90%)	42 (96%)	2 (4%)	24	51
28	AA	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	AB	51/52 (98%)	47 (92%)	4 (8%)	11	37
30	AC	34/34 (100%)	32 (94%)	2 (6%)	18	44
32	a	171/199 (86%)	168 (98%)	3 (2%)	51	67
33	b	152/190 (80%)	145 (95%)	7 (5%)	24	50
34	c	133/173 (77%)	127 (96%)	6 (4%)	24	51
35	d	117/126 (93%)	115 (98%)	2 (2%)	53	67
36	e	88/116 (76%)	85 (97%)	3 (3%)	32	57
37	f	77/147 (52%)	77 (100%)	0	100	100
38	g	104/105 (99%)	102 (98%)	2 (2%)	50	66
39	h	97/107 (91%)	92 (95%)	5 (5%)	21	48
40	i	80/90 (89%)	78 (98%)	2 (2%)	42	62
41	j	90/99 (91%)	87 (97%)	3 (3%)	33	57
42	k	93/104 (89%)	86 (92%)	7 (8%)	12	38
43	l	90/96 (94%)	88 (98%)	2 (2%)	45	63
44	m	83/84 (99%)	80 (96%)	3 (4%)	31	56
45	n	75/77 (97%)	71 (95%)	4 (5%)	20	47
46	o	65/65 (100%)	63 (97%)	2 (3%)	35	59
47	p	72/78 (92%)	67 (93%)	5 (7%)	14	40
48	q	47/65 (72%)	46 (98%)	1 (2%)	47	64
49	r	70/79 (89%)	66 (94%)	4 (6%)	18	45
50	s	64/66 (97%)	63 (98%)	1 (2%)	55	68
51	t	56/61 (92%)	55 (98%)	1 (2%)	51	67
All	All	4340/4768 (91%)	4173 (96%)	167 (4%)	30	54

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2	VAL
3	A	18	VAL
3	A	76	VAL
3	A	93	VAL
3	A	109	LEU
3	A	119	VAL
3	A	171	VAL

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Mol	Chain	Res	Type
3	A	173	LEU
3	A	175	LEU
3	A	183	VAL
3	A	228	ASP
4	B	5	VAL
4	B	26	VAL
4	B	34	VAL
4	B	43	ASP
4	B	189	VAL
4	B	203	VAL
5	C	14	VAL
5	C	156	ASN
5	C	176	ASP
5	C	186	VAL
6	D	6	TYR
6	D	7	TYR
6	D	97	GLU
6	D	142	TYR
6	D	151	LEU
6	D	158	THR
7	E	3	VAL
7	E	35	THR
7	E	88	LEU
7	E	102	ILE
7	E	104	LEU
7	E	161	VAL
8	F	4	ILE
8	F	11	ASN
8	F	21	VAL
8	F	30	LEU
9	G	73	VAL
9	G	78	THR
9	G	100	VAL
10	I	22	ILE
10	I	62	VAL
10	I	85	VAL
10	I	122	VAL
11	J	57	LEU
11	J	89	VAL
11	J	111	ILE
12	K	26	VAL
12	K	132	THR

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Mol	Chain	Res	Type
13	L	116	VAL
14	M	27	VAL
14	M	28	VAL
14	M	31	THR
14	M	54	VAL
14	M	106	LEU
15	N	3	ILE
15	N	25	VAL
15	N	27	VAL
15	N	45	VAL
15	N	46	VAL
15	N	59	THR
15	N	72	VAL
15	N	81	ASP
15	N	83	ILE
16	O	3	VAL
16	O	17	LEU
16	O	99	VAL
17	P	51	VAL
17	P	63	VAL
18	Q	20	VAL
18	Q	23	LEU
18	Q	71	VAL
18	Q	72	THR
18	Q	77	ASP
19	R	10	VAL
19	R	16	VAL
19	R	31	VAL
19	R	61	LEU
19	R	85	VAL
20	S	27	VAL
20	S	35	VAL
20	S	82	VAL
21	T	8	VAL
21	T	20	LEU
21	T	64	VAL
21	T	72	VAL
21	T	92	VAL
22	U	19	VAL
22	U	39	THR
23	V	15	ASN
23	V	29	LEU

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Mol	Chain	Res	Type
23	V	32	LEU
25	X	50	VAL
25	X	56	VAL
26	Y	2	VAL
26	Y	24	VAL
27	Z	10	LEU
27	Z	22	THR
29	AB	28	LEU
29	AB	30	HIS
29	AB	31	ILE
29	AB	53	ASP
30	AC	3	VAL
30	AC	25	VAL
32	a	185	ILE
32	a	186	VAL
32	a	198	VAL
33	b	65	VAL
33	b	66	THR
33	b	75	VAL
33	b	148	ILE
33	b	152	VAL
33	b	181	ILE
33	b	206	ILE
34	c	54	LEU
34	c	85	THR
34	c	116	LEU
34	c	122	ILE
34	c	146	GLU
34	c	190	LEU
35	d	87	VAL
35	d	114	LEU
36	e	18	VAL
36	e	54	LEU
36	e	61	LEU
38	g	103	VAL
38	g	126	CYS
39	h	21	LYS
39	h	28	VAL
39	h	55	ASP
39	h	57	VAL
39	h	103	VAL
40	i	58	ASN

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Mol	Chain	Res	Type
40	i	69	THR
41	j	31	VAL
41	j	34	THR
41	j	64	VAL
42	k	20	VAL
42	k	32	VAL
42	k	36	VAL
42	k	56	LEU
42	k	57	THR
42	k	113	ARG
42	k	118	VAL
43	l	6	ILE
43	l	24	VAL
44	m	33	VAL
44	m	45	LEU
44	m	53	ASP
45	n	21	THR
45	n	69	LEU
45	n	84	LEU
45	n	86	LEU
46	o	2	VAL
46	o	74	LEU
47	p	7	LEU
47	p	45	VAL
47	p	57	VAL
47	p	58	VAL
47	p	77	VAL
48	q	28	LEU
49	r	26	ASP
49	r	35	ARG
49	r	39	ILE
49	r	61	VAL
50	s	74	HIS
51	t	42	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	152	GLN
3	A	238	ASN
4	B	32	ASN
4	B	36	GLN

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Mol	Chain	Res	Type
4	B	136	ASN
4	B	150	GLN
4	B	173	GLN
5	C	90	GLN
5	C	195	GLN
6	D	4	HIS
6	D	62	GLN
7	E	37	ASN
7	E	47	ASN
7	E	63	GLN
7	E	87	GLN
8	F	2	GLN
9	G	40	HIS
9	G	80	HIS
9	G	136	GLN
11	J	93	ASN
12	K	88	ASN
13	L	31	HIS
13	L	73	ASN
13	L	81	ASN
14	M	38	GLN
16	O	43	GLN
16	O	71	ASN
17	P	91	GLN
18	Q	31	GLN
19	R	48	GLN
19	R	70	HIS
20	S	65	GLN
20	S	68	ASN
24	W	27	ASN
24	W	39	GLN
27	Z	18	HIS
32	a	145	ASN
33	b	7	ASN
33	b	99	GLN
34	c	73	ASN
34	c	130	ASN
34	c	135	GLN
36	e	17	GLN
37	f	27	ASN
37	f	121	ASN
38	g	17	GLN

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Mol	Chain	Res	Type
39	h	36	GLN
39	h	49	GLN
39	h	80	HIS
42	k	72	ASN
43	l	7	ASN
45	n	39	GLN
45	n	45	HIS
46	o	26	ASN
46	o	79	ASN
47	p	50	ASN
48	q	51	GLN
50	s	19	HIS
50	s	60	GLN
50	s	83	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	119/120 (99%)	33 (27%)	2 (1%)
2	5	75/76 (98%)	19 (25%)	0
31	2	2831/2903 (97%)	549 (19%)	9 (0%)
52	1	1505/1540 (97%)	303 (20%)	7 (0%)
53	4	42/93 (45%)	9 (21%)	0
All	All	4572/4732 (96%)	913 (19%)	18 (0%)

All (913) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	9	G
1	3	12	C
1	3	13	G
1	3	14	U
1	3	15	A
1	3	16	G
1	3	20	G
1	3	24	G
1	3	25	U
1	3	26	C
1	3	27	C
1	3	34	A
1	3	35	C

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Mol	Chain	Res	Type
1	3	42	C
1	3	44	G
1	3	45	A
1	3	50	A
1	3	51	G
1	3	52	A
1	3	53	A
1	3	57	A
1	3	59	A
1	3	64	G
1	3	66	A
1	3	67	G
1	3	69	G
1	3	87	U
1	3	88	C
1	3	89	U
1	3	90	C
1	3	108	A
1	3	110	C
1	3	112	G
2	5	17	C
2	5	19	G
2	5	20	U
2	5	21	A
2	5	22	G
2	5	23	A
2	5	26	A
2	5	30	G
2	5	31	A
2	5	37	A
2	5	43	C
2	5	45	U
2	5	46	G
2	5	47	U
2	5	61	C
2	5	69	G
2	5	70	G
2	5	73	A
2	5	76	A
31	2	4	U
31	2	14	A
31	2	23	G

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Mol	Chain	Res	Type
31	2	27	G
31	2	28	A
31	2	34	U
31	2	43	G
31	2	44	A
31	2	49	A
31	2	50	U
31	2	51	G
31	2	63	A
31	2	64	A
31	2	71	A
31	2	74	A
31	2	75	G
31	2	87	U
31	2	88	G
31	2	91	A
31	2	96	C
31	2	101	A
31	2	102	U
31	2	118	A
31	2	119	A
31	2	120	U
31	2	125	A
31	2	126	A
31	2	139	U
31	2	140	C
31	2	142	A
31	2	150	U
31	2	162	U
31	2	163	C
31	2	178	G
31	2	181	A
31	2	186	G
31	2	196	A
31	2	199	A
31	2	205	G
31	2	212	G
31	2	215	G
31	2	216	A
31	2	222	A
31	2	223	A
31	2	228	C

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Mol	Chain	Res	Type
31	2	229	C
31	2	230	G
31	2	233	A
31	2	238	C
31	2	239	C
31	2	242	G
31	2	248	G
31	2	255	A
31	2	265	A
31	2	266	G
31	2	267	C
31	2	268	C
31	2	271	G
31	2	275	C
31	2	276	U
31	2	277	G
31	2	281	C
31	2	284	U
31	2	286	U
31	2	289	G
31	2	290	U
31	2	291	G
31	2	292	U
31	2	311	A
31	2	322	A
31	2	323	C
31	2	329	G
31	2	330	A
31	2	343	C
31	2	345	A
31	2	347	A
31	2	348	A
31	2	349	U
31	2	350	G
31	2	354	A
31	2	356	G
31	2	357	C
31	2	358	U
31	2	362	A
31	2	365	U
31	2	369	U
31	2	370	G

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Mol	Chain	Res	Type
31	2	372	G
31	2	384	A
31	2	386	G
31	2	387	U
31	2	390	U
31	2	404	A
31	2	406	G
31	2	411	G
31	2	422	A
31	2	424	G
31	2	436	C
31	2	451	U
31	2	455	C
31	2	456	C
31	2	467	G
31	2	481	G
31	2	490	C
31	2	491	G
31	2	504	A
31	2	505	A
31	2	509	C
31	2	512	G
31	2	527	C
31	2	528	A
31	2	529	A
31	2	531	C
31	2	532	A
31	2	544	C
31	2	545	U
31	2	546	U
31	2	549	G
31	2	563	A
31	2	573	U
31	2	575	A
31	2	580	U
31	2	603	A
31	2	613	A
31	2	614	A
31	2	615	U
31	2	616	A
31	2	627	A
31	2	637	A

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Mol	Chain	Res	Type
31	2	643	A
31	2	644	A
31	2	647	G
31	2	653	U
31	2	654	A
31	2	669	G
31	2	675	A
31	2	686	U
31	2	695	G
31	2	711	G
31	2	714	U
31	2	721	A
31	2	726	G
31	2	727	A
31	2	730	A
31	2	734	A
31	2	737	C
31	2	738	G
31	2	740	C
31	2	747	C
31	2	748	G
31	2	765	C
31	2	775	G
31	2	776	G
31	2	782	A
31	2	783	A
31	2	784	G
31	2	785	G
31	2	790	U
31	2	792	A
31	2	805	G
31	2	810	U
31	2	812	C
31	2	819	A
31	2	827	U
31	2	828	U
31	2	846	U
31	2	847	U
31	2	857	G
31	2	858	G
31	2	859	G
31	2	860	U

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Mol	Chain	Res	Type
31	2	864	G
31	2	866	A
31	2	878	A
31	2	883	G
31	2	887	U
31	2	896	A
31	2	897	C
31	2	899	A
31	2	902	C
31	2	910	A
31	2	914	G
31	2	915	C
31	2	923	G
31	2	931	U
31	2	932	U
31	2	933	A
31	2	934	U
31	2	941	A
31	2	945	A
31	2	946	C
31	2	953	G
31	2	961	C
31	2	973	A
31	2	974	G
31	2	979	A
31	2	983	A
31	2	985	C
31	2	995	C
31	2	996	A
31	2	1009	A
31	2	1010	A
31	2	1012	U
31	2	1013	C
31	2	1022	G
31	2	1026	G
31	2	1033	U
31	2	1115	G
31	2	1122	G
31	2	1124	G
31	2	1132	U
31	2	1134	A
31	2	1135	C

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Mol	Chain	Res	Type
31	2	1141	U
31	2	1142	A
31	2	1143	A
31	2	1168	G
31	2	1169	A
31	2	1170	C
31	2	1171	G
31	2	1172	C
31	2	1173	U
31	2	1174	U
31	2	1175	A
31	2	1176	U
31	2	1180	U
31	2	1186	G
31	2	1211	C
31	2	1212	G
31	2	1236	G
31	2	1247	A
31	2	1248	G
31	2	1253	A
31	2	1256	G
31	2	1264	A
31	2	1265	A
31	2	1271	G
31	2	1272	A
31	2	1287	A
31	2	1289	C
31	2	1300	G
31	2	1301	A
31	2	1313	U
31	2	1329	U
31	2	1333	G
31	2	1341	G
31	2	1345	C
31	2	1346	G
31	2	1360	G
31	2	1365	A
31	2	1368	G
31	2	1378	A
31	2	1379	U
31	2	1395	A
31	2	1407	G

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Mol	Chain	Res	Type
31	2	1416	G
31	2	1419	A
31	2	1420	A
31	2	1421	G
31	2	1427	A
31	2	1428	C
31	2	1437	C
31	2	1438	U
31	2	1452	G
31	2	1455	G
31	2	1460	U
31	2	1461	C
31	2	1482	G
31	2	1490	A
31	2	1491	G
31	2	1504	A
31	2	1515	A
31	2	1522	A
31	2	1523	U
31	2	1524	G
31	2	1528	A
31	2	1530	G
31	2	1534	U
31	2	1535	A
31	2	1536	C
31	2	1537	G
31	2	1540	G
31	2	1541	C
31	2	1546	G
31	2	1548	A
31	2	1554	U
31	2	1559	U
31	2	1561	C
31	2	1566	A
31	2	1569	A
31	2	1578	U
31	2	1579	A
31	2	1584	U
31	2	1607	C
31	2	1608	A
31	2	1613	G
31	2	1639	C

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Mol	Chain	Res	Type
31	2	1646	C
31	2	1647	U
31	2	1648	U
31	2	1654	A
31	2	1663	G
31	2	1674	G
31	2	1695	G
31	2	1702	G
31	2	1721	G
31	2	1728	C
31	2	1729	U
31	2	1730	C
31	2	1732	C
31	2	1733	G
31	2	1738	G
31	2	1756	G
31	2	1764	C
31	2	1773	A
31	2	1782	U
31	2	1800	C
31	2	1801	A
31	2	1808	A
31	2	1816	C
31	2	1829	A
31	2	1835	G
31	2	1839	G
31	2	1845	G
31	2	1848	A
31	2	1849	G
31	2	1850	G
31	2	1856	U
31	2	1857	G
31	2	1858	A
31	2	1860	G
31	2	1867	G
31	2	1870	C
31	2	1876	A
31	2	1880	U
31	2	1883	U
31	2	1884	G
31	2	1885	A
31	2	1889	A

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Mol	Chain	Res	Type
31	2	1893	C
31	2	1906	G
31	2	1912	A
31	2	1913	A
31	2	1924	C
31	2	1926	U
31	2	1927	A
31	2	1929	G
31	2	1930	G
31	2	1936	A
31	2	1937	A
31	2	1938	A
31	2	1939	U
31	2	1940	U
31	2	1955	U
31	2	1964	G
31	2	1967	C
31	2	1970	A
31	2	1971	U
31	2	1972	G
31	2	1989	G
31	2	1991	U
31	2	1992	G
31	2	1993	U
31	2	1995	U
31	2	1996	C
31	2	1997	C
31	2	2022	U
31	2	2023	C
31	2	2031	A
31	2	2034	U
31	2	2043	C
31	2	2052	A
31	2	2055	C
31	2	2056	G
31	2	2060	A
31	2	2061	G
31	2	2062	A
31	2	2069	G
31	2	2093	G
31	2	2097	A
31	2	2098	U

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Mol	Chain	Res	Type
31	2	2106	U
31	2	2110	G
31	2	2112	G
31	2	2113	U
31	2	2118	U
31	2	2119	A
31	2	2120	G
31	2	2121	G
31	2	2124	G
31	2	2126	A
31	2	2127	G
31	2	2131	U
31	2	2132	U
31	2	2133	G
31	2	2134	A
31	2	2136	G
31	2	2138	G
31	2	2145	C
31	2	2146	C
31	2	2148	G
31	2	2149	U
31	2	2150	C
31	2	2152	G
31	2	2155	U
31	2	2156	G
31	2	2158	A
31	2	2159	G
31	2	2165	C
31	2	2171	A
31	2	2172	U
31	2	2173	A
31	2	2180	U
31	2	2189	U
31	2	2198	A
31	2	2204	G
31	2	2210	U
31	2	2213	U
31	2	2214	C
31	2	2225	A
31	2	2238	G
31	2	2239	G
31	2	2256	G

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Mol	Chain	Res	Type
31	2	2258	C
31	2	2266	A
31	2	2278	A
31	2	2283	C
31	2	2285	C
31	2	2287	A
31	2	2292	U
31	2	2305	U
31	2	2307	G
31	2	2309	A
31	2	2310	C
31	2	2311	A
31	2	2312	U
31	2	2313	C
31	2	2318	G
31	2	2322	A
31	2	2325	G
31	2	2326	C
31	2	2327	A
31	2	2336	A
31	2	2347	C
31	2	2350	C
31	2	2354	C
31	2	2361	G
31	2	2383	G
31	2	2385	C
31	2	2388	A
31	2	2390	U
31	2	2391	G
31	2	2402	U
31	2	2403	C
31	2	2406	A
31	2	2422	C
31	2	2423	U
31	2	2424	C
31	2	2427	C
31	2	2429	G
31	2	2430	A
31	2	2431	U
31	2	2433	A
31	2	2435	A
31	2	2436	G

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Mol	Chain	Res	Type
31	2	2441	U
31	2	2448	A
31	2	2464	G
31	2	2468	A
31	2	2471	A
31	2	2472	G
31	2	2473	U
31	2	2475	C
31	2	2476	A
31	2	2477	U
31	2	2478	A
31	2	2494	G
31	2	2498	C
31	2	2501	C
31	2	2503	A
31	2	2505	G
31	2	2511	U
31	2	2518	A
31	2	2520	C
31	2	2529	G
31	2	2534	A
31	2	2547	A
31	2	2554	U
31	2	2566	A
31	2	2567	G
31	2	2572	A
31	2	2582	G
31	2	2586	U
31	2	2602	A
31	2	2603	G
31	2	2609	U
31	2	2613	U
31	2	2615	U
31	2	2623	G
31	2	2629	U
31	2	2630	G
31	2	2639	A
31	2	2656	U
31	2	2661	G
31	2	2682	A
31	2	2685	G
31	2	2689	U

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Mol	Chain	Res	Type
31	2	2690	U
31	2	2714	G
31	2	2718	G
31	2	2722	G
31	2	2726	A
31	2	2733	A
31	2	2739	U
31	2	2744	G
31	2	2746	U
31	2	2748	A
31	2	2750	A
31	2	2752	C
31	2	2764	A
31	2	2765	A
31	2	2766	A
31	2	2776	A
31	2	2778	A
31	2	2779	U
31	2	2791	G
31	2	2793	C
31	2	2795	C
31	2	2796	U
31	2	2798	U
31	2	2799	A
31	2	2800	A
31	2	2801	G
31	2	2808	G
31	2	2818	U
31	2	2820	A
31	2	2836	U
31	2	2850	A
31	2	2859	G
31	2	2867	G
31	2	2872	A
31	2	2873	A
31	2	2879	A
31	2	2880	C
31	2	2883	A
31	2	2884	U
31	2	2885	G
31	2	2893	A
31	2	2902	C

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Mol	Chain	Res	Type
52	1	9	G
52	1	13	U
52	1	22	G
52	1	39	G
52	1	47	C
52	1	48	C
52	1	51	A
52	1	53	A
52	1	54	C
52	1	61	G
52	1	64	G
52	1	66	A
52	1	71	A
52	1	95	C
52	1	105	G
52	1	121	U
52	1	127	G
52	1	131	A
52	1	136	C
52	1	144	G
52	1	146	G
52	1	149	A
52	1	150	U
52	1	151	A
52	1	158	G
52	1	159	G
52	1	160	A
52	1	163	C
52	1	169	C
52	1	170	U
52	1	171	A
52	1	174	A
52	1	179	A
52	1	181	A
52	1	184	G
52	1	195	A
52	1	197	A
52	1	199	A
52	1	200	G
52	1	204	G
52	1	209	U
52	1	210	C

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Mol	Chain	Res	Type
52	1	215	C
52	1	220	G
52	1	226	G
52	1	240	G
52	1	244	U
52	1	245	U
52	1	247	G
52	1	251	G
52	1	266	G
52	1	267	C
52	1	268	U
52	1	281	G
52	1	289	G
52	1	305	G
52	1	306	A
52	1	316	C
52	1	320	A
52	1	328	C
52	1	330	C
52	1	339	C
52	1	346	G
52	1	347	G
52	1	352	C
52	1	363	A
52	1	367	U
52	1	369	G
52	1	372	C
52	1	373	A
52	1	376	G
52	1	388	G
52	1	390	U
52	1	398	U
52	1	406	G
52	1	411	A
52	1	413	G
52	1	418	C
52	1	420	U
52	1	421	U
52	1	422	C
52	1	423	G
52	1	424	G
52	1	429	U

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Mol	Chain	Res	Type
52	1	438	U
52	1	446	G
52	1	464	U
52	1	465	A
52	1	467	U
52	1	468	A
52	1	478	A
52	1	482	A
52	1	484	G
52	1	486	U
52	1	491	G
52	1	494	G
52	1	495	A
52	1	497	G
52	1	504	C
52	1	505	G
52	1	509	A
52	1	510	A
52	1	517	G
52	1	518	C
52	1	521	G
52	1	527	G
52	1	530	G
52	1	531	U
52	1	547	A
52	1	560	A
52	1	563	A
52	1	572	A
52	1	576	C
52	1	577	G
52	1	586	C
52	1	587	G
52	1	588	G
52	1	595	A
52	1	596	A
52	1	606	G
52	1	619	U
52	1	620	C
52	1	640	A
52	1	641	U
52	1	642	A
52	1	645	G

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Mol	Chain	Res	Type
52	1	649	A
52	1	653	U
52	1	654	G
52	1	660	C
52	1	661	G
52	1	662	U
52	1	665	A
52	1	681	A
52	1	686	U
52	1	688	G
52	1	694	A
52	1	695	A
52	1	701	U
52	1	702	A
52	1	703	G
52	1	711	G
52	1	718	A
52	1	719	C
52	1	721	G
52	1	723	U
52	1	724	G
52	1	731	G
52	1	747	A
52	1	755	G
52	1	757	U
52	1	758	C
52	1	760	G
52	1	777	A
52	1	781	A
52	1	794	A
52	1	797	C
52	1	799	G
52	1	812	G
52	1	815	A
52	1	817	C
52	1	820	U
52	1	821	G
52	1	832	G
52	1	838	G
52	1	839	C
52	1	849	G
52	1	872	A

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Mol	Chain	Res	Type
52	1	876	C
52	1	884	U
52	1	885	G
52	1	889	A
52	1	900	A
52	1	902	G
52	1	914	A
52	1	934	C
52	1	935	A
52	1	938	A
52	1	942	G
52	1	946	A
52	1	956	U
52	1	957	U
52	1	958	A
52	1	959	A
52	1	966	G
52	1	969	A
52	1	971	G
52	1	974	A
52	1	975	A
52	1	976	G
52	1	977	A
52	1	979	C
52	1	980	C
52	1	982	U
52	1	986	U
52	1	987	G
52	1	988	G
52	1	989	U
52	1	992	U
52	1	993	G
52	1	994	A
52	1	1004	A
52	1	1030	U
52	1	1031	C
52	1	1033	G
52	1	1034	G
52	1	1045	C
52	1	1053	G
52	1	1066	C
52	1	1088	G

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Mol	Chain	Res	Type
52	1	1094	G
52	1	1095	U
52	1	1101	A
52	1	1108	G
52	1	1130	A
52	1	1136	C
52	1	1137	C
52	1	1138	G
52	1	1139	G
52	1	1140	C
52	1	1141	C
52	1	1157	A
52	1	1158	C
52	1	1159	U
52	1	1168	U
52	1	1169	A
52	1	1182	G
52	1	1184	G
52	1	1191	A
52	1	1196	A
52	1	1197	A
52	1	1202	U
52	1	1205	U
52	1	1206	G
52	1	1212	U
52	1	1216	A
52	1	1217	C
52	1	1218	C
52	1	1219	A
52	1	1224	U
52	1	1225	A
52	1	1226	C
52	1	1227	A
52	1	1238	A
52	1	1240	U
52	1	1241	G
52	1	1256	A
52	1	1258	G
52	1	1261	A
52	1	1275	A
52	1	1278	G
52	1	1280	A

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Mol	Chain	Res	Type
52	1	1282	C
52	1	1287	A
52	1	1288	A
52	1	1289	A
52	1	1296	C
52	1	1297	G
52	1	1298	U
52	1	1300	G
52	1	1301	U
52	1	1302	C
52	1	1317	C
52	1	1331	G
52	1	1339	A
52	1	1340	A
52	1	1346	A
52	1	1347	G
52	1	1348	U
52	1	1363	A
52	1	1381	U
52	1	1394	A
52	1	1397	C
52	1	1403	C
52	1	1404	C
52	1	1408	A
52	1	1426	G
52	1	1429	A
52	1	1433	A
52	1	1438	G
52	1	1439	G
52	1	1440	U
52	1	1441	A
52	1	1446	A
52	1	1447	A
52	1	1448	C
52	1	1449	C
52	1	1451	U
52	1	1452	C
52	1	1453	G
52	1	1455	G
52	1	1492	A
52	1	1494	G
52	1	1495	U

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Mol	Chain	Res	Type
52	1	1497	G
52	1	1499	A
52	1	1502	A
52	1	1517	A
52	1	1519	A
52	1	1520	C
52	1	1529	G
52	1	1530	G
52	1	1532	U
53	4	51	U
53	4	53	U
53	4	56	G
53	4	58	G
53	4	59	A
53	4	60	A
53	4	61	G
53	4	62	A
53	4	63	U

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3	51	G
1	3	52	A
31	2	227	A
31	2	265	A
31	2	784	G
31	2	859	G
31	2	882	G
31	2	1179	G
31	2	1340	U
31	2	2581	G
31	2	2858	C
52	1	178	C
52	1	421	U
52	1	509	A
52	1	595	A
52	1	1190	G
52	1	1201	A
52	1	1300	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 55 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](#)

There are no chain breaks in this entry.

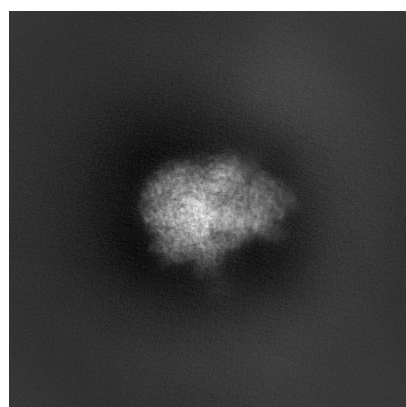
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21422. These allow visual inspection of the internal detail of the map and identification of artifacts.

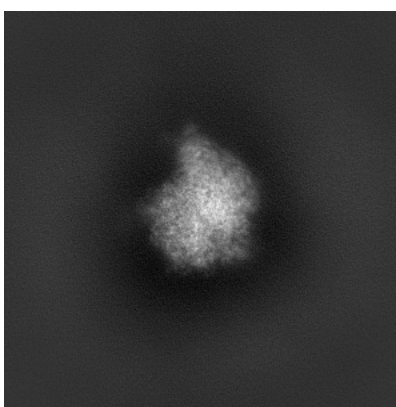
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

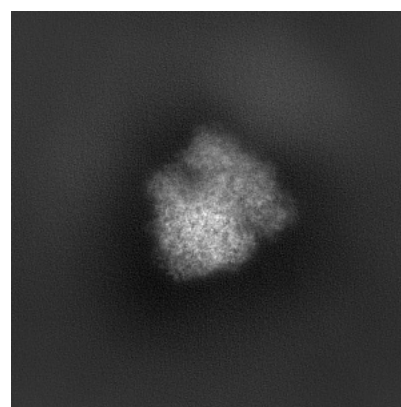
6.1.1 Primary map



X



Y

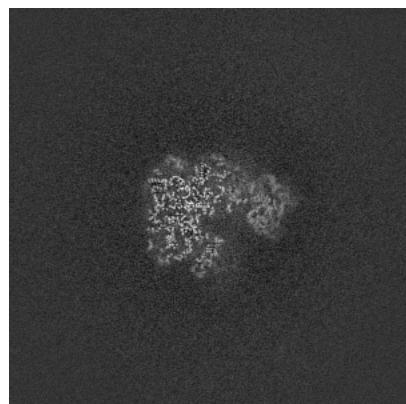


Z

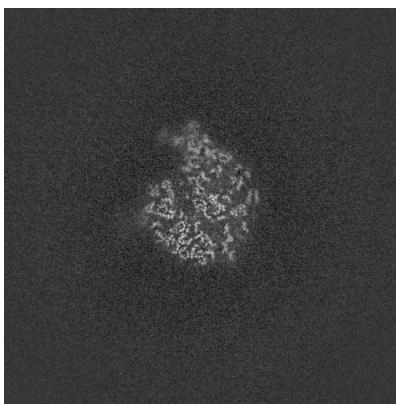
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

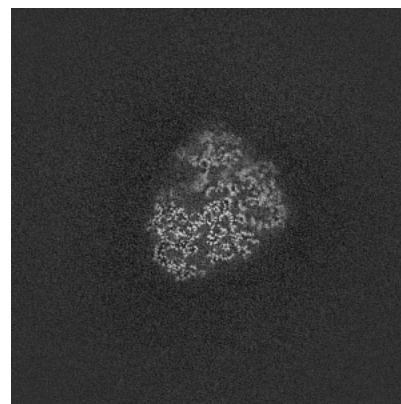
6.2.1 Primary map



X Index: 324



Y Index: 324

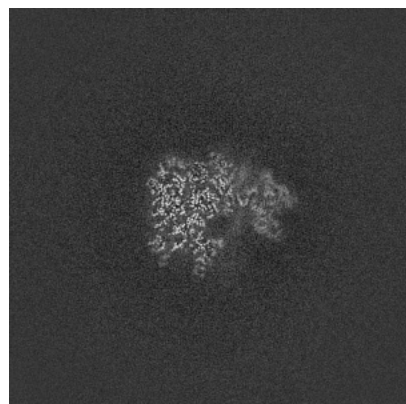


Z Index: 324

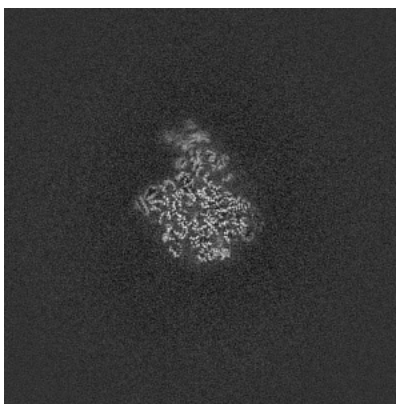
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

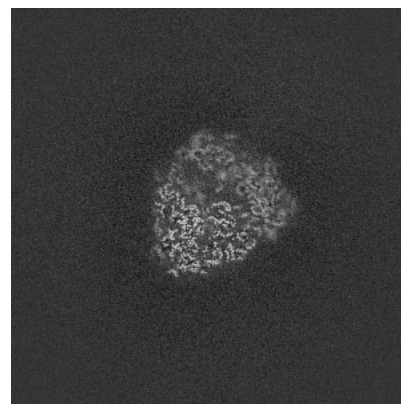
6.3.1 Primary map



X Index: 331



Y Index: 313

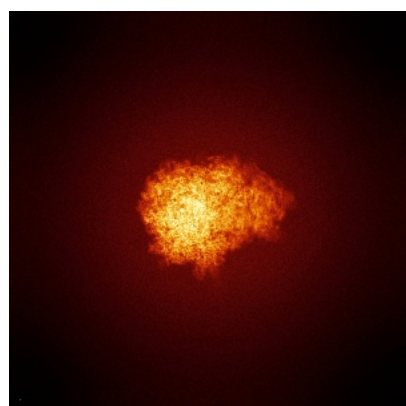


Z Index: 312

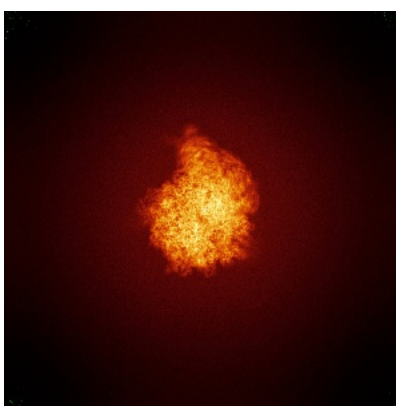
The images above show the largest variance slices of the map in three orthogonal directions.

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

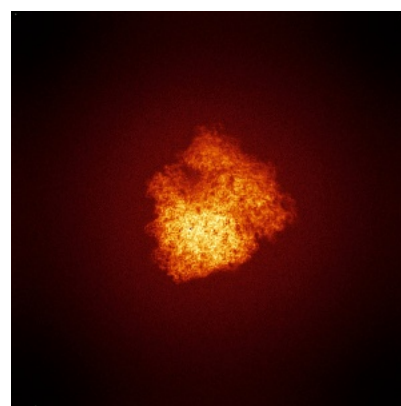
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

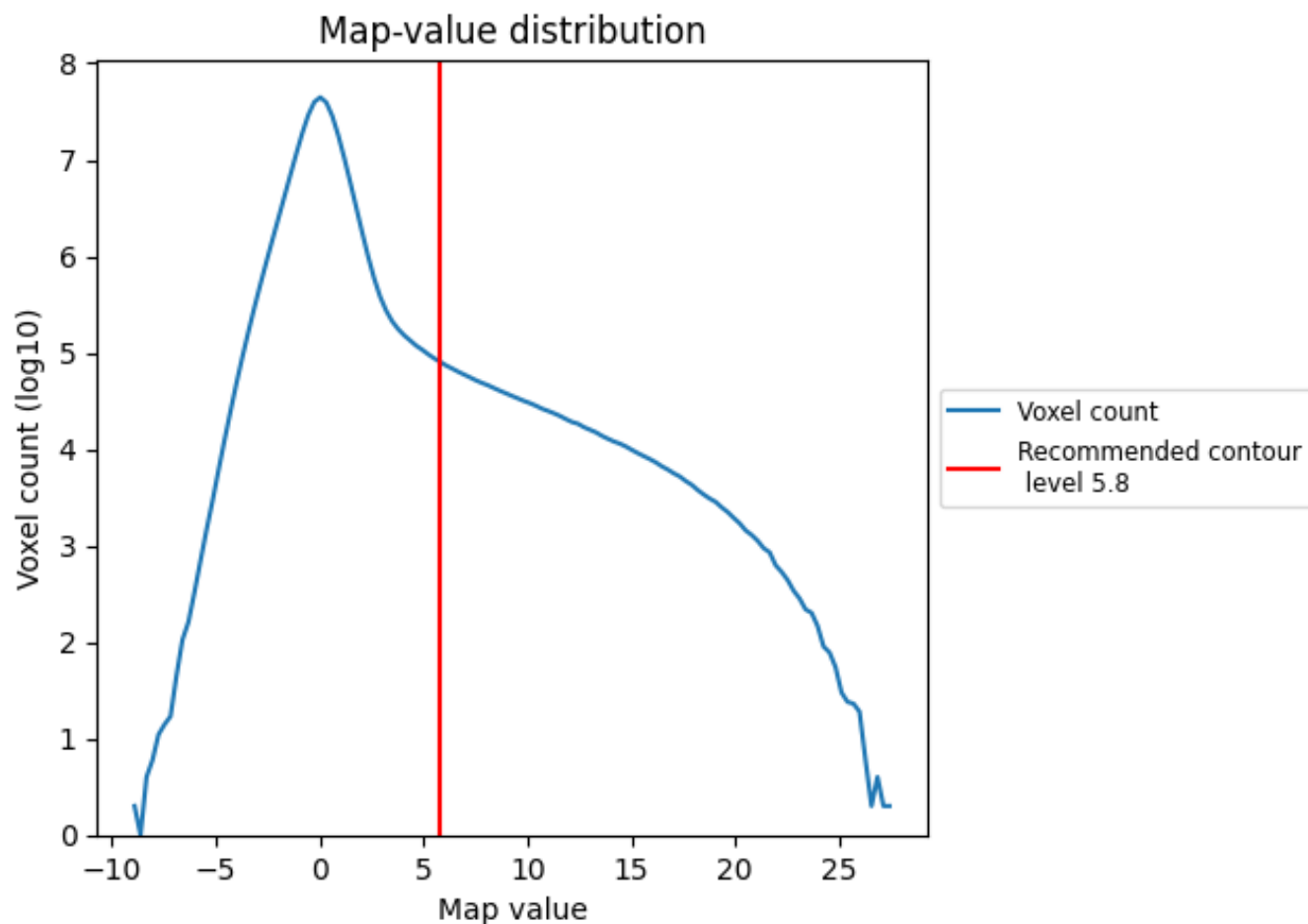
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

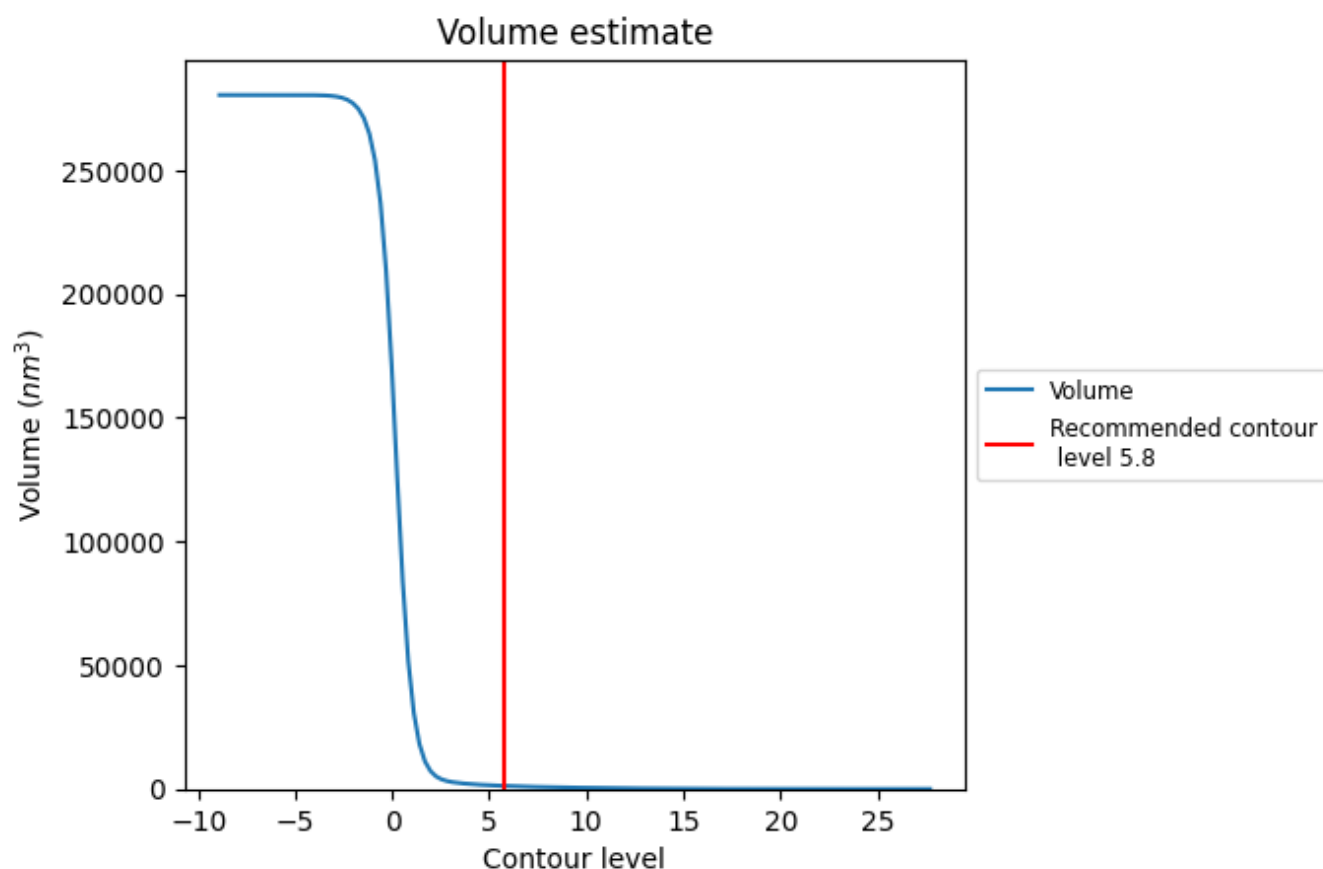
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

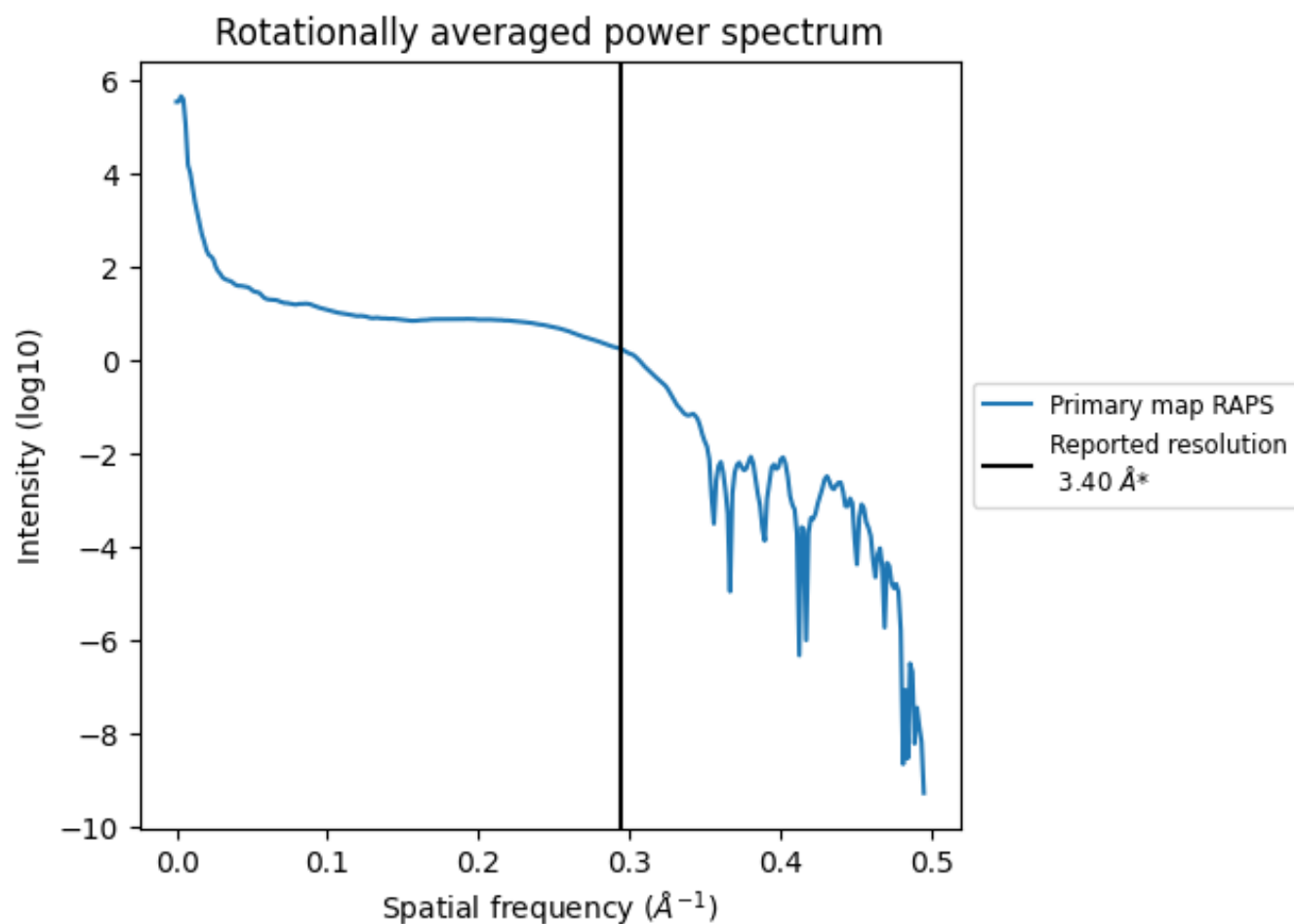
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1233 nm³; this corresponds to an approximate mass of 1114 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

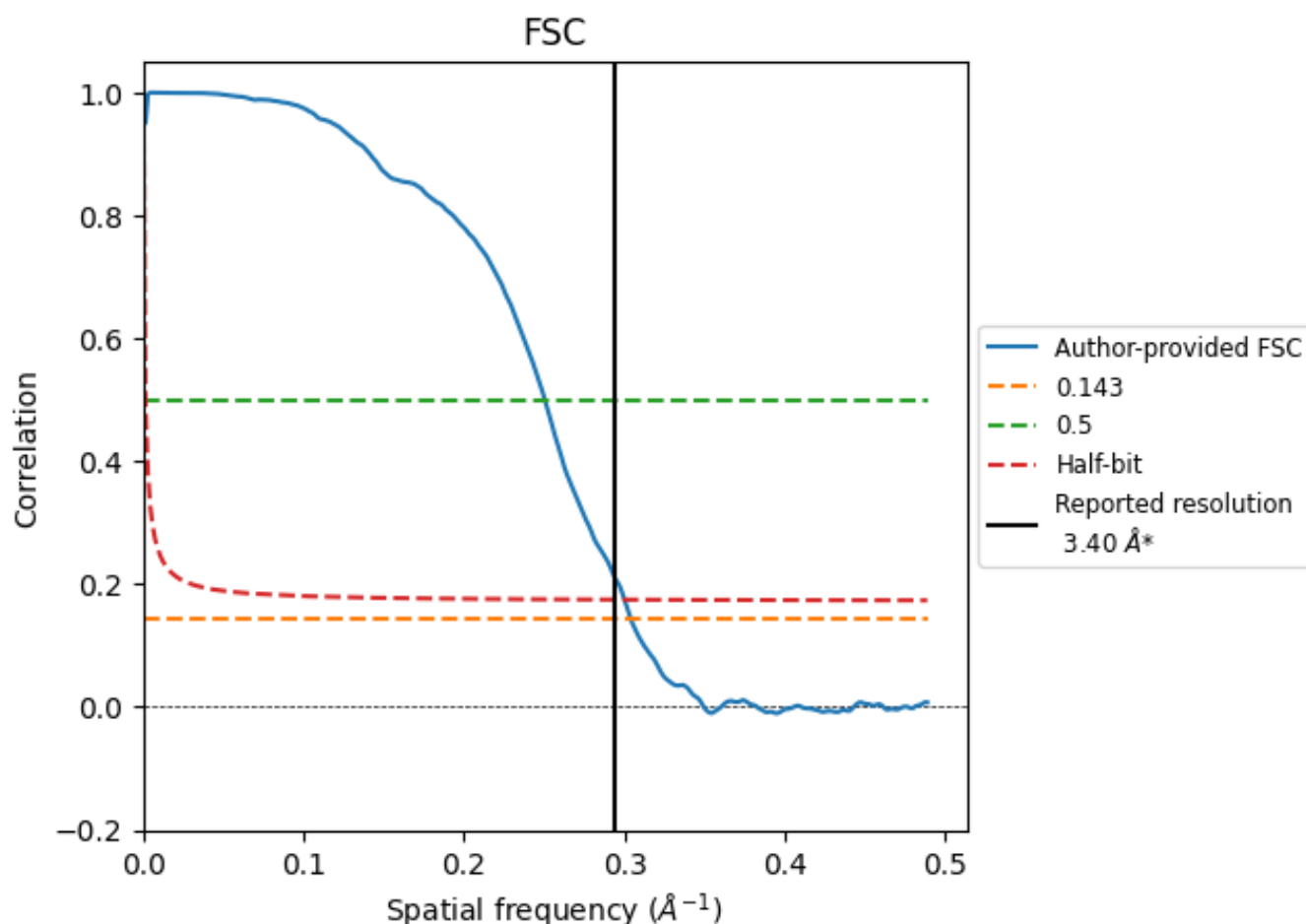


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

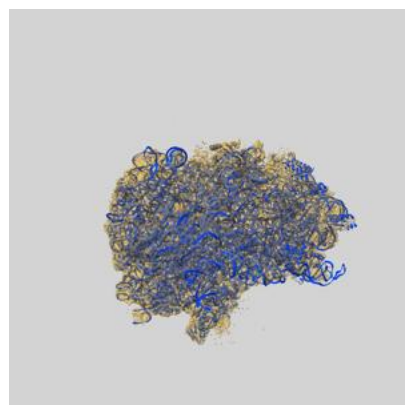
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.29	3.99	3.33
Unmasked-calculated*	-	-	-

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

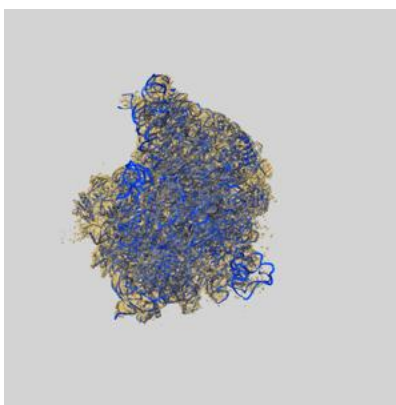
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21422 and PDB model 6VWN. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

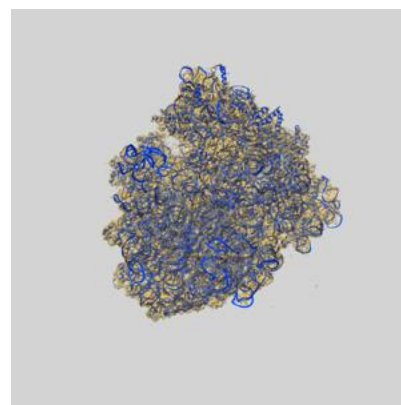
9.1 Map-model overlay [i](#)



X



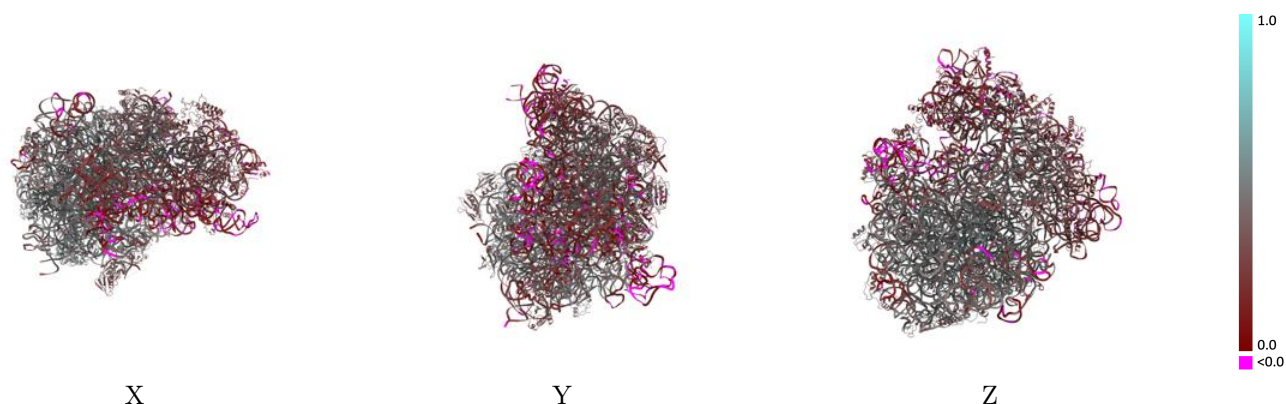
Y



Z

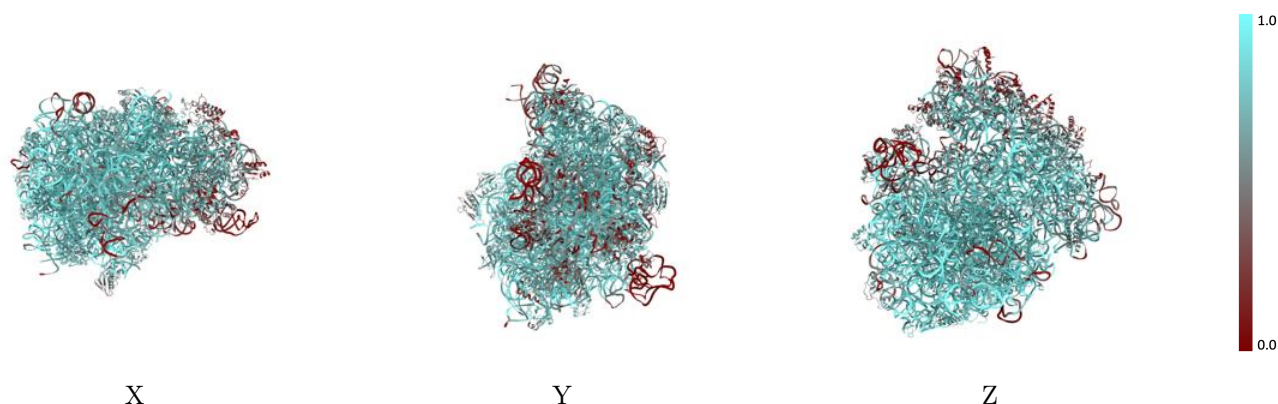
The images above show the 3D surface view of the map at the recommended contour level 5.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



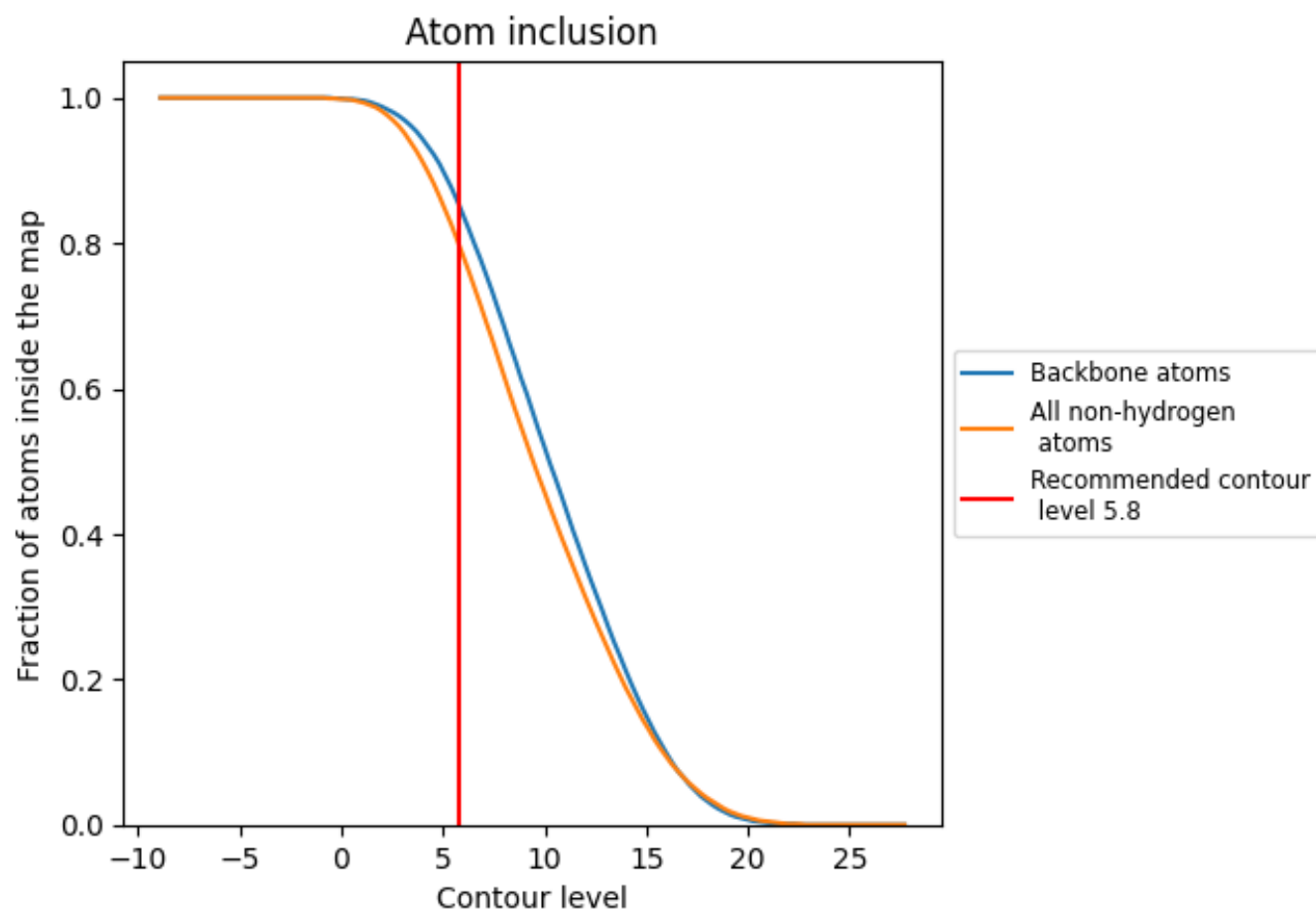
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (5.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7970	 0.3700
1	 0.7890	 0.2950
2	 0.8900	 0.4250
3	 0.8460	 0.3390
4	 0.3280	 0.0890
5	 0.5920	 0.1470
A	 0.8710	 0.4700
AA	 0.9240	 0.4960
AB	 0.8820	 0.4630
AC	 0.8190	 0.4100
B	 0.8170	 0.4810
C	 0.7680	 0.4510
D	 0.5120	 0.2570
E	 0.6000	 0.3360
F	 0.4850	 0.3540
G	 0.8520	 0.4700
I	 0.8340	 0.4590
J	 0.8100	 0.4660
K	 0.8490	 0.4510
L	 0.8920	 0.4790
M	 0.6870	 0.3540
N	 0.7970	 0.4390
O	 0.8560	 0.4740
P	 0.7830	 0.4680
Q	 0.8330	 0.4740
R	 0.8250	 0.4460
S	 0.7620	 0.4500
T	 0.7180	 0.4150
U	 0.8430	 0.4760
V	 0.8620	 0.4530
W	 0.7410	 0.4100
X	 0.7850	 0.4410
Y	 0.8500	 0.4770
Z	 0.4000	 0.3500
a	 0.3710	 0.2890



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Chain	Atom inclusion	Q-score
b	 0.5570	 0.2940
c	 0.4300	 0.2100
d	 0.7270	 0.3840
e	 0.6510	 0.3420
f	 0.4020	 0.1780
g	 0.7100	 0.3830
h	 0.4030	 0.1840
i	 0.3490	 0.2100
j	 0.6690	 0.3010
k	 0.5920	 0.2600
l	 0.4190	 0.1820
m	 0.5240	 0.2360
n	 0.7070	 0.3540
o	 0.5740	 0.2640
p	 0.6830	 0.3360
q	 0.7350	 0.3520
r	 0.3510	 0.1830
s	 0.6780	 0.2530
t	 0.5070	 0.2400