



## Full wwPDB EM Validation Report ⓘ

Apr 22, 2026 – 03:44 PM JST

PDB ID : 9JQ2 / pdb\_00009jq2  
EMDB ID : EMD-61720  
Title : Structure of the Bacterial Ribosome with human tRNA Lys(mcm5h2U34) and mRNA(AAG)  
Authors : Ishiguro, K.; Mo, Y.; Shirouzu, M.; Suzuki, T.  
Deposited on : 2024-09-27  
Resolution : 2.61 Å(reported)  
Based on initial model : 7y7e

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

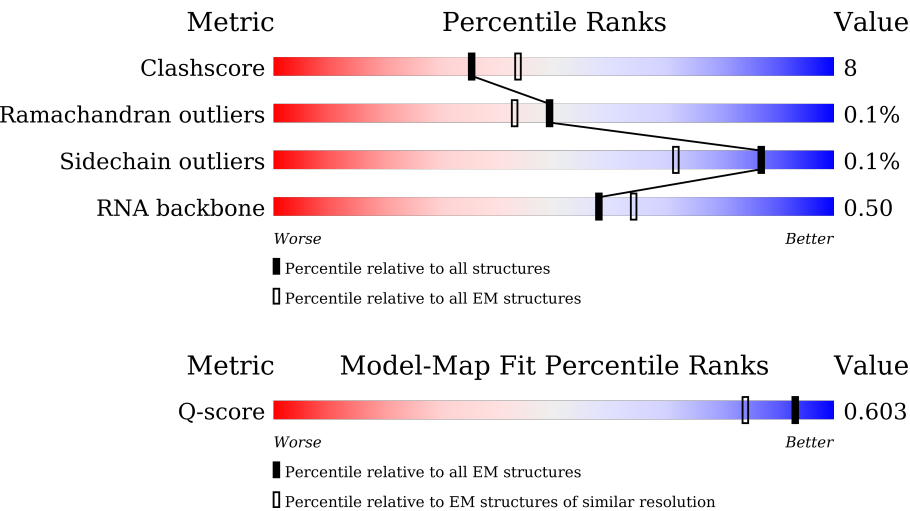
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
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 2.61 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	8735 ( 2.11 - 3.11 )

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

Mol	Chain	Length	Quality of chain
1	A	1542	<div><div></div><div>54%</div><div>37%</div><div>7%</div><div>.</div></div>
2	B	241	<div><div>78%</div><div>57%</div><div>36%</div><div>7%</div></div>
3	C	233	<div><div>64%</div><div>25%</div><div>12%</div></div>

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Mol	Chain	Length	Quality of chain
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	

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

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Mol	Chain	Length	Quality of chain
54	Z	77	<div><div></div><div>5%</div><div>60%</div><div>29%</div><div>12%</div></div>
55	V	76	<div><div></div><div>50%</div><div>32%</div><div>11%</div><div></div><div></div></div>

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 142029 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0
			32466	14487	5964	10503	1512		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2761	Total	C	N	O	P	0	0
			59301	26460	10925	19155	2761		

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called 50S ribosomal protein L17.

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

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	51	Total	C	N	O		0	0
			417	269	76	72			

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	11	Total	C	N	O	P	0	0
			234	105	41	77	11		

- Molecule 54 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Z	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 55 is a RNA chain called A-site tRNA-Lys.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	V	73	Total	C	N	O	P	S	0	0
			1578	712	279	514	72	1		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	107	Total	Mg	0
			107	107	
56	a	320	Total	Mg	0
			320	320	
56	b	6	Total	Mg	0
			6	6	
56	z	1	Total	Mg	0
			1	1	
56	Z	3	Total	Mg	0
			3	3	
56	V	1	Total	Mg	0
			1	1	

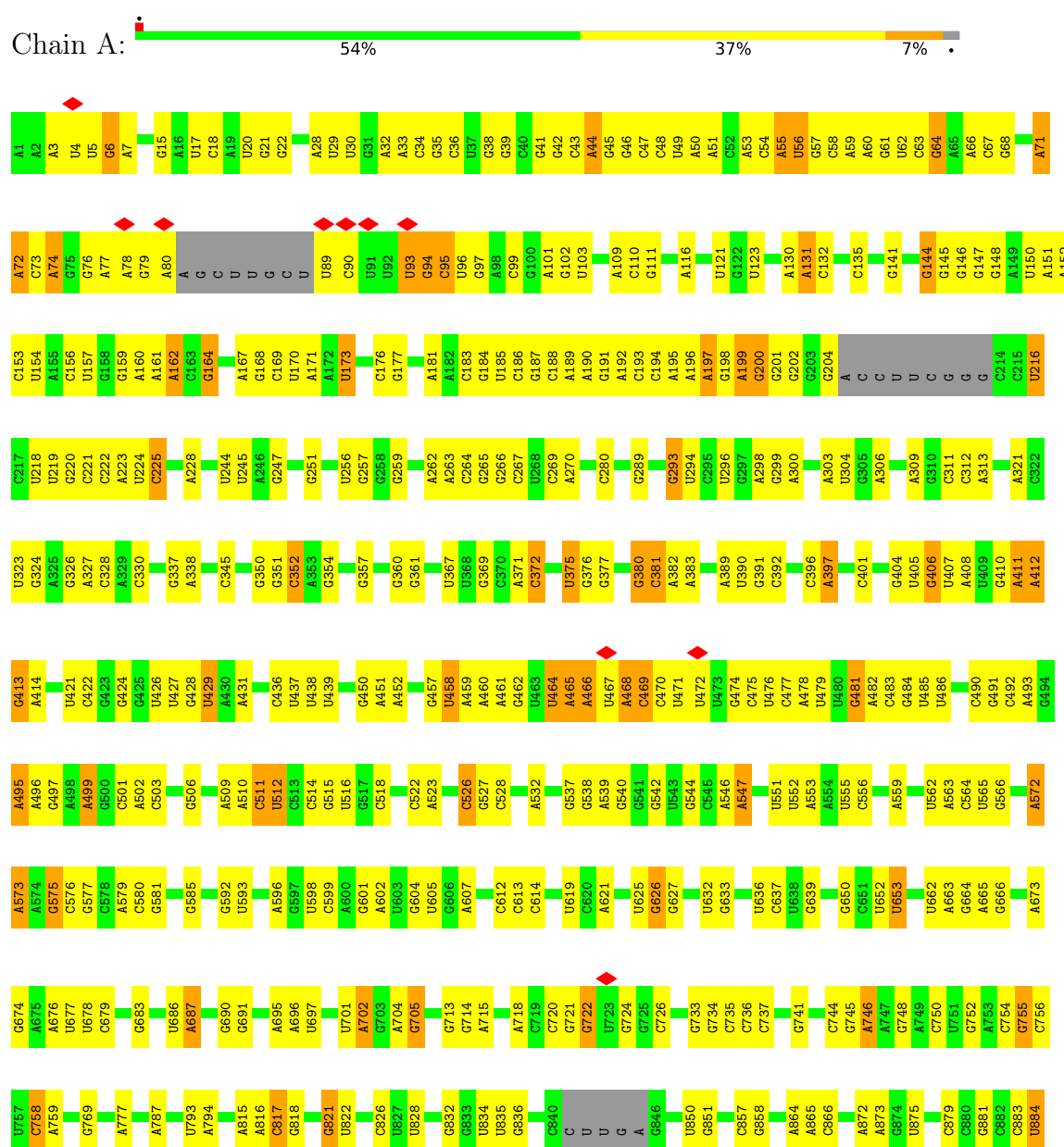
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

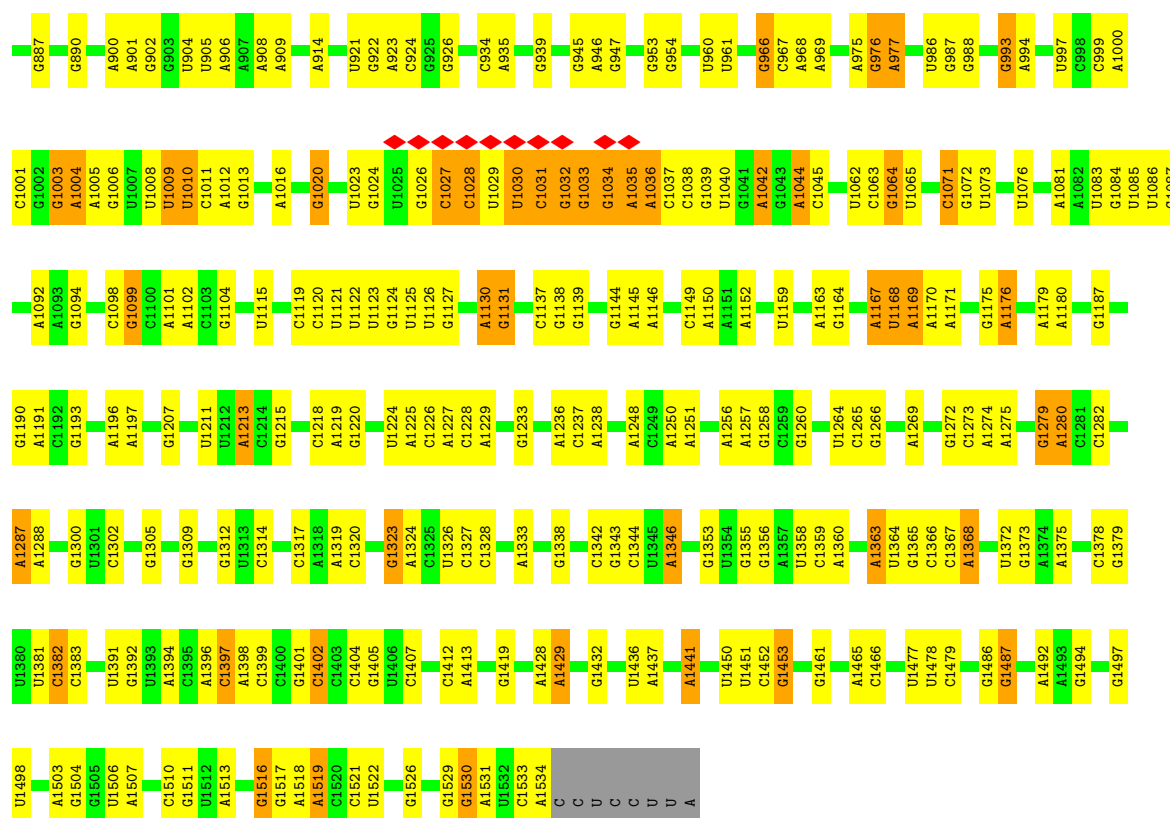
Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

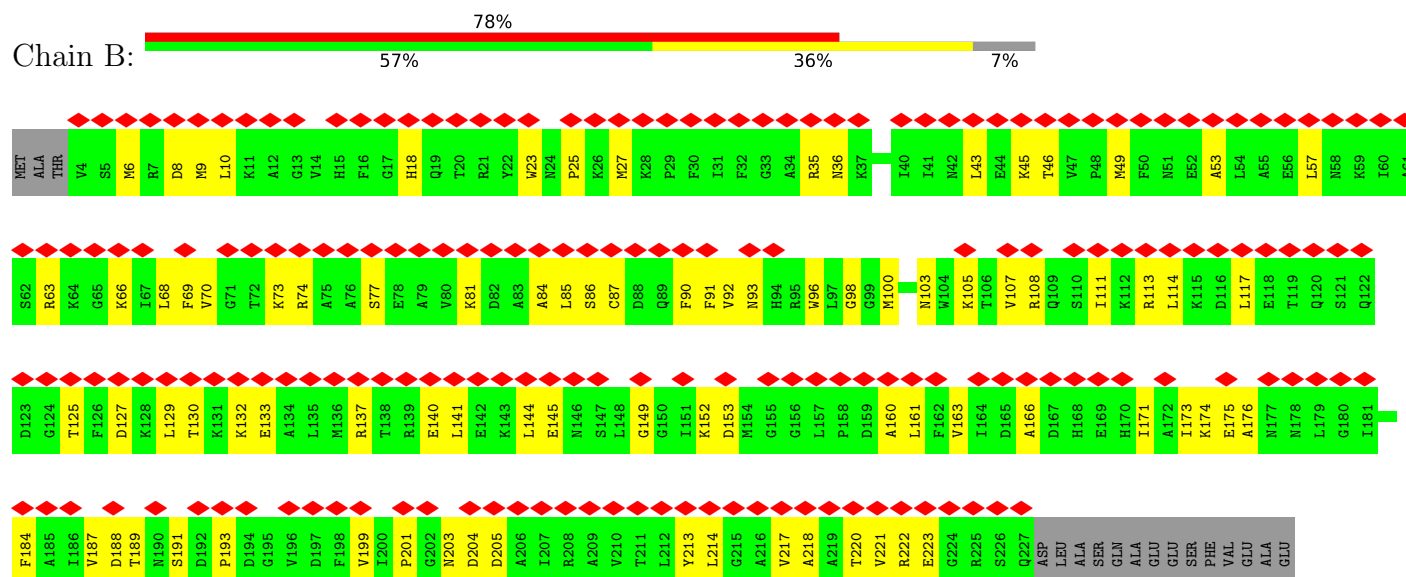
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 16S rRNA

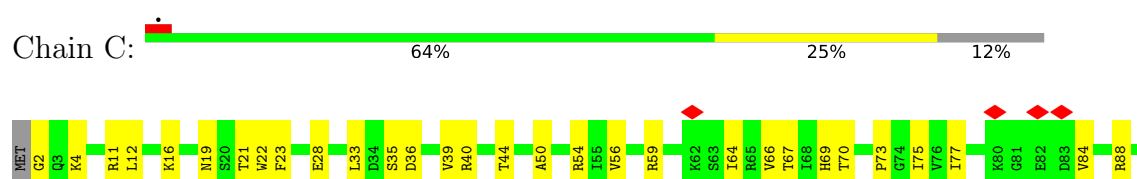




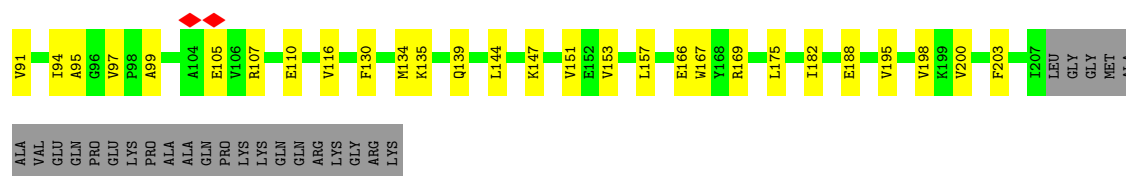
• Molecule 2: 30S ribosomal protein S2



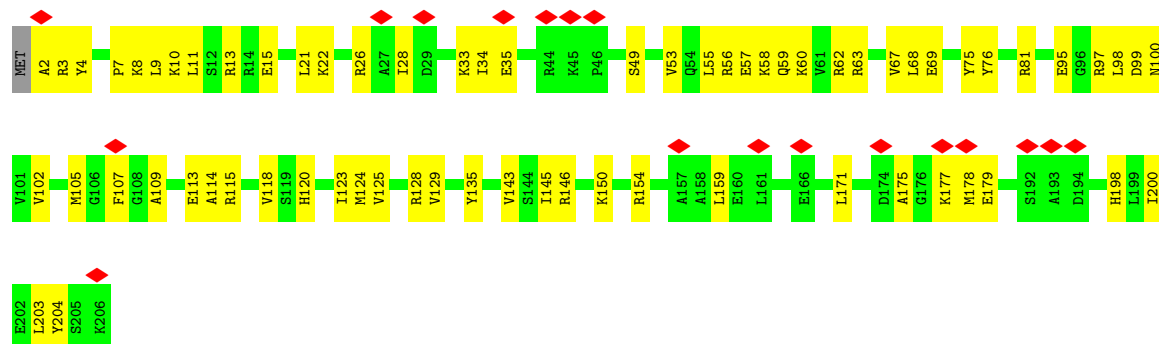
• Molecule 3: 30S ribosomal protein S3



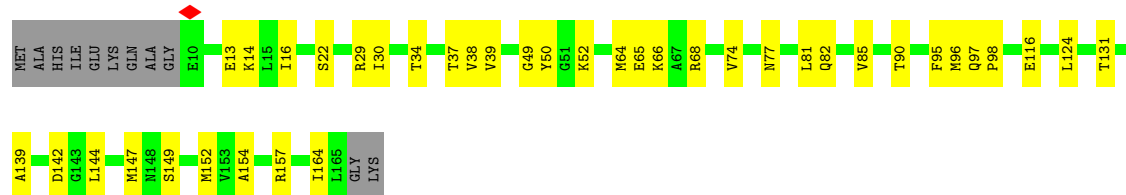




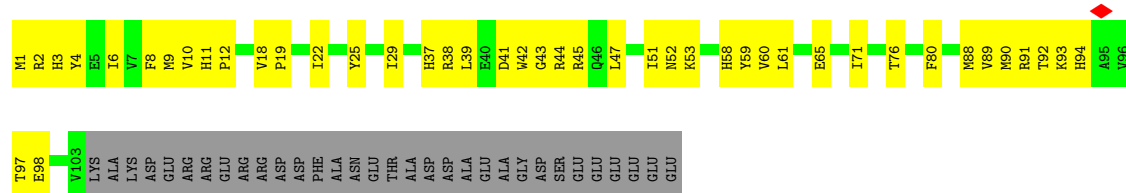
• Molecule 4: 30S ribosomal protein S4



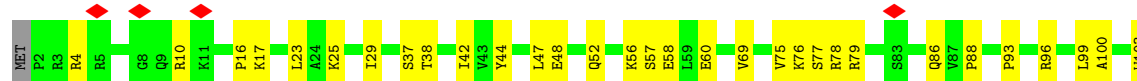
• Molecule 5: 30S ribosomal protein S5

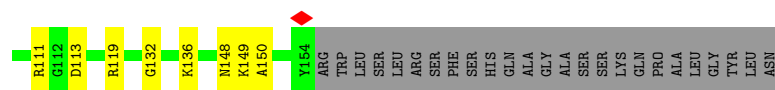


• Molecule 6: 30S ribosomal protein S6, fully modified isoform

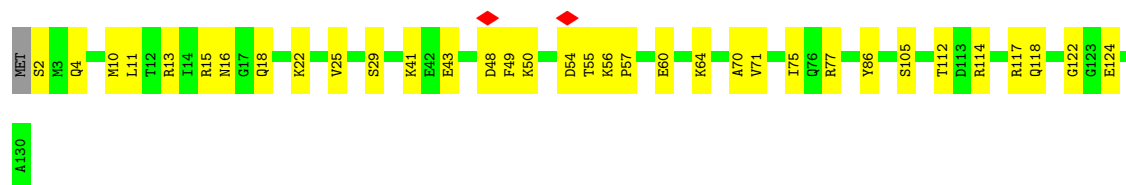


• Molecule 7: 30S ribosomal protein S7

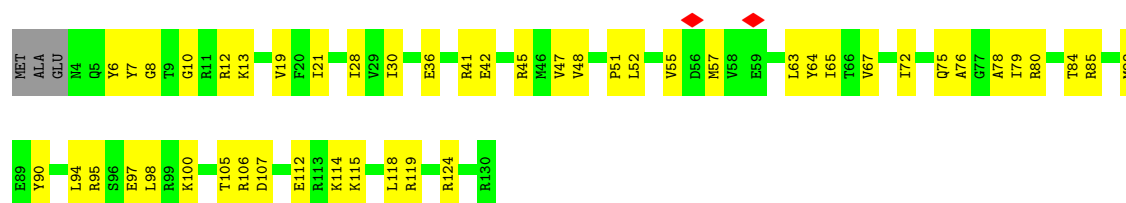




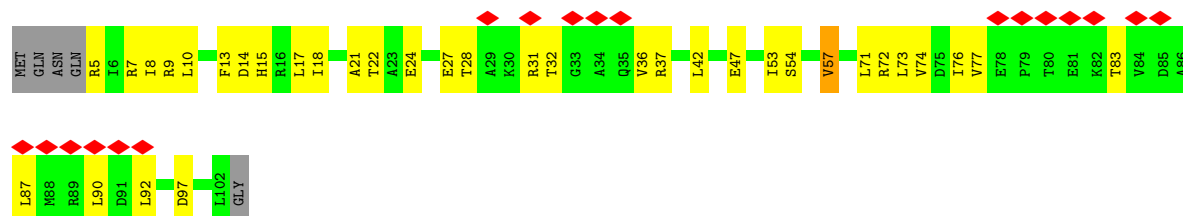
• Molecule 8: 30S ribosomal protein S8



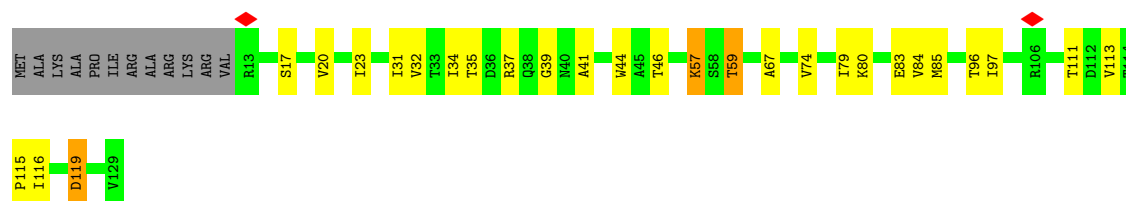
• Molecule 9: 30S ribosomal protein S9



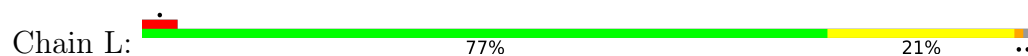
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12





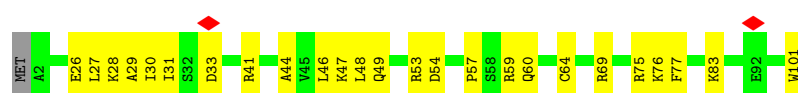
- Molecule 13: 30S ribosomal protein S13

Chain M: 69% 29%



- Molecule 14: 30S ribosomal protein S14

Chain N: 74% 25%



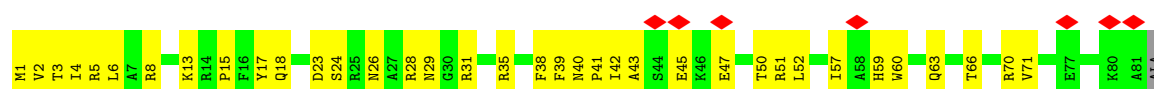
- Molecule 15: 30S ribosomal protein S15

Chain O: 73% 26%



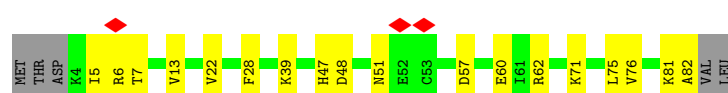
- Molecule 16: 30S ribosomal protein S16

Chain P: 9% 55% 44%



- Molecule 17: 30S ribosomal protein S17

Chain Q: 73% 21% 6%

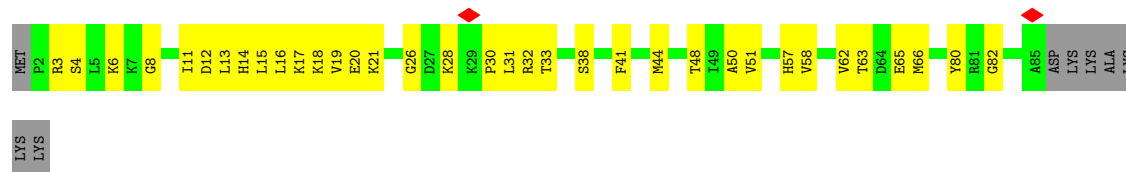


- Molecule 18: 30S ribosomal protein S18

Chain R: 8% 53% 35% 12%



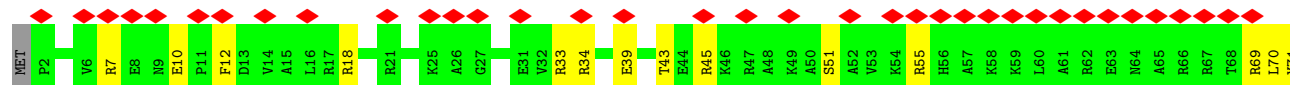
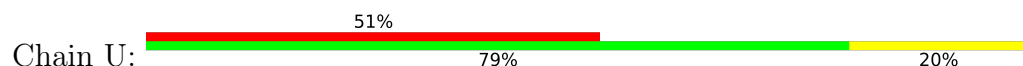
- Molecule 19: 30S ribosomal protein S19



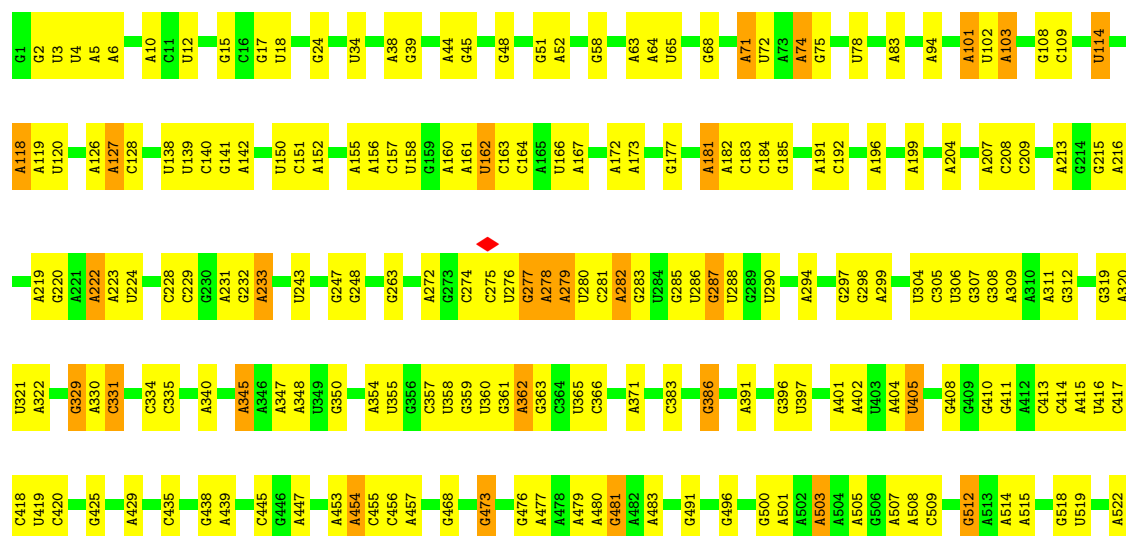
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21

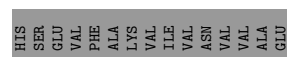


- Molecule 22: 23S rRNA

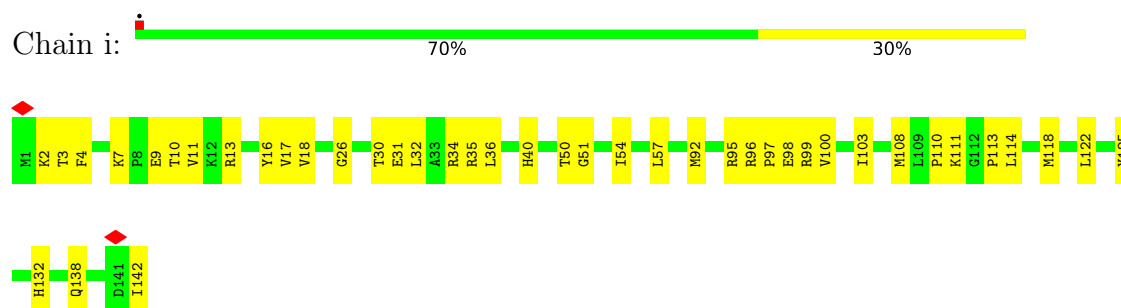


G1980	G1864	G1738	A1580	C1483	C1386	A1264	G1149	G989	G881	U755	G619	A529
A1981	U1865	A1739	A1583	A1494	A1387	A1269	C1150	G993	G882	G775	G620	G530
U1982	A1866	G1740	U1584	A1495	G1388	G1270	C1153	C994	G883	G776	A627	C531
U1991	G1869	A1744	C1585	A1496	A1392	G1271	G1157	C995	U884	A782	G636	A532
G1992	C1870	A1745	A1586	C1498	U1397	G1272	G1157	A996	C885	A783	A637	A533
U1993	A1871	A1746	U1589	C1499	C1398	A1274	G1168	C998	A886	G784	G638	U534
U2011	G1873	C1747	A1591	G1500	U1397	A1275	A1169	U999	U887	G785	G639	A538
G2012	A1874	C1748	U1592	G1501	C1398	A1276	U1168	A1000	C888	G786	C840	
A2013	G1875	A1757	A1593	U1506	G1401	A1286	C1172	A1001	C889	C791	U841	C544
A2014	U1880	C1760	A1594	C1507	U1402	G1289	U	G891	G890	C796	C645	U545
A2015	C1881	C1761	U1594	A1508	U1405	C1290	U	A892	U846		U546	U547
C2021	U1882	C1762	A1595	A1509	U1406	C1291	A	C893	G847	G805	U648	A547
U2022	G1902	A1773	U1599	G1510	G1407	G1292	U	U894	G847	G806	U649	G548
C2023	G1903	U1778	C1600	U1513	G1408	C1293	U	U895	U807	U807	U653	G549
G2024	G1904	A1603	A1603	A1514	U1409	G1296	G1177	A1010	U808	U810	A654	C550
C2025	G1905	C1607	U1523	U1515	G1410	G1297	C1178	U1011	A896	U811	U657	G551
U2026	G1906	U1607	A1525	G1514	C1414	G1300	G1179	U1012	C897	U812	U658	
G2027	G1907	A1608	A1526	U1515	U1415	A1301	U1180	C1013	C898	C812	U659	
U2028	A1784	G1632	G1527	G1514	G1416	A1302	U1181	U1014	A899	U813	G859	
G2029	A1785	G1633	A1528	G1527	G1417	G1311	U1182	U1015	A900	C914	A563	
A2030	A1786	A1634	G1538	A1528	A1419	C1315	U1183	U1016	C901			
A2031	C1790	A1618	U1534	G1529	A1420	U1188	U1188	A1021	C902	U827	U666	
G2032	A1791	G1622	U1535	U1529	G1421	G1197	G1197	G1022	G907	U828	U567	
U2033	G1792	A1626	A1536	U1534	A1427	U1198	U1198	U1023	A910	A829	U568	
G2034	G1793	A1627	A1537	U1535	C1428	U1199	U1199	G1024	G914	A833	U573	
U2035	A1794	A1632	G1538	U1536	G1429	U1203	U1203	G1025	G915	G834	A574	
G2036	C1795	G1632	G1539	U1537	A1429	A1204	A1204	A1027	C916	U839	A575	
U2037	A1796	A1633	G1540	G1537	G1430	C1330	U1210	A1028	G917	C840	U703	
G2038	U1798	A1634	G1541	G1538	A1431	G1331	G1211	U1033	A920	G843	G708	
A2039	G1799	A1637	U1542	U1539	A1434	G1334	C1211	C921	C922	A844	U709	
G2040	A1800	U1647	A1545	U1540	G1435	G1337	G1212	A1040	A927	A845	U710	
C2041	A1801	U1648	A1546	U1541	C1437	A1342	G1223	C1045	A928	U846	A715	
U2042	A1802	G1674	C1547	U1542	U1438	G1343	A1226	A1046	U931	U847	A716	
G2043	A1803	U1682	A1548	U1543	U1443	A1344	U1230	G1047	U932	C948	C717	
C2044	G1807	U1683	C1550	U1544	G1444	C1345	U1231	A1048	U933	U850	A718	
A2045	A1808	U1684	G1556	U1545	G1445	U1352	U1234	C1052	U934	U852	C719	
G2046	A1809	U1685	U1557	U1546	C1446	A1353	U1235	C	A946		A721	
C2047	A1810	A1713	G1558	U1557	C1447	A1354	G1236	A	C947	G856	A722	
U2048	C1816	U1714	C1559	U1558	U1460	A1355	A1237	G	A948	G857	C723	
G2049	A1829	G1715	U1560	U1559	U1461	G1356	A1238	U	C949	G858	U724	
C2050	G1835	U1720	U1561	U1560	U1462	G1357	U1242	A	U955	U860	G729	
G2051	G1836	G1721	U1562	U1561	U1463	C1358	C1243	U	U956	A861	A730	
A2052	U1842	G1724	U1563	U1562	A1469	G1364	G1250	U	C959	G862	C610	
C2053	A1847	U1729	U1564	U1563	A1470	A1365	U1132	G	A960	A742	C611	
G2054	A1848	C1730	A1570	U1564	U1475	A1366	A1133	U	C961	A743	G612	
C2055	U1856	G1731	A1571	U1565	G1476	A1367	C1135	C	U973	U871	A613	
A2056	G1857	U1736	U1572	U1566	G1477	U1379	G1138	U	G974	U872	A614	
G2057	A1858	G1737	U1573	U1567	U1478	A1383	U1141	U	A983	C876	U747	
U2058			U1574	U1568	U1482		A1142	G	A984	A877	U754	
C2059			U1575	U1569								
A2060			U1576	U1570								
G2061			U1577	U1571								
C2062			U1578	U1572								
U2063			U1579	U1573								
G2064												
C2065												
U2066												
A2067												
C2068												
U2069												
G2070												
A2071												
C2072												
U2073												
G2074												
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A2121												
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G2164												
A2165												

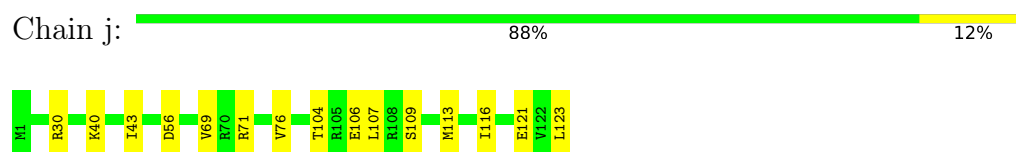




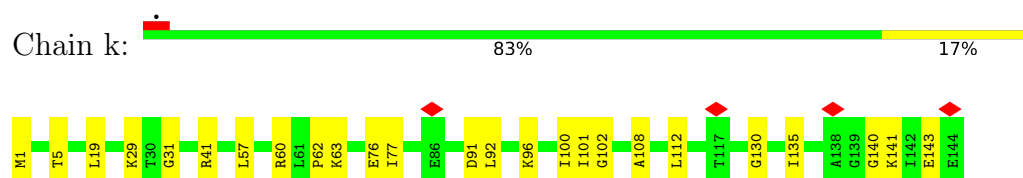
- Molecule 30: 50S ribosomal protein L13



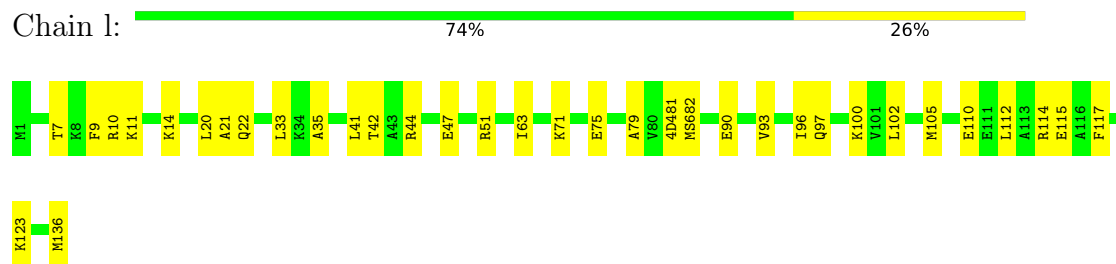
- Molecule 31: 50S ribosomal protein L14



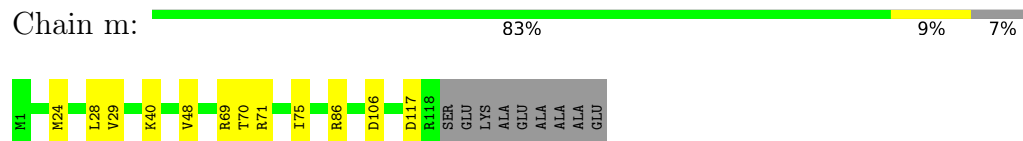
- Molecule 32: 50S ribosomal protein L15



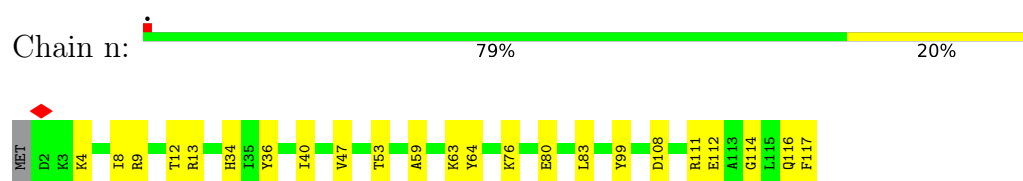
- Molecule 33: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L17

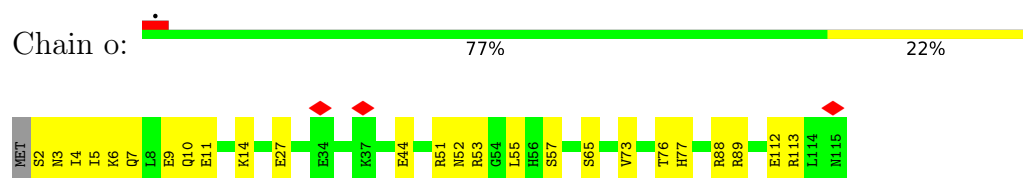


- Molecule 35: 50S ribosomal protein L18

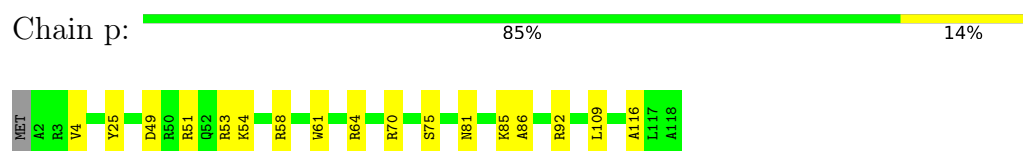




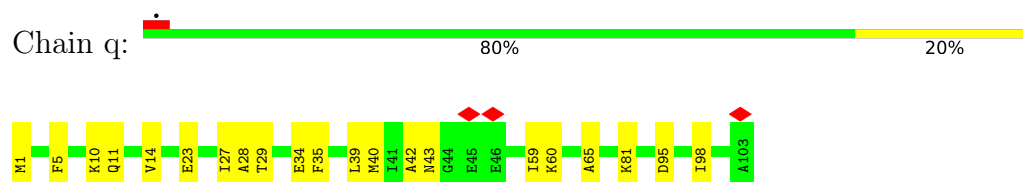
- Molecule 36: 50S ribosomal protein L19



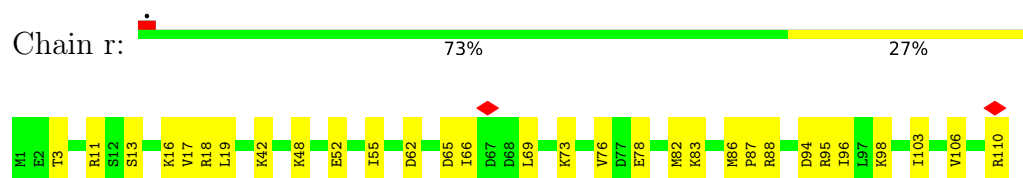
- Molecule 37: 50S ribosomal protein L20



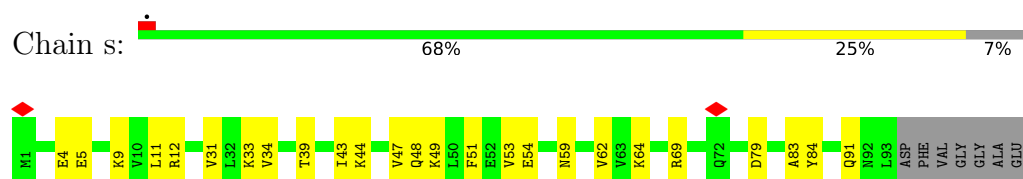
- Molecule 38: 50S ribosomal protein L21



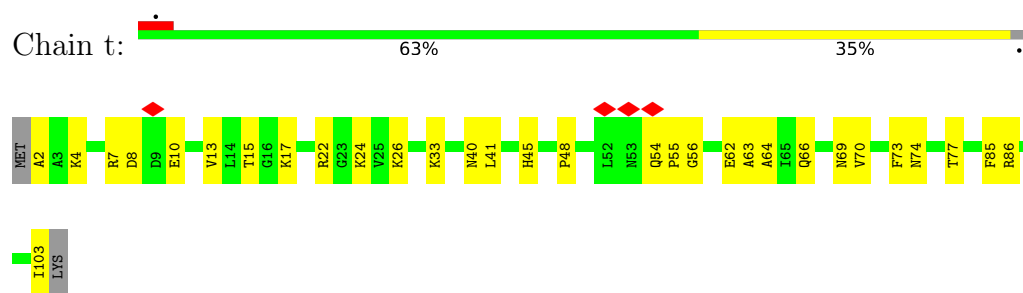
- Molecule 39: 50S ribosomal protein L22



- Molecule 40: 50S ribosomal protein L23

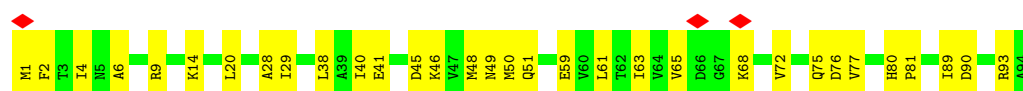


- Molecule 41: 50S ribosomal protein L24




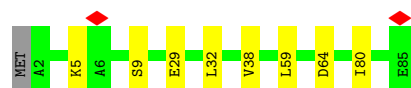
- Molecule 42: 50S ribosomal protein L25

Chain u:  66% 34%




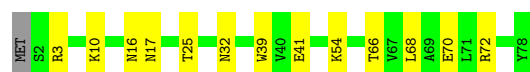
- Molecule 43: 50S ribosomal protein L27

Chain v:  89% 9%



- Molecule 44: 50S ribosomal protein L28

Chain w:  82% 17%




- Molecule 45: 50S ribosomal protein L29

Chain x:  5% 67% 32%



- Molecule 46: 50S ribosomal protein L30

Chain y:  5% 81% 17%




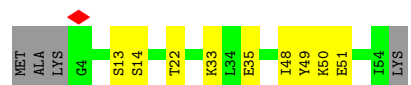
- Molecule 47: 50S ribosomal protein L32

Chain z:  70% 28%




- Molecule 48: 50S ribosomal protein L33

Chain 0:  76% 16% 7%




- Molecule 49: 50S ribosomal protein L34

Chain 1:  87% 13%




- Molecule 50: 50S ribosomal protein L35

Chain 2:  78% 17% . .



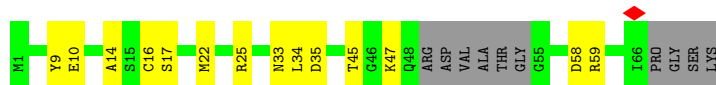
- Molecule 51: 50S ribosomal protein L36

Chain 3:  79% 21%



- Molecule 52: 50S ribosomal protein L31

Chain 4:  66% 20% 14%



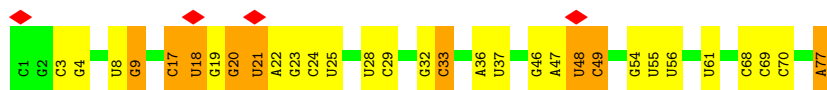
- Molecule 53: mRNA

Chain X:  29% 69%



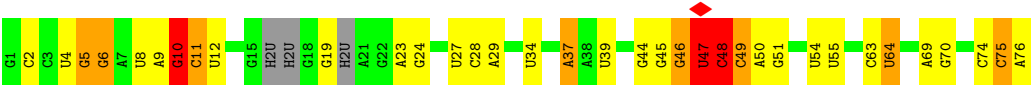
- Molecule 54: P-site tRNA-fMet

Chain Z:  5% 60% 29% 12%



- Molecule 55: A-site tRNA-Lys

Chain V:  50% 32% 11% . .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	278889	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0119	Depositor
Map size (Å)	439.10498, 439.10498, 439.10498	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8285, 0.8285, 0.8285	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, OMC, 1MG, UR3, 2MA, 1MA, MA6, IAS, D2T, 5MC, 4SU, PSU, H2U, MEQ, 4D4, OMG, G7M, 6MZ, OMU, 2MG, 4OC, A1L4U, MS6, ZN, 5MU, 2MU, 12A, 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	A	0.44	0/36073	0.42	1/56264 (0.0%)
2	B	0.25	0/1784	0.56	0/2403
3	C	0.36	0/1651	0.55	0/2225
4	D	0.30	0/1665	0.55	0/2227
5	E	0.39	0/1165	0.60	0/1568
6	F	0.36	0/858	0.55	0/1160
7	G	0.33	0/1219	0.52	0/1635
8	H	0.36	0/989	0.60	2/1326 (0.2%)
9	I	0.39	0/1034	0.61	0/1375
10	J	0.39	0/796	0.69	2/1077 (0.2%)
11	K	0.39	0/884	0.59	0/1191
12	L	0.39	0/960	0.53	0/1286
13	M	0.35	0/900	0.50	0/1204
14	N	0.39	0/817	0.53	0/1088
15	O	0.39	0/722	0.57	0/964
16	P	0.34	0/653	0.59	0/877
17	Q	0.36	0/650	0.48	0/871
18	R	0.34	0/553	0.52	0/742
19	S	0.44	0/685	0.57	0/922
20	T	0.34	0/676	0.53	0/895
21	U	0.22	0/597	0.47	0/792
22	a	0.54	0/65842	0.43	2/102711 (0.0%)
23	b	0.41	0/2850	0.38	0/4444
24	c	0.46	0/2121	0.53	0/2852
25	d	0.45	0/1576	0.48	0/2119
26	e	0.38	0/1571	0.52	0/2113
27	f	0.34	0/1434	0.49	0/1926
28	g	0.33	0/1343	0.58	1/1816 (0.1%)
29	h	0.27	0/306	0.54	0/413
30	i	0.43	0/1152	0.50	0/1551
31	j	0.45	0/955	0.49	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	k	0.43	0/1062	0.57	0/1413
33	l	0.44	0/1073	0.53	0/1433
34	m	0.47	0/958	0.53	0/1281
35	n	0.35	0/902	0.56	0/1209
36	o	0.42	0/929	0.50	0/1242
37	p	0.51	0/960	0.51	0/1278
38	q	0.44	0/829	0.61	0/1107
39	r	0.44	0/864	0.57	0/1156
40	s	0.38	0/744	0.60	0/994
41	t	0.34	0/787	0.57	0/1051
42	u	0.38	0/766	0.59	0/1025
43	v	0.43	0/642	0.44	0/848
44	w	0.43	0/635	0.54	0/848
45	x	0.35	0/502	0.55	0/667
46	y	0.38	0/453	0.52	0/605
47	z	0.45	0/450	0.51	0/599
48	0	0.42	0/424	0.58	0/565
49	1	0.46	0/380	0.55	0/498
50	2	0.45	0/513	0.56	0/676
51	3	0.46	0/303	0.61	0/397
52	4	0.31	0/488	0.45	0/649
53	X	0.45	0/261	0.34	0/404
54	Z	0.37	0/1725	0.38	0/2687
55	V	0.34	0/1429	0.38	0/2217
All	All	0.47	0/152560	0.46	8/228165 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
13	M	0	1
44	w	0	1
50	2	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	g	112	PRO	CA-N-CD	-8.01	100.79	112.00
8	H	4	GLN	CA-C-N	-7.34	113.39	122.42
8	H	4	GLN	C-N-CA	-7.34	113.39	122.42
10	J	53	ILE	CA-C-N	-6.57	108.51	123.15
10	J	53	ILE	C-N-CA	-6.57	108.51	123.15
22	a	512	G	O4'-C1'-N9	5.73	116.80	108.20
22	a	2501	C	C4'-C3'-O3'	5.34	117.41	109.40
1	A	572	A	C4'-C3'-O3'	-5.22	105.17	113.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	31	HIS	Peptide
12	L	101	ALA	Peptide
13	M	65	VAL	Peptide
44	w	16	ASN	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32466	0	16359	427	0
2	B	1753	0	1780	63	0
3	C	1624	0	1696	47	0
4	D	1643	0	1707	57	0
5	E	1152	0	1196	34	0
6	F	839	0	833	33	0
7	G	1203	0	1254	36	0
8	H	979	0	1031	25	0
9	I	1022	0	1070	46	0
10	J	786	0	828	25	0
11	K	877	0	884	21	0
12	L	957	0	1017	20	0
13	M	891	0	952	27	0
14	N	805	0	844	23	0
15	O	714	0	734	20	0
16	P	643	0	661	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	641	0	682	11	0
18	R	544	0	565	20	0
19	S	668	0	693	27	0
20	T	670	0	719	21	0
21	U	589	0	629	12	0
22	a	59301	0	29850	491	0
23	b	2549	0	1291	17	0
24	c	2082	0	2154	30	0
25	d	1566	0	1618	19	0
26	e	1552	0	1619	39	0
27	f	1410	0	1444	30	0
28	g	1323	0	1371	37	0
29	h	303	0	327	8	0
30	i	1129	0	1162	29	0
31	j	946	0	1023	13	0
32	k	1053	0	1129	20	0
33	l	1075	0	1144	21	0
34	m	945	0	989	7	0
35	n	892	0	923	16	0
36	o	917	0	962	17	0
37	p	947	0	1019	16	0
38	q	816	0	839	15	0
39	r	857	0	922	21	0
40	s	738	0	807	22	0
41	t	779	0	831	27	0
42	u	753	0	780	23	0
43	v	634	0	653	7	0
44	w	625	0	652	7	0
45	x	501	0	531	13	0
46	y	449	0	488	7	0
47	z	444	0	458	12	0
48	0	417	0	451	6	0
49	1	377	0	418	6	0
50	2	504	0	572	12	0
51	3	302	0	340	6	0
52	4	480	0	478	13	0
53	X	234	0	118	0	0
54	Z	1645	0	842	14	0
55	V	1578	0	806	16	0
56	A	107	0	0	0	0
56	V	1	0	0	0	0
56	Z	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	a	320	0	0	0	0
56	b	6	0	0	0	0
56	z	1	0	0	0	0
57	3	1	0	0	0	0
57	4	1	0	0	0	0
All	All	142029	0	95145	1816	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 8.

All (1816) 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)
1:A:1127:G:H1	1:A:1145:A:N6	1.62	0.96
22:a:1168:G:H1	22:a:1181:U:H3	1.12	0.96
19:S:41:PHE:H	19:S:44:MET:HE3	1.31	0.94
14:N:49:GLN:HE22	19:S:13:LEU:H	1.00	0.93
41:t:15:THR:OG1	41:t:69:ASN:ND2	2.03	0.91
1:A:1127:G:H1	1:A:1145:A:H61	0.93	0.90
6:F:88:MET:HE1	18:R:61:ARG:HG2	1.52	0.89
1:A:198:G:H1	1:A:219:U:H3	1.21	0.89
4:D:145:ILE:HD13	4:D:178:MET:HB3	1.54	0.88
16:P:52:LEU:HD12	16:P:57:ILE:HD11	1.56	0.88
11:K:20:VAL:HG12	11:K:83:GLU:HB2	1.56	0.87
1:A:427:U:OP1	4:D:13:ARG:NH2	2.07	0.86
22:a:1153:C:OP1	37:p:92:ARG:NH2	2.08	0.85
22:a:1607:C:N4	22:a:1622:G:OP2	2.09	0.85
1:A:636:U:OP1	17:Q:6:ARG:NH1	2.09	0.84
1:A:76:G:H1	1:A:93:U:H3	0.86	0.83
1:A:1280:A:OP1	10:J:9:ARG:NH1	2.13	0.82
9:I:115:LYS:HB2	9:I:118:LEU:HD12	1.60	0.82
19:S:15:LEU:HD13	19:S:33:THR:HG21	1.61	0.82
22:a:1365:A:OP1	44:w:3:ARG:NH2	2.12	0.82
6:F:2:ARG:HD3	6:F:91:ARG:HE	1.45	0.81
19:S:19:VAL:HG21	19:S:44:MET:HG2	1.58	0.81
26:e:125:SER:O	26:e:137:LYS:NZ	2.14	0.81
5:E:157:ARG:NH2	8:H:43:GLU:OE2	2.13	0.80
1:A:1086:U:H3	1:A:1099:G:H22	1.30	0.80
17:Q:7:THR:OG1	17:Q:60:GLU:OE2	2.00	0.80
11:K:35:THR:HG22	11:K:41:ALA:HA	1.63	0.80
22:a:545:U:HO2'	22:a:548:G:H1	1.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:U:H3	1:A:1020:G:H1	1.29	0.80
5:E:14:LYS:NZ	5:E:116:GLU:OE2	2.15	0.80
3:C:35:SER:OG	3:C:59:ARG:NH2	2.16	0.79
13:M:82:ASP:OD1	22:a:888:C:N4	2.16	0.79
30:i:125:TYR:OH	30:i:132:HIS:NE2	2.15	0.79
1:A:836:G:H1	1:A:850:U:H3	1.31	0.79
7:G:86:GLN:HB2	7:G:148:ASN:HD22	1.47	0.78
2:B:114:LEU:HD12	2:B:144:LEU:HB3	1.63	0.78
22:a:2796:U:H3	22:a:2799:A:H61	1.31	0.78
3:C:11:ARG:NH2	3:C:175:LEU:O	2.17	0.78
2:B:35:ARG:NH1	2:B:36:ASN:OD1	2.16	0.77
1:A:1526:G:OP1	21:U:45:ARG:NH2	2.18	0.77
24:c:135:ILE:O	24:c:167:ARG:NH1	2.17	0.77
2:B:73:LYS:NZ	2:B:205:ASP:OD1	2.17	0.77
19:S:11:ILE:HD12	19:S:38:SER:HB3	1.65	0.77
47:z:53:LYS:NZ	47:z:55:ILE:O	2.17	0.77
4:D:4:TYR:OH	4:D:7:PRO:O	2.03	0.76
27:f:30:ARG:H	27:f:159:THR:HG22	1.48	0.76
1:A:71:A:N6	1:A:99:C:O2	2.18	0.76
22:a:68:G:N2	22:a:74:A:OP2	2.19	0.76
1:A:324:G:N1	1:A:327:A:OP2	2.18	0.76
28:g:95:ARG:HG2	28:g:106:SER:HB3	1.68	0.76
9:I:55:VAL:HG23	9:I:57:MET:HG3	1.68	0.75
9:I:106:ARG:NH1	9:I:107:ASP:O	2.19	0.75
22:a:1864:U:OP1	22:a:2410:G:O2'	2.04	0.75
1:A:55:A:OP2	1:A:352:C:N4	2.20	0.75
1:A:526:C:OP1	12:L:88:LYS:NZ	2.16	0.75
1:A:673:A:H2'	1:A:674:G:C8	2.21	0.75
1:A:1027:C:H2'	1:A:1028:C:C6	2.22	0.75
1:A:1229:A:OP2	13:M:113:ARG:NH1	2.18	0.75
1:A:1328:C:H5''	13:M:28:THR:HG21	1.68	0.75
24:c:107:PRO:HD2	24:c:110:LEU:HD22	1.69	0.75
22:a:1724:G:H1	22:a:1736:U:H3	1.35	0.74
1:A:73:C:HO2'	1:A:74:A:H8	1.32	0.74
4:D:105:MET:HE2	4:D:171:LEU:HD11	1.69	0.74
1:A:677:U:H3	1:A:713:G:H22	1.36	0.74
1:A:76:G:N2	1:A:93:U:O2	2.18	0.73
1:A:1003:G:H21	1:A:1005:A:H5'	1.52	0.73
19:S:14:HIS:HA	19:S:17:LYS:HE3	1.70	0.73
22:a:881:G:H1	22:a:895:U:H3	0.76	0.73
22:a:995:C:OP2	37:p:54:LYS:NZ	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:e:149:ILE:HB	26:e:188:MET:HG2	1.68	0.73
1:A:1004:A:H2'	1:A:1005:A:C8	2.23	0.73
4:D:124:MET:HE2	4:D:146:ARG:HG2	1.70	0.73
18:R:71:THR:HG23	18:R:73:ARG:H	1.53	0.73
22:a:993:G:OP2	37:p:51:ARG:NH2	2.21	0.73
17:Q:57:ASP:OD1	17:Q:82:ALA:N	2.20	0.73
30:i:114:LEU:HG	30:i:118:MET:HE3	1.70	0.73
42:u:76:ASP:OD1	42:u:90:ASP:HB2	1.87	0.73
4:D:28:ILE:HG23	4:D:34:ILE:HD11	1.70	0.72
26:e:21:ARG:NH1	26:e:107:SER:OG	2.22	0.72
27:f:102:ARG:NH2	52:4:9:TYR:OH	2.20	0.72
40:s:12:ARG:HD3	45:x:29:ARG:HD2	1.70	0.72
14:N:49:GLN:HE22	19:S:13:LEU:N	1.83	0.72
7:G:48:GLU:O	7:G:52:GLN:NE2	2.23	0.72
26:e:111:GLU:OE1	26:e:114:ARG:NH1	2.23	0.72
6:F:41:ASP:OD1	6:F:58:HIS:NE2	2.23	0.72
22:a:2095:A:O5'	29:h:11:ASN:ND2	2.22	0.72
2:B:117:LEU:HB3	2:B:141:LEU:HD13	1.72	0.71
1:A:1382:C:O2'	7:G:79:ARG:NH1	2.23	0.71
4:D:109:ALA:HB3	4:D:113:GLU:HG3	1.71	0.71
7:G:76:LYS:HE3	7:G:78:ARG:HE	1.55	0.71
1:A:404:G:O6	4:D:2:ALA:N	2.23	0.71
4:D:128:ARG:NH1	4:D:129:VAL:O	2.24	0.71
30:i:4:PHE:O	37:p:64:ARG:NH2	2.19	0.71
22:a:1045:C:O2	22:a:1111:A:N6	2.23	0.71
22:a:1799:G:N7	24:c:178:SER:OG	2.23	0.71
1:A:4:U:H2'	1:A:5:U:H2'	1.73	0.71
13:M:33:ILE:HD13	13:M:60:VAL:HG22	1.71	0.71
22:a:2102:G:H1	22:a:2187:U:H3	1.26	0.71
2:B:86:SER:O	2:B:222:ARG:NH2	2.24	0.70
10:J:47:GLU:OE1	14:N:76:LYS:NZ	2.23	0.70
22:a:1590:A:H2'	22:a:1591:A:C8	2.27	0.70
3:C:105:GLU:O	3:C:107:ARG:NH1	2.25	0.70
52:4:16:CYS:HA	52:4:34:LEU:HB2	1.72	0.70
1:A:28:A:O2'	1:A:296:U:OP1	2.08	0.70
1:A:437:U:O2'	4:D:120:HIS:ND1	2.25	0.69
28:g:91:GLY:O	28:g:94:TYR:HD2	1.75	0.69
22:a:856:G:H2'	22:a:857:G:C8	2.27	0.69
7:G:113:ASP:HB2	7:G:119:ARG:HG2	1.73	0.69
1:A:946:A:H2'	1:A:947:G:C8	2.28	0.69
48:0:33:LYS:HD3	48:0:51:GLU:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:6:LEU:HD22	45:x:56:LEU:HD12	1.75	0.69
1:A:756:C:HO2'	8:H:2:SER:N	1.90	0.69
30:i:92:MET:HE1	30:i:103:ILE:HD12	1.74	0.69
1:A:311:C:OP1	16:P:31:ARG:NH2	2.25	0.69
1:A:1062:U:H2'	1:A:1063:C:C6	2.27	0.69
5:E:65:GLU:HG3	5:E:68:ARG:HH21	1.57	0.68
5:E:95:PHE:HE2	5:E:97:GLN:NE2	1.89	0.68
22:a:1212:G:O2'	22:a:1236:G:N2	2.24	0.68
3:C:54:ARG:HB3	3:C:69:HIS:HB2	1.74	0.68
12:L:87:VAL:HG11	12:L:90:LEU:HD12	1.75	0.68
2:B:100:MET:HA	2:B:107:VAL:HG21	1.76	0.68
36:o:5:ILE:O	36:o:9:GLU:HG3	1.94	0.68
14:N:49:GLN:NE2	19:S:13:LEU:H	1.84	0.68
22:a:1800:C:OP2	24:c:182:ARG:NH1	2.26	0.68
2:B:18:HIS:ND1	2:B:188:ASP:OD2	2.25	0.68
7:G:48:GLU:OE2	7:G:52:GLN:NE2	2.26	0.68
13:M:79:ARG:NE	19:S:65:GLU:OE2	2.26	0.68
22:a:1311:G:H21	22:a:1603:A:H62	1.40	0.68
22:a:1434:A:H2'	22:a:1435:G:C8	2.29	0.68
1:A:544:G:OP1	4:D:56:ARG:NH2	2.25	0.68
4:D:75:TYR:OH	4:D:97:ARG:NH1	2.26	0.68
1:A:299:G:H2'	1:A:300:A:C8	2.29	0.68
3:C:77:ILE:HA	3:C:84:VAL:HG13	1.74	0.68
22:a:1434:A:H2'	22:a:1435:G:H8	1.58	0.68
42:u:2:PHE:HB2	42:u:61:LEU:HD22	1.76	0.68
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.75	0.67
7:G:25:LYS:O	7:G:29:ILE:HG12	1.94	0.67
1:A:490:C:H2'	1:A:491:G:H8	1.59	0.67
22:a:1405:U:H2'	22:a:1406:U:C6	2.29	0.67
33:l:75:GLU:HB2	33:l:90:GLU:HG3	1.76	0.67
38:q:11:GLN:HE21	38:q:39:LEU:HG	1.58	0.67
1:A:1314:C:OP2	19:S:4:SER:OG	2.11	0.67
9:I:112:GLU:OE2	9:I:115:LYS:NZ	2.27	0.67
3:C:175:LEU:HD23	3:C:182:ILE:HD13	1.77	0.67
2:B:217:VAL:O	2:B:221:VAL:HG22	1.95	0.67
1:A:1073:U:O2	2:B:103:ASN:ND2	2.26	0.67
14:N:41:ARG:NH1	19:S:6:LYS:O	2.28	0.67
26:e:23:PHE:HB2	26:e:114:ARG:HH12	1.60	0.67
42:u:20:LEU:HD11	42:u:41:GLU:HG2	1.76	0.67
1:A:76:G:O6	1:A:93:U:O4	2.14	0.66
2:B:70:VAL:HG12	2:B:92:VAL:HB	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.10	0.66
37:p:109:LEU:HD11	38:q:40:MET:HE1	1.77	0.66
22:a:2204:G:OP2	24:c:147:LYS:NZ	2.28	0.66
1:A:202:G:H21	1:A:466:A:H61	1.42	0.66
9:I:48:VAL:HG22	9:I:79:ILE:HG21	1.78	0.66
22:a:2102:G:N2	22:a:2187:U:O2	2.28	0.66
33:l:14:LYS:O	33:l:71:LYS:NZ	2.18	0.66
45:x:20:ASN:HA	45:x:23:ARG:HH11	1.61	0.66
1:A:492:C:H2'	1:A:493:A:C8	2.31	0.66
22:a:639:U:H2'	22:a:640:C:C6	2.31	0.66
20:T:55:GLN:HB2	20:T:76:LYS:HE2	1.77	0.66
24:c:142:HIS:ND1	24:c:193:GLY:O	2.20	0.66
20:T:79:LEU:O	20:T:83:ILE:HG13	1.96	0.65
31:j:107:LEU:HB2	31:j:116:ILE:HD11	1.78	0.65
1:A:666:G:H5'	1:A:726:C:H1'	1.78	0.65
15:O:26:GLU:HG3	15:O:81:LEU:HD13	1.78	0.65
27:f:162:SER:N	27:f:165:GLU:OE2	2.29	0.65
22:a:2328:A:H2'	22:a:2329:U:C6	2.31	0.65
1:A:1126:U:H5	10:J:7:ARG:HH12	1.42	0.65
20:T:35:VAL:HG21	20:T:54:MET:HG2	1.78	0.65
31:j:121:GLU:OE2	36:o:65:SER:OG	2.14	0.65
32:k:141:LYS:NZ	32:k:143:GLU:OE2	2.29	0.65
1:A:714:G:H2'	1:A:715:A:C8	2.32	0.65
32:k:91:ASP:OD1	32:k:92:LEU:N	2.28	0.65
18:R:34:THR:OG1	18:R:35:GLU:OE1	2.14	0.65
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.79	0.65
1:A:613:C:OP1	4:D:81:ARG:HD3	1.97	0.64
22:a:881:G:O6	22:a:895:U:O4	2.15	0.64
25:d:184:ARG:NH2	36:o:11:GLU:OE1	2.30	0.64
26:e:41:GLN:HG2	26:e:43:THR:HG23	1.80	0.64
1:A:259:G:OP1	20:T:36:TYR:OH	2.11	0.64
1:A:475:C:H2'	1:A:476:U:H6	1.62	0.64
2:B:218:ALA:O	2:B:222:ARG:HG2	1.98	0.64
38:q:65:ALA:HB3	38:q:95:ASP:HB2	1.80	0.64
1:A:451:A:OP2	16:P:70:ARG:NH2	2.30	0.64
8:H:54:ASP:OD1	8:H:55:THR:N	2.29	0.64
27:f:29:PRO:HB2	27:f:169:LEU:HD22	1.80	0.64
27:f:106:ILE:HD12	52:4:34:LEU:HD21	1.78	0.64
33:l:35:ALA:HB2	33:l:102:LEU:HD11	1.78	0.64
45:x:39:GLN:HG2	45:x:41:HIS:HE1	1.62	0.64
1:A:147:G:H2'	1:A:148:G:C8	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:A:H5'	3:C:4:LYS:HE3	1.81	0.63
2:B:133:GLU:OE2	2:B:137:ARG:NH2	2.31	0.63
6:F:61:LEU:HD11	18:R:24:LYS:HE3	1.79	0.63
35:n:83:LEU:HD11	35:n:114:GLY:HA3	1.80	0.63
1:A:426:U:OP1	4:D:33:LYS:NZ	2.21	0.63
16:P:39:PHE:HD1	16:P:50:THR:HG1	1.46	0.63
18:R:57:ARG:HB3	18:R:61:ARG:HH21	1.63	0.63
40:s:48:GLN:HE22	40:s:54:GLU:HA	1.62	0.63
12:L:68:GLY:O	12:L:99:ARG:NH1	2.32	0.63
1:A:71:A:N1	1:A:99:C:O2'	2.30	0.63
6:F:88:MET:HE2	6:F:90:MET:SD	2.39	0.63
9:I:52:LEU:HD11	9:I:63:LEU:HD11	1.81	0.63
22:a:2537:U:H2'	22:a:2538:C:C6	2.34	0.63
22:a:286:U:H2'	22:a:287:G:H8	1.64	0.63
22:a:807:U:OP2	32:k:41:ARG:NH1	2.31	0.63
13:M:12:HIS:O	13:M:44:LYS:NZ	2.25	0.62
18:R:41:PRO:HG2	18:R:44:ILE:HG12	1.81	0.62
5:E:34:THR:HG22	5:E:52:LYS:HG2	1.80	0.62
41:t:13:VAL:HA	41:t:70:VAL:HG12	1.81	0.62
4:D:55:LEU:O	4:D:59:GLN:HG2	2.00	0.62
9:I:84:THR:HG22	9:I:88:MET:HE1	1.81	0.62
16:P:41:PRO:HG2	16:P:42:ILE:HD12	1.80	0.62
22:a:138:U:O2'	22:a:141:G:O6	2.12	0.62
22:a:2377:A:O2'	35:n:117:PHE:O	2.13	0.62
42:u:48:MET:SD	42:u:51:GLN:NE2	2.72	0.62
1:A:437:U:C2	1:A:495:A:N7	2.67	0.62
1:A:1004:A:H1'	1:A:1036:A:H62	1.64	0.62
22:a:347:A:H2'	22:a:348:A:H8	1.64	0.62
23:b:66:A:H61	23:b:107:G:H2'	1.65	0.62
1:A:1187:G:H5'	9:I:115:LYS:HE2	1.80	0.62
22:a:2327:A:H2'	22:a:2328:A:C8	2.34	0.62
26:e:97:ASN:HB2	26:e:100:MET:HG3	1.81	0.62
9:I:47:VAL:HG13	9:I:80:ARG:HD3	1.80	0.62
1:A:437:U:O2	1:A:495:A:N7	2.33	0.62
22:a:290:U:O2	22:a:350:G:O6	2.17	0.62
1:A:627:G:OP2	16:P:35:ARG:NH2	2.33	0.62
18:R:42:SER:HB2	18:R:52:GLN:HG2	1.80	0.62
41:t:86:ARG:NH2	41:t:100:SER:OG	2.33	0.62
22:a:2:G:H2'	22:a:3:U:C6	2.35	0.61
10:J:36:VAL:HG12	10:J:76:ILE:HG12	1.81	0.61
16:P:18:GLN:OE1	16:P:35:ARG:HD2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:40:ASN:HB3	16:P:43:ALA:HB2	1.81	0.61
1:A:375:U:OP1	16:P:70:ARG:NE	2.33	0.61
7:G:88:PRO:HG3	7:G:149:LYS:HA	1.81	0.61
44:w:39:TRP:NE1	44:w:41:GLU:OE2	2.30	0.61
45:x:5:GLU:O	45:x:9:LYS:NZ	2.32	0.61
7:G:75:VAL:HB	7:G:86:GLN:HB3	1.81	0.61
24:c:120:VAL:HG12	24:c:131:PRO:HG2	1.81	0.61
27:f:158:THR:HG22	27:f:160:ALA:H	1.66	0.61
1:A:201:G:N2	1:A:216:U:O2	2.33	0.61
1:A:464:U:O4	1:A:468:A:N7	2.33	0.61
8:H:48:ASP:OD1	8:H:49:PHE:N	2.33	0.61
33:l:79:ALA:HB3	43:v:5:LYS:NZ	2.15	0.61
1:A:459:A:H2'	1:A:460:A:H8	1.64	0.61
1:A:1031:C:O2'	1:A:1033:G:N2	2.33	0.61
1:A:1344:C:OP1	9:I:124:ARG:HD3	2.01	0.61
3:C:88:ARG:HA	3:C:91:VAL:HG12	1.83	0.61
38:q:35:PHE:HB2	38:q:59:ILE:HB	1.83	0.61
1:A:404:G:OP2	4:D:115:ARG:NH2	2.23	0.61
7:G:150:ALA:HB1	11:K:59:THR:HG21	1.82	0.61
22:a:278:A:N6	22:a:362:A:N7	2.48	0.61
1:A:459:A:H2'	1:A:460:A:C8	2.36	0.61
1:A:653:U:C4	8:H:56:LYS:HG2	2.35	0.61
1:A:1323:G:H2'	1:A:1324:A:C8	2.35	0.61
54:Z:17:C:OP1	54:Z:61:U:O2'	2.16	0.61
22:a:276:U:O2'	22:a:277:G:O5'	2.18	0.61
1:A:575:G:O2'	1:A:821:G:OP2	2.16	0.61
26:e:2:GLU:OE2	26:e:11:ALA:HB1	2.01	0.61
27:f:50:LEU:HD21	27:f:67:ILE:HD12	1.83	0.61
2:B:66:LYS:HD3	2:B:90:PHE:HE2	1.65	0.60
12:L:76:GLU:HG2	12:L:77:HIS:ND1	2.15	0.60
22:a:127:A:H5''	22:a:128:C:C6	2.36	0.60
4:D:125:VAL:HG22	4:D:143:VAL:HG22	1.82	0.60
40:s:48:GLN:NE2	40:s:53:VAL:O	2.33	0.60
8:H:114:ARG:O	8:H:118:GLN:HG2	2.02	0.60
25:d:46:ARG:NH2	25:d:88:GLU:O	2.26	0.60
33:l:47:GLU:OE2	33:l:51:ARG:NE	2.34	0.60
22:a:1141:U:H4'	22:a:1142:A:O4'	2.01	0.60
1:A:1119:C:OP1	9:I:85:ARG:NH1	2.31	0.60
3:C:134:MET:HE1	3:C:166:GLU:OE1	2.00	0.60
29:h:34:GLY:O	29:h:36:ALA:N	2.35	0.60
38:q:34:GLU:OE1	38:q:60:LYS:NZ	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:G:H22	1:A:741:G:H1	1.50	0.60
4:D:57:GLU:OE2	4:D:200:ILE:HG13	2.02	0.60
22:a:2291:U:H2'	22:a:2292:U:C6	2.37	0.60
12:L:110:ARG:HB3	12:L:119:VAL:HG21	1.83	0.60
22:a:1590:A:H2'	22:a:1591:A:H8	1.65	0.60
1:A:350:G:H2'	1:A:351:G:C8	2.37	0.60
1:A:1073:U:O2'	2:B:103:ASN:OD1	2.13	0.60
22:a:357:C:H2'	22:a:358:U:C6	2.37	0.60
42:u:20:LEU:HD21	42:u:41:GLU:HG3	1.83	0.60
18:R:35:GLU:OE1	18:R:35:GLU:N	2.33	0.60
22:a:276:U:O2	22:a:362:A:N6	2.35	0.60
22:a:1397:U:OP2	22:a:1398:C:N4	2.28	0.60
1:A:360:G:H2'	1:A:361:G:C8	2.36	0.60
9:I:97:GLU:HA	9:I:100:LYS:HG2	1.84	0.60
18:R:28:THR:HG22	18:R:32:TYR:HE2	1.67	0.60
22:a:2303:G:O2'	27:f:121:SER:O	2.19	0.60
1:A:653:U:H5'	8:H:56:LYS:NZ	2.16	0.59
4:D:102:VAL:HG13	4:D:114:ALA:HB1	1.84	0.59
22:a:887:U:O2'	22:a:889:C:OP2	2.11	0.59
47:z:28:LEU:HD12	47:z:37:LYS:HD3	1.84	0.59
6:F:37:HIS:HB3	6:F:97:THR:HG22	1.84	0.59
7:G:38:THR:O	7:G:42:ILE:HG13	2.03	0.59
25:d:108:ASP:OD1	25:d:173:GLN:HA	2.02	0.59
41:t:54:GLN:HG2	41:t:55:PRO:HD3	1.82	0.59
1:A:662:U:OP1	6:F:93:LYS:NZ	2.33	0.59
22:a:2481:G:HO2'	22:a:2482:A:H8	1.50	0.59
41:t:33:LYS:HB3	41:t:64:ALA:HB1	1.83	0.59
41:t:66:GLN:HB2	41:t:69:ASN:OD1	2.02	0.59
1:A:376:G:O3'	16:P:5:ARG:NH1	2.36	0.59
6:F:43:GLY:HA2	6:F:58:HIS:CE1	2.37	0.59
55:V:23:A:H2'	55:V:24:G:C8	2.37	0.59
3:C:116:VAL:HG21	3:C:200:VAL:HG11	1.85	0.59
27:f:16:LEU:HD13	27:f:29:PRO:HD2	1.84	0.59
22:a:299:A:N1	22:a:322:A:O2'	2.32	0.59
22:a:568:U:O4	38:q:81:LYS:NZ	2.35	0.59
40:s:39:THR:O	40:s:43:ILE:HD12	2.02	0.59
55:V:75:C:H2'	55:V:76:A:C8	2.38	0.59
1:A:1098:C:O2'	21:U:71:TYR:O	2.17	0.59
1:A:1363:A:O2'	1:A:1365:G:N7	2.29	0.59
23:b:5:U:OP1	23:b:61:G:O2'	2.18	0.59
1:A:490:C:H2'	1:A:491:G:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:A:H5''	20:T:29:ARG:HH12	1.68	0.59
7:G:37:SER:HA	9:I:41:ARG:HH12	1.67	0.59
22:a:224:U:OP2	22:a:408:G:N2	2.29	0.59
24:c:133:ARG:NH1	24:c:187:ASP:OD1	2.30	0.59
1:A:78:A:H2'	1:A:79:G:C8	2.37	0.59
1:A:553:A:H5''	12:L:21:VAL:HG21	1.84	0.59
1:A:1516:2MG:N1	1:A:1519:MA6:OP2	2.34	0.59
13:M:39:ILE:HD12	13:M:56:LEU:HD11	1.85	0.59
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.84	0.59
1:A:1030:U:H5'	1:A:1031:C:H5''	1.82	0.59
40:s:5:GLU:N	40:s:5:GLU:OE1	2.36	0.59
1:A:411:A:OP1	4:D:26:ARG:NH1	2.36	0.58
2:B:45:LYS:HE3	2:B:49:MET:HE3	1.85	0.58
20:T:45:ALA:HB1	20:T:49:LYS:NZ	2.18	0.58
22:a:1570:A:H2'	22:a:1571:A:C8	2.38	0.58
22:a:2547:A:H2'	22:a:2548:U:C6	2.38	0.58
26:e:154:ASP:OD2	26:e:157:LEU:N	2.34	0.58
30:i:16:TYR:HB2	30:i:54:ILE:HD13	1.86	0.58
1:A:1533:C:H4'	1:A:1534:A:C8	2.38	0.58
1:A:1031:C:O3'	1:A:1032:G:N2	2.36	0.58
22:a:340:A:O2'	26:e:162:ARG:NH1	2.36	0.58
22:a:2845:U:H5''	36:o:52:ASN:O	2.03	0.58
35:n:99:TYR:OH	35:n:111:ARG:NH1	2.37	0.58
1:A:78:A:H2'	1:A:79:G:H8	1.68	0.58
1:A:193:C:H2'	1:A:194:C:C6	2.39	0.58
15:O:64:ARG:NH2	15:O:68:ASP:OD1	2.34	0.58
22:a:997:G:OP2	37:p:58:ARG:NH1	2.37	0.58
22:a:1223:G:N2	22:a:1226:A:OP2	2.32	0.58
41:t:94:ARG:HE	41:t:103:ILE:HD13	1.69	0.58
48:O:14:SER:OG	48:O:50:LYS:NZ	2.36	0.58
1:A:1530:G:H2'	1:A:1531:A:C8	2.39	0.58
4:D:69:GLU:OE2	4:D:204:TYR:OH	2.22	0.58
22:a:1567:G:OP2	24:c:83:TYR:OH	2.18	0.58
41:t:97:LYS:O	41:t:98:SER:OG	2.20	0.58
5:E:77:ASN:HB2	5:E:82:GLN:NE2	2.19	0.57
22:a:78:U:OP1	45:x:7:ARG:NH2	2.37	0.57
22:a:995:C:O2	30:i:3:THR:OG1	2.22	0.57
30:i:32:LEU:HD22	30:i:54:ILE:HG21	1.85	0.57
22:a:703:U:H2'	22:a:704:G:O4'	2.05	0.57
14:N:49:GLN:OE1	19:S:12:ASP:HA	2.05	0.57
40:s:11:LEU:O	40:s:12:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:C:H4'	20:T:56:PRO:HG3	1.85	0.57
1:A:429:U:H3'	4:D:9:LEU:HD12	1.85	0.57
22:a:103:A:H8	22:a:103:A:OP1	1.88	0.57
22:a:276:U:O2'	22:a:278:A:N7	2.37	0.57
33:l:79:ALA:HB3	43:v:5:LYS:HZ2	1.70	0.57
6:F:12:PRO:HB2	6:F:44:ARG:HH12	1.70	0.57
14:N:28:LYS:HA	14:N:31:ILE:HD12	1.86	0.57
33:l:10:ARG:HG3	33:l:11:LYS:HG3	1.87	0.57
33:l:22:GLN:O	33:l:100:LYS:NZ	2.35	0.57
1:A:458:U:O2	1:A:474:G:O6	2.22	0.57
1:A:464:U:O2'	1:A:465:A:O5'	2.21	0.57
2:B:23:TRP:CZ3	2:B:25:PRO:HA	2.40	0.57
4:D:98:LEU:HB2	4:D:135:TYR:HB3	1.87	0.57
9:I:51:PRO:O	9:I:55:VAL:HG22	2.05	0.57
30:i:9:GLU:HG3	30:i:10:THR:HG23	1.86	0.57
2:B:85:LEU:C	2:B:87:CYS:H	2.13	0.57
22:a:1746:A:H2'	22:a:1747:U:C6	2.39	0.57
1:A:544:G:P	4:D:56:ARG:HH22	2.26	0.57
9:I:21:ILE:HD11	9:I:90:TYR:HB2	1.87	0.57
1:A:613:C:H2'	1:A:614:C:C6	2.40	0.57
1:A:908:A:H2'	1:A:909:A:C8	2.40	0.57
1:A:1119:C:H2'	1:A:1120:C:H6	1.70	0.57
10:J:28:THR:HG21	10:J:90:LEU:HD22	1.86	0.57
20:T:32:ILE:HD13	20:T:75:HIS:CE1	2.40	0.57
22:a:641:U:O2'	22:a:2350:C:OP1	2.22	0.57
22:a:2834:G:H2'	22:a:2879:A:H61	1.69	0.57
1:A:1391:U:H2'	1:A:1392:G:C8	2.40	0.56
24:c:145:GLU:HB2	24:c:188:CYS:HB3	1.87	0.56
41:t:41:LEU:HD23	41:t:62:GLU:HB3	1.86	0.56
1:A:683:G:N2	11:K:39:GLY:O	2.37	0.56
1:A:720:C:H5''	18:R:41:PRO:HA	1.87	0.56
28:g:94:TYR:CD1	28:g:107:LEU:HA	2.39	0.56
1:A:475:C:H2'	1:A:476:U:C6	2.41	0.56
1:A:477:C:H2'	1:A:478:A:C8	2.40	0.56
1:A:1360:A:OP2	14:N:75:ARG:NH2	2.36	0.56
13:M:66:GLU:HB3	13:M:70:ARG:NH1	2.21	0.56
22:a:1011:G:OP1	37:p:75:SER:OG	2.16	0.56
22:a:1534:U:O3'	22:a:1535:A:H2'	2.04	0.56
35:n:4:LYS:O	35:n:8:ILE:HG12	2.06	0.56
40:s:4:GLU:OE2	40:s:49:LYS:HE2	2.06	0.56
5:E:85:VAL:HG23	5:E:96:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:6:ILE:HG12	6:F:89:VAL:HG22	1.86	0.56
22:a:361:G:H8	22:a:361:G:OP2	1.89	0.56
46:y:4:THR:HB	46:y:37:GLU:OE1	2.04	0.56
1:A:542:G:OP1	4:D:10:LYS:NZ	2.39	0.56
9:I:12:ARG:HG3	9:I:13:LYS:H	1.70	0.56
13:M:88:GLY:O	13:M:92:ARG:HG3	2.06	0.56
22:a:1311:G:N2	22:a:1603:A:H62	2.03	0.56
22:a:2071:A:H2'	22:a:2072:C:C6	2.40	0.56
22:a:2100:G:H1	22:a:2189:U:H3	1.52	0.56
24:c:232:HIS:HA	24:c:242:LYS:HE3	1.86	0.56
1:A:1193:G:O6	3:C:2:GLY:N	2.38	0.56
18:R:26:ILE:HD11	18:R:67:LEU:HD23	1.87	0.56
22:a:2273:A:H2'	22:a:2274:A:C8	2.40	0.56
1:A:34:C:H2'	1:A:35:G:C8	2.40	0.56
1:A:1412:C:H2'	1:A:1413:A:C8	2.41	0.56
14:N:27:LEU:CD2	14:N:48:LEU:HB2	2.35	0.56
22:a:2:G:H2'	22:a:3:U:H6	1.68	0.56
22:a:549:G:H2'	22:a:550:C:C6	2.41	0.56
32:k:77:ILE:HD11	32:k:108:ALA:HB1	1.88	0.56
1:A:754:C:OP1	15:O:72:ARG:NH2	2.39	0.56
6:F:1:MET:N	6:F:65:GLU:OE2	2.24	0.56
20:T:17:ALA:O	20:T:21:ASN:HB2	2.05	0.56
22:a:544:C:H2'	22:a:545:U:O4'	2.05	0.56
22:a:1475:G:O2'	22:a:1514:G:O6	2.23	0.56
22:a:2898:U:H2'	22:a:2899:A:C8	2.41	0.56
26:e:168:ASP:CG	26:e:170:ARG:HH22	2.14	0.56
42:u:4:ILE:HB	42:u:63:ILE:HG13	1.88	0.56
1:A:653:U:H5'	8:H:56:LYS:HZ3	1.71	0.56
22:a:549:G:H2'	22:a:550:C:H6	1.71	0.56
23:b:52:A:N7	35:n:64:TYR:OH	2.27	0.56
31:j:71:ARG:NH2	31:j:123:LEU:O	2.39	0.56
33:l:42:THR:HG22	33:l:93:VAL:HG12	1.88	0.56
39:r:73:LYS:HB2	39:r:106:VAL:HB	1.87	0.56
47:z:54:VAL:HG23	47:z:55:ILE:HG12	1.86	0.56
4:D:15:GLU:HG2	4:D:60:LYS:HB3	1.88	0.56
22:a:577:G:O2'	22:a:1254:A:OP1	2.24	0.56
36:o:2:SER:O	36:o:6:LYS:HG3	2.05	0.56
1:A:666:G:O4'	1:A:726:C:O2'	2.22	0.55
22:a:172:A:H2'	22:a:173:A:C8	2.41	0.55
22:a:550:C:H2'	22:a:551:G:H8	1.70	0.55
22:a:2394:C:H5''	32:k:63:LYS:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:77:VAL:HG12	42:u:89:ILE:HG12	1.88	0.55
43:v:59:LEU:HD12	43:v:80:ILE:HD12	1.87	0.55
1:A:993:G:O2'	1:A:994:A:N7	2.40	0.55
1:A:1010:U:H2'	1:A:1011:C:C6	2.41	0.55
20:T:27:MET:HE1	20:T:61:GLN:HE21	1.72	0.55
22:a:2097:A:H2'	22:a:2098:U:C6	2.41	0.55
22:a:2657:A:O3'	28:g:160:LYS:NZ	2.38	0.55
26:e:111:GLU:OE2	26:e:115:GLN:NE2	2.35	0.55
30:i:18:VAL:HG21	30:i:142:ILE:HD12	1.88	0.55
1:A:836:G:O6	1:A:850:U:O4	2.23	0.55
22:a:17:G:H2'	22:a:18:U:C6	2.41	0.55
39:r:18:ARG:HG3	39:r:76:VAL:HB	1.88	0.55
1:A:1035:A:C8	1:A:1036:A:H2	2.25	0.55
22:a:1357:C:H2'	22:a:1358:G:O4'	2.07	0.55
22:a:2661:G:H2'	22:a:2662:A:C8	2.41	0.55
34:m:69:ARG:O	34:m:70:THR:OG1	2.21	0.55
42:u:46:LYS:O	42:u:50:MET:HG3	2.06	0.55
22:a:500:G:N1	22:a:503:A:OP2	2.39	0.55
47:z:33:THR:HG22	47:z:51:GLY:HA2	1.89	0.55
1:A:464:U:H3	1:A:468:A:H62	1.54	0.55
5:E:16:ILE:HD11	5:E:38:VAL:HG13	1.89	0.55
17:Q:60:GLU:OE1	17:Q:76:VAL:HB	2.06	0.55
52:4:16:CYS:SG	52:4:17:SER:N	2.80	0.55
1:A:35:G:O2'	12:L:115:SER:O	2.18	0.55
1:A:1004:A:H1'	1:A:1036:A:N6	2.22	0.55
22:a:2646:C:OP2	22:a:2732:G:O2'	2.25	0.55
27:f:13:VAL:O	27:f:17:MET:HG2	2.05	0.55
54:Z:9:G:H21	54:Z:46:G:H3'	1.72	0.55
54:Z:20:G:H4'	54:Z:21:H2U:OP2	2.07	0.55
1:A:745:G:H2'	1:A:746:A:C8	2.41	0.55
26:e:141:MET:HE3	26:e:143:LEU:HD12	1.88	0.55
15:O:75:VAL:O	15:O:79:THR:HG23	2.07	0.55
16:P:59:HIS:O	16:P:63:GLN:HG3	2.06	0.55
17:Q:47:HIS:HB2	17:Q:71:LYS:HD3	1.88	0.55
22:a:347:A:H2'	22:a:348:A:C8	2.40	0.55
22:a:1242:U:H2'	22:a:1243:C:C6	2.42	0.55
25:d:46:ARG:NH1	25:d:85:ALA:O	2.39	0.55
33:l:41:LEU:HG	33:l:96:ILE:HG13	1.87	0.55
36:o:2:SER:OG	36:o:3:ASN:N	2.40	0.55
1:A:592:G:H2'	1:A:593:U:H6	1.72	0.55
14:N:27:LEU:HD21	14:N:44:ALA:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2021:C:OP1	37:p:25:TYR:OH	2.25	0.55
40:s:64:LYS:HA	40:s:79:ASP:OD1	2.07	0.55
3:C:12:LEU:HA	3:C:16:LYS:HB2	1.90	0.54
5:E:49:GLY:HA2	5:E:66:LYS:HZ2	1.72	0.54
5:E:65:GLU:HG3	5:E:68:ARG:NH2	2.23	0.54
10:J:10:LEU:O	10:J:71:LEU:HA	2.07	0.54
22:a:2102:G:O6	22:a:2187:U:O4	2.24	0.54
22:a:2419:U:H4'	48:0:22:THR:HG21	1.88	0.54
24:c:155:ALA:HB2	24:c:162:VAL:HG23	1.89	0.54
26:e:88:ARG:HH21	26:e:88:ARG:HG3	1.71	0.54
36:o:27:GLU:OE2	36:o:44:GLU:HG2	2.06	0.54
2:B:8:ASP:OD1	2:B:9:MET:N	2.39	0.54
3:C:50:ALA:HA	3:C:75:ILE:HD11	1.89	0.54
22:a:2305:U:H5''	27:f:131:GLY:HA3	1.88	0.54
24:c:180:GLU:HB2	24:c:269:ARG:O	2.07	0.54
1:A:573:A:N3	1:A:883:C:O2'	2.39	0.54
1:A:662:U:H2'	1:A:663:A:C8	2.42	0.54
4:D:8:LYS:HD3	4:D:21:LEU:HD21	1.89	0.54
14:N:27:LEU:HD11	14:N:47:LYS:HB2	1.89	0.54
22:a:322:A:OP2	26:e:163:ASN:HB2	2.07	0.54
22:a:995:C:N4	30:i:2:LYS:HD2	2.22	0.54
22:a:1548:A:H2'	22:a:1549:A:C8	2.42	0.54
1:A:1397:C:OP2	5:E:29:ARG:NH2	2.40	0.54
17:Q:81:LYS:NZ	17:Q:82:ALA:O	2.41	0.54
30:i:97:PRO:O	30:i:100:VAL:HG22	2.08	0.54
39:r:48:LYS:O	39:r:52:GLU:OE1	2.26	0.54
39:r:86:MET:HE2	39:r:96:ILE:HD11	1.89	0.54
3:C:91:VAL:HA	3:C:94:ILE:HG22	1.89	0.54
4:D:177:LYS:HE2	4:D:179:GLU:HG2	1.88	0.54
13:M:83:LEU:HD11	19:S:66:MET:CG	2.37	0.54
22:a:548:G:H2'	22:a:549:G:O4'	2.08	0.54
22:a:848:C:H2'	22:a:849:A:H8	1.72	0.54
54:Z:48:U:H5''	54:Z:49:C:H5'	1.88	0.54
1:A:407:U:O2'	4:D:113:GLU:OE2	2.21	0.54
8:H:114:ARG:CZ	8:H:117:ARG:HH21	2.21	0.54
22:a:156:A:H2'	22:a:157:C:O4'	2.08	0.54
22:a:796:C:OP1	26:e:57:LYS:NZ	2.31	0.54
22:a:2255:G:H21	43:v:9:SER:HB3	1.72	0.54
1:A:202:G:N2	1:A:466:A:H61	2.04	0.54
3:C:130:PHE:O	3:C:134:MET:HG3	2.07	0.54
6:F:22:ILE:HG23	6:F:39:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:m:24:MET:HE1	34:m:40:LYS:HD3	1.89	0.54
1:A:1035:A:H4'	1:A:1036:A:OP1	2.07	0.54
9:I:88:MET:HG3	9:I:95:ARG:HG2	1.88	0.54
22:a:191:A:H2'	22:a:192:C:C6	2.43	0.54
22:a:1210:G:H4'	22:a:1211:C:H5''	1.90	0.54
33:l:63:ILE:HG12	33:l:105:MET:HG3	1.89	0.54
39:r:52:GLU:HA	39:r:55:ILE:HD12	1.89	0.54
40:s:44:LYS:O	40:s:48:GLN:HG2	2.08	0.54
6:F:3:HIS:ND1	6:F:65:GLU:HG2	2.23	0.54
18:R:70:TYR:HB2	18:R:74:HIS:CE1	2.43	0.54
33:l:20:LEU:HD13	42:u:81:PRO:HG3	1.90	0.54
34:m:106:ASP:OD1	34:m:106:ASP:N	2.41	0.54
1:A:1149:C:H2'	1:A:1150:A:C8	2.42	0.54
1:A:1530:G:H2'	1:A:1531:A:H8	1.73	0.54
3:C:110:GLU:HB2	3:C:144:LEU:HD12	1.90	0.54
16:P:6:LEU:HD22	16:P:17:TYR:HB3	1.90	0.54
28:g:105:LEU:HB2	28:g:113:VAL:HG13	1.90	0.54
5:E:149:SER:H	5:E:152:MET:HE2	1.73	0.53
22:a:182:A:H2'	22:a:183:C:H6	1.72	0.53
22:a:2101:A:H2'	22:a:2102:G:C8	2.43	0.53
1:A:41:G:H2'	1:A:42:G:H8	1.73	0.53
1:A:269:C:H2'	1:A:270:A:C8	2.43	0.53
7:G:37:SER:OG	9:I:41:ARG:NH1	2.41	0.53
20:T:21:ASN:OD1	20:T:66:LEU:HD13	2.08	0.53
28:g:112:PRO:HD2	28:g:112:PRO:O	2.07	0.53
1:A:592:G:H2'	1:A:593:U:C6	2.42	0.53
6:F:4:TYR:CD2	6:F:71:ILE:HG13	2.43	0.53
22:a:639:U:H2'	22:a:640:C:H6	1.71	0.53
22:a:1469:A:H2'	22:a:1470:A:C8	2.43	0.53
45:x:39:GLN:HG2	45:x:41:HIS:CE1	2.43	0.53
1:A:201:G:H1	1:A:216:U:H3	1.56	0.53
2:B:69:PHE:O	2:B:91:PHE:HA	2.08	0.53
2:B:188:ASP:CG	2:B:189:THR:H	2.17	0.53
3:C:153:VAL:HG22	3:C:198:VAL:HG22	1.89	0.53
15:O:7:ALA:O	15:O:11:ILE:HG12	2.08	0.53
19:S:16:LEU:O	19:S:19:VAL:HG12	2.09	0.53
22:a:279:A:N6	22:a:361:G:H1'	2.23	0.53
23:b:48:U:H2'	23:b:49:C:C6	2.44	0.53
22:a:183:C:H42	22:a:213:A:H61	1.55	0.53
50:2:62:LEU:HD22	50:2:65:ALA:HB2	1.90	0.53
5:E:81:LEU:HD11	5:E:96:MET:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:881:G:N2	22:a:895:U:O2	2.27	0.53
22:a:1494:A:H2'	22:a:1495:A:C8	2.44	0.53
23:b:66:A:N6	23:b:107:G:H2'	2.23	0.53
40:s:54:GLU:OE2	40:s:91:GLN:NE2	2.39	0.53
1:A:686:U:O2'	1:A:687:A:OP2	2.24	0.53
1:A:1436:U:H2'	1:A:1437:A:C8	2.43	0.53
11:K:37:ARG:HG3	11:K:37:ARG:HH21	1.74	0.53
22:a:83:A:N6	22:a:101:A:O2'	2.35	0.53
22:a:612:G:H21	22:a:616:A:H62	1.57	0.53
1:A:1510:C:H2'	1:A:1511:G:C8	2.44	0.53
13:M:53:ILE:O	13:M:57:ARG:HG3	2.09	0.53
15:O:64:ARG:HH12	15:O:89:ARG:C	2.17	0.53
22:a:1720:U:H2'	22:a:1721:G:O4'	2.08	0.53
22:a:1870:C:O2'	22:a:1871:A:H8	1.92	0.53
27:f:106:ILE:HD11	52:4:22:MET:SD	2.49	0.53
1:A:157:U:O2	1:A:164:G:O6	2.27	0.53
1:A:410:G:H2'	1:A:429:U:C5	2.44	0.53
3:C:50:ALA:O	3:C:70:THR:OG1	2.26	0.53
9:I:36:GLU:HA	9:I:45:ARG:HE	1.74	0.53
14:N:46:LEU:HD12	19:S:13:LEU:HB2	1.91	0.53
22:a:391:A:O2'	22:a:410:G:OP1	2.25	0.53
22:a:1019:U:H2'	22:a:1020:A:C8	2.44	0.53
22:a:1419:A:O2'	22:a:1421:G:N7	2.31	0.53
23:b:79:G:N7	42:u:14:LYS:NZ	2.56	0.53
39:r:83:LYS:HD3	39:r:95:ARG:NH1	2.24	0.53
41:t:85:PHE:CE1	41:t:94:ARG:HG2	2.43	0.53
1:A:176:C:H2'	1:A:177:G:N3	2.23	0.53
22:a:126:A:OP1	49:1:45:SER:OG	2.25	0.53
22:a:2193:G:H2'	22:a:2194:U:C6	2.43	0.53
22:a:2848:G:O2'	22:a:2867:G:N2	2.30	0.53
1:A:49:U:O2'	1:A:50:A:H2'	2.09	0.52
1:A:377:G:H5''	16:P:24:SER:OG	2.09	0.52
22:a:2830:C:H5''	25:d:56:LYS:HE3	1.90	0.52
1:A:159:G:N2	1:A:162:A:OP2	2.32	0.52
22:a:419:U:H2'	22:a:420:C:C6	2.44	0.52
41:t:8:ASP:O	41:t:24:LYS:NZ	2.42	0.52
45:x:32:ALA:HB2	45:x:37:LEU:HD23	1.92	0.52
1:A:713:G:H2'	1:A:714:G:C8	2.43	0.52
16:P:15:PRO:HD2	16:P:42:ILE:CD1	2.39	0.52
22:a:181:A:H1'	22:a:435:C:H5'	1.91	0.52
22:a:849:A:H2'	22:a:850:U:C6	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1047:G:HO2'	22:a:1110:G:H1	1.54	0.52
22:a:1572:A:H2'	22:a:1573:G:C8	2.43	0.52
28:g:60:ASP:N	28:g:60:ASP:OD1	2.42	0.52
1:A:35:G:H2'	1:A:36:C:C6	2.43	0.52
1:A:64:G:H2'	1:A:99:C:H41	1.74	0.52
1:A:1013:G:N2	1:A:1016:A:OP2	2.30	0.52
10:J:27:GLU:HB3	10:J:31:ARG:HH21	1.74	0.52
11:K:97:ILE:HG22	21:U:12:PHE:HZ	1.74	0.52
14:N:29:ALA:O	14:N:33:ASP:HB2	2.10	0.52
33:l:110:GLU:O	33:l:114:ARG:HG3	2.08	0.52
35:n:53:THR:O	35:n:59:ALA:HB2	2.09	0.52
1:A:192:A:H2'	1:A:193:C:C6	2.45	0.52
22:a:1012:U:OP2	37:p:70:ARG:NH2	2.30	0.52
41:t:7:ARG:NH2	41:t:26:LYS:O	2.37	0.52
46:y:3:LYS:HE2	46:y:40:ASP:OD2	2.09	0.52
22:a:1199:U:H1'	37:p:4:VAL:HG22	1.89	0.52
22:a:2481:G:O2'	22:a:2482:A:H8	1.93	0.52
27:f:160:ALA:HB1	27:f:165:GLU:HG2	1.92	0.52
1:A:312:C:H2'	1:A:313:A:C8	2.45	0.52
1:A:750:C:O2'	15:O:21:ASP:OD1	2.24	0.52
22:a:851:C:H2'	22:a:852:U:C6	2.45	0.52
22:a:2790:U:H5'	22:a:2893:A:H62	1.75	0.52
23:b:28:C:OP1	35:n:36:TYR:OH	2.25	0.52
27:f:44:ILE:HG21	27:f:79:ILE:HG22	1.91	0.52
38:q:29:THR:HG22	38:q:29:THR:O	2.09	0.52
46:y:44:ILE:HA	46:y:47:MET:HE3	1.91	0.52
1:A:821:G:H2'	1:A:822:U:C6	2.45	0.52
22:a:1198:U:H2'	22:a:1199:U:C6	2.45	0.52
22:a:1799:G:OP1	24:c:258:ARG:NH1	2.35	0.52
29:h:6:LEU:HD11	29:h:37:VAL:HG13	1.90	0.52
39:r:83:LYS:HD3	39:r:95:ARG:HH11	1.75	0.52
1:A:195:A:H1'	1:A:222:C:O2'	2.09	0.52
1:A:546:A:OP1	4:D:69:GLU:N	2.42	0.52
1:A:755:G:OP2	15:O:65:LYS:HD3	2.10	0.52
3:C:19:ASN:O	3:C:40:ARG:NH2	2.43	0.52
10:J:42:LEU:HD11	10:J:73:LEU:HD12	1.91	0.52
22:a:718:A:H2'	22:a:719:C:O4'	2.10	0.52
22:a:848:C:H2'	22:a:849:A:C8	2.45	0.52
22:a:1027:A:C2	22:a:2488:G:H5'	2.45	0.52
26:e:149:ILE:HG23	26:e:171:ASP:O	2.09	0.52
35:n:114:GLY:O	35:n:116:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:t:48:PRO:HG3	41:t:56:GLY:H	1.75	0.52
1:A:537:G:H2'	1:A:538:G:C8	2.45	0.52
22:a:354:A:H2'	22:a:355:U:O4'	2.10	0.52
22:a:593:U:H2'	22:a:594:U:C6	2.44	0.52
22:a:920:A:OP1	46:y:19:LYS:NZ	2.43	0.52
22:a:2740:A:H2'	22:a:2741:A:C8	2.45	0.52
27:f:94:GLU:O	27:f:98:GLU:HG3	2.10	0.52
30:i:11:VAL:HG21	30:i:50:THR:HA	1.92	0.52
1:A:461:A:H2'	1:A:462:G:H8	1.74	0.51
1:A:539:A:H2'	1:A:540:G:C8	2.45	0.51
1:A:1180:A:OP1	9:I:105:THR:OG1	2.22	0.51
6:F:45:ARG:HD3	6:F:59:TYR:CE1	2.45	0.51
22:a:48:G:O2'	22:a:118:A:N1	2.40	0.51
22:a:48:G:H22	22:a:177:G:H2'	1.74	0.51
22:a:610:C:H2'	22:a:611:C:H6	1.75	0.51
22:a:1572:A:H2'	22:a:1573:G:H8	1.74	0.51
22:a:2430:A:N3	22:a:2430:A:H2'	2.25	0.51
1:A:224:U:H2'	1:A:225:C:C6	2.45	0.51
1:A:1121:U:H2'	1:A:1122:U:C6	2.45	0.51
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.91	0.51
52:4:14:ALA:HB1	52:4:34:LEU:HD11	1.92	0.51
1:A:56:U:H2'	1:A:57:G:C8	2.45	0.51
1:A:57:G:H2'	1:A:58:C:C6	2.46	0.51
33:l:33:LEU:HD13	33:l:117:PHE:HB3	1.92	0.51
1:A:857:C:H2'	1:A:858:G:O4'	2.10	0.51
1:A:1010:U:H2'	1:A:1011:C:H6	1.74	0.51
13:M:23:TYR:HB3	13:M:66:GLU:HG3	1.93	0.51
22:a:2636:C:H2'	22:a:2637:U:C6	2.46	0.51
31:j:43:ILE:HD12	31:j:56:ASP:HB2	1.93	0.51
39:r:3:THR:OG1	39:r:62:ASP:OD2	2.27	0.51
39:r:82:MET:HB2	39:r:98:LYS:HB2	1.93	0.51
1:A:377:G:H5'	16:P:5:ARG:HH12	1.75	0.51
1:A:410:G:N1	1:A:431:A:OP2	2.26	0.51
11:K:67:ALA:HB2	11:K:96:THR:HG23	1.92	0.51
27:f:164:GLU:HG2	27:f:165:GLU:N	2.25	0.51
28:g:127:THR:HG22	28:g:128:GLN:H	1.74	0.51
40:s:47:VAL:HG13	40:s:51:PHE:HD2	1.76	0.51
1:A:1326:U:H2'	1:A:1327:C:H6	1.76	0.51
5:E:50:TYR:H	5:E:66:LYS:CE	2.24	0.51
22:a:340:A:HO2'	26:e:162:ARG:HH12	1.58	0.51
22:a:849:A:H2'	22:a:850:U:H6	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2591:C:H2'	22:a:2592:G:C8	2.46	0.51
10:J:32:THR:HG21	10:J:83:THR:HG23	1.93	0.51
15:O:57:LEU:HD21	22:a:715:A:N6	2.25	0.51
25:d:39:ASP:OD1	25:d:39:ASP:N	2.43	0.51
55:V:4:U:O2'	55:V:5:G:H8	1.94	0.51
1:A:413:G:O2'	1:A:428:G:N2	2.43	0.51
1:A:1034:G:O2'	1:A:1035:A:O5'	2.29	0.51
3:C:167:TRP:HZ3	3:C:169:ARG:HB2	1.76	0.51
22:a:1579:A:H2'	22:a:1580:A:C8	2.46	0.51
22:a:2636:C:H2'	22:a:2637:U:H6	1.75	0.51
24:c:87:ARG:HG3	24:c:89:ALA:H	1.76	0.51
33:l:136:MET:HE1	42:u:75:GLN:O	2.11	0.51
1:A:1124:G:H1'	1:A:1125:U:H5	1.76	0.51
1:A:1368:A:OP2	9:I:114:LYS:NZ	2.40	0.51
15:O:56:LEU:HA	15:O:59:MET:HE2	1.93	0.51
16:P:4:ILE:O	16:P:71:VAL:HG21	2.11	0.51
22:a:627:A:N1	22:a:636:G:O2'	2.36	0.51
22:a:1923:U:OP1	54:Z:25:U:O2'	2.26	0.51
27:f:38:MET:HG3	27:f:57:LEU:HD22	1.93	0.51
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.92	0.50
6:F:41:ASP:CG	6:F:58:HIS:HE2	2.15	0.50
28:g:11:VAL:HG13	28:g:15:VAL:HG23	1.93	0.50
31:j:69:VAL:HG21	31:j:104:THR:HG21	1.92	0.50
3:C:116:VAL:HG23	3:C:200:VAL:HG21	1.94	0.50
6:F:38:ARG:HG3	6:F:97:THR:HA	1.93	0.50
20:T:35:VAL:HG22	20:T:50:ALA:HB1	1.93	0.50
22:a:2478:A:H5'	51:3:32:LYS:HD3	1.93	0.50
22:a:2883:A:H5''	22:a:2884:U:H5'	1.93	0.50
1:A:34:C:H2'	1:A:35:G:H8	1.76	0.50
2:B:87:CYS:SG	2:B:221:VAL:HG21	2.51	0.50
22:a:851:C:H2'	22:a:852:U:H6	1.76	0.50
22:a:917:A:H5''	22:a:2268:A:H61	1.75	0.50
22:a:2052:A:H4'	25:d:148:GLN:O	2.11	0.50
22:a:2099:U:H2'	22:a:2100:G:H8	1.77	0.50
1:A:102:G:H2'	1:A:103:U:H6	1.76	0.50
1:A:1005:A:H8	1:A:1005:A:O5'	1.94	0.50
2:B:27:MET:HE2	2:B:193:PRO:HG3	1.93	0.50
11:K:34:ILE:HD13	11:K:74:VAL:HG21	1.93	0.50
13:M:83:LEU:HD11	19:S:66:MET:HG2	1.92	0.50
22:a:550:C:H2'	22:a:551:G:C8	2.47	0.50
22:a:2522:U:O2'	22:a:2647:U:OP1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2674:G:H4'	31:j:30:ARG:HD2	1.94	0.50
1:A:162:A:O5'	1:A:162:A:H8	1.95	0.50
5:E:144:LEU:O	5:E:147:MET:HG2	2.10	0.50
22:a:839:U:H2'	22:a:840:C:C6	2.47	0.50
22:a:1126:A:OP1	22:a:1126:A:H8	1.95	0.50
22:a:1526:C:H2'	22:a:1527:G:O4'	2.11	0.50
36:o:89:ARG:NH2	36:o:113:ARG:O	2.44	0.50
54:Z:69:C:H2'	54:Z:70:C:C6	2.46	0.50
1:A:1092:A:H5''	7:G:4:ARG:HH12	1.76	0.50
2:B:111:ILE:HD12	2:B:152:LYS:HA	1.92	0.50
9:I:28:ILE:HG12	9:I:63:LEU:HD12	1.94	0.50
10:J:15:HIS:HA	10:J:18:ILE:HG22	1.93	0.50
19:S:63:THR:H	19:S:66:MET:HE3	1.77	0.50
22:a:24:G:O2'	39:r:78:GLU:O	2.29	0.50
22:a:263:G:O2'	22:a:429:A:N3	2.43	0.50
22:a:1509:A:O2'	22:a:1510:G:OP2	2.27	0.50
55:V:44:G:H2'	55:V:45:G:O4'	2.10	0.50
1:A:437:U:H2'	1:A:438:U:C6	2.47	0.50
1:A:1373:G:N7	9:I:13:LYS:NZ	2.59	0.50
14:N:64:CYS:HB3	14:N:69:ARG:H	1.76	0.50
22:a:1980:G:O2'	22:a:1982:U:OP2	2.28	0.50
22:a:2809:A:H2'	22:a:2810:A:C8	2.47	0.50
26:e:170:ARG:HH21	26:e:170:ARG:HG3	1.77	0.50
52:4:45:THR:OG1	52:4:47:LYS:HG2	2.11	0.50
52:4:58:ASP:OD1	52:4:59:ARG:N	2.44	0.50
54:Z:17:C:N4	54:Z:18:U:O4	2.44	0.50
16:P:15:PRO:HD2	16:P:42:ILE:HD11	1.94	0.50
22:a:222:A:N1	22:a:233:A:H5'	2.27	0.50
41:t:94:ARG:HB2	41:t:103:ILE:HD13	1.94	0.50
1:A:1037:C:H2'	1:A:1038:C:C6	2.47	0.50
9:I:55:VAL:HG11	9:I:94:LEU:HD23	1.92	0.50
22:a:207:A:H2'	22:a:208:C:O4'	2.12	0.50
22:a:996:A:OP2	38:q:10:LYS:HG2	2.12	0.50
22:a:1506:U:H2'	22:a:1507:C:C6	2.47	0.50
22:a:1594:U:H2'	22:a:1595:C:C6	2.47	0.50
23:b:29:A:H2'	23:b:30:C:C6	2.46	0.50
27:f:2:ALA:HB2	27:f:94:GLU:OE1	2.12	0.50
42:u:6:ALA:HB3	42:u:65:VAL:HG22	1.94	0.50
42:u:45:ASP:O	42:u:49:ASN:ND2	2.45	0.50
1:A:17:U:H2'	1:A:18:C:C6	2.46	0.49
1:A:95:C:H2'	1:A:96:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:C:H2'	1:A:265:G:O4'	2.11	0.49
1:A:309:A:O2'	1:A:607:A:N1	2.42	0.49
1:A:407:U:H2'	1:A:408:A:C8	2.47	0.49
10:J:5:ARG:HG3	10:J:77:VAL:HG12	1.94	0.49
24:c:132:MET:O	24:c:167:ARG:NH1	2.45	0.49
1:A:109:A:H5'	1:A:110:C:C5	2.47	0.49
1:A:1152:A:OP1	10:J:72:ARG:NH2	2.28	0.49
7:G:77:SER:OG	7:G:86:GLN:OE1	2.23	0.49
9:I:12:ARG:O	9:I:13:LYS:C	2.55	0.49
22:a:914:G:H3'	22:a:915:C:H5''	1.94	0.49
25:d:35:THR:N	25:d:49:GLN:O	2.39	0.49
41:t:74:ASN:HB3	41:t:77:THR:HG22	1.94	0.49
4:D:8:LYS:HB3	4:D:21:LEU:HD22	1.93	0.49
21:U:34:ARG:HG2	21:U:34:ARG:HH11	1.78	0.49
22:a:927:A:H2'	22:a:928:A:C8	2.46	0.49
22:a:998:C:H2'	22:a:999:U:O4'	2.11	0.49
22:a:1000:A:H2'	22:a:1001:A:C8	2.46	0.49
22:a:2469:A:H2'	22:a:2470:G:O4'	2.13	0.49
23:b:39:A:H2'	23:b:40:U:C6	2.47	0.49
24:c:157:SER:O	24:c:160:THR:OG1	2.26	0.49
36:o:7:GLN:O	36:o:11:GLU:HG3	2.13	0.49
38:q:10:LYS:NZ	38:q:23:GLU:OE2	2.45	0.49
48:0:13:SER:HB2	48:0:49:TYR:CZ	2.46	0.49
54:Z:24:C:H2'	54:Z:25:U:C6	2.46	0.49
1:A:636:U:H2'	1:A:637:C:C6	2.47	0.49
7:G:56:LYS:HG3	7:G:57:SER:H	1.76	0.49
8:H:41:LYS:HD2	8:H:48:ASP:HA	1.94	0.49
8:H:64:LYS:HG3	8:H:71:VAL:HG21	1.94	0.49
26:e:111:GLU:O	26:e:115:GLN:HG3	2.12	0.49
1:A:38:G:H4'	1:A:547:A:N6	2.27	0.49
1:A:522:C:OP2	12:L:66:TYR:OH	2.24	0.49
1:A:601:G:H2'	1:A:602:A:C8	2.48	0.49
20:T:51:PHE:HA	20:T:54:MET:HG3	1.94	0.49
22:a:1177:G:H2'	22:a:1178:C:C6	2.48	0.49
40:s:64:LYS:N	40:s:64:LYS:HD2	2.28	0.49
1:A:1115:U:O2'	14:N:101:TRP:O	2.24	0.49
9:I:48:VAL:HG22	9:I:79:ILE:CG2	2.42	0.49
10:J:17:LEU:H	10:J:17:LEU:HD23	1.78	0.49
22:a:183:C:H42	22:a:213:A:N6	2.10	0.49
22:a:2243:U:H2'	22:a:2244:U:C6	2.47	0.49
25:d:74:GLU:N	25:d:74:GLU:OE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:121:SER:HB2	27:f:128:TYR:CE1	2.47	0.49
1:A:562:U:H5'	1:A:563:A:C5	2.48	0.49
1:A:864:A:H2'	1:A:865:A:C8	2.47	0.49
1:A:1032:G:N2	1:A:1033:G:N3	2.60	0.49
1:A:1076:U:OP1	2:B:174:LYS:NZ	2.31	0.49
1:A:1130:A:H2'	1:A:1131:G:C8	2.48	0.49
4:D:150:LYS:NZ	4:D:178:MET:HB2	2.27	0.49
22:a:871:U:H2'	22:a:872:U:C6	2.48	0.49
22:a:1028:A:H2'	22:a:1029:A:C8	2.47	0.49
22:a:1342:A:O2'	22:a:1344:U:OP2	2.31	0.49
22:a:2099:U:H2'	22:a:2100:G:C8	2.47	0.49
22:a:2300:C:H2'	22:a:2301:C:H6	1.77	0.49
1:A:67:C:H2'	1:A:68:G:H8	1.78	0.49
1:A:406:G:O6	1:A:495:A:H2'	2.13	0.49
1:A:501:C:H2'	1:A:502:A:C8	2.48	0.49
1:A:923:A:O2'	1:A:1399:C:OP2	2.30	0.49
1:A:1346:A:O2'	7:G:10:ARG:NH2	2.46	0.49
5:E:95:PHE:CE2	5:E:97:GLN:NE2	2.76	0.49
6:F:61:LEU:HD11	18:R:24:LYS:CE	2.42	0.49
8:H:105:SER:OG	8:H:124:GLU:HB2	2.12	0.49
22:a:611:C:H2'	22:a:612:G:O4'	2.12	0.49
55:V:50:A:H2'	55:V:51:G:C8	2.47	0.49
1:A:945:G:C2	1:A:946:A:C8	3.01	0.49
7:G:37:SER:CA	9:I:41:ARG:HH12	2.26	0.49
22:a:682:G:H5'	49:1:26:ASN:ND2	2.27	0.49
22:a:1866:A:N6	22:a:1875:G:O2'	2.45	0.49
4:D:81:ARG:HD2	4:D:81:ARG:C	2.38	0.49
22:a:581:C:H2'	22:a:582:A:C8	2.48	0.49
22:a:933:A:H5'	22:a:934:U:OP2	2.13	0.49
26:e:2:GLU:OE2	26:e:12:LEU:N	2.46	0.49
32:k:112:LEU:HD12	32:k:130:GLY:HA3	1.95	0.49
39:r:17:VAL:HG11	39:r:103:ILE:HG12	1.95	0.49
41:t:41:LEU:HA	41:t:62:GLU:HA	1.93	0.49
42:u:29:ILE:HD12	42:u:38:LEU:O	2.13	0.49
19:S:62:VAL:HA	19:S:66:MET:HE3	1.95	0.48
22:a:922:C:O2'	43:v:29:GLU:OE1	2.27	0.48
22:a:2012:G:OP1	39:r:11:ARG:NH2	2.33	0.48
26:e:145:ASP:HA	26:e:166:LYS:O	2.13	0.48
28:g:45:HIS:CG	28:g:45:HIS:O	2.65	0.48
34:m:28:LEU:HD23	34:m:48:VAL:HG21	1.93	0.48
1:A:151:A:C5	1:A:152:A:C8	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:A:H2'	1:A:264:C:C6	2.48	0.48
1:A:1167:A:O2'	1:A:1169:A:N7	2.43	0.48
7:G:111:ARG:O	7:G:119:ARG:NE	2.46	0.48
22:a:94:A:H8	22:a:94:A:O5'	1.97	0.48
36:o:6:LYS:O	36:o:10:GLN:HG2	2.13	0.48
10:J:83:THR:O	10:J:87:LEU:HG	2.13	0.48
19:S:26:GLY:O	19:S:28:LYS:N	2.47	0.48
22:a:184:C:H2'	22:a:185:G:C8	2.49	0.48
22:a:320:A:N3	26:e:163:ASN:ND2	2.61	0.48
22:a:483:A:C8	41:t:45:HIS:HD2	2.31	0.48
22:a:2557:G:H2'	22:a:2558:C:C6	2.48	0.48
27:f:16:LEU:HD12	27:f:28:VAL:HG13	1.94	0.48
35:n:40:ILE:HG13	35:n:47:VAL:HG22	1.93	0.48
55:V:10:2MG:H2'	55:V:11:C:C6	2.48	0.48
1:A:511:C:O2'	1:A:512:U:OP2	2.27	0.48
4:D:49:SER:O	4:D:53:VAL:HG23	2.14	0.48
22:a:306:U:H2'	22:a:307:G:O4'	2.12	0.48
22:a:312:G:H5'	22:a:331:C:O2'	2.13	0.48
22:a:476:G:N1	22:a:479:A:OP2	2.43	0.48
22:a:2898:U:H2'	22:a:2899:A:H8	1.78	0.48
29:h:30:LEU:HB3	29:h:36:ALA:HB3	1.93	0.48
1:A:483:C:O2	16:P:13:LYS:NZ	2.42	0.48
1:A:676:A:H2'	1:A:677:U:H6	1.78	0.48
1:A:875:U:O2'	8:H:15:ARG:HD2	2.13	0.48
1:A:1119:C:H2'	1:A:1120:C:C6	2.48	0.48
9:I:6:TYR:HB2	9:I:21:ILE:HG12	1.93	0.48
9:I:118:LEU:CD2	9:I:124:ARG:HG2	2.42	0.48
16:P:38:PHE:HE2	16:P:51:ARG:NH1	2.12	0.48
21:U:7:ARG:O	21:U:10:GLU:HB3	2.14	0.48
22:a:876:C:H2'	22:a:877:A:O4'	2.13	0.48
22:a:2636:C:O2'	25:d:45:TYR:OH	2.28	0.48
1:A:160:A:H2'	1:A:161:A:O4'	2.12	0.48
1:A:1087:G:N2	21:U:70:LEU:O	2.41	0.48
1:A:1213:A:O2'	1:A:1215:G:N7	2.43	0.48
22:a:282:A:H2'	22:a:283:G:C8	2.48	0.48
22:a:1046:A:H3'	22:a:1047:G:H5'	1.95	0.48
1:A:381:C:H2'	1:A:382:A:O4'	2.13	0.48
1:A:652:U:O4	1:A:752:G:O2'	2.26	0.48
1:A:977:A:N6	1:A:1224:U:O5'	2.47	0.48
4:D:198:HIS:O	4:D:201:VAL:N	2.47	0.48
5:E:131:THR:HG22	5:E:131:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:113:VAL:O	11:K:113:VAL:HG12	2.13	0.48
22:a:2752:C:H2'	22:a:2753:A:O4'	2.14	0.48
26:e:145:ASP:OD1	26:e:183:PHE:HD1	1.95	0.48
40:s:62:VAL:O	40:s:64:LYS:NZ	2.45	0.48
1:A:401:C:O2'	1:A:621:A:N3	2.43	0.48
1:A:585:G:O2'	1:A:879:C:OP1	2.25	0.48
3:C:135:LYS:HB3	3:C:139:GLN:NE2	2.28	0.48
1:A:7:A:C8	5:E:124:LEU:HD23	2.49	0.48
1:A:1450:U:O2'	1:A:1453:G:O6	2.28	0.48
7:G:93:PRO:HA	7:G:96:ARG:HD2	1.96	0.48
11:K:17:SER:HB2	11:K:80:LYS:HE2	1.96	0.48
21:U:51:SER:HB2	21:U:55:ARG:HH12	1.78	0.48
22:a:358:U:H2'	22:a:359:G:H8	1.78	0.48
22:a:861:A:H2'	22:a:862:G:O4'	2.14	0.48
22:a:1549:A:H2'	22:a:1550:C:C6	2.48	0.48
22:a:2392:A:OP2	50:2:31:HIS:NE2	2.46	0.48
23:b:48:U:H2'	23:b:49:C:H6	1.79	0.48
1:A:159:G:N2	1:A:161:A:H3'	2.29	0.48
8:H:112:THR:HG22	8:H:114:ARG:H	1.79	0.48
10:J:14:ASP:N	10:J:14:ASP:OD1	2.47	0.48
21:U:10:GLU:CD	21:U:18:ARG:HH21	2.22	0.48
22:a:2086:U:H2'	22:a:2087:G:C8	2.49	0.48
22:a:2095:A:C5'	29:h:11:ASN:HD21	2.25	0.48
22:a:2298:A:OP1	27:f:71:ARG:NH2	2.45	0.48
22:a:2718:G:O2'	22:a:2847:U:OP1	2.27	0.48
22:a:161:A:OP2	22:a:162:U:O2'	2.19	0.47
22:a:577:G:H2'	22:a:578:G:C8	2.48	0.47
22:a:1405:U:H2'	22:a:1406:U:H6	1.77	0.47
22:a:2031:A:C6	22:a:2498:OMC:H1'	2.49	0.47
1:A:131:A:H2'	1:A:132:C:C6	2.49	0.47
1:A:199:A:H2'	1:A:200:G:C8	2.49	0.47
1:A:1248:A:H2	9:I:72:ILE:HD11	1.79	0.47
17:Q:5:ILE:HD12	17:Q:62:ARG:HD3	1.95	0.47
22:a:286:U:H2'	22:a:287:G:C8	2.47	0.47
22:a:610:C:H2'	22:a:611:C:C6	2.49	0.47
22:a:883:G:H2'	22:a:884:U:C6	2.49	0.47
22:a:959:A:H2'	22:a:960:A:C8	2.49	0.47
22:a:1915:3TD:O5'	22:a:1915:3TD:H6	2.14	0.47
24:c:133:ARG:O	24:c:167:ARG:NH2	2.47	0.47
28:g:94:TYR:HD1	28:g:107:LEU:HD23	1.79	0.47
31:j:109:SER:O	31:j:113:MET:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:U:O2'	1:A:30:U:H5'	2.14	0.47
1:A:337:G:H2'	1:A:338:A:C8	2.49	0.47
4:D:95:GLU:OE2	4:D:100:ASN:ND2	2.43	0.47
12:L:42:PRO:HG2	12:L:46:ASN:O	2.14	0.47
22:a:1203:U:OP2	22:a:1204:A:O2'	2.31	0.47
22:a:1296:G:OP1	22:a:2709:G:O2'	2.25	0.47
22:a:2014:A:H2'	22:a:2015:A:C8	2.49	0.47
28:g:44:LYS:O	28:g:50:LEU:HA	2.14	0.47
40:s:12:ARG:HB2	40:s:33:LYS:O	2.14	0.47
40:s:59:ASN:HB2	40:s:84:TYR:HB2	1.95	0.47
1:A:223:A:H2'	1:A:224:U:C6	2.49	0.47
1:A:502:A:H2'	1:A:503:C:O4'	2.14	0.47
11:K:17:SER:HA	11:K:79:ILE:HA	1.95	0.47
13:M:66:GLU:HB3	13:M:70:ARG:HH12	1.78	0.47
22:a:1796:U:H2'	22:a:1797:G:C8	2.49	0.47
22:a:1856:U:H2'	22:a:1857:G:O4'	2.14	0.47
22:a:1880:U:H2'	22:a:1881:C:C6	2.49	0.47
22:a:1946:U:H2'	22:a:1947:C:C6	2.50	0.47
30:i:92:MET:HE3	30:i:99:ARG:HG3	1.95	0.47
1:A:883:C:O2'	1:A:884:U:H5'	2.14	0.47
9:I:42:GLU:H	9:I:42:GLU:CD	2.21	0.47
11:K:23:ILE:HD12	11:K:96:THR:HG21	1.96	0.47
22:a:414:C:H2'	22:a:415:A:C8	2.49	0.47
22:a:810:U:C4	32:k:29:LYS:O	2.68	0.47
22:a:1682:G:H2'	22:a:1683:U:C6	2.49	0.47
26:e:129:PRO:HD3	26:e:156:ASN:OD1	2.14	0.47
30:i:13:ARG:HG3	30:i:51:GLY:O	2.13	0.47
32:k:57:LEU:HA	32:k:60:ARG:HG2	1.97	0.47
1:A:152:A:H3'	1:A:153:C:H6	1.78	0.47
3:C:56:VAL:O	3:C:66:VAL:HA	2.14	0.47
6:F:38:ARG:HD3	6:F:98:GLU:H	1.79	0.47
7:G:99:LEU:HD22	7:G:103:TRP:CZ2	2.49	0.47
22:a:83:A:OP1	41:t:2:ALA:HB2	2.15	0.47
22:a:305:C:H2'	22:a:306:U:C6	2.50	0.47
22:a:2745:C:H2'	22:a:2746:U:C6	2.50	0.47
27:f:105:THR:HG22	27:f:106:ILE:HD13	1.95	0.47
32:k:5:THR:O	32:k:5:THR:HG22	2.15	0.47
37:p:86:ALA:HB2	37:p:116:ALA:HB2	1.96	0.47
1:A:202:G:H1'	1:A:468:A:H2	1.78	0.47
1:A:382:A:H2'	1:A:383:A:C8	2.50	0.47
1:A:464:U:H3	1:A:468:A:N6	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:G:O2'	1:A:1190:G:N2	2.47	0.47
1:A:1168:U:O5'	1:A:1168:U:H6	1.97	0.47
1:A:1273:C:H2'	1:A:1274:A:O4'	2.15	0.47
2:B:43:LEU:HA	2:B:46:THR:HB	1.95	0.47
2:B:66:LYS:HD3	2:B:90:PHE:CE2	2.47	0.47
4:D:105:MET:HB3	4:D:171:LEU:HD21	1.96	0.47
7:G:48:GLU:CD	7:G:52:GLN:HE22	2.23	0.47
9:I:67:VAL:CG2	9:I:75:GLN:HG3	2.44	0.47
22:a:454:A:H4'	22:a:455:C:OP2	2.15	0.47
22:a:638:G:H2'	22:a:639:U:C6	2.49	0.47
22:a:2101:A:H2'	22:a:2102:G:H8	1.80	0.47
22:a:2847:U:H2'	22:a:2848:G:O4'	2.15	0.47
30:i:95:ARG:CZ	30:i:96:ARG:HH22	2.27	0.47
32:k:77:ILE:CD1	32:k:108:ALA:HB1	2.45	0.47
55:V:47:H2U:O2'	55:V:48:5MC:H5'	2.15	0.47
2:B:145:GLU:O	2:B:149:GLY:HA3	2.15	0.47
15:O:17:ARG:HG2	15:O:17:ARG:O	2.14	0.47
22:a:1428:C:C5	22:a:1569:A:H5''	2.49	0.47
22:a:2312:U:H5'	27:f:85:ILE:HD11	1.96	0.47
31:j:104:THR:HG22	31:j:106:GLU:OE1	2.15	0.47
42:u:29:ILE:HG22	42:u:90:ASP:OD1	2.14	0.47
1:A:73:C:O2'	1:A:74:A:H8	1.95	0.47
1:A:881:G:OP2	12:L:6:GLN:NE2	2.34	0.47
1:A:1521:C:H2'	1:A:1522:U:C6	2.50	0.47
6:F:9:MET:HE2	6:F:9:MET:HB3	1.78	0.47
9:I:76:ALA:O	9:I:79:ILE:HG22	2.14	0.47
15:O:14:GLU:HG2	15:O:84:ARG:NH2	2.30	0.47
22:a:1334:G:OP1	40:s:69:ARG:NH2	2.48	0.47
22:a:2064:C:H2'	22:a:2065:C:C6	2.50	0.47
24:c:60:GLN:HG2	24:c:85:PRO:HB2	1.96	0.47
26:e:170:ARG:HG3	26:e:170:ARG:NH2	2.30	0.47
1:A:323:U:H2'	1:A:324:G:O4'	2.15	0.47
1:A:503:C:O2'	1:A:510:A:N1	2.45	0.47
7:G:17:LYS:HD3	7:G:44:TYR:CD1	2.49	0.47
22:a:5:A:H2'	22:a:6:A:C8	2.50	0.47
22:a:231:A:H2'	22:a:232:G:O4'	2.15	0.47
22:a:742:A:H2'	22:a:743:A:C8	2.50	0.47
22:a:1869:G:H5'	22:a:1870:C:OP2	2.15	0.47
27:f:69:LYS:HA	27:f:84:PRO:HA	1.97	0.47
32:k:100:ILE:HG22	32:k:101:ILE:HG23	1.96	0.47
41:t:4:LYS:O	41:t:94:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:t:10:GLU:OE2	41:t:22:ARG:HG2	2.15	0.47
47:z:48:TYR:CE1	47:z:53:LYS:HD3	2.49	0.47
1:A:20:U:H2'	1:A:21:G:O4'	2.15	0.46
1:A:123:U:OP1	1:A:312:C:H5'	2.14	0.46
1:A:1009:U:O4	1:A:1020:G:O6	2.32	0.46
5:E:50:TYR:H	5:E:66:LYS:HE3	1.80	0.46
9:I:85:ARG:HA	9:I:88:MET:HE2	1.98	0.46
22:a:243:U:OP2	50:2:8:ARG:NH1	2.48	0.46
22:a:813:U:H2'	22:a:814:C:C6	2.50	0.46
22:a:1794:A:H2'	22:a:1795:C:C6	2.49	0.46
22:a:2074:U:H2'	22:a:2075:U:C6	2.49	0.46
28:g:52:PHE:CE1	28:g:72:LEU:HD12	2.49	0.46
1:A:718:A:H5'	11:K:119:IAS:C	2.45	0.46
1:A:816:A:OP2	1:A:817:C:O2'	2.19	0.46
2:B:161:LEU:HD11	2:B:176:ALA:HB2	1.97	0.46
2:B:187:VAL:HG11	2:B:199:VAL:HG13	1.98	0.46
15:O:26:GLU:OE1	15:O:26:GLU:N	2.48	0.46
22:a:2340:A:H5'	23:b:41:G:H21	1.81	0.46
22:a:2788:C:H2'	22:a:2789:C:C6	2.51	0.46
41:t:62:GLU:N	41:t:62:GLU:OE1	2.48	0.46
1:A:999:C:N3	1:A:1042:A:N6	2.64	0.46
1:A:1144:G:N2	1:A:1146:A:H62	2.12	0.46
22:a:286:U:C2	22:a:287:G:C8	3.04	0.46
22:a:892:A:C6	22:a:893:C:C4	3.03	0.46
22:a:1263:U:H2'	22:a:1264:A:C8	2.48	0.46
22:a:2680:U:O2'	22:a:2681:C:H5'	2.15	0.46
1:A:102:G:H2'	1:A:103:U:C6	2.50	0.46
1:A:405:U:O4	4:D:3:ARG:N	2.47	0.46
1:A:1477:U:H2'	1:A:1478:U:C6	2.51	0.46
5:E:74:VAL:HG21	5:E:144:LEU:HD22	1.98	0.46
8:H:13:ARG:HB3	8:H:25:VAL:HG11	1.97	0.46
11:K:85:MET:SD	11:K:111:THR:HB	2.55	0.46
22:a:160:A:N3	22:a:2208:C:O2'	2.48	0.46
22:a:1507:C:H2'	22:a:1508:A:O4'	2.16	0.46
33:l:7:THR:HG22	33:l:9:PHE:H	1.79	0.46
40:s:34:VAL:HG11	40:s:43:ILE:HG12	1.97	0.46
48:0:33:LYS:CD	48:0:51:GLU:HG2	2.43	0.46
1:A:826:C:O2	8:H:16:ASN:ND2	2.48	0.46
1:A:1233:G:OP1	9:I:119:ARG:NH1	2.48	0.46
3:C:56:VAL:HB	3:C:67:THR:HB	1.97	0.46
12:L:38:TYR:CE2	12:L:40:THR:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:83:LYS:HD3	14:N:83:LYS:HA	1.78	0.46
21:U:39:GLU:HG2	21:U:43:THR:HB	1.98	0.46
26:e:176:ASP:OD1	26:e:179:SER:HB3	2.16	0.46
39:r:13:SER:O	39:r:17:VAL:HG23	2.16	0.46
1:A:201:G:H2'	1:A:202:G:C8	2.50	0.46
1:A:501:C:H2'	1:A:502:A:H8	1.81	0.46
22:a:345:A:N3	22:a:347:A:N6	2.64	0.46
22:a:1790:C:H2'	22:a:1791:A:C5	2.51	0.46
22:a:2796:U:H3	22:a:2799:A:N6	2.07	0.46
1:A:1130:A:H2'	1:A:1131:G:H8	1.81	0.46
3:C:39:VAL:HG22	3:C:91:VAL:HG23	1.98	0.46
3:C:153:VAL:HG12	3:C:157:LEU:HD21	1.97	0.46
20:T:43:ASP:OD1	20:T:44:LYS:N	2.47	0.46
22:a:64:A:H2'	22:a:65:U:C6	2.50	0.46
22:a:401:A:H2'	22:a:402:A:C8	2.50	0.46
22:a:1292:G:H2'	22:a:1293:C:C6	2.50	0.46
22:a:1809:A:H2'	22:a:1810:A:C8	2.51	0.46
22:a:2899:A:H2'	22:a:2900:A:C8	2.51	0.46
35:n:76:LYS:O	35:n:80:GLU:OE1	2.34	0.46
55:V:10:2MG:O2'	55:V:11:C:OP1	2.31	0.46
1:A:67:C:H2'	1:A:68:G:C8	2.50	0.46
3:C:130:PHE:HD2	3:C:134:MET:HE2	1.81	0.46
7:G:69:VAL:HG23	7:G:100:ALA:HB1	1.96	0.46
22:a:1315:C:O2'	22:a:1392:A:N3	2.47	0.46
22:a:1800:C:P	24:c:263:THR:HG21	2.56	0.46
22:a:2100:G:H2'	22:a:2101:A:C8	2.51	0.46
37:p:58:ARG:HA	37:p:61:TRP:CE3	2.51	0.46
43:v:38:VAL:HG12	43:v:59:LEU:HB2	1.98	0.46
1:A:173:U:H5''	1:A:197:A:O4'	2.16	0.46
1:A:1272:G:H2'	1:A:1273:C:O4'	2.16	0.46
2:B:90:PHE:HE1	2:B:153:ASP:OD1	1.99	0.46
7:G:93:PRO:HA	7:G:96:ARG:HG2	1.97	0.46
22:a:566:U:H2'	22:a:567:U:O4'	2.16	0.46
22:a:594:U:H2'	22:a:595:C:C6	2.51	0.46
22:a:720:U:H2'	22:a:721:A:C8	2.51	0.46
22:a:1443:U:H2'	22:a:1444:G:H8	1.81	0.46
26:e:15:SER:OG	26:e:17:THR:OG1	2.30	0.46
35:n:34:HIS:ND1	35:n:53:THR:OG1	2.44	0.46
42:u:1:MET:HG3	42:u:59:GLU:OE2	2.16	0.46
42:u:9:ARG:HG2	42:u:41:GLU:CD	2.41	0.46
22:a:2484:G:OP1	33:l:44:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2639:A:H2'	22:a:2640:G:O4'	2.16	0.46
32:k:96:LYS:HE2	32:k:102:GLY:O	2.16	0.46
41:t:33:LYS:HE3	41:t:64:ALA:HB3	1.98	0.46
50:2:32:ILE:HG13	50:2:32:ILE:O	2.16	0.46
1:A:482:A:H2'	1:A:483:C:O4'	2.16	0.45
1:A:522:C:H41	12:L:50:ARG:NH2	2.13	0.45
2:B:63:ARG:O	2:B:63:ARG:HD3	2.15	0.45
22:a:38:A:H2'	22:a:39:G:O4'	2.16	0.45
22:a:155:A:H2'	22:a:156:A:C8	2.51	0.45
22:a:1048:A:N7	22:a:1111:A:C6	2.84	0.45
22:a:1180:U:H2'	22:a:1181:U:O4'	2.15	0.45
22:a:2474:U:OP2	22:a:2475:C:N4	2.38	0.45
42:u:72:VAL:HG12	42:u:93:ARG:HA	1.98	0.45
49:1:18:PHE:HA	49:1:43:THR:HG21	1.99	0.45
51:3:16:ILE:HD13	51:3:25:VAL:HG22	1.98	0.45
1:A:864:A:H4'	5:E:90:THR:HG23	1.99	0.45
3:C:147:LYS:HB2	3:C:203:PHE:CD2	2.50	0.45
22:a:729:G:C6	24:c:207:LYS:HB2	2.51	0.45
22:a:1197:G:H2'	22:a:1198:U:H6	1.81	0.45
22:a:1870:C:HO2'	22:a:1871:A:H8	1.62	0.45
22:a:2514:U:H2'	22:a:2515:C:C6	2.50	0.45
22:a:2820:A:N3	22:a:2820:A:H2'	2.31	0.45
40:s:5:GLU:HG3	45:x:22:LEU:CD1	2.45	0.45
1:A:834:U:H2'	1:A:835:U:C6	2.52	0.45
1:A:968:A:C6	1:A:1062:U:O2'	2.69	0.45
1:A:1359:C:H3'	14:N:75:ARG:NH2	2.32	0.45
1:A:1428:A:H2'	1:A:1429:A:O4'	2.16	0.45
4:D:57:GLU:O	4:D:60:LYS:HG2	2.16	0.45
8:H:50:LYS:NZ	8:H:60:GLU:OE1	2.47	0.45
22:a:640:C:H2'	22:a:641:U:C6	2.51	0.45
22:a:2552:OMU:HM23	22:a:2554:U:C6	2.52	0.45
22:a:2698:U:H2'	22:a:2699:C:C6	2.51	0.45
22:a:2849:U:H4'	22:a:2868:A:C2	2.51	0.45
26:e:171:ASP:OD2	26:e:173:THR:OG1	2.24	0.45
1:A:43:C:H2'	1:A:44:A:O4'	2.16	0.45
1:A:109:A:H5'	1:A:110:C:H5	1.82	0.45
1:A:724:G:OP2	1:A:724:G:H8	1.99	0.45
1:A:1011:C:H2'	1:A:1012:A:C8	2.51	0.45
1:A:1104:G:H5'	2:B:113:ARG:HH22	1.81	0.45
1:A:1127:G:N2	1:A:1145:A:N1	2.52	0.45
1:A:1437:A:H5''	20:T:29:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1465:A:H2'	1:A:1466:C:C6	2.52	0.45
3:C:64:ILE:O	3:C:99:ALA:HA	2.17	0.45
20:T:45:ALA:HB1	20:T:49:LYS:HZ3	1.82	0.45
22:a:297:G:H2'	22:a:298:G:O4'	2.17	0.45
22:a:881:G:H2'	22:a:882:G:H8	1.80	0.45
22:a:1025:G:O2'	22:a:1026:G:OP1	2.30	0.45
22:a:1446:C:H2'	22:a:1447:C:C6	2.52	0.45
22:a:1545:A:H2'	22:a:1546:G:O4'	2.17	0.45
22:a:1739:A:H2'	22:a:1740:G:O4'	2.16	0.45
44:w:66:THR:O	44:w:70:GLU:OE1	2.35	0.45
55:V:50:A:H2'	55:V:51:G:H8	1.80	0.45
1:A:201:G:O2'	1:A:469:C:O2'	2.21	0.45
1:A:1169:A:H2'	1:A:1170:A:C8	2.52	0.45
2:B:53:ALA:O	2:B:57:LEU:HD23	2.16	0.45
5:E:13:GLU:HG2	5:E:39:VAL:HG23	1.99	0.45
22:a:754:U:H2'	22:a:755:U:C6	2.52	0.45
22:a:1509:A:N3	22:a:1510:G:C8	2.85	0.45
22:a:2102:G:N1	22:a:2187:U:N3	2.37	0.45
23:b:1:U:H2'	23:b:2:G:H8	1.80	0.45
32:k:135:ILE:HG12	32:k:140:GLY:HA3	1.98	0.45
1:A:198:G:O6	1:A:219:U:O4	2.35	0.45
1:A:632:U:H5''	1:A:633:G:C8	2.52	0.45
1:A:1138:G:H3'	1:A:1138:G:N3	2.32	0.45
3:C:28:GLU:N	3:C:28:GLU:OE1	2.49	0.45
5:E:81:LEU:HD13	5:E:85:VAL:HG22	1.97	0.45
14:N:57:PRO:HA	14:N:60:GLN:OE1	2.17	0.45
22:a:74:A:N3	22:a:74:A:H5''	2.31	0.45
22:a:2395:C:H2'	22:a:2396:G:O4'	2.16	0.45
28:g:105:LEU:HB3	28:g:107:LEU:HG	1.99	0.45
34:m:29:VAL:HG11	34:m:75:ILE:HG23	1.97	0.45
2:B:130:THR:O	2:B:132:LYS:N	2.50	0.45
2:B:166:ALA:HB3	2:B:191:SER:OG	2.17	0.45
5:E:81:LEU:HB2	5:E:98:PRO:HG3	1.99	0.45
22:a:829:A:N7	22:a:2248:C:H5'	2.31	0.45
22:a:989:G:OP2	46:y:12:SER:OG	2.25	0.45
28:g:164:TYR:HB2	28:g:167:GLU:HB2	1.99	0.45
35:n:108:ASP:O	35:n:112:GLU:OE1	2.34	0.45
47:z:29:SER:O	47:z:37:LYS:HA	2.17	0.45
1:A:604:G:H2'	1:A:605:U:O4'	2.17	0.45
7:G:113:ASP:HB2	7:G:119:ARG:CG	2.45	0.45
9:I:10:GLY:HA3	9:I:78:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:84:VAL:HG11	11:K:97:ILE:HG12	1.99	0.45
12:L:55:VAL:HG21	12:L:80:ILE:HD11	1.98	0.45
14:N:26:GLU:O	14:N:30:ILE:HG12	2.17	0.45
22:a:3:U:H2'	22:a:4:U:C6	2.52	0.45
50:2:50:VAL:HG12	50:2:55:LEU:HD22	1.97	0.45
1:A:676:A:H5''	11:K:115:PRO:HB3	1.99	0.45
1:A:745:G:H2'	1:A:746:A:H8	1.82	0.45
19:S:30:PRO:HB3	19:S:48:THR:HG23	1.99	0.45
20:T:28:MET:HE2	20:T:61:GLN:HG3	1.98	0.45
22:a:108:G:H2'	22:a:109:C:O4'	2.17	0.45
22:a:481:G:O2'	22:a:507:A:N1	2.41	0.45
22:a:1792:G:H5'	24:c:204:VAL:HG13	1.99	0.45
44:w:10:LYS:HE3	44:w:54:LYS:HD3	1.99	0.45
1:A:1220:G:OP2	14:N:53:ARG:NH1	2.50	0.45
2:B:77:SER:HB3	2:B:93:ASN:HB2	1.99	0.45
4:D:99:ASP:OD1	4:D:100:ASN:N	2.50	0.45
6:F:9:MET:HE3	6:F:59:TYR:CZ	2.52	0.45
22:a:166:U:H2'	22:a:167:A:C8	2.52	0.45
22:a:2030:6MZ:C2	22:a:2499:C:H5''	2.47	0.45
24:c:66:ASP:OD2	24:c:102:ARG:NH1	2.48	0.45
36:o:51:ARG:HG2	36:o:53:ARG:HG2	1.99	0.45
1:A:151:A:OP2	1:A:169:C:N4	2.50	0.44
1:A:499:A:H62	4:D:2:ALA:N	2.15	0.44
1:A:704:A:H3'	1:A:705:G:H8	1.82	0.44
1:A:883:C:C2'	1:A:884:U:H5'	2.47	0.44
4:D:107:PHE:CG	4:D:145:ILE:HD11	2.52	0.44
4:D:118:VAL:HG22	4:D:123:ILE:HG13	1.98	0.44
22:a:598:U:H2'	22:a:599:A:C8	2.52	0.44
22:a:627:A:O2'	32:k:76:GLU:OE2	2.33	0.44
22:a:1591:A:H2'	22:a:1592:C:C6	2.52	0.44
22:a:1932:A:H2'	22:a:1933:G:O4'	2.17	0.44
28:g:42:GLU:HG3	28:g:55:ARG:HD3	1.98	0.44
1:A:900:A:H2'	1:A:901:A:C8	2.52	0.44
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.52	0.44
12:L:108:LYS:HB3	12:L:108:LYS:HE3	1.90	0.44
13:M:66:GLU:CD	13:M:66:GLU:H	2.25	0.44
22:a:1138:G:N2	30:i:108:MET:HE2	2.33	0.44
22:a:1386:C:H2'	22:a:1387:A:C8	2.53	0.44
22:a:1563:U:H2'	22:a:1564:C:C6	2.53	0.44
22:a:2193:G:H2'	22:a:2194:U:H6	1.81	0.44
30:i:26:GLY:O	30:i:30:THR:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:29:LYS:O	32:k:29:LYS:HG2	2.16	0.44
33:l:112:LEU:O	33:l:115:GLU:HG3	2.17	0.44
40:s:9:LYS:HE3	40:s:12:ARG:HH22	1.82	0.44
1:A:186:C:H2'	1:A:187:G:O4'	2.18	0.44
1:A:195:A:O2'	1:A:196:A:O4'	2.34	0.44
1:A:197:A:C6	1:A:221:C:H5'	2.53	0.44
1:A:1000:A:H2'	1:A:1001:C:C6	2.53	0.44
2:B:217:VAL:O	2:B:220:THR:HG22	2.17	0.44
3:C:134:MET:HE1	3:C:166:GLU:CD	2.42	0.44
16:P:2:VAL:HG11	16:P:60:TRP:CE3	2.52	0.44
16:P:8:ARG:NH1	16:P:15:PRO:HG3	2.33	0.44
22:a:290:U:O2	22:a:350:G:C6	2.70	0.44
22:a:468:G:OP2	49:1:37:LYS:NZ	2.43	0.44
22:a:538:A:H4'	30:i:7:LYS:HG2	1.98	0.44
22:a:580:U:H2'	22:a:581:C:C6	2.52	0.44
22:a:888:C:H2'	22:a:889:C:C6	2.52	0.44
22:a:1269:A:H2'	22:a:1270:C:C6	2.52	0.44
22:a:1800:C:OP2	24:c:263:THR:HG21	2.17	0.44
24:c:24:LEU:HD13	24:c:83:TYR:HB2	2.00	0.44
30:i:31:GLU:HG2	30:i:142:ILE:HG23	1.99	0.44
36:o:9:GLU:HB3	36:o:55:LEU:HB2	1.99	0.44
1:A:33:A:H2'	1:A:34:C:C6	2.52	0.44
1:A:537:G:H2'	1:A:538:G:H8	1.81	0.44
1:A:580:C:H2'	1:A:581:G:O4'	2.18	0.44
1:A:695:A:H2'	1:A:696:A:C8	2.53	0.44
1:A:736:C:H2'	1:A:737:C:C6	2.53	0.44
1:A:923:A:H2'	1:A:924:C:O4'	2.17	0.44
1:A:1287:A:H2'	1:A:1288:A:C8	2.52	0.44
6:F:12:PRO:HB2	6:F:44:ARG:NH1	2.33	0.44
22:a:365:U:H2'	22:a:366:C:C6	2.52	0.44
22:a:1418:G:N1	22:a:1579:A:OP2	2.46	0.44
22:a:1589:U:H2'	22:a:1590:A:C8	2.52	0.44
22:a:2501:C:H4'	22:a:2502:G:OP2	2.17	0.44
22:a:2901:C:H2'	22:a:2902:C:C6	2.52	0.44
31:j:106:GLU:OE1	31:j:106:GLU:N	2.51	0.44
34:m:86:ARG:HH21	34:m:117:ASP:CG	2.24	0.44
42:u:6:ALA:HB1	42:u:40:ILE:HB	2.00	0.44
1:A:769:G:H4'	1:A:1513:A:H4'	2.00	0.44
1:A:1382:C:HO2'	7:G:79:ARG:HH11	1.65	0.44
2:B:130:THR:C	2:B:132:LYS:H	2.25	0.44
13:M:52:GLN:O	13:M:55:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:21:ASP:OD2	15:O:24:SER:OG	2.27	0.44
22:a:415:A:H2'	22:a:416:U:C6	2.52	0.44
22:a:1328:A:H2'	22:a:1330:C:C4	2.53	0.44
22:a:1589:U:H2'	22:a:1590:A:H8	1.82	0.44
26:e:6:LYS:HE3	26:e:119:ILE:HG23	2.00	0.44
30:i:17:VAL:HG12	30:i:138:GLN:O	2.18	0.44
54:Z:32:G:H2'	54:Z:33:OMC:H6	1.82	0.44
1:A:1032:G:H22	1:A:1033:G:H21	1.66	0.44
3:C:135:LYS:HB3	3:C:135:LYS:HE3	1.86	0.44
13:M:71:ARG:O	13:M:75:MET:HG2	2.17	0.44
18:R:49:ALA:O	18:R:53:ARG:HG3	2.18	0.44
22:a:278:A:H2	22:a:361:G:N2	2.15	0.44
22:a:1047:G:O2'	22:a:1110:G:N1	2.43	0.44
22:a:1168:G:H2'	22:a:1169:A:C8	2.53	0.44
22:a:1168:G:O6	22:a:1181:U:O4	2.36	0.44
28:g:16:ASP:HB3	28:g:27:LYS:HB2	2.00	0.44
32:k:57:LEU:HD22	50:2:54:ASP:HB3	1.99	0.44
1:A:68:G:H5'	1:A:171:A:O2'	2.18	0.44
1:A:151:A:C2	1:A:152:A:H1'	2.52	0.44
1:A:581:G:O6	1:A:758:C:H3'	2.17	0.44
4:D:76:TYR:CE2	4:D:204:TYR:HB3	2.53	0.44
5:E:82:GLN:HG2	5:E:147:MET:CE	2.48	0.44
9:I:76:ALA:HA	9:I:79:ILE:HG22	2.00	0.44
15:O:64:ARG:NH1	15:O:89:ARG:HD2	2.33	0.44
16:P:8:ARG:CZ	16:P:15:PRO:HG3	2.47	0.44
22:a:438:G:H2'	22:a:439:A:C8	2.52	0.44
22:a:534:U:O2'	37:p:49:ASP:OD2	2.33	0.44
25:d:12:THR:OG1	25:d:13:ARG:N	2.51	0.44
41:t:40:ASN:HB3	41:t:63:ALA:O	2.18	0.44
1:A:110:C:H2'	1:A:111:G:O4'	2.18	0.44
1:A:451:A:H4'	1:A:452:A:O5'	2.18	0.44
1:A:514:C:H2'	1:A:515:G:H8	1.83	0.44
1:A:522:C:H41	12:L:50:ARG:HH22	1.65	0.44
1:A:1366:C:H2'	1:A:1367:C:C6	2.53	0.44
1:A:1404:C:H2'	1:A:1405:G:C8	2.53	0.44
1:A:1441:A:H62	1:A:1461:G:H21	1.66	0.44
3:C:151:VAL:HG22	3:C:200:VAL:HG22	1.99	0.44
22:a:784:G:H5'	22:a:785:G:OP1	2.17	0.44
22:a:1407:G:H2'	22:a:1408:G:C8	2.53	0.44
22:a:1778:U:H2'	22:a:1784:A:N6	2.33	0.44
22:a:2300:C:H2'	22:a:2301:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2302:U:H2'	22:a:2303:G:H8	1.83	0.44
22:a:2329:U:H2'	22:a:2330:G:C8	2.51	0.44
22:a:2649:C:H2'	22:a:2650:U:H6	1.82	0.44
25:d:152:PRO:HG3	25:d:156:PHE:CZ	2.53	0.44
29:h:17:ASP:N	29:h:17:ASP:OD1	2.49	0.44
55:V:11:C:H2'	55:V:12:U:C6	2.53	0.44
1:A:555:U:H2'	1:A:556:C:C6	2.53	0.44
1:A:1071:C:H2'	1:A:1072:G:C8	2.53	0.44
6:F:18:VAL:HB	6:F:19:PRO:HD3	2.00	0.44
14:N:27:LEU:HD22	14:N:48:LEU:HB2	1.98	0.44
18:R:16:GLU:HG2	18:R:18:VAL:HG23	2.00	0.44
22:a:2047:C:H2'	22:a:2048:G:H8	1.82	0.44
28:g:89:LEU:HD23	28:g:94:TYR:HB3	1.98	0.44
32:k:63:LYS:HG2	50:2:13:ARG:HG3	2.00	0.44
37:p:81:ASN:HD21	37:p:85:LYS:NZ	2.16	0.44
41:t:99:ASN:C	41:t:99:ASN:OD1	2.60	0.44
44:w:68:LEU:O	44:w:72:ARG:HG3	2.18	0.44
1:A:45:G:H2'	1:A:46:G:C8	2.53	0.43
1:A:470:C:H2'	1:A:471:U:C6	2.53	0.43
1:A:678:U:H2'	1:A:679:C:C6	2.53	0.43
1:A:1083:U:O2'	1:A:1102:A:OP2	2.30	0.43
20:T:8:LYS:O	20:T:12:ILE:HG13	2.17	0.43
22:a:219:A:H2'	22:a:220:G:O4'	2.18	0.43
23:b:27:C:C4	23:b:28:C:C4	3.05	0.43
1:A:6:G:H2'	5:E:124:LEU:HD21	2.00	0.43
1:A:144:G:H2'	1:A:145:G:O4'	2.17	0.43
1:A:599:C:H4'	8:H:122:GLY:C	2.43	0.43
22:a:287:G:H2'	22:a:288:U:C6	2.52	0.43
22:a:1614:A:C6	39:r:87:PRO:HB3	2.53	0.43
22:a:2467:C:H2'	22:a:2468:A:O4'	2.18	0.43
38:q:1:MET:HA	38:q:42:ALA:O	2.18	0.43
1:A:4:U:C2'	1:A:5:U:H2'	2.46	0.43
1:A:64:G:C8	1:A:99:C:N4	2.86	0.43
1:A:1218:C:H2'	1:A:1219:A:C8	2.53	0.43
2:B:68:LEU:HG	2:B:70:VAL:HG13	2.00	0.43
22:a:1508:A:H2	22:a:1509:A:N6	2.16	0.43
22:a:2532:G:N2	22:a:2663:G:O2'	2.51	0.43
22:a:2625:G:H2'	22:a:2626:C:O4'	2.19	0.43
30:i:111:LYS:HD2	30:i:111:LYS:N	2.32	0.43
5:E:77:ASN:HB2	5:E:82:GLN:HE22	1.83	0.43
10:J:18:ILE:O	10:J:22:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:59:ASP:OD2	20:T:76:LYS:NZ	2.38	0.43
22:a:71:A:N1	22:a:114:U:H1'	2.33	0.43
22:a:659:G:O2'	26:e:95:LYS:O	2.34	0.43
22:a:2039:U:H2'	22:a:2040:G:C8	2.53	0.43
22:a:2421:G:OP2	50:2:32:ILE:HG22	2.17	0.43
28:g:60:ASP:O	28:g:62:TRP:N	2.49	0.43
38:q:5:PHE:HE1	38:q:14:VAL:HG21	1.83	0.43
42:u:68:LYS:HE2	42:u:68:LYS:HA	2.00	0.43
1:A:1309:G:H5'	13:M:77:ILE:HD11	1.99	0.43
2:B:160:ALA:HB1	2:B:184:PHE:HE2	1.84	0.43
2:B:199:VAL:HG12	2:B:201:PRO:HD3	2.00	0.43
3:C:54:ARG:HB3	3:C:69:HIS:CD2	2.53	0.43
5:E:139:ALA:O	5:E:142:ASP:HB3	2.18	0.43
19:S:32:ARG:HA	19:S:50:ALA:HB3	2.01	0.43
22:a:687:C:H5''	49:1:2:LYS:HE2	1.99	0.43
22:a:1541:C:H2'	22:a:1542:U:O4'	2.18	0.43
28:g:94:TYR:HA	28:g:106:SER:O	2.18	0.43
1:A:471:U:H2'	1:A:472:U:C6	2.53	0.43
1:A:922:G:N3	1:A:1398:A:H2	2.17	0.43
18:R:72:ASP:OD1	18:R:72:ASP:N	2.45	0.43
40:s:31:VAL:HG22	40:s:84:TYR:CD1	2.54	0.43
45:x:27:ASN:O	45:x:31:GLN:HG3	2.18	0.43
50:2:27:ALA:O	50:2:28:ASN:HB2	2.17	0.43
52:4:22:MET:HE2	52:4:22:MET:HB3	1.77	0.43
1:A:551:U:H2'	1:A:552:U:O4'	2.19	0.43
1:A:619:U:O4'	4:D:128:ARG:NH2	2.51	0.43
1:A:1035:A:H1'	1:A:1036:A:O5'	2.18	0.43
2:B:133:GLU:O	2:B:137:ARG:HG2	2.19	0.43
2:B:163:VAL:HG11	2:B:173:ILE:HD11	2.00	0.43
4:D:22:LYS:HD3	4:D:22:LYS:HA	1.81	0.43
6:F:92:THR:HG22	6:F:94:HIS:H	1.84	0.43
11:K:57:LYS:HE3	11:K:57:LYS:HB3	1.68	0.43
13:M:2:ALA:HB2	13:M:53:ILE:HD13	2.01	0.43
18:R:14:THR:HB	18:R:48:ARG:HE	1.83	0.43
22:a:204:A:H8	22:a:204:A:OP1	2.02	0.43
22:a:362:A:C4	22:a:363:G:C8	3.07	0.43
22:a:538:A:H5''	30:i:7:LYS:HE3	2.01	0.43
22:a:989:G:OP1	46:y:32:ILE:HD12	2.19	0.43
22:a:2052:A:O2'	25:d:148:GLN:O	2.35	0.43
30:i:35:ARG:HG2	30:i:40:HIS:CE1	2.53	0.43
38:q:43:ASN:O	38:q:43:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:0:35:GLU:OE2	48:0:48:ILE:HG23	2.19	0.43
1:A:89:U:H2'	1:A:90:C:C6	2.54	0.43
1:A:1266:G:N2	1:A:1269:A:OP2	2.33	0.43
7:G:132:GLY:O	7:G:136:LYS:HG2	2.19	0.43
17:Q:48:ASP:OD2	17:Q:51:ASN:HA	2.19	0.43
22:a:279:A:H2'	22:a:280:U:O4'	2.19	0.43
22:a:1495:A:H2'	22:a:1496:A:C8	2.53	0.43
22:a:1499:C:H2'	22:a:1500:G:H8	1.83	0.43
22:a:2025:C:H2'	22:a:2026:U:C6	2.54	0.43
27:f:60:ILE:HA	27:f:140:GLU:OE2	2.17	0.43
1:A:167:A:H2'	1:A:168:G:C8	2.53	0.43
1:A:436:C:O2'	4:D:154:ARG:HD3	2.19	0.43
2:B:98:GLY:HA2	2:B:171:ILE:HD11	2.01	0.43
19:S:18:LYS:HB3	19:S:31:LEU:HD23	2.00	0.43
22:a:590:A:H2'	22:a:591:U:C6	2.54	0.43
31:j:71:ARG:HH22	31:j:123:LEU:C	2.27	0.43
40:s:12:ARG:HD3	40:s:12:ARG:HA	1.77	0.43
45:x:13:GLU:O	45:x:16:THR:HG22	2.19	0.43
1:A:986:U:H2'	1:A:987:G:O4'	2.19	0.43
1:A:1326:U:H2'	1:A:1327:C:C6	2.53	0.43
1:A:1372:U:H2'	1:A:1373:G:O4'	2.19	0.43
3:C:188:GLU:OE1	3:C:195:VAL:HG11	2.19	0.43
14:N:54:ASP:OD1	14:N:59:ARG:NH2	2.48	0.43
22:a:44:A:H2'	22:a:45:G:O4'	2.19	0.43
22:a:1632:A:H2'	22:a:1633:G:C8	2.53	0.43
43:v:32:LEU:HA	43:v:64:ASP:OD1	2.19	0.43
1:A:61:G:H2'	1:A:62:U:O4'	2.20	0.42
1:A:625:U:O2'	1:A:626:G:H5'	2.19	0.42
1:A:690:G:H2'	1:A:691:G:O4'	2.19	0.42
1:A:722:G:H2'	1:A:722:G:N3	2.34	0.42
2:B:70:VAL:HG11	2:B:96:TRP:HZ3	1.84	0.42
6:F:25:TYR:O	6:F:29:ILE:HG12	2.19	0.42
8:H:11:LEU:HD22	8:H:75:ILE:HD11	2.00	0.42
15:O:36:ILE:O	15:O:40:GLN:HG2	2.19	0.42
22:a:891:G:C2	22:a:892:A:N7	2.87	0.42
22:a:1178:C:O5'	22:a:1178:C:H6	2.01	0.42
22:a:1437:C:H2'	22:a:1438:U:C6	2.54	0.42
22:a:1478:G:H1	22:a:1513:U:H3	1.66	0.42
22:a:2335:A:OP1	35:n:13:ARG:NE	2.38	0.42
28:g:107:LEU:HD12	28:g:113:VAL:HG11	2.01	0.42
28:g:149:ARG:HG3	28:g:162:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Z:28:U:H2'	54:Z:29:C:H6	1.84	0.42
1:A:62:U:H2'	1:A:63:C:C6	2.54	0.42
1:A:76:G:H2'	1:A:77:A:C8	2.54	0.42
1:A:968:A:C8	1:A:1062:U:H4'	2.54	0.42
3:C:88:ARG:NH2	3:C:99:ALA:O	2.52	0.42
5:E:22:SER:HA	5:E:30:ILE:O	2.18	0.42
8:H:18:GLN:NE2	8:H:70:ALA:HB1	2.34	0.42
13:M:59:GLU:HA	13:M:62:LYS:NZ	2.34	0.42
22:a:883:G:N1	22:a:894:U:C2	2.88	0.42
22:a:1446:C:H2'	22:a:1447:C:H6	1.84	0.42
22:a:1637:A:H5'	22:a:1760:C:O2'	2.19	0.42
27:f:147:ASP:OD1	27:f:147:ASP:N	2.44	0.42
28:g:72:LEU:HD23	28:g:75:MET:SD	2.58	0.42
38:q:11:GLN:NE2	38:q:39:LEU:HG	2.29	0.42
2:B:203:ASN:OD1	2:B:204:ASP:N	2.52	0.42
3:C:23:PHE:CD2	10:J:97:ASP:HB2	2.55	0.42
5:E:50:TYR:H	5:E:66:LYS:NZ	2.18	0.42
22:a:184:C:H2'	22:a:185:G:H8	1.84	0.42
22:a:208:C:H2'	22:a:209:C:C6	2.54	0.42
22:a:2751:G:O4'	28:g:3:ARG:HD2	2.19	0.42
26:e:31:VAL:HG22	26:e:96:VAL:HG11	2.00	0.42
28:g:40:ALA:HA	28:g:58:TYR:HD2	1.84	0.42
55:V:28:C:H2'	55:V:29:A:H8	1.84	0.42
1:A:946:A:O2'	1:A:1333:A:N3	2.42	0.42
1:A:1170:A:H2'	1:A:1171:A:O4'	2.20	0.42
1:A:1309:G:OP2	13:M:98:ARG:NH2	2.45	0.42
2:B:105:LYS:HA	2:B:108:ARG:NH1	2.33	0.42
6:F:42:TRP:CZ2	6:F:61:LEU:HD13	2.54	0.42
11:K:32:VAL:O	11:K:44:TRP:HA	2.19	0.42
16:P:28:ARG:NE	16:P:29:ASN:OD1	2.41	0.42
21:U:33:ARG:HG2	21:U:34:ARG:HH22	1.84	0.42
22:a:151:C:H2'	22:a:152:A:H8	1.84	0.42
22:a:708:G:H2'	22:a:709:U:C6	2.54	0.42
22:a:1168:G:H2'	22:a:1169:A:H8	1.84	0.42
22:a:1414:C:H2'	22:a:1415:U:O4'	2.20	0.42
22:a:1874:C:H2'	22:a:1875:G:O4'	2.18	0.42
22:a:2335:A:P	35:n:13:ARG:HE	2.42	0.42
22:a:2562:U:OP1	31:j:40:LYS:NZ	2.44	0.42
26:e:111:GLU:HG2	32:k:1:MET:HB2	2.01	0.42
28:g:90:VAL:HG12	28:g:91:GLY:H	1.84	0.42
39:r:66:ILE:HA	39:r:69:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:V:37:12A:N1	55:V:37:12A:N	2.64	0.42
1:A:293:G:C6	1:A:294:U:C4	3.08	0.42
1:A:1250:A:H2'	1:A:1251:A:C8	2.55	0.42
3:C:73:PRO:HG3	3:C:105:GLU:HG2	2.00	0.42
15:O:60:VAL:HG11	22:a:715:A:C8	2.54	0.42
22:a:1870:C:O2'	22:a:1871:A:O4'	2.37	0.42
32:k:62:PRO:O	50:2:13:ARG:HG2	2.20	0.42
41:t:22:ARG:HD2	41:t:73:PHE:CD2	2.55	0.42
54:Z:69:C:H2'	54:Z:70:C:H6	1.84	0.42
1:A:167:A:H2'	1:A:168:G:H8	1.83	0.42
1:A:188:C:H2'	1:A:189:A:O4'	2.20	0.42
1:A:461:A:H2'	1:A:462:G:C8	2.53	0.42
1:A:701:U:OP1	1:A:702:A:O2'	2.27	0.42
3:C:22:TRP:CG	3:C:59:ARG:HD2	2.54	0.42
4:D:67:VAL:HG12	4:D:68:LEU:O	2.20	0.42
15:O:56:LEU:HD21	22:a:715:A:C2	2.53	0.42
16:P:45:GLU:C	16:P:47:GLU:H	2.27	0.42
22:a:222:A:C2	22:a:233:A:H5'	2.54	0.42
22:a:290:U:C2	22:a:350:G:O6	2.72	0.42
22:a:693:A:O2'	22:a:1353:A:N3	2.48	0.42
22:a:1263:U:OP1	47:z:13:ARG:NH1	2.53	0.42
23:b:51:G:H5'	35:n:63:LYS:NZ	2.35	0.42
28:g:17:VAL:HG12	28:g:26:ILE:HD12	2.02	0.42
29:h:34:GLY:C	29:h:36:ALA:H	2.28	0.42
1:A:150:U:H2'	1:A:151:A:H8	1.84	0.42
1:A:202:G:H1'	1:A:468:A:C2	2.55	0.42
1:A:1006:G:H1	1:A:1023:U:H3	1.67	0.42
2:B:6:MET:HE3	2:B:10:LEU:HD22	2.01	0.42
2:B:129:LEU:HD12	2:B:133:GLU:HB3	2.02	0.42
2:B:214:LEU:HA	2:B:217:VAL:HG22	2.01	0.42
7:G:17:LYS:HD3	7:G:44:TYR:CE1	2.55	0.42
9:I:30:ILE:HA	9:I:65:ILE:HB	2.02	0.42
22:a:518:G:H2'	22:a:519:U:C6	2.54	0.42
22:a:2028:U:H2'	22:a:2029:G:O4'	2.20	0.42
22:a:2443:C:OP1	26:e:63:LYS:HD3	2.19	0.42
30:i:31:GLU:OE2	30:i:34:ARG:NH1	2.45	0.42
36:o:14:LYS:HD2	36:o:77:HIS:HA	2.02	0.42
44:w:17:ASN:HB2	44:w:25:THR:OG1	2.20	0.42
45:x:2:LYS:HB3	45:x:52:ARG:HH21	1.83	0.42
45:x:14:LEU:HA	45:x:14:LEU:HD23	1.67	0.42
47:z:34:SER:OG	47:z:36:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:V:9:A:H5'	55:V:46:G7M:H1'	2.01	0.42
1:A:135:C:N3	16:P:1:MET:HB3	2.35	0.42
1:A:144:G:C6	1:A:145:G:C5	3.07	0.42
1:A:184:G:H2'	1:A:185:U:C6	2.55	0.42
1:A:303:A:H2'	1:A:304:U:O4'	2.20	0.42
1:A:1120:C:H2'	1:A:1121:U:C6	2.54	0.42
1:A:1163:A:H2'	1:A:1164:G:C8	2.54	0.42
1:A:1355:G:H2'	1:A:1356:G:C8	2.53	0.42
2:B:203:ASN:OD1	2:B:205:ASP:N	2.52	0.42
3:C:167:TRP:CZ3	3:C:169:ARG:HB2	2.55	0.42
6:F:3:HIS:CE1	6:F:65:GLU:HG2	2.55	0.42
22:a:1354:A:H2'	22:a:1355:G:O4'	2.20	0.42
26:e:124:PHE:HZ	26:e:138:LEU:HD11	1.84	0.42
28:g:103:ILE:HG22	28:g:105:LEU:HD22	2.02	0.42
39:r:65:ASP:OD1	39:r:65:ASP:N	2.53	0.42
47:z:52:ARG:O	47:z:54:VAL:HG13	2.20	0.42
50:2:11:ALA:HA	50:2:62:LEU:HD21	2.02	0.42
54:Z:36:A:H2'	54:Z:37:U:C6	2.55	0.42
1:A:865:A:H2'	1:A:866:C:C6	2.55	0.42
1:A:1023:U:H2'	1:A:1024:G:O4'	2.20	0.42
1:A:1175:G:H2'	1:A:1176:A:H8	1.84	0.42
2:B:187:VAL:O	2:B:201:PRO:HA	2.20	0.42
2:B:217:VAL:HA	2:B:220:THR:HG22	2.01	0.42
7:G:16:PRO:HG3	9:I:42:GLU:HG2	2.02	0.42
12:L:38:TYR:CE1	12:L:52:VAL:HG23	2.54	0.42
16:P:8:ARG:HB2	16:P:17:TYR:CE1	2.55	0.42
22:a:843:G:H2'	22:a:844:A:C8	2.54	0.42
22:a:1364:G:N2	22:a:1367:A:OP2	2.32	0.42
22:a:2816:G:N3	22:a:2883:A:O2'	2.46	0.42
24:c:145:GLU:HG2	24:c:151:GLY:C	2.45	0.42
28:g:99:LYS:O	28:g:102:VAL:HG22	2.20	0.42
40:s:31:VAL:HA	40:s:83:ALA:O	2.20	0.42
1:A:976:G:OP2	1:A:1358:U:O2'	2.36	0.42
1:A:1179:A:H2'	1:A:1180:A:O4'	2.20	0.42
4:D:11:LEU:HD13	4:D:63:ARG:HG2	2.02	0.42
6:F:47:LEU:HD13	6:F:51:ILE:HD13	2.01	0.42
7:G:93:PRO:HA	7:G:96:ARG:CD	2.50	0.42
22:a:453:A:N3	22:a:457:A:O2'	2.53	0.42
22:a:657:U:H2'	22:a:658:U:C6	2.55	0.42
22:a:1212:G:H1'	22:a:1237:A:N6	2.35	0.42
22:a:2365:G:N7	50:2:39:LYS:NZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:d:25:THR:HG21	25:d:193:VAL:HG22	2.01	0.42
26:e:88:ARG:HG3	26:e:88:ARG:NH2	2.33	0.42
28:g:105:LEU:HD12	28:g:107:LEU:HD21	2.02	0.42
39:r:88:ARG:HG3	39:r:94:ASP:OD2	2.19	0.42
51:3:15:LYS:NZ	51:3:26:ILE:HD11	2.35	0.42
1:A:53:A:H2'	1:A:54:C:O4'	2.19	0.41
1:A:953:G:H2'	1:A:954:G:O4'	2.20	0.41
1:A:1035:A:C4	1:A:1036:A:H2	2.37	0.41
1:A:1236:A:H2'	1:A:1237:C:C6	2.55	0.41
2:B:81:LYS:O	2:B:85:LEU:HD23	2.20	0.41
4:D:35:GLU:OE1	4:D:35:GLU:N	2.53	0.41
5:E:85:VAL:HG11	5:E:147:MET:HB3	2.02	0.41
5:E:96:MET:HE3	5:E:96:MET:HB2	1.87	0.41
15:O:64:ARG:HH12	15:O:89:ARG:HD2	1.85	0.41
22:a:358:U:C4	22:a:359:G:N7	2.88	0.41
22:a:612:G:O2'	22:a:614:A:N7	2.50	0.41
22:a:1149:G:H2'	22:a:1150:C:C6	2.55	0.41
22:a:1203:U:C4	22:a:1204:A:C5	3.09	0.41
22:a:1599:U:H2'	22:a:1600:C:C6	2.55	0.41
22:a:1902:C:H4'	24:c:242:LYS:O	2.19	0.41
22:a:2635:A:O2'	25:d:81:GLU:OE1	2.21	0.41
42:u:80:HIS:CG	42:u:81:PRO:HD2	2.55	0.41
52:4:33:ASN:C	52:4:34:LEU:HD12	2.44	0.41
1:A:406:G:N7	1:A:495:A:O2'	2.39	0.41
1:A:1071:C:H2'	1:A:1072:G:H8	1.85	0.41
1:A:1122:U:H2'	1:A:1123:U:C6	2.55	0.41
3:C:23:PHE:HA	10:J:13:PHE:CE2	2.55	0.41
6:F:8:PHE:CZ	6:F:60:VAL:HB	2.55	0.41
9:I:7:TYR:CG	9:I:8:GLY:N	2.87	0.41
19:S:20:GLU:OE2	19:S:21:LYS:HG3	2.19	0.41
22:a:413:C:H2'	22:a:414:C:C6	2.55	0.41
22:a:447:A:O2'	22:a:473:G:N7	2.46	0.41
22:a:2649:C:H2'	22:a:2650:U:C6	2.55	0.41
22:a:2884:U:H5	47:z:41:HIS:CD2	2.37	0.41
27:f:104:ILE:HD11	27:f:175:PHE:CE1	2.55	0.41
28:g:127:THR:HG22	28:g:128:GLN:N	2.33	0.41
39:r:13:SER:HB3	39:r:16:LYS:HD2	2.02	0.41
46:y:4:THR:HA	46:y:38:ARG:O	2.20	0.41
55:V:69:A:H2'	55:V:70:G:C8	2.55	0.41
1:A:244:U:O4	1:A:906:A:H1'	2.19	0.41
1:A:490:C:C2	1:A:491:G:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:A:H2'	1:A:677:U:C6	2.54	0.41
1:A:904:U:H2'	1:A:905:U:C6	2.55	0.41
1:A:1086:U:H3	1:A:1099:G:N2	2.09	0.41
1:A:1225:A:H2'	1:A:1226:C:C6	2.54	0.41
2:B:84:ALA:CB	2:B:91:PHE:HB3	2.50	0.41
6:F:76:THR:HG23	6:F:80:PHE:HE2	1.85	0.41
7:G:23:LEU:HD21	7:G:47:LEU:HD11	2.02	0.41
7:G:47:LEU:HB3	7:G:58:GLU:OE2	2.19	0.41
22:a:150:U:H2'	22:a:151:C:C6	2.56	0.41
22:a:682:G:H5'	49:1:26:ASN:CG	2.45	0.41
22:a:1802:A:H2'	22:a:1803:A:C8	2.55	0.41
24:c:41:GLY:O	24:c:43:ARG:HD2	2.19	0.41
25:d:157:LYS:HB2	25:d:157:LYS:HE3	1.82	0.41
31:j:71:ARG:HH21	31:j:104:THR:HG23	1.86	0.41
33:l:21:ALA:HB2	33:l:97:GLN:HB2	2.03	0.41
52:4:10:GLU:C	52:4:25:ARG:HG3	2.45	0.41
1:A:523:A:N6	12:L:89:D2T:OD2	2.44	0.41
1:A:1144:G:O2'	1:A:1145:A:H5'	2.20	0.41
5:E:37:THR:HG21	5:E:64:MET:HE2	2.03	0.41
10:J:37:ARG:HD2	10:J:37:ARG:HA	1.72	0.41
11:K:115:PRO:O	11:K:116:ILE:HD13	2.20	0.41
13:M:85:CYS:O	13:M:89:LEU:HD23	2.21	0.41
17:Q:13:VAL:HG23	17:Q:22:VAL:HG13	2.02	0.41
22:a:12:U:O2	22:a:2626:C:H4'	2.20	0.41
22:a:329:G:H1	41:t:17:LYS:HZ2	1.68	0.41
22:a:371:A:H61	22:a:401:A:H3'	1.84	0.41
22:a:2483:C:N3	33:l:123:LYS:NZ	2.65	0.41
22:a:2602:A:C6	54:Z:77:A:H4'	2.56	0.41
41:t:85:PHE:HE1	41:t:94:ARG:HG2	1.86	0.41
52:4:35:ASP:OD1	52:4:35:ASP:N	2.52	0.41
1:A:195:A:H2'	1:A:196:A:C8	2.55	0.41
1:A:298:A:H2'	1:A:299:G:C8	2.56	0.41
1:A:437:U:H3	1:A:495:A:H8	1.51	0.41
1:A:1342:C:H2'	1:A:1343:G:C8	2.55	0.41
2:B:140:GLU:HG3	2:B:144:LEU:HD13	2.03	0.41
9:I:72:ILE:H	9:I:72:ILE:HD12	1.85	0.41
10:J:21:ALA:HB1	10:J:92:LEU:HD12	2.03	0.41
22:a:321:U:O3'	26:e:162:ARG:NH1	2.50	0.41
22:a:1506:U:H2'	22:a:1507:C:H6	1.85	0.41
22:a:1747:U:H2'	22:a:1748:C:C6	2.55	0.41
22:a:2328:A:H2'	22:a:2329:U:H6	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2530:A:H62	28:g:172:LYS:NZ	2.18	0.41
30:i:57:LEU:HD23	30:i:57:LEU:HA	1.88	0.41
30:i:98:GLU:H	30:i:98:GLU:CD	2.28	0.41
34:m:71:ARG:HD2	34:m:71:ARG:HA	1.90	0.41
1:A:71:A:C4	1:A:72:A:C8	3.08	0.41
1:A:1039:G:H2'	1:A:1040:U:C6	2.55	0.41
1:A:1436:U:H2'	1:A:1437:A:H8	1.83	0.41
2:B:220:THR:O	2:B:223:GLU:HG2	2.20	0.41
9:I:67:VAL:HG21	9:I:75:GLN:HG3	2.02	0.41
22:a:277:G:H4'	22:a:278:A:C4	2.55	0.41
22:a:576:U:H2'	22:a:577:G:C8	2.55	0.41
22:a:833:A:H2'	22:a:834:G:C8	2.55	0.41
22:a:1715:G:N2	22:a:1744:A:OP2	2.39	0.41
26:e:48:THR:HG22	26:e:86:ALA:HB3	2.03	0.41
28:g:42:GLU:HB3	28:g:44:LYS:NZ	2.35	0.41
38:q:27:ILE:HG22	38:q:28:ALA:O	2.20	0.41
54:Z:3:C:H2'	54:Z:4:G:H8	1.85	0.41
1:A:101:A:C6	1:A:102:G:N7	2.89	0.41
1:A:678:U:H2'	1:A:679:C:H6	1.84	0.41
1:A:1035:A:C5	1:A:1036:A:H2	2.39	0.41
1:A:1264:U:H2'	1:A:1265:C:C6	2.56	0.41
1:A:1355:G:H2'	1:A:1356:G:H8	1.86	0.41
4:D:58:LYS:HD3	4:D:203:LEU:HD23	2.01	0.41
9:I:19:VAL:HG22	9:I:79:ILE:HD12	2.02	0.41
13:M:83:LEU:HD11	19:S:66:MET:HG3	2.02	0.41
15:O:32:LEU:HA	15:O:32:LEU:HD23	1.86	0.41
17:Q:60:GLU:O	17:Q:75:LEU:HD12	2.21	0.41
22:a:404:A:H1'	22:a:405:U:OP2	2.20	0.41
22:a:512:G:OP1	22:a:1234:U:O2'	2.34	0.41
22:a:612:G:C2	22:a:614:A:H5''	2.55	0.41
22:a:1407:G:H2'	22:a:1408:G:H8	1.86	0.41
22:a:2216:G:H2'	22:a:2217:G:C8	2.55	0.41
22:a:2900:A:H2'	22:a:2901:C:O4'	2.20	0.41
30:i:110:PRO:C	30:i:111:LYS:HD2	2.46	0.41
36:o:4:ILE:H	36:o:4:ILE:HD12	1.84	0.41
42:u:28:ALA:HB3	42:u:40:ILE:HG13	2.01	0.41
47:z:43:ILE:HG22	47:z:49:TYR:HB2	2.01	0.41
1:A:412:A:H3'	1:A:412:A:P	2.61	0.41
1:A:1123:U:O2'	1:A:1124:G:H5'	2.19	0.41
1:A:1478:U:H2'	1:A:1479:C:C6	2.56	0.41
1:A:1504:G:OP2	1:A:1507:A:O2'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:LEU:HB2	2:B:144:LEU:HD23	2.02	0.41
3:C:22:TRP:NE1	3:C:36:ASP:OD2	2.52	0.41
20:T:51:PHE:CD1	20:T:51:PHE:C	2.98	0.41
22:a:723:C:H2'	22:a:724:U:O4'	2.20	0.41
22:a:1387:A:H2'	22:a:1388:G:C8	2.56	0.41
22:a:1401:G:H2'	22:a:1402:U:O4'	2.21	0.41
22:a:1954:G:O2'	22:a:1956:U:O4	2.37	0.41
22:a:2591:C:H2'	22:a:2592:G:H8	1.85	0.41
31:j:76:VAL:HG12	36:o:73:VAL:HB	2.03	0.41
1:A:63:C:H4'	1:A:380:G:O2'	2.21	0.41
1:A:197:A:N1	1:A:220:G:O2'	2.46	0.41
1:A:371:A:H2'	1:A:372:C:O4'	2.21	0.41
1:A:396:C:H2'	1:A:397:A:H5''	2.02	0.41
1:A:481:G:O2'	1:A:483:C:N4	2.54	0.41
1:A:908:A:H2'	1:A:909:A:H8	1.84	0.41
1:A:1044:A:C5	1:A:1045:C:H1'	2.56	0.41
2:B:125:THR:C	2:B:127:ASP:H	2.28	0.41
4:D:159:LEU:HD23	4:D:175:ALA:HB1	2.02	0.41
7:G:57:SER:OG	7:G:60:GLU:HB2	2.21	0.41
8:H:22:LYS:HE2	8:H:22:LYS:HA	2.02	0.41
11:K:31:ILE:HG23	11:K:46:THR:HG22	2.01	0.41
13:M:40:ALA:HB3	13:M:43:VAL:HG23	2.03	0.41
13:M:66:GLU:OE2	13:M:66:GLU:N	2.52	0.41
16:P:1:MET:HE2	16:P:66:THR:HG21	2.02	0.41
19:S:80:TYR:CZ	19:S:82:GLY:HA2	2.56	0.41
22:a:182:A:H2'	22:a:183:C:C6	2.54	0.41
22:a:228:C:H4'	22:a:229:C:H5''	2.01	0.41
22:a:514:A:H2'	22:a:515:A:O4'	2.21	0.41
22:a:558:U:OP1	30:i:113:PRO:HD2	2.20	0.41
22:a:901:C:C4	22:a:902:C:C4	3.09	0.41
22:a:948:C:H1'	22:a:984:A:C8	2.56	0.41
22:a:1230:A:H2'	22:a:1231:U:O4'	2.21	0.41
22:a:1904:G:O2'	22:a:1928:A:N1	2.48	0.41
22:a:2011:U:OP1	39:r:42:LYS:NZ	2.38	0.41
22:a:2217:G:C6	22:a:2218:G:N7	2.89	0.41
22:a:2516:A:O2'	22:a:2517:C:H5'	2.21	0.41
23:b:1:U:H2'	23:b:2:G:C8	2.56	0.41
25:d:181:ASP:OD2	25:d:184:ARG:HG3	2.21	0.41
27:f:91:LEU:C	27:f:96:MET:HB2	2.46	0.41
28:g:52:PHE:HE1	28:g:72:LEU:HD12	1.86	0.41
28:g:90:VAL:HG12	28:g:91:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:o:88:ARG:NH2	36:o:112:GLU:HB2	2.35	0.41
39:r:110:ARG:HA	39:r:110:ARG:HD2	1.90	0.41
42:u:9:ARG:HA	42:u:41:GLU:OE2	2.21	0.41
51:3:26:ILE:O	51:3:26:ILE:HG13	2.19	0.41
55:V:63:C:H2'	55:V:64:U:C6	2.56	0.41
1:A:598:U:H4'	8:H:86:TYR:CG	2.55	0.41
1:A:939:G:N3	1:A:1375:A:H2	2.19	0.41
1:A:1127:G:H5'	1:A:1280:A:O2'	2.21	0.41
3:C:21:THR:HG22	3:C:21:THR:O	2.21	0.41
3:C:33:LEU:CD1	14:N:77:PHE:HB3	2.51	0.41
13:M:49:SER:N	13:M:52:GLN:OE1	2.33	0.41
18:R:24:LYS:O	18:R:26:ILE:HG12	2.21	0.41
22:a:247:G:H4'	22:a:386:G:C5	2.55	0.41
22:a:319:G:H2'	22:a:320:A:O4'	2.20	0.41
22:a:1730:C:O2'	22:a:1731:G:O4'	2.39	0.41
25:d:1:MET:HA	25:d:88:GLU:OE2	2.21	0.41
37:p:53:ARG:HH11	37:p:53:ARG:HD2	1.76	0.41
51:3:7:VAL:HG12	51:3:35:GLN:HB3	2.03	0.41
1:A:109:A:C6	1:A:326:G:C6	3.10	0.40
1:A:687:A:C2	1:A:704:A:C5	3.09	0.40
1:A:735:C:H5'	18:R:60:LYS:HD3	2.03	0.40
1:A:744:C:H2'	1:A:745:G:C8	2.56	0.40
2:B:74:ARG:NH2	21:U:69:ARG:HH12	2.19	0.40
6:F:10:VAL:HG12	6:F:11:HIS:O	2.22	0.40
6:F:52:ASN:O	6:F:53:LYS:HB2	2.21	0.40
13:M:3:ARG:NH1	52:4:35:ASP:OD2	2.53	0.40
22:a:157:C:H2'	22:a:158:U:O4'	2.22	0.40
22:a:1430:G:H2'	22:a:1431:A:O4'	2.21	0.40
22:a:1548:A:H2'	22:a:1549:A:H8	1.84	0.40
22:a:2690:U:O2'	22:a:2872:A:H1'	2.21	0.40
30:i:36:LEU:HD11	30:i:122:LEU:HB2	2.02	0.40
32:k:19:LEU:HD13	32:k:31:GLY:HA3	2.02	0.40
37:p:81:ASN:OD1	37:p:85:LYS:HE2	2.21	0.40
55:V:69:A:H2'	55:V:70:G:H8	1.85	0.40
1:A:1126:U:C5	10:J:7:ARG:NH1	2.88	0.40
1:A:1264:U:H2'	1:A:1265:C:H6	1.86	0.40
1:A:1486:G:H2'	1:A:1487:G:O4'	2.20	0.40
3:C:95:ALA:O	3:C:97:VAL:HG23	2.21	0.40
4:D:62:ARG:HH21	4:D:69:GLU:N	2.19	0.40
8:H:10:MET:HE2	8:H:10:MET:HB3	1.97	0.40
8:H:11:LEU:HD12	8:H:77:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:64:TYR:C	9:I:65:ILE:HD13	2.46	0.40
10:J:21:ALA:HA	10:J:24:GLU:OE2	2.22	0.40
10:J:54:SER:OG	10:J:57:VAL:O	2.39	0.40
22:a:183:C:N4	22:a:213:A:H61	2.18	0.40
22:a:617:G:OP1	26:e:102:ARG:NH2	2.54	0.40
22:a:709:U:H2'	22:a:710:U:C6	2.56	0.40
22:a:2096:C:H2'	22:a:2097:A:C8	2.56	0.40
23:b:75:G:H2'	23:b:76:G:O4'	2.21	0.40
27:f:42:GLU:N	27:f:42:GLU:CD	2.79	0.40
28:g:170:ARG:NH1	51:3:29:ALA:O	2.54	0.40
1:A:153:C:H2'	1:A:154:U:C6	2.56	0.40
1:A:190:A:H2'	1:A:191:G:O4'	2.22	0.40
1:A:300:A:H1'	1:A:565:U:O2	2.21	0.40
1:A:404:G:N7	4:D:2:ALA:HB3	2.36	0.40
1:A:562:U:O2'	12:L:13:ALA:O	2.17	0.40
1:A:1028:C:C4	1:A:1033:G:O6	2.75	0.40
3:C:40:ARG:O	3:C:44:THR:HG23	2.21	0.40
4:D:21:LEU:O	4:D:21:LEU:HD23	2.20	0.40
6:F:88:MET:CE	18:R:61:ARG:HG2	2.37	0.40
10:J:8:ILE:HB	10:J:74:VAL:CG1	2.52	0.40
12:L:7:LEU:HD23	12:L:7:LEU:HA	1.82	0.40
16:P:23:ASP:HB3	16:P:26:ASN:OD1	2.20	0.40
16:P:51:ARG:C	16:P:52:LEU:HD22	2.46	0.40
17:Q:28:PHE:CD1	17:Q:39:LYS:HG3	2.57	0.40
22:a:417:C:H2'	22:a:418:C:C6	2.57	0.40
22:a:1003:G:O2'	22:a:1010:A:N1	2.48	0.40
22:a:1182:G:H2'	22:a:1183:U:O4'	2.21	0.40
22:a:1881:C:H2'	22:a:1882:U:O4'	2.21	0.40
27:f:142:ASP:O	27:f:146:VAL:HG23	2.22	0.40
29:h:4:ILE:HD11	29:h:18:GLN:NE2	2.36	0.40
47:z:48:TYR:CZ	47:z:53:LYS:HD3	2.56	0.40
1:A:94:G:N2	1:A:97:G:O6	2.49	0.40
1:A:256:U:H2'	1:A:257:G:C8	2.56	0.40
1:A:612:C:H2'	1:A:613:C:H6	1.85	0.40
1:A:1279:G:OP1	10:J:9:ARG:NH2	2.55	0.40
4:D:8:LYS:HB3	4:D:21:LEU:CD2	2.52	0.40
5:E:154:ALA:HB2	5:E:164:ILE:HG13	2.02	0.40
7:G:23:LEU:HD12	7:G:23:LEU:HA	1.81	0.40
11:K:97:ILE:HG22	21:U:12:PHE:CZ	2.56	0.40
12:L:39:THR:HA	12:L:50:ARG:O	2.22	0.40
20:T:55:GLN:HA	20:T:58:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:397:U:H5''	44:w:32:ASN:HB2	2.03	0.40
22:a:973:A:H5'	22:a:1188:U:H1'	2.03	0.40
22:a:1289:C:H2'	22:a:1290:C:H6	1.87	0.40
28:g:19:ILE:HD13	28:g:43:VAL:HG13	2.03	0.40
33:l:20:LEU:HD23	33:l:20:LEU:HA	1.92	0.40
36:o:57:SER:O	36:o:76:THR:HG22	2.22	0.40
38:q:14:VAL:HB	38:q:98:ILE:CD1	2.51	0.40
39:r:19:LEU:HA	39:r:19:LEU:HD23	1.78	0.40
1:A:696:A:H2'	1:A:697:U:H6	1.86	0.40
1:A:1510:C:H2'	1:A:1511:G:H8	1.84	0.40
2:B:171:ILE:O	2:B:175:GLU:HG3	2.21	0.40
2:B:203:ASN:O	2:B:213:TYR:HE2	2.05	0.40
2:B:213:TYR:O	2:B:217:VAL:HG22	2.21	0.40
4:D:145:ILE:CD1	4:D:178:MET:HB3	2.39	0.40
9:I:36:GLU:HG3	9:I:45:ARG:NE	2.36	0.40
16:P:1:MET:O	16:P:3:THR:HG23	2.21	0.40
19:S:3:ARG:HD3	19:S:8:GLY:O	2.22	0.40
19:S:51:VAL:O	19:S:57:HIS:HA	2.22	0.40
22:a:308:G:H2'	22:a:309:A:C8	2.57	0.40
22:a:359:G:H2'	22:a:360:U:H6	1.86	0.40
22:a:2097:A:H2'	22:a:2098:U:H6	1.83	0.40
23:b:24:G:N7	23:b:56:G:H2'	2.36	0.40
24:c:115:GLN:O	24:c:125:LYS:NZ	2.52	0.40
25:d:32:ASN:HD22	25:d:52:THR:HB	1.85	0.40
35:n:9:ARG:O	35:n:12:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	202 (91%)	20 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	204/233 (88%)	188 (92%)	16 (8%)	0	100	100
4	D	203/206 (98%)	192 (95%)	11 (5%)	0	100	100
5	E	154/167 (92%)	146 (95%)	8 (5%)	0	100	100
6	F	101/135 (75%)	94 (93%)	7 (7%)	0	100	100
7	G	151/179 (84%)	139 (92%)	12 (8%)	0	100	100
8	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
9	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
10	J	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	12	26
11	K	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
12	L	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
13	M	113/118 (96%)	105 (93%)	8 (7%)	0	100	100
14	N	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
17	Q	77/84 (92%)	67 (87%)	10 (13%)	0	100	100
18	R	64/75 (85%)	58 (91%)	5 (8%)	1 (2%)	7	15
19	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
20	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
24	c	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
25	d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	44
26	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
27	f	175/179 (98%)	172 (98%)	3 (2%)	0	100	100
28	g	174/177 (98%)	156 (90%)	18 (10%)	0	100	100
29	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
30	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
31	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
32	k	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
33	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
34	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
35	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
37	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
38	q	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
39	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
40	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
41	t	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
42	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
43	v	82/85 (96%)	80 (98%)	2 (2%)	0	100	100
44	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
45	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
47	z	54/57 (95%)	54 (100%)	0	0	100	100
48	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	7	15
51	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
52	4	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
All	All	5487/5913 (93%)	5203 (95%)	280 (5%)	4 (0%)	49	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL
25	d	149	ASN
18	R	23	TYR
50	2	32	ILE

### 5.3.2 Protein sidechains ⓘ

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	89/98 (91%)	87 (98%)	2 (2%)	45	70
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	71 (99%)	1 (1%)	59	80
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
24	c	216/218 (99%)	216 (100%)	0	100	100
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	137/138 (99%)	137 (100%)	0	100	100
29	h	32/114 (28%)	32 (100%)	0	100	100
30	i	116/116 (100%)	116 (100%)	0	100	100
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	107/107 (100%)	107 (100%)	0	100	100
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100
39	r	93/93 (100%)	93 (100%)	0	100	100
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	83 (100%)	0	100	100
42	u	78/78 (100%)	78 (100%)	0	100	100
43	v	62/63 (98%)	62 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	54 (100%)	0	100	100
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100
48	0	46/49 (94%)	46 (100%)	0	100	100
49	1	38/38 (100%)	38 (100%)	0	100	100
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	55/62 (89%)	55 (100%)	0	100	100
All	All	4576/4825 (95%)	4573 (100%)	3 (0%)	87	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	57	LYS
11	K	59	THR
19	S	58	VAL

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

Mol	Chain	Res	Type
2	B	58	ASN
2	B	122	GLN
2	B	168	HIS
3	C	3	GLN
3	C	139	GLN
4	D	152	GLN

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Mol	Chain	Res	Type
5	E	70	ASN
7	G	52	GLN
7	G	148	ASN
9	I	31	ASN
9	I	110	GLN
11	K	40	ASN
12	L	75	GLN
13	M	8	ASN
14	N	49	GLN
15	O	62	GLN
19	S	53	ASN
20	T	48	GLN
21	U	64	ASN
24	c	25	HIS
24	c	53	HIS
24	c	143	ASN
25	d	173	GLN
26	e	115	GLN
27	f	5	HIS
28	g	64	GLN
30	i	86	GLN
33	l	60	GLN
35	n	100	HIS
36	o	15	GLN
37	p	81	ASN
38	q	11	GLN
40	s	48	GLN
41	t	69	ASN
42	u	12	GLN
43	v	76	ASN
44	w	17	ASN
45	x	45	GLN
46	y	49	ASN
50	2	28	ASN
52	4	65	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1542 (97%)	259 (17%)	5 (0%)
22	a	2757/2904 (94%)	374 (13%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	b	118/120 (98%)	13 (11%)	0
53	X	10/35 (28%)	1 (10%)	0
54	Z	76/77 (98%)	13 (17%)	0
55	V	68/76 (89%)	12 (17%)	1 (1%)
All	All	4537/4754 (95%)	672 (14%)	6 (0%)

All (672) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	6	G
1	A	15	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	44	A
1	A	47	C
1	A	48	C
1	A	51	A
1	A	55	A
1	A	56	U
1	A	59	A
1	A	60	A
1	A	64	G
1	A	66	A
1	A	71	A
1	A	72	A
1	A	74	A
1	A	80	A
1	A	93	U
1	A	94	G
1	A	95	C
1	A	116	A
1	A	121	U
1	A	130	A
1	A	131	A
1	A	141	G
1	A	144	G
1	A	146	G
1	A	156	C
1	A	162	A
1	A	164	G

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Mol	Chain	Res	Type
1	A	170	U
1	A	173	U
1	A	181	A
1	A	183	C
1	A	197	A
1	A	199	A
1	A	200	G
1	A	204	G
1	A	216	U
1	A	218	U
1	A	225	C
1	A	228	A
1	A	245	U
1	A	247	G
1	A	251	G
1	A	262	A
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	293	G
1	A	306	A
1	A	321	A
1	A	328	C
1	A	330	C
1	A	345	C
1	A	352	C
1	A	354	G
1	A	357	G
1	A	367	U
1	A	369	G
1	A	372	C
1	A	375	U
1	A	380	G
1	A	381	C
1	A	389	A
1	A	390	U
1	A	391	G
1	A	392	C
1	A	397	A
1	A	406	G
1	A	411	A

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Mol	Chain	Res	Type
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	439	U
1	A	450	G
1	A	457	G
1	A	458	U
1	A	464	U
1	A	465	A
1	A	466	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	479	U
1	A	481	G
1	A	484	G
1	A	485	U
1	A	486	U
1	A	495	A
1	A	496	A
1	A	497	G
1	A	499	A
1	A	506	G
1	A	509	A
1	A	511	C
1	A	512	U
1	A	518	C
1	A	526	C
1	A	528	C
1	A	532	A
1	A	547	A
1	A	559	A
1	A	564	C
1	A	566	G
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	C

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Mol	Chain	Res	Type
1	A	577	G
1	A	579	A
1	A	596	A
1	A	626	G
1	A	639	G
1	A	650	G
1	A	653	U
1	A	665	A
1	A	687	A
1	A	702	A
1	A	705	G
1	A	721	G
1	A	722	G
1	A	733	G
1	A	734	G
1	A	746	A
1	A	748	G
1	A	755	G
1	A	758	C
1	A	759	A
1	A	777	A
1	A	787	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	818	G
1	A	821	G
1	A	828	U
1	A	832	G
1	A	851	G
1	A	872	A
1	A	873	A
1	A	884	U
1	A	887	G
1	A	890	G
1	A	902	G
1	A	914	A
1	A	921	U
1	A	926	G
1	A	934	C
1	A	935	A

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Mol	Chain	Res	Type
1	A	960	U
1	A	961	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	988	G
1	A	993	G
1	A	997	U
1	A	1003	G
1	A	1004	A
1	A	1008	U
1	A	1009	U
1	A	1010	U
1	A	1020	G
1	A	1027	C
1	A	1028	C
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1035	A
1	A	1036	A
1	A	1042	A
1	A	1044	A
1	A	1064	G
1	A	1065	U
1	A	1071	C
1	A	1081	A
1	A	1084	G
1	A	1085	U
1	A	1094	G
1	A	1099	G
1	A	1101	A
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1139	G
1	A	1159	U

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Mol	Chain	Res	Type
1	A	1167	A
1	A	1168	U
1	A	1169	A
1	A	1176	A
1	A	1196	A
1	A	1197	A
1	A	1211	U
1	A	1213	A
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1256	A
1	A	1257	A
1	A	1258	G
1	A	1260	G
1	A	1275	A
1	A	1279	G
1	A	1280	A
1	A	1282	C
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1323	G
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1364	U
1	A	1368	A
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1382	C
1	A	1383	C
1	A	1394	A
1	A	1396	A
1	A	1397	C

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Mol	Chain	Res	Type
1	A	1419	G
1	A	1429	A
1	A	1432	G
1	A	1441	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1487	G
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
22	a	10	A
22	a	15	G
22	a	34	U
22	a	51	G
22	a	52	A
22	a	58	G
22	a	63	A
22	a	71	A
22	a	72	U
22	a	74	A
22	a	75	G
22	a	101	A
22	a	102	U
22	a	103	A
22	a	114	U
22	a	118	A
22	a	119	A
22	a	120	U
22	a	127	A
22	a	139	U
22	a	140	C
22	a	142	A
22	a	162	U
22	a	163	C
22	a	164	C
22	a	181	A

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Mol	Chain	Res	Type
22	a	196	A
22	a	199	A
22	a	215	G
22	a	216	A
22	a	222	A
22	a	223	A
22	a	233	A
22	a	248	G
22	a	272	A
22	a	274	C
22	a	275	C
22	a	277	G
22	a	278	A
22	a	279	A
22	a	281	C
22	a	282	A
22	a	285	G
22	a	287	G
22	a	294	A
22	a	304	U
22	a	311	A
22	a	329	G
22	a	330	A
22	a	331	C
22	a	334	C
22	a	335	C
22	a	345	A
22	a	362	A
22	a	383	C
22	a	386	G
22	a	396	G
22	a	405	U
22	a	411	G
22	a	425	G
22	a	445	C
22	a	454	A
22	a	456	C
22	a	473	G
22	a	477	A
22	a	480	A
22	a	481	G
22	a	491	G

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Mol	Chain	Res	Type
22	a	496	G
22	a	501	A
22	a	503	A
22	a	505	A
22	a	508	A
22	a	509	C
22	a	522	A
22	a	529	A
22	a	530	G
22	a	531	C
22	a	532	A
22	a	544	C
22	a	546	U
22	a	547	A
22	a	548	G
22	a	549	G
22	a	563	A
22	a	568	U
22	a	573	U
22	a	575	A
22	a	592	A
22	a	600	G
22	a	603	A
22	a	613	A
22	a	614	A
22	a	615	U
22	a	618	G
22	a	620	G
22	a	627	A
22	a	637	A
22	a	645	C
22	a	647	G
22	a	653	U
22	a	654	A
22	a	659	G
22	a	685	A
22	a	686	U
22	a	717	C
22	a	721	A
22	a	730	A
22	a	747	5MU
22	a	775	G

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Mol	Chain	Res	Type
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	791	C
22	a	805	G
22	a	811	U
22	a	812	C
22	a	827	U
22	a	828	U
22	a	845	A
22	a	846	U
22	a	847	U
22	a	859	G
22	a	866	A
22	a	884	U
22	a	888	C
22	a	891	G
22	a	892	A
22	a	895	U
22	a	896	A
22	a	897	C
22	a	899	A
22	a	902	C
22	a	907	G
22	a	910	A
22	a	915	C
22	a	916	G
22	a	931	U
22	a	932	U
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	989	G
22	a	996	A
22	a	997	G
22	a	1006	C
22	a	1012	U
22	a	1013	C
22	a	1018	U
22	a	1022	G

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Mol	Chain	Res	Type
22	a	1033	U
22	a	1040	A
22	a	1047	G
22	a	1108	U
22	a	1111	A
22	a	1112	G
22	a	1116	G
22	a	1122	G
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1141	U
22	a	1142	A
22	a	1157	G
22	a	1169	A
22	a	1204	A
22	a	1212	G
22	a	1236	G
22	a	1250	G
22	a	1253	A
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1273	U
22	a	1275	A
22	a	1286	A
22	a	1289	C
22	a	1300	G
22	a	1301	A
22	a	1315	C
22	a	1321	A
22	a	1327	A
22	a	1328	A
22	a	1329	U
22	a	1331	G
22	a	1337	G
22	a	1345	C
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1410	G

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Mol	Chain	Res	Type
22	a	1416	G
22	a	1427	A
22	a	1428	C
22	a	1452	G
22	a	1453	A
22	a	1460	U
22	a	1482	G
22	a	1493	C
22	a	1497	U
22	a	1508	A
22	a	1510	G
22	a	1515	A
22	a	1523	U
22	a	1524	G
22	a	1529	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1560	G
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1586	A
22	a	1608	A
22	a	1626	A
22	a	1634	A
22	a	1647	U
22	a	1648	U
22	a	1674	G
22	a	1713	A
22	a	1715	G
22	a	1729	U
22	a	1730	C
22	a	1738	G
22	a	1744	A
22	a	1757	A
22	a	1764	C
22	a	1773	A

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Mol	Chain	Res	Type
22	a	1782	U
22	a	1786	A
22	a	1800	C
22	a	1801	A
22	a	1807	G
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1842	G
22	a	1847	A
22	a	1848	A
22	a	1858	A
22	a	1865	U
22	a	1866	A
22	a	1871	A
22	a	1872	A
22	a	1906	G
22	a	1913	A
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1965	C
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2021	C
22	a	2023	C
22	a	2027	G
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M

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Mol	Chain	Res	Type
22	a	2190	G
22	a	2191	A
22	a	2198	A
22	a	2199	A
22	a	2203	U
22	a	2204	G
22	a	2210	U
22	a	2211	A
22	a	2212	A
22	a	2225	A
22	a	2238	G
22	a	2239	G
22	a	2283	C
22	a	2287	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2341	G
22	a	2345	G
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2371	G
22	a	2377	A
22	a	2378	A
22	a	2383	G
22	a	2385	C
22	a	2402	U
22	a	2403	C
22	a	2404	U
22	a	2406	A
22	a	2410	G
22	a	2419	U
22	a	2424	C
22	a	2425	A
22	a	2429	G
22	a	2430	A
22	a	2435	A
22	a	2441	U
22	a	2447	G

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Mol	Chain	Res	Type
22	a	2448	A
22	a	2475	C
22	a	2476	A
22	a	2478	A
22	a	2482	A
22	a	2491	U
22	a	2501	C
22	a	2502	G
22	a	2505	G
22	a	2518	A
22	a	2525	G
22	a	2529	G
22	a	2547	A
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2582	G
22	a	2586	U
22	a	2602	A
22	a	2609	U
22	a	2613	U
22	a	2629	U
22	a	2630	G
22	a	2661	G
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2716	C
22	a	2726	A
22	a	2733	A
22	a	2739	U
22	a	2744	G
22	a	2748	A
22	a	2750	A
22	a	2752	C
22	a	2757	A
22	a	2765	A
22	a	2777	G
22	a	2778	A
22	a	2797	U
22	a	2798	U
22	a	2799	A

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Mol	Chain	Res	Type
22	a	2801	G
22	a	2820	A
22	a	2821	A
22	a	2835	A
22	a	2849	U
22	a	2873	A
22	a	2879	A
22	a	2880	C
22	a	2884	U
22	a	2885	G
22	a	2898	U
22	a	2899	A
23	b	13	G
23	b	35	C
23	b	42	C
23	b	44	G
23	b	53	A
23	b	56	G
23	b	67	G
23	b	89	U
23	b	90	C
23	b	92	C
23	b	99	A
23	b	105	G
23	b	109	A
53	X	17	A
54	Z	9	G
54	Z	17	C
54	Z	18	U
54	Z	19	G
54	Z	20	G
54	Z	22	A
54	Z	23	G
54	Z	47	A
54	Z	48	U
54	Z	49	C
54	Z	54	G
54	Z	68	C
54	Z	77	A
55	V	2	C
55	V	5	G
55	V	6	2MG

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Mol	Chain	Res	Type
55	V	8	U
55	V	11	C
55	V	19	G
55	V	47	H2U
55	V	48	5MC
55	V	49	5MC
55	V	64	U
55	V	74	C
55	V	75	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	758	C
1	A	817	C
1	A	1026	G
1	A	1034	G
1	A	1035	A
55	V	10	2MG

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	5MU	a	747	22	19,22,23	4.53	7 (36%)	28,32,35	3.79	10 (35%)
22	PSU	a	2605	22	18,21,22	1.08	1 (5%)	22,30,33	1.77	2 (9%)
1	2MG	A	1207	1	23,26,27	2.56	6 (26%)	32,38,41	2.19	9 (28%)
12	D2T	L	89	12	7,9,10	1.04	0	6,11,13	1.21	1 (16%)
22	2MG	a	1835	22	23,26,27	2.49	7 (30%)	32,38,41	2.19	9 (28%)
1	2MG	A	966	1	23,26,27	2.52	6 (26%)	32,38,41	2.25	10 (31%)
22	6MZ	a	2030	22	23,25,26	2.59	4 (17%)	29,36,39	2.51	10 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	2MG	V	6	55	23,26,27	2.66	7 (30%)	32,38,41	2.20	9 (28%)
55	2MG	V	10	55	23,26,27	2.59	6 (26%)	32,38,41	2.19	10 (31%)
55	12A	V	37	56,55	33,36,37	1.06	2 (6%)	47,52,55	1.30	4 (8%)
11	IAS	K	119	11	6,7,8	0.97	0	6,8,10	1.42	2 (33%)
55	H2U	V	47	55	18,21,22	1.04	2 (11%)	21,30,33	0.74	0
22	OMC	a	2498	56,22	19,22,23	2.67	7 (36%)	26,31,34	0.92	1 (3%)
25	MEQ	d	150	25	8,9,10	1.19	0	5,10,12	1.09	0
54	OMC	Z	33	54	19,22,23	2.74	7 (36%)	26,31,34	0.75	0
54	PSU	Z	56	54	18,21,22	1.05	1 (5%)	22,30,33	1.67	3 (13%)
54	4SU	Z	8	54	18,21,22	3.98	8 (44%)	26,30,33	2.37	5 (19%)
22	G7M	a	2069	22	23,26,27	2.65	9 (39%)	35,39,42	1.83	11 (31%)
55	A1L4U	V	34	53,55	20,25,26	0.89	2 (10%)	30,35,38	1.31	3 (10%)
1	2MG	A	1516	1	23,26,27	2.51	7 (30%)	32,38,41	2.03	10 (31%)
1	MA6	A	1518	1	23,26,27	1.48	5 (21%)	34,38,41	2.30	10 (29%)
55	PSU	V	39	55	18,21,22	1.11	1 (5%)	22,30,33	1.78	4 (18%)
33	MS6	l	82	33	5,7,8	1.24	1 (20%)	2,7,9	1.89	1 (50%)
54	5MU	Z	55	54	19,22,23	4.52	6 (31%)	28,32,35	3.80	9 (32%)
1	5MC	A	1407	1	18,22,23	3.39	7 (38%)	26,32,35	1.12	2 (7%)
55	2MU	V	54	55	20,23,24	1.41	5 (25%)	28,33,36	2.01	9 (32%)
22	5MU	a	1939	22	19,22,23	4.48	7 (36%)	28,32,35	3.79	9 (32%)
22	PSU	a	1911	22	18,21,22	1.06	1 (5%)	22,30,33	1.98	5 (22%)
22	2MG	a	2445	22	23,26,27	2.47	7 (30%)	32,38,41	2.14	9 (28%)
22	PSU	a	2580	22	18,21,22	1.19	2 (11%)	22,30,33	2.01	6 (27%)
22	OMG	a	2251	54,22	23,26,27	2.58	9 (39%)	33,38,41	2.03	8 (24%)
1	4OC	A	1402	56,1	20,23,24	2.85	8 (40%)	26,32,35	1.09	3 (11%)
22	6MZ	a	1618	22	23,25,26	2.54	4 (17%)	29,36,39	2.42	12 (41%)
22	3TD	a	1915	22	18,22,23	3.95	7 (38%)	22,32,35	1.71	2 (9%)
1	UR3	A	1498	1	19,22,23	2.62	6 (31%)	26,32,35	1.43	3 (11%)
22	PSU	a	2504	22	18,21,22	1.11	2 (11%)	22,30,33	1.70	4 (18%)
22	OMU	a	2552	22	19,22,23	2.62	6 (31%)	26,31,34	1.84	5 (19%)
55	PSU	V	27	55	18,21,22	1.03	1 (5%)	22,30,33	1.74	3 (13%)
55	5MC	V	48	55	18,22,23	3.67	8 (44%)	26,32,35	0.96	1 (3%)
55	PSU	V	55	55	18,21,22	1.01	1 (5%)	22,30,33	1.88	4 (18%)
1	PSU	A	516	56,1	18,21,22	1.08	2 (11%)	22,30,33	1.82	5 (22%)
22	1MG	a	745	22	22,26,27	2.45	7 (31%)	33,39,42	1.67	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	4D4	l	81	33	9,11,12	1.55	1 (11%)	8,13,15	2.14	3 (37%)
22	PSU	a	2604	22	18,21,22	1.05	1 (5%)	22,30,33	1.90	4 (18%)
55	1MA	V	58	55	21,25,26	0.72	0	31,37,40	0.76	0
22	5MC	a	1962	22	18,22,23	3.46	7 (38%)	26,32,35	1.14	2 (7%)
22	2MA	a	2503	56,22	22,25,26	3.74	10 (45%)	33,37,40	2.85	9 (27%)
1	G7M	A	527	1	23,26,27	2.71	8 (34%)	35,39,42	1.76	9 (25%)
55	5MC	V	49	55	18,22,23	3.62	8 (44%)	26,32,35	1.01	2 (7%)
22	PSU	a	955	22	18,21,22	1.12	1 (5%)	22,30,33	1.74	2 (9%)
1	MA6	A	1519	1	23,26,27	1.52	5 (21%)	34,38,41	2.27	10 (29%)
22	H2U	a	2449	22	18,21,22	1.23	2 (11%)	21,30,33	0.85	1 (4%)
55	G7M	V	46	55	23,26,27	2.78	8 (34%)	35,39,42	1.69	9 (25%)
54	H2U	Z	21	54	18,21,22	1.05	2 (11%)	21,30,33	1.27	4 (19%)
22	PSU	a	2457	22	18,21,22	1.20	3 (16%)	22,30,33	1.96	4 (18%)
22	PSU	a	1917	22	18,21,22	1.07	2 (11%)	22,30,33	2.01	5 (22%)
22	PSU	a	746	56,22	18,21,22	1.16	3 (16%)	22,30,33	1.56	2 (9%)
1	5MC	A	967	1	18,22,23	3.60	8 (44%)	26,32,35	0.99	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
12	D2T	L	89	12	-	2/7/12/14	-
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
1	2MG	A	966	1	-	2/9/27/28	0/3/3/3
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
55	2MG	V	6	55	-	2/9/27/28	0/3/3/3
55	2MG	V	10	55	-	0/9/27/28	0/3/3/3
55	12A	V	37	56,55	-	4/25/43/44	0/3/3/3
11	IAS	K	119	11	-	0/7/7/8	-
55	H2U	V	47	55	-	7/7/38/39	0/2/2/2
22	OMC	a	2498	56,22	-	0/9/27/28	0/2/2/2
25	MEQ	d	150	25	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	OMC	Z	33	54	-	0/9/27/28	0/2/2/2
54	PSU	Z	56	54	-	0/7/25/26	0/2/2/2
54	4SU	Z	8	54	-	0/7/25/26	0/2/2/2
22	G7M	a	2069	22	-	1/7/25/26	0/3/3/3
55	A1L4U	V	34	53,55	-	2/13/31/32	0/2/2/2
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
55	PSU	V	39	55	-	0/7/25/26	0/2/2/2
33	MS6	l	82	33	-	0/4/6/8	-
54	5MU	Z	55	54	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
55	2MU	V	54	55	-	0/9/27/28	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	2MG	a	2445	22	-	0/9/27/28	0/3/3/3
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
22	OMG	a	2251	54,22	-	0/9/27/28	0/3/3/3
1	4OC	A	1402	56,1	-	0/9/29/30	0/2/2/2
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
22	PSU	a	2504	22	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
55	PSU	V	27	55	-	0/7/25/26	0/2/2/2
55	5MC	V	48	55	-	2/7/25/26	0/2/2/2
55	PSU	V	55	55	-	0/7/25/26	0/2/2/2
1	PSU	A	516	56,1	-	0/7/25/26	0/2/2/2
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
33	4D4	l	81	33	-	3/11/12/14	-
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
55	1MA	V	58	55	-	0/7/25/26	0/3/3/3
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
22	2MA	a	2503	56,22	-	2/7/25/26	0/3/3/3
1	G7M	A	527	1	-	3/7/25/26	0/3/3/3
55	5MC	V	49	55	-	3/7/25/26	0/2/2/2
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	2/11/29/30	0/3/3/3
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
55	G7M	V	46	55	-	0/7/25/26	0/3/3/3
54	H2U	Z	21	54	-	3/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
22	PSU	a	746	56,22	-	1/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2

All (261) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C6-C5	11.87	1.49	1.35
22	a	2503	2MA	C4-N3	11.52	1.48	1.34
22	a	2030	6MZ	C6-N6	10.48	1.45	1.34
22	a	1618	6MZ	C6-N6	10.46	1.45	1.34
54	Z	55	5MU	C6-N1	10.34	1.55	1.38
22	a	747	5MU	C6-N1	10.22	1.55	1.38
22	a	1939	5MU	C6-N1	10.16	1.55	1.38
54	Z	55	5MU	C2-N1	9.83	1.54	1.38
22	a	747	5MU	C2-N1	9.47	1.53	1.38
22	a	1939	5MU	C2-N1	9.37	1.53	1.38
55	V	48	5MC	C6-C5	9.27	1.49	1.34
54	Z	8	4SU	C4-N3	9.16	1.47	1.37
1	A	967	5MC	C6-C5	9.15	1.49	1.34
22	a	1962	5MC	C6-C5	9.05	1.49	1.34
55	V	49	5MC	C6-C5	9.04	1.49	1.34
54	Z	55	5MU	C4-C5	8.99	1.59	1.44
1	A	1407	5MC	C6-C5	8.89	1.49	1.34
22	a	747	5MU	C4-C5	8.82	1.59	1.44
22	a	1939	5MU	C4-C5	8.35	1.58	1.44
22	a	1915	3TD	C2-N1	8.29	1.48	1.37
22	a	1939	5MU	C4-N3	-8.10	1.23	1.38
22	a	747	5MU	C4-N3	-7.92	1.24	1.38
55	V	6	2MG	C2-N3	7.75	1.46	1.31
55	V	10	2MG	C2-N3	7.55	1.46	1.31
54	Z	55	5MU	C4-N3	-7.54	1.24	1.38
1	A	1207	2MG	C2-N3	7.35	1.46	1.31
1	A	966	2MG	C2-N3	7.26	1.45	1.31
54	Z	8	4SU	C2-N1	7.10	1.49	1.38
55	V	48	5MC	C4-N3	7.02	1.46	1.34
55	V	49	5MC	C4-N3	7.01	1.46	1.34
22	a	1835	2MG	C2-N3	6.91	1.45	1.31
1	A	1516	2MG	C2-N3	6.90	1.45	1.31
22	a	2251	OMG	C4-N3	6.86	1.50	1.34
22	a	2503	2MA	C2-N3	6.83	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C4-N3	6.76	1.45	1.34
22	a	2445	2MG	C2-N3	6.69	1.44	1.31
1	A	1207	2MG	C4-N3	6.62	1.50	1.34
1	A	1498	UR3	C2-N1	6.59	1.48	1.38
55	V	6	2MG	C4-N3	6.53	1.49	1.34
55	V	10	2MG	C4-N3	6.48	1.49	1.34
54	Z	8	4SU	C2-N3	6.44	1.49	1.38
55	V	46	G7M	C2-N2	6.39	1.49	1.34
22	a	1962	5MC	C4-N3	6.39	1.44	1.34
55	V	49	5MC	C2-N3	6.35	1.49	1.36
1	A	1402	4OC	C4-N3	6.32	1.43	1.32
55	V	46	G7M	C4-N3	6.25	1.49	1.34
55	V	48	5MC	C2-N3	6.22	1.49	1.36
1	A	527	G7M	C4-N3	6.21	1.49	1.34
1	A	967	5MC	C2-N3	6.14	1.48	1.36
1	A	966	2MG	C4-N3	6.13	1.48	1.34
1	A	1516	2MG	C4-N3	6.12	1.48	1.34
22	a	1939	5MU	C6-C5	6.10	1.44	1.34
54	Z	55	5MU	C6-C5	6.09	1.44	1.34
22	a	747	5MU	C6-C5	6.05	1.44	1.34
1	A	527	G7M	C2-N2	6.05	1.48	1.34
22	a	2552	OMU	C2-N1	6.02	1.48	1.38
1	A	1407	5MC	C4-N3	5.99	1.44	1.34
22	a	2069	G7M	C2-N2	5.97	1.48	1.34
22	a	1835	2MG	C4-N3	5.95	1.48	1.34
54	Z	33	OMC	C2-N3	5.89	1.48	1.36
22	a	2069	G7M	C4-N3	5.87	1.48	1.34
22	a	2445	2MG	C4-N3	5.87	1.48	1.34
1	A	1498	UR3	C6-C5	5.80	1.48	1.35
22	a	2503	2MA	C2-N1	5.77	1.44	1.34
54	Z	8	4SU	C6-C5	5.75	1.48	1.35
1	A	1402	4OC	C6-C5	5.71	1.48	1.35
22	a	1962	5MC	C2-N3	5.69	1.47	1.36
22	a	745	1MG	C4-N3	5.62	1.47	1.34
54	Z	8	4SU	C4-S4	-5.52	1.57	1.68
1	A	1407	5MC	C2-N3	5.51	1.47	1.36
54	Z	33	OMC	C6-C5	5.50	1.47	1.35
55	V	46	G7M	C2-N3	5.46	1.46	1.33
22	a	1915	3TD	C6-N1	5.44	1.45	1.36
22	a	2552	OMU	C2-N3	5.42	1.47	1.38
1	A	527	G7M	C2-N3	5.39	1.46	1.33
22	a	2498	OMC	C2-N3	5.39	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2552	OMU	C6-C5	5.38	1.47	1.35
22	a	2498	OMC	C6-C5	5.35	1.47	1.35
22	a	745	1MG	C2-N2	5.34	1.43	1.34
22	a	2503	2MA	C6-N6	-5.33	1.20	1.34
1	A	1402	4OC	C2-N3	5.24	1.47	1.36
22	a	2251	OMG	C2-N3	5.12	1.45	1.33
22	a	745	1MG	C2-N3	5.11	1.43	1.34
55	V	48	5MC	C6-N1	5.09	1.46	1.38
22	a	2069	G7M	C5-N7	-4.99	1.33	1.39
22	a	2503	2MA	C5-C6	4.88	1.54	1.41
55	V	6	2MG	C2-N1	4.88	1.44	1.36
1	A	967	5MC	C6-N1	4.86	1.46	1.38
55	V	49	5MC	C6-N1	4.81	1.46	1.38
54	Z	8	4SU	C5-C4	4.76	1.48	1.42
22	a	2069	G7M	C2-N3	4.73	1.44	1.33
55	V	10	2MG	C2-N1	4.67	1.44	1.36
22	a	2251	OMG	C2-N2	4.63	1.45	1.34
22	a	1962	5MC	C6-N1	4.60	1.45	1.38
1	A	1407	5MC	C6-N1	4.58	1.45	1.38
54	Z	33	OMC	C4-N3	4.53	1.43	1.34
55	V	46	G7M	C5-N7	-4.51	1.33	1.39
54	Z	33	OMC	C4-N4	4.50	1.44	1.33
1	A	527	G7M	C5-N7	-4.47	1.34	1.39
22	a	2498	OMC	C4-N4	4.46	1.44	1.33
1	A	1498	UR3	C2-N3	4.45	1.47	1.39
1	A	966	2MG	C2-N1	4.41	1.43	1.36
1	A	1516	2MG	C2-N1	4.36	1.43	1.36
22	a	1835	2MG	C2-N1	4.30	1.43	1.36
1	A	1207	2MG	C2-N1	4.16	1.43	1.36
22	a	2498	OMC	C2-N1	4.13	1.49	1.40
1	A	1402	4OC	C4-N4	4.05	1.44	1.35
55	V	49	5MC	C4-N4	4.01	1.44	1.34
55	V	48	5MC	C4-N4	4.01	1.44	1.34
22	a	2498	OMC	C4-N3	4.00	1.42	1.34
22	a	1915	3TD	C2-N3	4.00	1.47	1.38
1	A	967	5MC	C2-N1	3.94	1.48	1.40
22	a	2445	2MG	C2-N1	3.94	1.43	1.36
55	V	48	5MC	C2-N1	3.90	1.48	1.40
1	A	967	5MC	C4-N4	3.90	1.44	1.34
22	a	2251	OMG	C5-N7	-3.89	1.31	1.39
22	a	1962	5MC	C4-N4	3.81	1.44	1.34
55	V	46	G7M	C5-C6	3.81	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C2-N1	3.78	1.48	1.40
54	Z	33	OMC	C2-N1	3.77	1.48	1.40
22	a	2503	2MA	C5-N7	-3.75	1.31	1.39
1	A	527	G7M	C5-C6	3.73	1.53	1.43
22	a	2251	OMG	O6-C6	-3.73	1.16	1.23
22	a	2445	2MG	C5-N7	-3.70	1.31	1.39
1	A	1407	5MC	C4-N4	3.69	1.43	1.34
22	a	745	1MG	C5-N7	-3.65	1.32	1.39
22	a	1835	2MG	C5-N7	-3.65	1.32	1.39
55	V	49	5MC	C2-N1	3.62	1.47	1.40
1	A	1518	MA6	C5-C4	-3.59	1.32	1.39
1	A	1519	MA6	C5-C4	-3.55	1.32	1.39
1	A	966	2MG	C5-N7	-3.51	1.32	1.39
54	Z	8	4SU	O2-C2	-3.50	1.16	1.23
22	a	2552	OMU	O2-C2	-3.48	1.16	1.23
1	A	1516	2MG	C5-N7	-3.39	1.32	1.39
22	a	2069	G7M	C5-C6	3.35	1.52	1.43
55	V	37	12A	CA-C	3.35	1.57	1.52
1	A	1402	4OC	O2-C2	-3.30	1.17	1.23
22	a	2503	2MA	C6-N1	3.30	1.39	1.35
22	a	2552	OMU	O4-C4	-3.29	1.18	1.24
22	a	2030	6MZ	C5-C4	-3.28	1.32	1.39
1	A	1402	4OC	C5-C4	3.26	1.47	1.40
54	Z	56	PSU	C6-C5	3.25	1.39	1.35
55	V	6	2MG	C5-N7	-3.25	1.32	1.39
55	V	39	PSU	C6-C5	3.24	1.39	1.35
1	A	1407	5MC	C2-N1	3.24	1.47	1.40
22	a	2069	G7M	O6-C6	-3.23	1.17	1.23
33	l	81	4D4	OB-CB	-3.22	1.36	1.43
22	a	1618	6MZ	C5-C4	-3.20	1.33	1.39
22	a	2498	OMC	O2-C2	-3.19	1.17	1.23
22	a	2449	H2U	C2-N3	-3.16	1.32	1.38
22	a	2449	H2U	C4-N3	-3.15	1.32	1.37
1	A	1518	MA6	C5-N7	-3.13	1.33	1.39
55	V	10	2MG	C5-N7	-3.11	1.33	1.39
1	A	1407	5MC	O2-C2	-3.10	1.18	1.23
54	Z	33	OMC	O2-C2	-3.08	1.18	1.23
22	a	1962	5MC	C2-N1	3.08	1.46	1.40
1	A	1519	MA6	C6-N6	3.06	1.45	1.36
22	a	2445	2MG	O6-C6	-3.06	1.17	1.23
22	a	1962	5MC	O2-C2	-3.02	1.18	1.23
22	a	2504	PSU	C6-C5	3.01	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C5-N7	-2.99	1.33	1.39
55	V	27	PSU	C6-C5	2.98	1.38	1.35
22	a	2030	6MZ	C5-N7	-2.98	1.33	1.39
1	A	1519	MA6	C5-N7	-2.98	1.33	1.39
22	a	747	5MU	O2-C2	-2.97	1.17	1.23
55	V	46	G7M	C2-N1	2.93	1.44	1.37
22	a	1835	2MG	O6-C6	-2.90	1.18	1.23
1	A	1518	MA6	C8-N9	-2.89	1.32	1.37
22	a	745	1MG	C4-N9	-2.88	1.30	1.38
22	a	1939	5MU	O2-C2	-2.88	1.17	1.23
1	A	1518	MA6	C6-N6	2.85	1.45	1.36
54	Z	8	4SU	C6-N1	2.85	1.44	1.38
55	V	55	PSU	C6-C5	2.84	1.38	1.35
55	V	46	G7M	C6-N1	2.84	1.44	1.38
1	A	1498	UR3	O2-C2	-2.84	1.17	1.22
1	A	527	G7M	O6-C6	-2.83	1.18	1.23
54	Z	21	H2U	C2-N3	-2.82	1.32	1.38
1	A	1516	2MG	O6-C6	-2.81	1.18	1.23
22	a	2030	6MZ	C8-N9	-2.81	1.32	1.37
1	A	1498	UR3	O4-C4	-2.81	1.17	1.23
22	a	2498	OMC	C6-N1	2.80	1.44	1.38
1	A	1207	2MG	O6-C6	-2.79	1.18	1.23
55	V	54	2MU	C4-N3	-2.78	1.33	1.38
1	A	1519	MA6	C8-N9	-2.78	1.32	1.37
22	a	745	1MG	O6-C6	-2.71	1.17	1.23
1	A	527	G7M	C2-N1	2.70	1.44	1.37
22	a	745	1MG	C5-C6	2.70	1.52	1.45
55	V	47	H2U	C2-N3	-2.70	1.33	1.38
1	A	1498	UR3	C6-N1	2.70	1.44	1.38
33	l	82	MS6	CB-CA	2.69	1.57	1.53
22	a	955	PSU	C6-C5	2.69	1.38	1.35
1	A	516	PSU	C6-C5	2.67	1.38	1.35
1	A	1402	4OC	C6-N1	2.67	1.44	1.38
22	a	746	PSU	C6-C5	2.66	1.38	1.35
55	V	47	H2U	C4-N3	-2.66	1.33	1.37
22	a	2445	2MG	C4-N9	-2.65	1.31	1.38
22	a	1618	6MZ	C5-N7	-2.65	1.34	1.39
1	A	966	2MG	O6-C6	-2.65	1.18	1.23
55	V	54	2MU	C2-N1	2.61	1.42	1.38
55	V	46	G7M	O6-C6	-2.61	1.18	1.23
1	A	1516	2MG	C4-N9	-2.60	1.31	1.38
54	Z	21	H2U	C4-N3	-2.60	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Z	33	OMC	C6-N1	2.59	1.44	1.38
22	a	1618	6MZ	C8-N9	-2.55	1.32	1.37
1	A	527	G7M	C6-N1	2.53	1.43	1.38
22	a	1911	PSU	C6-C5	2.53	1.38	1.35
22	a	1939	5MU	O4-C4	-2.51	1.18	1.23
22	a	1915	3TD	O4-C4	-2.51	1.17	1.23
22	a	2580	PSU	C6-C5	2.50	1.38	1.35
55	V	10	2MG	C5-C6	2.50	1.53	1.44
22	a	2457	PSU	C6-C5	2.50	1.38	1.35
1	A	967	5MC	O2-C2	-2.49	1.19	1.23
22	a	2251	OMG	C8-N9	-2.47	1.32	1.37
22	a	2552	OMU	C4-N3	2.47	1.43	1.38
22	a	1917	PSU	C6-C5	2.46	1.38	1.35
55	V	49	5MC	O2-C2	-2.46	1.19	1.23
1	A	1519	MA6	C4-N9	-2.44	1.32	1.37
22	a	2251	OMG	C5-C6	2.44	1.53	1.44
22	a	2605	PSU	C6-C5	2.42	1.38	1.35
55	V	6	2MG	C6-N1	2.42	1.43	1.38
55	V	48	5MC	O2-C2	-2.41	1.19	1.23
55	V	6	2MG	C5-C6	2.41	1.53	1.44
22	a	747	5MU	O4-C4	-2.37	1.19	1.23
22	a	1915	3TD	C4-N3	2.37	1.45	1.40
22	a	1835	2MG	C5-C6	2.36	1.53	1.44
1	A	1207	2MG	C5-C6	2.33	1.53	1.44
55	V	10	2MG	O6-C6	-2.33	1.19	1.23
22	a	2604	PSU	C6-C5	2.31	1.38	1.35
22	a	746	PSU	C4-C5	-2.30	1.37	1.44
22	a	2069	G7M	C2-N1	2.30	1.43	1.37
1	A	1516	2MG	C5-C6	2.29	1.52	1.44
54	Z	55	5MU	O2-C2	-2.27	1.18	1.23
1	A	966	2MG	C5-C6	2.26	1.52	1.44
22	a	2445	2MG	C5-C6	2.25	1.52	1.44
22	a	1915	3TD	O2-C2	-2.25	1.18	1.23
55	V	54	2MU	C6-C5	2.22	1.38	1.34
22	a	2251	OMG	C4-N9	-2.21	1.32	1.38
1	A	516	PSU	C4-C5	-2.21	1.37	1.44
22	a	1835	2MG	C4-N9	-2.20	1.32	1.38
22	a	2503	2MA	CM2-C2	2.20	1.56	1.49
55	V	6	2MG	O6-C6	-2.20	1.19	1.23
55	V	54	2MU	C2-N3	-2.18	1.34	1.38
22	a	2580	PSU	O4'-C1'	-2.17	1.40	1.43
22	a	2503	2MA	C8-N9	-2.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	54	2MU	C4-C5	2.16	1.48	1.44
55	V	49	5MC	CM5-C5	2.16	1.56	1.50
1	A	1518	MA6	C4-N9	-2.15	1.32	1.37
22	a	2457	PSU	C4-C5	-2.15	1.38	1.44
22	a	2069	G7M	C6-N1	2.09	1.42	1.38
55	V	34	A1L4U	C5M-C8	2.07	1.54	1.51
22	a	2457	PSU	O4'-C1'	-2.07	1.41	1.43
55	V	48	5MC	CM5-C5	2.07	1.55	1.50
1	A	967	5MC	CM5-C5	2.06	1.55	1.50
55	V	37	12A	CC-N6	2.06	1.41	1.37
22	a	1917	PSU	O4'-C1'	-2.05	1.41	1.43
22	a	2069	G7M	C4-N9	-2.05	1.32	1.38
22	a	746	PSU	O4'-C1'	-2.04	1.41	1.43
55	V	34	A1L4U	O9-C8	2.04	1.39	1.33
22	a	2503	2MA	C5-C4	-2.02	1.35	1.39
22	a	2251	OMG	C2-N1	2.02	1.42	1.37
22	a	2504	PSU	C4-C5	-2.01	1.38	1.44

All (297) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	1939	5MU	C5-C4-N3	12.91	126.33	115.31
54	Z	55	5MU	C5-C4-N3	12.51	125.99	115.31
22	a	747	5MU	C5-C4-N3	12.14	125.67	115.31
54	Z	55	5MU	C5-C6-N1	-11.00	112.02	123.34
22	a	747	5MU	C5-C6-N1	-10.59	112.44	123.34
22	a	1939	5MU	C5-C6-N1	-10.48	112.56	123.34
22	a	2503	2MA	C5-C4-N3	-8.68	117.43	127.19
54	Z	8	4SU	C4-N3-C2	-8.17	119.40	127.34
22	a	1835	2MG	C2-N3-C4	6.63	120.26	112.04
1	A	966	2MG	C2-N3-C4	6.51	120.11	112.04
22	a	2445	2MG	C2-N3-C4	6.50	120.10	112.04
22	a	2503	2MA	C4-N9-C1'	-6.47	111.17	126.59
55	V	6	2MG	C2-N3-C4	6.38	119.95	112.04
22	a	2503	2MA	C1'-N9-C8	6.38	141.54	127.14
55	V	10	2MG	C2-N3-C4	6.32	119.88	112.04
1	A	1207	2MG	C2-N3-C4	6.08	119.58	112.04
22	a	2503	2MA	N3-C4-N9	6.01	135.33	126.99
1	A	1518	MA6	N1-C2-N3	-5.93	119.33	128.60
22	a	2251	OMG	C5-C4-N3	-5.89	118.90	128.46
22	a	2552	OMU	C4-N3-C2	-5.79	118.94	126.58
1	A	1516	2MG	C2-N3-C4	5.78	119.21	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2030	6MZ	N1-C2-N3	-5.73	119.64	128.60
1	A	966	2MG	C5-C4-N3	-5.70	119.22	128.46
22	a	1915	3TD	N1-C2-N3	5.63	120.58	116.14
1	A	1519	MA6	N1-C2-N3	-5.61	119.82	128.60
55	V	6	2MG	C5-C4-N3	-5.53	119.49	128.46
55	V	34	A1L4U	O9-C8-C5M	5.49	121.44	111.27
22	a	1618	6MZ	C5-C4-N3	-5.49	119.59	126.75
22	a	1939	5MU	O4-C4-C5	-5.46	118.57	124.90
22	a	1618	6MZ	N1-C2-N3	-5.41	120.14	128.60
22	a	1835	2MG	C5-C4-N3	-5.41	119.69	128.46
22	a	2030	6MZ	C5-C4-N3	-5.40	119.70	126.75
22	a	2457	PSU	N1-C2-N3	5.36	121.20	115.13
22	a	2030	6MZ	C9-N6-C6	-5.32	118.29	122.87
22	a	1939	5MU	C4-N3-C2	-5.30	120.49	127.35
22	a	1911	PSU	N1-C2-N3	5.29	121.13	115.13
1	A	1207	2MG	C5-C4-N3	-5.25	119.94	128.46
22	a	747	5MU	C4-N3-C2	-5.21	120.61	127.35
22	a	1917	PSU	N1-C2-N3	5.20	121.02	115.13
54	Z	55	5MU	C4-N3-C2	-5.18	120.64	127.35
22	a	2580	PSU	N1-C2-N3	5.14	120.96	115.13
1	A	1498	UR3	C4-N3-C2	-5.14	119.72	124.56
22	a	1911	PSU	C4-N3-C2	-5.10	119.00	126.34
55	V	10	2MG	C5-C4-N3	-5.08	120.21	128.46
22	a	1917	PSU	C4-N3-C2	-5.04	119.08	126.34
22	a	2604	PSU	C4-N3-C2	-5.00	119.14	126.34
22	a	2604	PSU	N1-C2-N3	4.99	120.78	115.13
22	a	2580	PSU	C4-N3-C2	-4.98	119.17	126.34
54	Z	8	4SU	C5-C4-N3	4.97	119.30	114.69
55	V	55	PSU	N1-C2-N3	4.96	120.75	115.13
22	a	2445	2MG	C5-C4-N3	-4.94	120.44	128.46
1	A	966	2MG	C2-N1-C6	-4.94	118.80	124.48
22	a	747	5MU	O4-C4-C5	-4.94	119.18	124.90
1	A	1519	MA6	N9-C8-N7	-4.87	107.26	113.91
22	a	747	5MU	N3-C2-N1	4.86	121.34	114.89
1	A	516	PSU	C4-N3-C2	-4.86	119.34	126.34
22	a	2457	PSU	C4-N3-C2	-4.85	119.36	126.34
1	A	1207	2MG	C2-N1-C6	-4.81	118.95	124.48
22	a	1939	5MU	N3-C2-N1	4.80	121.26	114.89
22	a	955	PSU	C4-N3-C2	-4.80	119.43	126.34
22	a	2069	G7M	C2-N3-C4	4.78	120.81	112.30
54	Z	55	5MU	O4-C4-C5	-4.77	119.37	124.90
1	A	1518	MA6	C5-C4-N3	-4.77	120.53	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	V	54	2MU	N3-C2-N1	4.74	121.18	114.89
1	A	1518	MA6	N9-C8-N7	-4.73	107.44	113.91
22	a	2605	PSU	C4-N3-C2	-4.67	119.60	126.34
22	a	2504	PSU	C4-N3-C2	-4.65	119.64	126.34
1	A	1519	MA6	C2-N1-C6	4.64	122.71	111.75
55	V	39	PSU	C4-N3-C2	-4.64	119.66	126.34
55	V	55	PSU	C4-N3-C2	-4.63	119.66	126.34
55	V	39	PSU	N1-C2-N3	4.62	120.36	115.13
22	a	2605	PSU	N1-C2-N3	4.60	120.35	115.13
55	V	27	PSU	C4-N3-C2	-4.59	119.72	126.34
55	V	37	12A	CA-N-CC	-4.57	114.33	121.94
22	a	1835	2MG	C2-N1-C6	-4.55	119.24	124.48
22	a	2251	OMG	C2-N3-C4	4.55	120.41	112.30
22	a	955	PSU	N1-C2-N3	4.53	120.26	115.13
22	a	747	5MU	C5M-C5-C6	-4.47	116.88	122.85
54	Z	56	PSU	C4-N3-C2	-4.43	119.96	126.34
22	a	745	1MG	C5-C4-N3	-4.43	121.28	128.46
1	A	1518	MA6	C4-C5-C6	4.39	120.79	115.88
1	A	1518	MA6	C2-N1-C6	4.38	122.11	111.75
22	a	2030	6MZ	N9-C8-N7	-4.38	107.92	113.91
22	a	1618	6MZ	N9-C8-N7	-4.38	107.93	113.91
1	A	516	PSU	N1-C2-N3	4.37	120.08	115.13
22	a	2504	PSU	N1-C2-N3	4.37	120.08	115.13
1	A	1516	2MG	C5-C4-N3	-4.36	121.39	128.46
22	a	2251	OMG	N9-C4-N3	4.36	134.69	125.94
55	V	6	2MG	C2-N1-C6	-4.33	119.50	124.48
55	V	27	PSU	N1-C2-N3	4.31	120.02	115.13
22	a	2552	OMU	N3-C2-N1	4.29	120.59	114.89
54	Z	55	5MU	C5M-C5-C6	-4.29	117.12	122.85
54	Z	55	5MU	N3-C2-N1	4.29	120.59	114.89
1	A	1519	MA6	C4-C5-C6	4.29	120.68	115.88
1	A	1519	MA6	C5-C4-N3	-4.28	121.17	126.75
55	V	46	G7M	C2-N3-C4	4.24	119.85	112.30
54	Z	8	4SU	N3-C2-N1	4.23	120.51	114.89
22	a	746	PSU	C4-N3-C2	-4.23	120.24	126.34
55	V	54	2MU	C4-N3-C2	-4.22	121.89	127.35
54	Z	56	PSU	N1-C2-N3	4.21	119.90	115.13
22	a	2069	G7M	C5-C6-N1	4.19	120.55	111.79
55	V	10	2MG	C2-N1-C6	-4.19	119.66	124.48
22	a	747	5MU	C5M-C5-C4	4.18	123.37	118.77
1	A	527	G7M	C2-N3-C4	4.18	119.75	112.30
22	a	2445	2MG	C2-N1-C6	-4.16	119.69	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Z	8	4SU	C5-C4-S4	-4.13	119.15	124.47
22	a	1618	6MZ	C9-N6-C6	-4.12	119.32	122.87
22	a	1962	5MC	C5-C6-N1	-4.12	119.10	123.34
22	a	1915	3TD	C4-N3-C2	-4.09	120.17	124.61
54	Z	55	5MU	C5M-C5-C4	4.03	123.21	118.77
22	a	746	PSU	N1-C2-N3	3.98	119.64	115.13
1	A	527	G7M	C5-C6-N1	3.95	120.03	111.79
55	V	46	G7M	C5-C6-N1	3.92	119.97	111.79
55	V	6	2MG	N9-C4-N3	3.92	133.80	125.94
55	V	54	2MU	C5-C4-N3	3.86	118.60	115.31
22	a	2552	OMU	C5-C4-N3	3.82	120.55	114.84
22	a	2030	6MZ	C4-C5-C6	3.80	119.75	116.81
1	A	527	G7M	C5-C4-N3	-3.77	120.91	128.15
1	A	1518	MA6	C5-N7-C8	3.76	108.85	103.51
22	a	2030	6MZ	C2-N3-C4	3.75	120.61	111.75
1	A	1519	MA6	C5-N7-C8	3.74	108.82	103.51
1	A	1207	2MG	N9-C4-N3	3.73	133.43	125.94
33	l	81	4D4	NE-CZ-NH2	3.73	127.25	120.70
22	a	1618	6MZ	C2-N3-C4	3.71	120.51	111.75
22	a	2069	G7M	C5-C4-N3	-3.70	121.05	128.15
55	V	46	G7M	C5-C4-N3	-3.69	121.08	128.15
22	a	1618	6MZ	C4-C5-C6	3.68	119.66	116.81
22	a	745	1MG	C2-N3-C4	3.66	120.21	111.98
22	a	2251	OMG	C2-N1-C6	-3.66	118.43	125.10
1	A	1516	2MG	C2-N1-C6	-3.65	120.28	124.48
1	A	966	2MG	N9-C4-N3	3.62	133.21	125.94
22	a	2503	2MA	N9-C8-N7	-3.62	108.97	113.91
1	A	1407	5MC	C5-C6-N1	-3.60	119.63	123.34
22	a	1835	2MG	N9-C4-N3	3.54	133.05	125.94
22	a	2445	2MG	N9-C8-N7	-3.52	106.77	113.39
1	A	1516	2MG	N9-C8-N7	-3.44	106.91	113.39
55	V	10	2MG	N9-C8-N7	-3.43	106.92	113.39
1	A	1518	MA6	C2-N3-C4	3.42	119.83	111.75
55	V	49	5MC	C5-C6-N1	-3.38	119.86	123.34
54	Z	21	H2U	C4-N3-C2	-3.38	122.99	125.79
55	V	10	2MG	N9-C4-N3	3.36	132.68	125.94
22	a	1939	5MU	C5M-C5-C6	-3.32	118.42	122.85
1	A	527	G7M	O6-C6-C5	-3.31	120.59	128.06
55	V	55	PSU	O2-C2-N1	-3.31	119.14	122.79
22	a	2030	6MZ	C5-N7-C8	3.31	108.21	103.51
55	V	48	5MC	C5-C6-N1	-3.30	119.95	123.34
55	V	54	2MU	O4-C4-C5	-3.29	121.08	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	745	1MG	N9-C8-N7	-3.28	107.21	113.39
22	a	1939	5MU	C5M-C5-C4	3.27	122.37	118.77
22	a	1618	6MZ	C5-N7-C8	3.27	108.16	103.51
22	a	2069	G7M	O6-C6-C5	-3.26	120.70	128.06
1	A	527	G7M	CN7-N7-C5	3.25	130.81	126.77
22	a	2445	2MG	N9-C4-N3	3.24	132.45	125.94
55	V	46	G7M	O6-C6-C5	-3.24	120.75	128.06
1	A	1207	2MG	N9-C8-N7	-3.23	107.32	113.39
55	V	6	2MG	N9-C8-N7	-3.21	107.35	113.39
22	a	2580	PSU	O2-C2-N1	-3.18	119.28	122.79
22	a	747	5MU	O2-C2-N1	-3.18	118.56	122.79
22	a	2251	OMG	N9-C8-N7	-3.14	107.48	113.39
22	a	2503	2MA	N3-C2-N1	-3.14	119.95	125.72
22	a	1618	6MZ	N3-C4-N9	3.13	132.24	127.08
22	a	1939	5MU	O2-C2-N1	-3.13	118.62	122.79
1	A	1519	MA6	C2-N3-C4	3.12	119.12	111.75
1	A	967	5MC	C5-C6-N1	-3.11	120.14	123.34
1	A	527	G7M	N9-C4-N3	3.09	132.14	125.94
22	a	1917	PSU	O2-C2-N1	-3.07	119.41	122.79
22	a	1835	2MG	N9-C8-N7	-3.07	107.61	113.39
1	A	1207	2MG	C5-C6-N1	3.05	120.93	113.19
55	V	46	G7M	C2-N1-C6	-3.04	119.55	125.10
1	A	527	G7M	C2-N1-C6	-3.03	119.57	125.10
55	V	54	2MU	C5M-C5-C4	3.03	122.10	118.77
22	a	2503	2MA	C5-N7-C8	3.03	107.81	103.51
22	a	2251	OMG	C5-C6-N1	3.02	120.87	113.19
1	A	966	2MG	N9-C8-N7	-3.02	107.70	113.39
1	A	1519	MA6	C4-C5-N7	-3.01	106.95	110.62
22	a	2503	2MA	C6-C5-C4	3.01	121.23	117.18
33	l	81	4D4	CB-CA-C	-2.93	107.10	111.77
22	a	2030	6MZ	N3-C4-N9	2.92	131.90	127.08
55	V	39	PSU	O2-C2-N1	-2.91	119.58	122.79
54	Z	55	5MU	O2-C2-N1	-2.88	118.95	122.79
22	a	2251	OMG	O6-C6-C5	-2.87	118.98	126.60
54	Z	55	5MU	O4-C4-N3	-2.86	114.64	120.12
22	a	2069	G7M	C2-N1-C6	-2.86	119.89	125.10
22	a	2069	G7M	N9-C4-N3	2.81	131.58	125.94
1	A	1207	2MG	O6-C6-C5	-2.81	119.15	126.60
1	A	966	2MG	C5-C6-N1	2.80	120.30	113.19
22	a	2445	2MG	C5-C6-N1	2.77	120.23	113.19
55	V	10	2MG	C5-C6-N1	2.75	120.18	113.19
1	A	1518	MA6	C4-C5-N7	-2.74	107.29	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Z	8	4SU	O2-C2-N1	-2.72	119.17	122.79
22	a	1835	2MG	C5-C6-N1	2.72	120.10	113.19
22	a	745	1MG	C5-C6-N1	2.71	120.15	114.91
22	a	1962	5MC	CM5-C5-C6	-2.71	119.23	122.85
55	V	55	PSU	C6-N1-C2	-2.71	119.92	122.68
55	V	6	2MG	O6-C6-C5	-2.70	119.44	126.60
22	a	2457	PSU	C6-N1-C2	-2.70	119.93	122.68
33	l	82	MS6	CE-SD-CG	2.66	109.55	100.40
1	A	966	2MG	O6-C6-C5	-2.66	119.54	126.60
55	V	46	G7M	N9-C4-N3	2.64	131.23	125.94
22	a	2069	G7M	CN7-N7-C5	2.63	130.04	126.77
1	A	1518	MA6	N3-C4-N9	2.63	131.41	127.08
1	A	1516	2MG	N9-C4-N3	2.63	131.21	125.94
22	a	1939	5MU	O4-C4-N3	-2.62	115.09	120.12
1	A	1516	2MG	C5-C6-N1	2.60	119.80	113.19
22	a	747	5MU	O4-C4-N3	-2.59	115.15	120.12
55	V	27	PSU	O2-C2-N1	-2.57	119.96	122.79
22	a	2445	2MG	N1-C2-N3	-2.56	119.99	123.95
22	a	2457	PSU	O2-C2-N1	-2.55	119.98	122.79
1	A	1402	4OC	O2-C2-N3	-2.55	118.19	122.33
1	A	1407	5MC	CM5-C5-C6	-2.53	119.47	122.85
55	V	6	2MG	C5-C6-N1	2.52	119.60	113.19
1	A	1516	2MG	N1-C2-N3	-2.52	120.05	123.95
33	l	81	4D4	O-C-CA	-2.49	118.25	124.78
1	A	527	G7M	CN7-N7-C8	-2.49	120.99	124.84
22	a	1917	PSU	C6-C5-C4	2.49	119.94	118.20
22	a	2552	OMU	O4-C4-C5	-2.49	120.79	125.16
12	L	89	D2T	O-C-CA	-2.48	118.28	124.78
55	V	10	2MG	N1-C2-N3	-2.47	120.13	123.95
22	a	2580	PSU	O4'-C1'-C2'	2.47	108.63	105.14
22	a	2030	6MZ	C4-C5-N7	-2.46	107.62	110.62
1	A	1519	MA6	C4-N9-C8	2.46	108.39	105.73
55	V	37	12A	N6-CC-N	2.45	117.18	113.76
22	a	2498	OMC	O2-C2-N3	-2.44	118.37	122.33
1	A	1498	UR3	C6-N1-C2	-2.43	119.61	121.79
1	A	1518	MA6	C4-N9-C8	2.43	108.36	105.73
54	Z	21	H2U	C5-C6-N1	-2.42	103.63	111.61
55	V	54	2MU	C6-N1-C2	-2.42	118.84	121.30
55	V	37	12A	OG1-CB-CA	2.41	113.97	109.13
1	A	1519	MA6	C5-C4-N9	2.40	108.58	105.78
22	a	1911	PSU	O2-C2-N1	-2.39	120.16	122.79
55	V	10	2MG	C8-N7-C5	2.38	108.54	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2069	G7M	N9-C8-N7	-2.36	106.38	112.21
22	a	2604	PSU	O2-C2-N1	-2.36	120.20	122.79
22	a	1835	2MG	O6-C6-C5	-2.35	120.35	126.60
55	V	54	2MU	O2-C2-N3	-2.35	117.13	121.50
1	A	516	PSU	O4'-C1'-C2'	2.34	108.45	105.14
22	a	745	1MG	C1'-N9-C8	-2.33	120.06	126.70
22	a	2445	2MG	C8-N7-C5	2.33	108.45	104.24
22	a	1835	2MG	C8-N7-C5	2.32	108.44	104.24
22	a	2069	G7M	N1-C2-N3	-2.32	118.99	123.32
1	A	1516	2MG	C1'-N9-C4	-2.32	119.61	126.50
55	V	39	PSU	C6-N1-C2	-2.32	120.31	122.68
1	A	1516	2MG	O6-C6-C5	-2.32	120.45	126.60
22	a	1618	6MZ	C4-C5-N7	-2.31	107.80	110.62
11	K	119	IAS	OXT-C-CA	2.31	121.25	113.38
54	Z	56	PSU	O2-C2-N1	-2.31	120.25	122.79
55	V	6	2MG	N1-C2-N3	-2.31	120.38	123.95
1	A	1498	UR3	C1'-N1-C2	2.30	120.87	116.99
22	a	2604	PSU	C6-N1-C2	-2.29	120.34	122.68
55	V	6	2MG	C8-N7-C5	2.29	108.38	104.24
22	a	1835	2MG	N1-C2-N3	-2.29	120.42	123.95
22	a	2552	OMU	O2-C2-N1	-2.28	119.75	122.79
22	a	1917	PSU	C6-N1-C2	-2.26	120.37	122.68
22	a	1911	PSU	C6-N1-C2	-2.25	120.39	122.68
22	a	2030	6MZ	C5-C4-N9	2.25	108.40	105.78
22	a	745	1MG	N9-C4-N3	2.25	130.45	125.94
22	a	2503	2MA	CM2-C2-N3	2.23	120.64	117.15
55	V	46	G7M	N9-C8-N7	-2.23	106.70	112.21
55	V	46	G7M	CN7-N7-C5	2.23	129.53	126.77
22	a	1911	PSU	C6-C5-C4	2.22	119.75	118.20
1	A	1402	4OC	CM4-N4-C4	-2.22	118.12	122.45
1	A	966	2MG	C8-N7-C5	2.21	108.25	104.24
22	a	2445	2MG	O6-C6-C5	-2.21	120.74	126.60
1	A	516	PSU	O2-C2-N1	-2.21	120.36	122.79
22	a	745	1MG	C8-N7-C5	2.20	108.23	104.24
1	A	1516	2MG	C8-N7-C5	2.20	108.22	104.24
55	V	49	5MC	CM5-C5-C6	-2.20	119.91	122.85
55	V	10	2MG	O6-C6-C5	-2.20	120.77	126.60
22	a	2069	G7M	CN7-N7-C8	-2.19	121.45	124.84
22	a	2069	G7M	N2-C2-N1	2.17	121.33	116.71
54	Z	21	H2U	O4-C4-N3	2.16	123.70	120.28
54	Z	21	H2U	N3-C2-N1	-2.16	114.38	116.65
1	A	516	PSU	C6-N1-C2	-2.15	120.49	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2251	OMG	C8-N7-C5	2.15	108.13	104.24
55	V	34	A1L4U	O9-C8-O8	-2.12	116.50	123.14
55	V	54	2MU	C5M-C5-C6	-2.11	120.03	122.85
22	a	2504	PSU	O2-C2-N1	-2.11	120.47	122.79
22	a	1618	6MZ	C5-C6-N1	2.11	120.45	118.20
11	K	119	IAS	OXT-C-O	-2.10	119.31	124.09
1	A	1402	4OC	C6-C5-C4	2.09	119.52	116.96
22	a	2504	PSU	C6-N1-C2	-2.08	120.56	122.68
22	a	747	5MU	C6-C5-C4	2.05	119.74	118.03
1	A	1207	2MG	N1-C2-N3	-2.05	120.78	123.95
22	a	1618	6MZ	C5-C4-N9	2.04	108.16	105.78
1	A	966	2MG	N1-C2-N3	-2.04	120.79	123.95
22	a	1618	6MZ	C4-N9-C8	2.04	107.94	105.73
55	V	37	12A	CB-CA-N	-2.04	106.51	111.72
1	A	527	G7M	N9-C8-N7	-2.03	107.19	112.21
55	V	10	2MG	O3'-C3'-C2'	2.03	118.39	111.82
55	V	34	A1L4U	C6-N1-C2	-2.03	116.93	119.20
22	a	2449	H2U	O4-C4-N3	2.02	123.48	120.28
22	a	2580	PSU	C6-C5-C4	2.02	119.61	118.20
55	V	54	2MU	O3'-C3'-C2'	2.02	116.89	111.17
1	A	1207	2MG	C8-N7-C5	2.01	107.89	104.24
22	a	2580	PSU	C6-N1-C2	-2.01	120.63	122.68
55	V	46	G7M	CN7-N7-C8	-2.00	121.74	124.84
1	A	966	2MG	CM2-N2-C2	-2.00	119.44	123.86

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	2MG	C3'-C4'-C5'-O5'
25	d	150	MEQ	C-CA-CB-CG
25	d	150	MEQ	O-C-CA-CB
54	Z	21	H2U	O4'-C1'-N1-C2
54	Z	21	H2U	O4'-C1'-N1-C6
55	V	6	2MG	C3'-C4'-C5'-O5'
55	V	37	12A	N-CA-CB-OG1
55	V	37	12A	N-CA-CB-CG2
55	V	37	12A	C-CA-CB-OG1
55	V	37	12A	C-CA-CB-CG2
55	V	47	H2U	O4'-C1'-N1-C6
55	V	47	H2U	C2'-C1'-N1-C2
55	V	47	H2U	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
55	V	48	5MC	O4'-C4'-C5'-O5'
55	V	48	5MC	C3'-C4'-C5'-O5'
55	V	49	5MC	O4'-C4'-C5'-O5'
55	V	34	A1L4U	O4'-C1'-N1-C2
1	A	966	2MG	O4'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
22	a	2030	6MZ	O4'-C4'-C5'-O5'
55	V	49	5MC	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
55	V	6	2MG	O4'-C4'-C5'-O5'
25	d	150	MEQ	NE2-CD-CG-CB
25	d	150	MEQ	OE1-CD-CG-CB
55	V	47	H2U	C3'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
55	V	47	H2U	O4'-C4'-C5'-O5'
55	V	47	H2U	O4'-C1'-N1-C2
55	V	34	A1L4U	C4-C5-C5M-C8
25	d	150	MEQ	N-CA-CB-CG
12	L	89	D2T	CA-CB-CG-OD2
1	A	527	G7M	C4'-C5'-O5'-P
55	V	49	5MC	C4'-C5'-O5'-P
33	l	81	4D4	OB-CB-CG-CD
22	a	2503	2MA	C4'-C5'-O5'-P
33	l	81	4D4	CA-CB-CG-CD
55	V	47	H2U	C4'-C5'-O5'-P
1	A	527	G7M	O4'-C4'-C5'-O5'
12	L	89	D2T	CG-CB-SB-CB1
22	a	746	PSU	O4'-C1'-C5-C6
22	a	2069	G7M	O4'-C4'-C5'-O5'
54	Z	21	H2U	C2'-C1'-N1-C6
22	a	2503	2MA	O4'-C4'-C5'-O5'
33	l	81	4D4	O-C-CA-CB

There are no ring outliers.

16 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	89	D2T	1	0
22	a	2030	6MZ	2	0
55	V	10	2MG	2	0
55	V	37	12A	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	119	IAS	1	0
55	V	47	H2U	1	0
22	a	2498	OMC	1	0
54	Z	33	OMC	1	0
1	A	1516	2MG	1	0
1	A	1402	4OC	1	0
22	a	1915	3TD	1	0
22	a	2552	OMU	1	0
55	V	48	5MC	1	0
1	A	1519	MA6	1	0
55	V	46	G7M	1	0
54	Z	21	H2U	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 440 ligands modelled in this entry, 440 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.



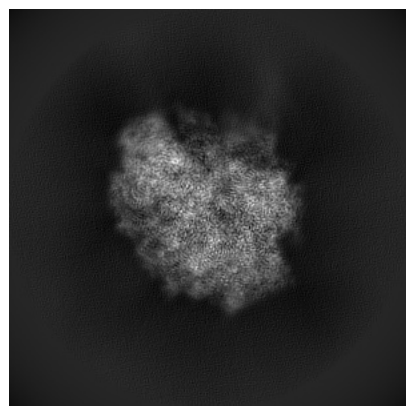
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61720. These allow visual inspection of the internal detail of the map and identification of artifacts.

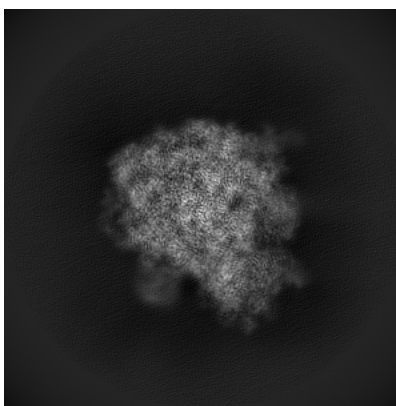
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

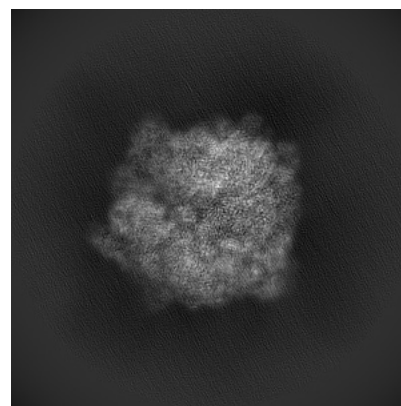
#### 6.1.1 Primary map



X

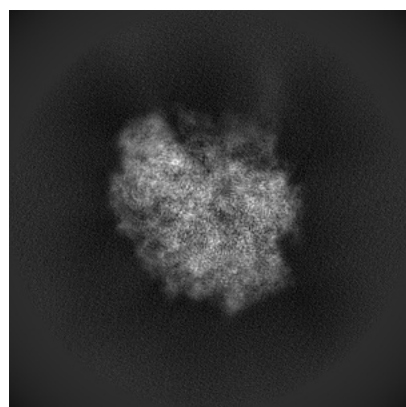


Y

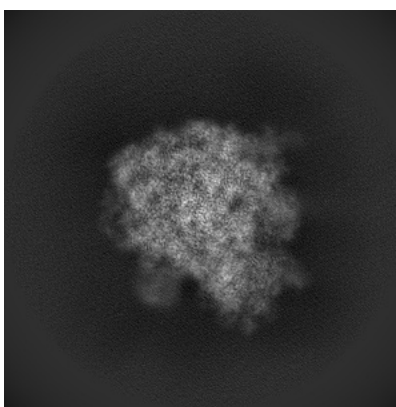


Z

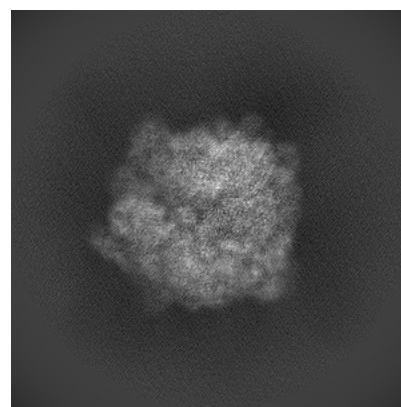
#### 6.1.2 Raw map



X



Y



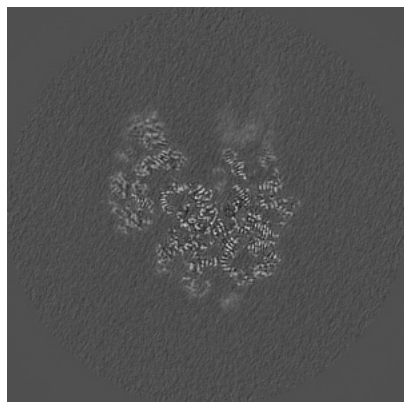
Z

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

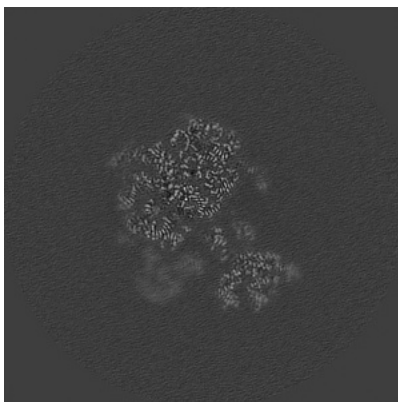


## 6.2 Central slices [i](#)

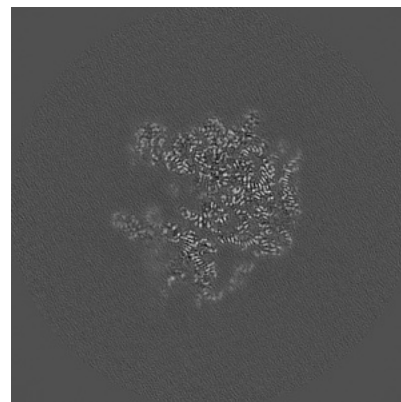
### 6.2.1 Primary map



X Index: 265

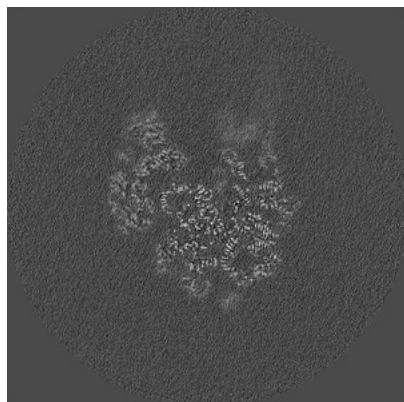


Y Index: 265

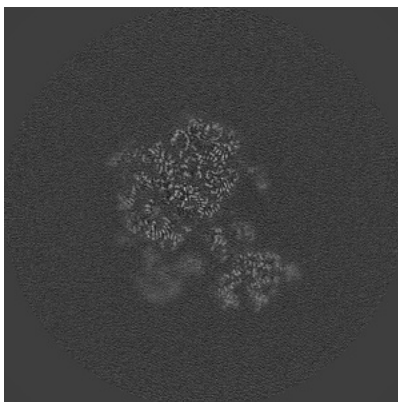


Z Index: 265

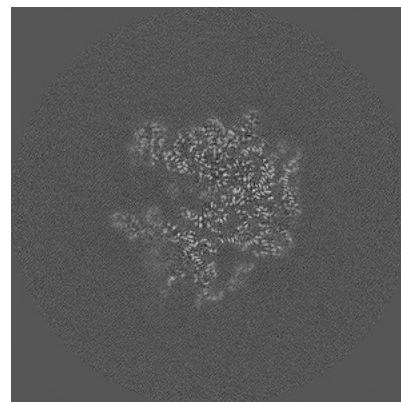
### 6.2.2 Raw map



X Index: 265



Y Index: 265

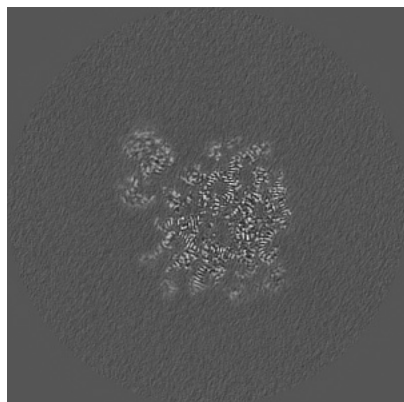


Z Index: 265

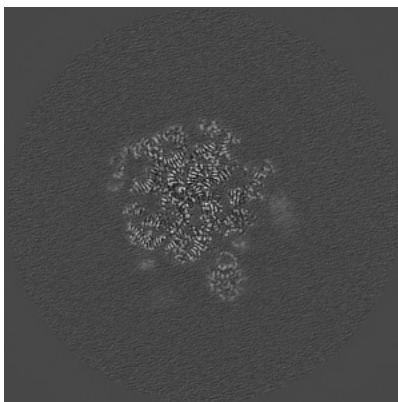
The images above show central slices of the map in three orthogonal directions.

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

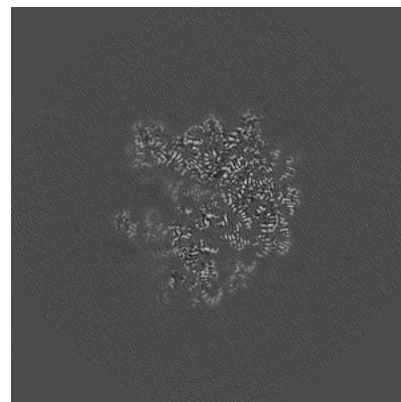
### 6.3.1 Primary map



X Index: 298

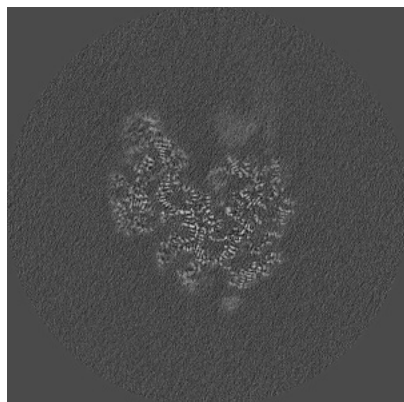


Y Index: 317

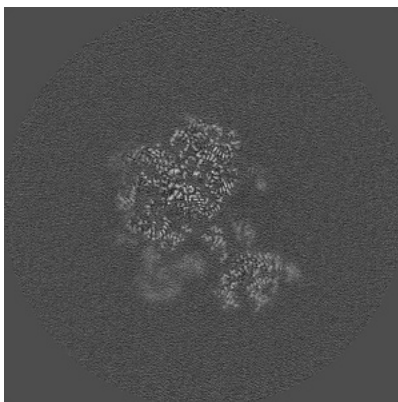


Z Index: 270

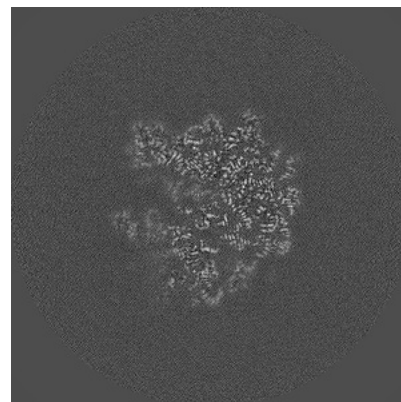
### 6.3.2 Raw map



X Index: 259



Y Index: 264

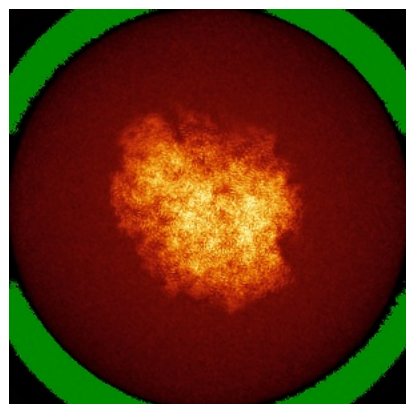


Z Index: 270

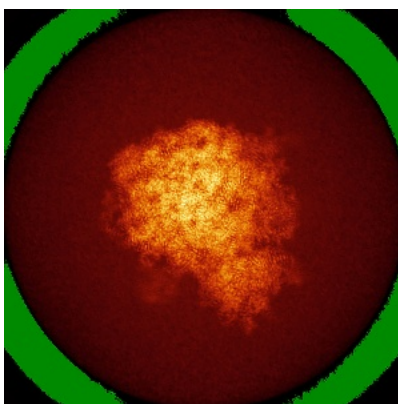
The images above show the largest variance slices of the map in three orthogonal directions.

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

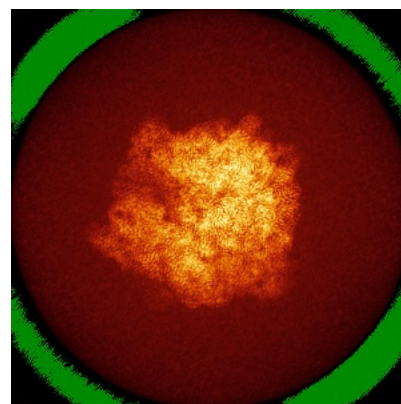
### 6.4.1 Primary map



X

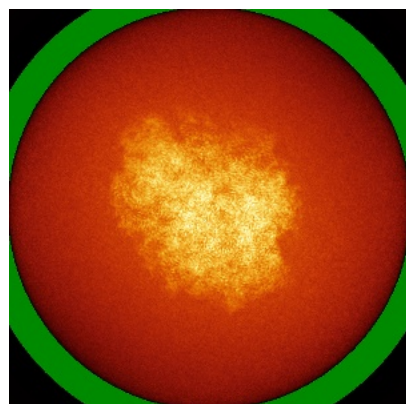


Y

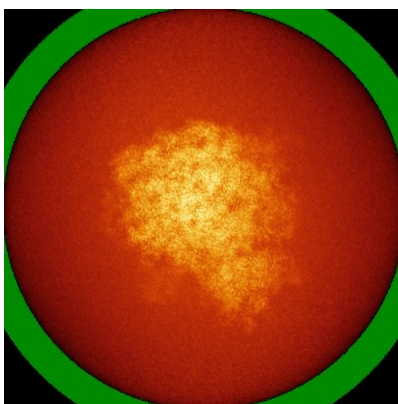


Z

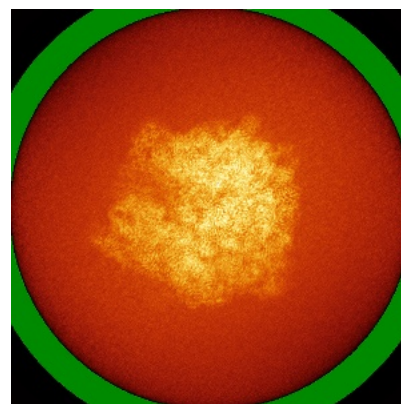
### 6.4.2 Raw map



X



Y

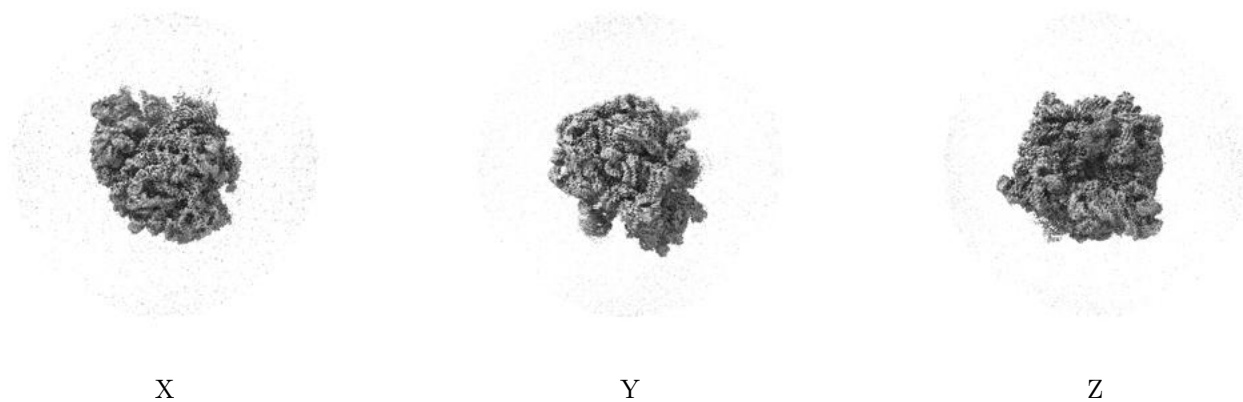


Z

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

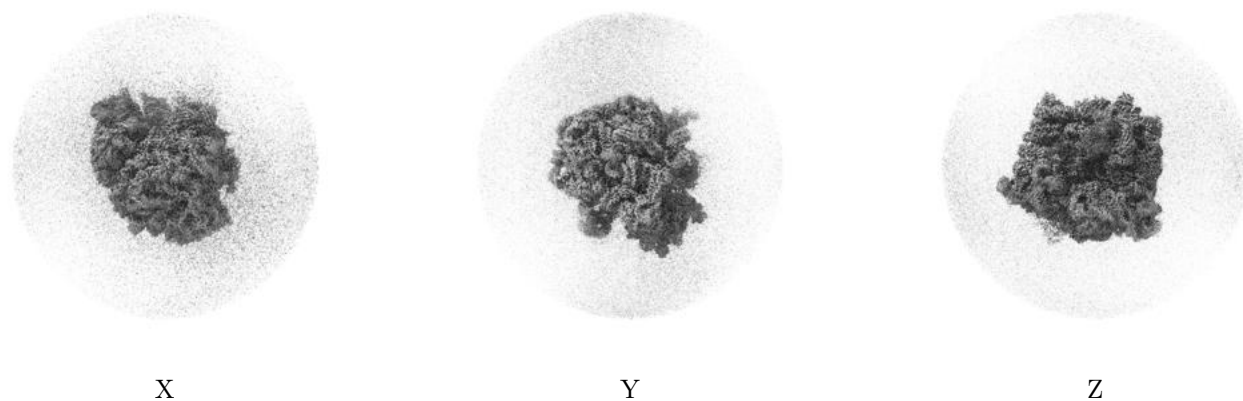
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0119. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

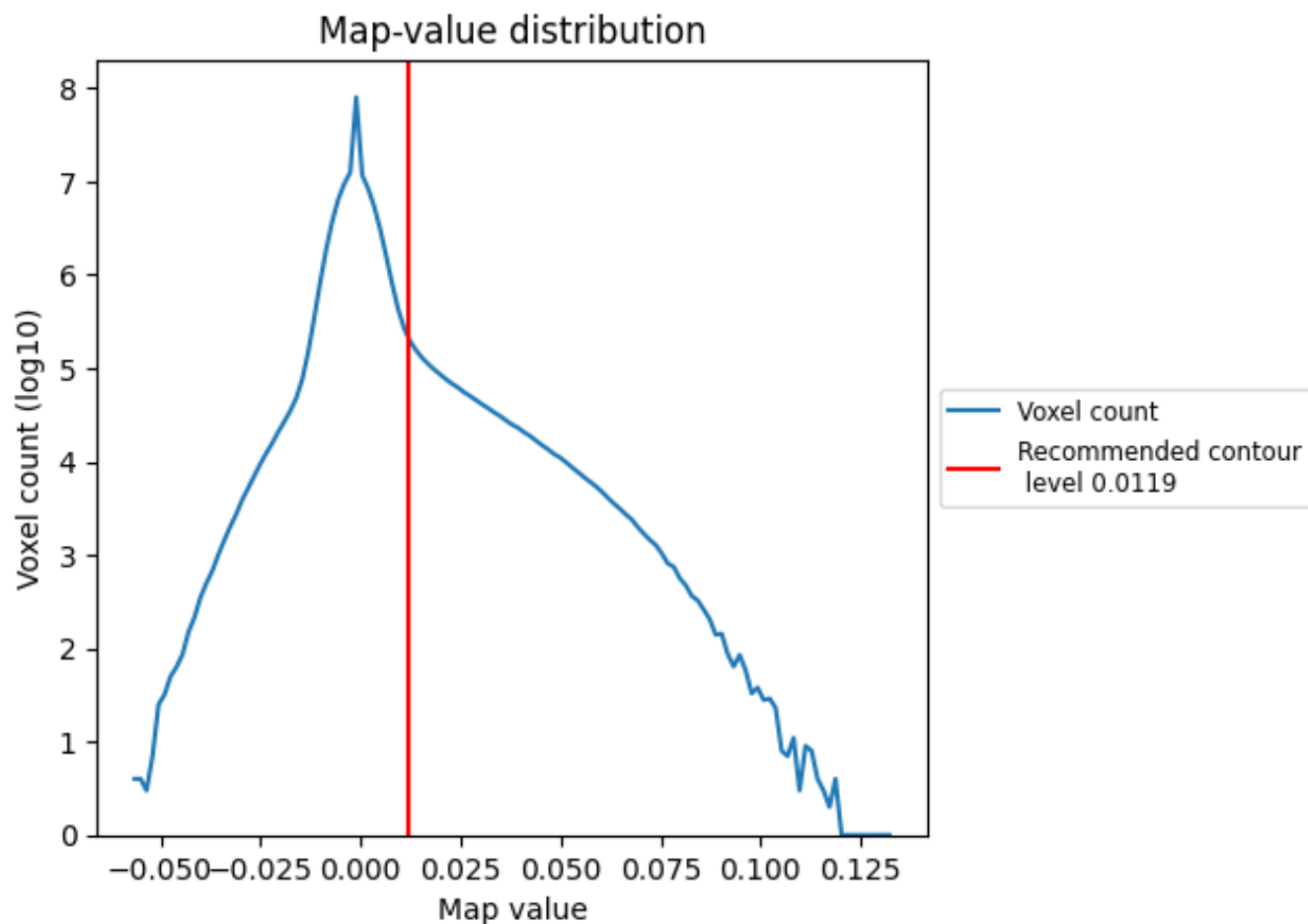
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

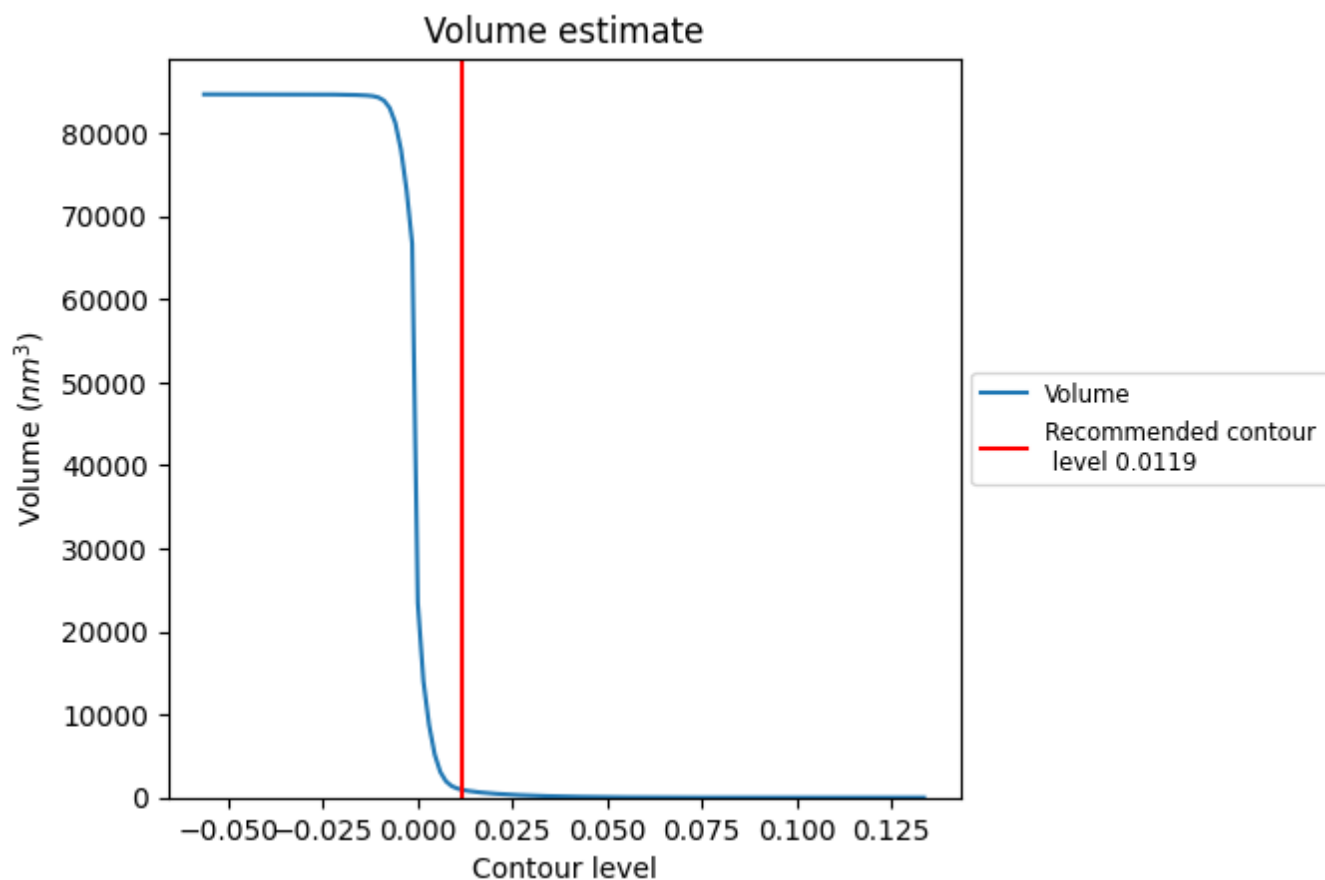
This section contains the results of statistical analysis of the map.

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



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

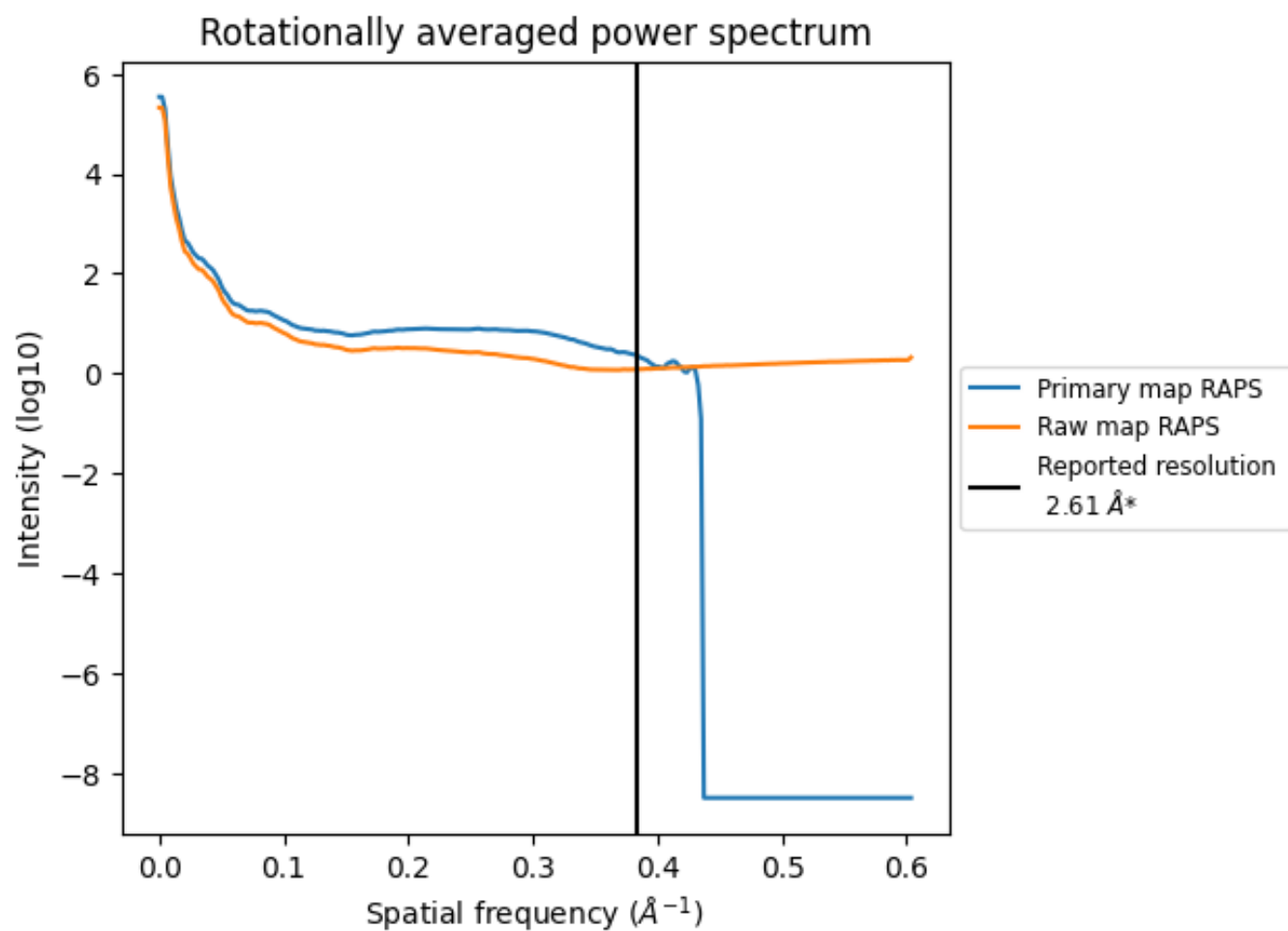
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 921  $\text{nm}^3$ ; this corresponds to an approximate mass of 832 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 ⓘ

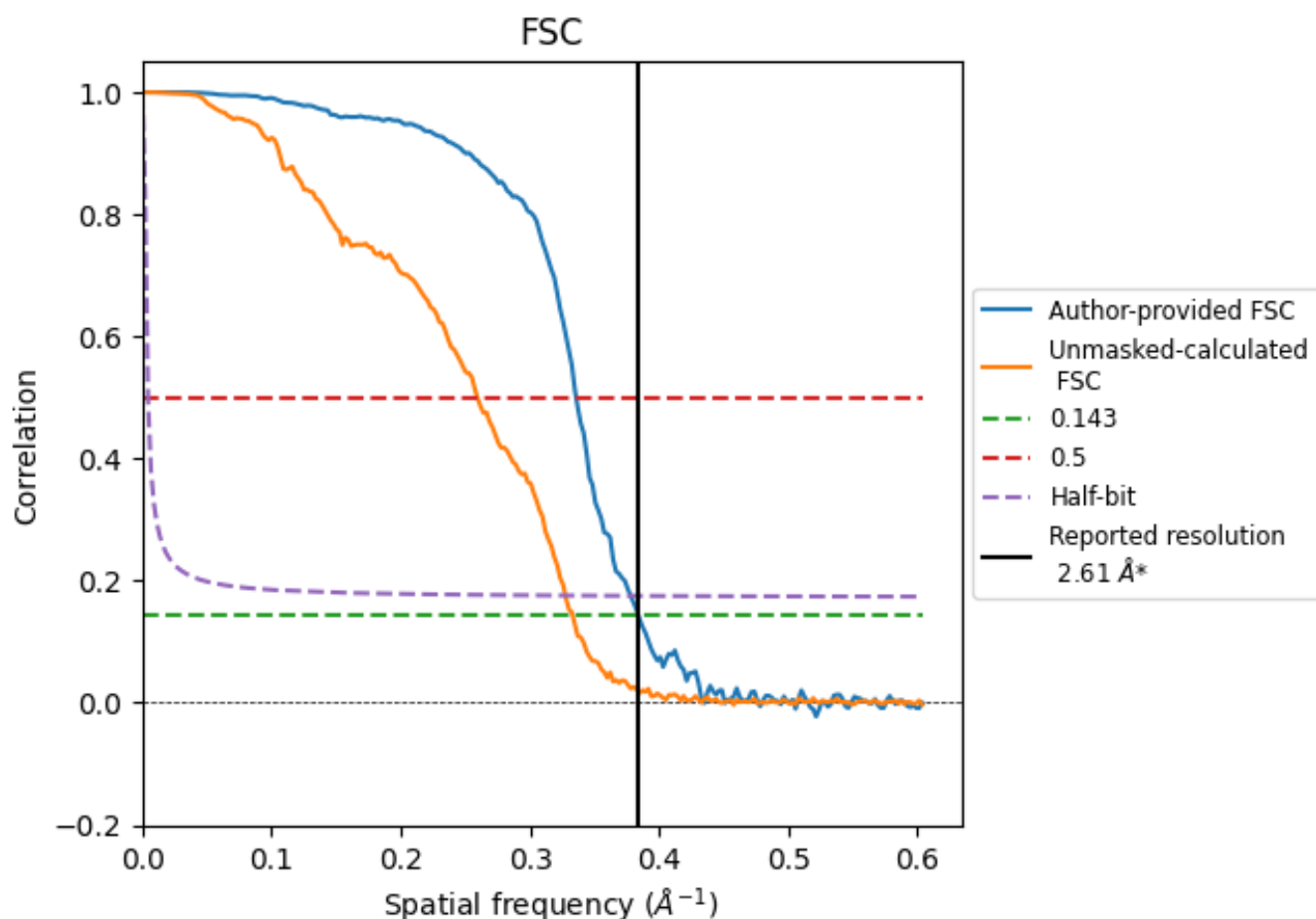


\*Reported resolution corresponds to spatial frequency of 0.383  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.383  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

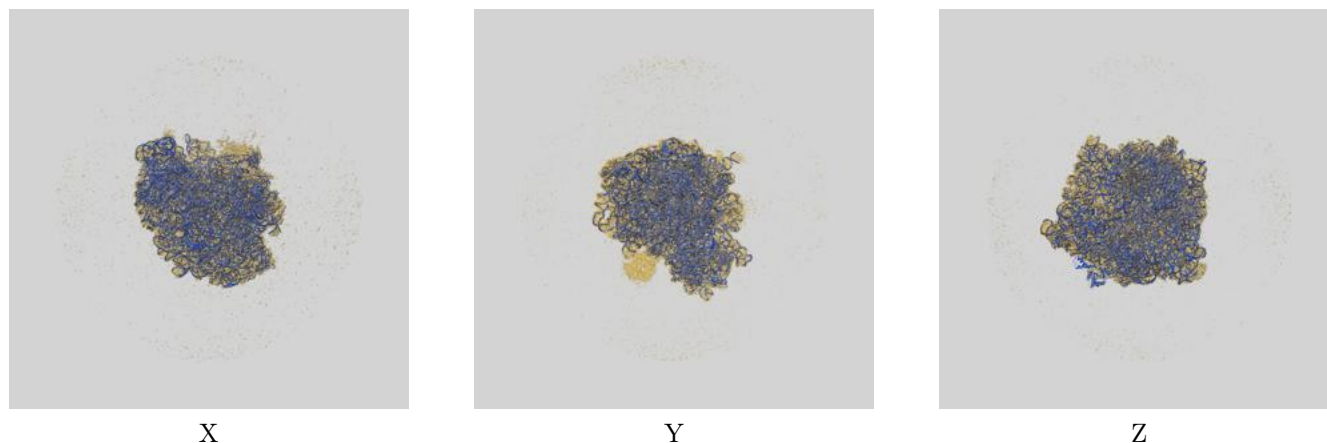
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	2.60	2.98	2.65
Unmasked-calculated*	3.00	3.86	3.05

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.61 by more than 10 %

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

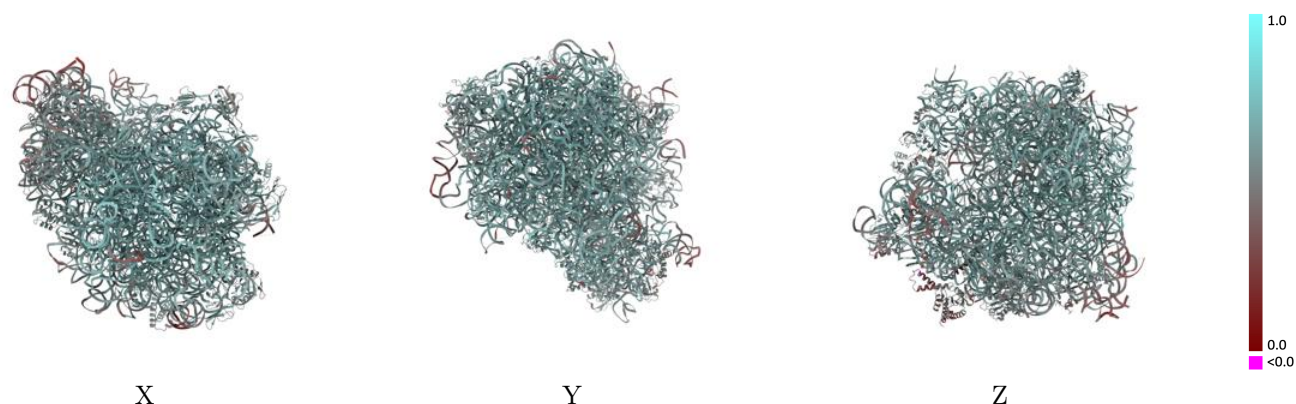
This section contains information regarding the fit between EMDB map EMD-61720 and PDB model 9JQ2. Per-residue inclusion information can be found in section [3](#) on page [15](#).

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



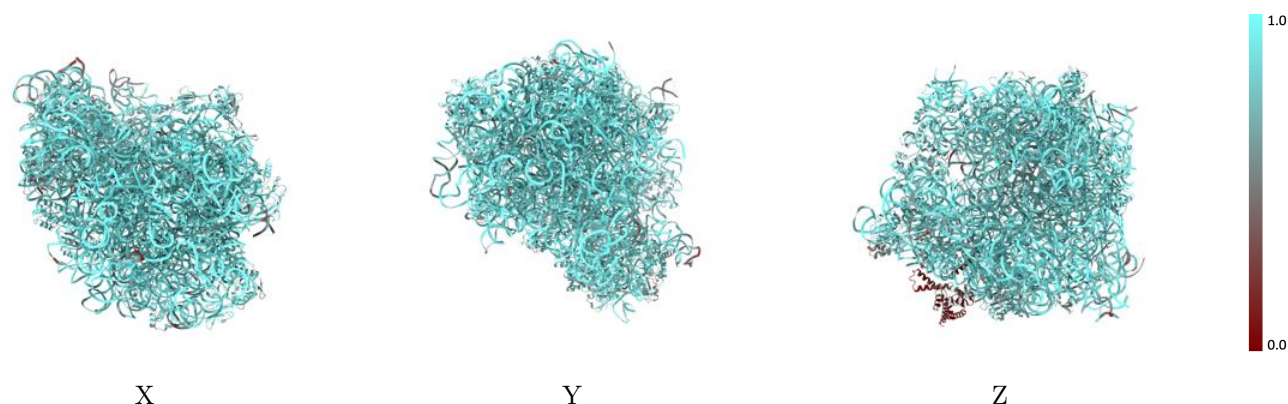
The images above show the 3D surface view of the map at the recommended contour level 0.0119 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



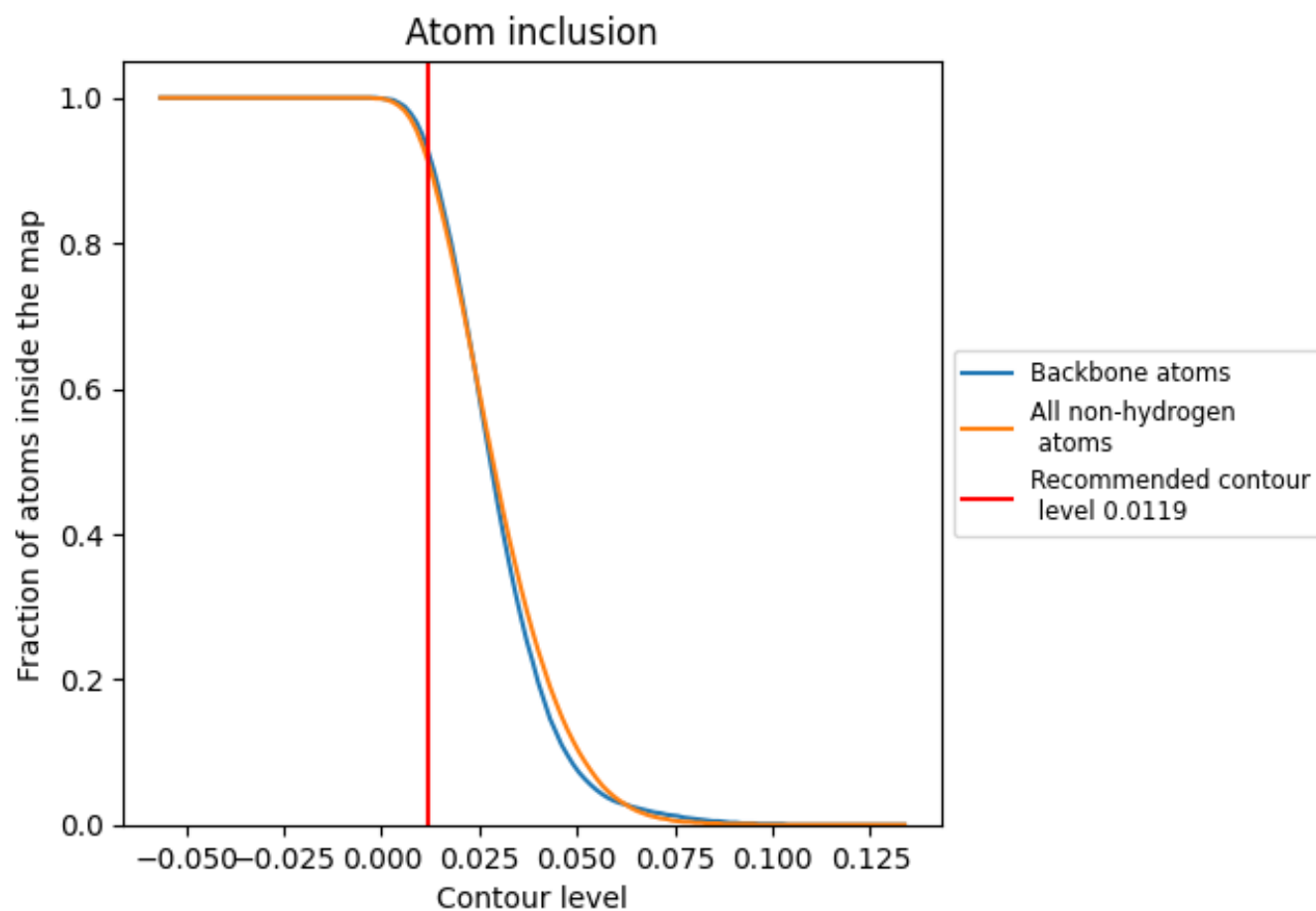
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0119).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ











































The table lists the average atom inclusion at the recommended contour level (0.0119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.6030
0	 0.8870	 0.6160
1	 0.9490	 0.6620
2	 0.9670	 0.6610
3	 0.9110	 0.6270
4	 0.7610	 0.5050
A	 0.9350	 0.5870
B	 0.2050	 0.4090
C	 0.8390	 0.5580
D	 0.7140	 0.5090
E	 0.8470	 0.5720
F	 0.8020	 0.5380
G	 0.7910	 0.5510
H	 0.8590	 0.5680
I	 0.8250	 0.5650
J	 0.6860	 0.5100
K	 0.8310	 0.5840
L	 0.8840	 0.6160
M	 0.8410	 0.5740
N	 0.8570	 0.5800
O	 0.8540	 0.5760
P	 0.7620	 0.5020
Q	 0.8140	 0.5570
R	 0.8070	 0.5470
S	 0.8300	 0.5620
T	 0.7570	 0.5320
U	 0.3860	 0.4150
V	 0.8750	 0.5710
X	 0.9400	 0.6150
Z	 0.8670	 0.5830
a	 0.9660	 0.6310
b	 0.9600	 0.6020
c	 0.9530	 0.6560
d	 0.9320	 0.6470
e	 0.8380	 0.5800



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Chain	Atom inclusion	Q-score
f	 0.8320	 0.5750
g	 0.7560	 0.5360
h	 0.5500	 0.5060
i	 0.9140	 0.6240
j	 0.9300	 0.6510
k	 0.8960	 0.6090
l	 0.9160	 0.6390
m	 0.9720	 0.6670
n	 0.8750	 0.5890
o	 0.9090	 0.6340
p	 0.9500	 0.6300
q	 0.8630	 0.5840
r	 0.9040	 0.6270
s	 0.8230	 0.5700
t	 0.8190	 0.5340
u	 0.8560	 0.5890
v	 0.9290	 0.6490
w	 0.9180	 0.6180
x	 0.7690	 0.5160
y	 0.8950	 0.6030
z	 0.9160	 0.6390